An Overview of Symbolic Explainability

Joao Marques-Silva

ICREA, Univ. Lleida, Catalunya, Spain

VTSA, Luxembourg, July 2024

Context – my team's recent & not so recent work...

- SAT Solving (Clause learning, UIPs, ...)
- Quantification & CEGAR (QBF, QMaxSAT, etc.)
- Function Synthesis (Min DNF cover, ...)
- Inconsistency (MUS, MCS, etc.)
- Certification of Reasoners
- Model Checking, Synthesizing Invariants, ATPG, Reconfiguration
- Optimization (MaxSAT, MinSAT, PBO, WBO, etc.)
- Propositional Encodings, Backbones, Autarkies, Minimal models, etc.
- Enumeration (MUSes, MCSes, etc.)
- Proof Systems (DRMaxSAT, etc.)
- Primes, Abduction, DLs, etc.

Context – new area of research, since circa 2018...

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Enhancing ML by exploiting AR & FM !

Proof Systems
(DRMaxSAT, etc.)

Primes, Abduction, DLs, etc.

Explainability & Interpretability in ML

Recent & ongoing ML successes

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

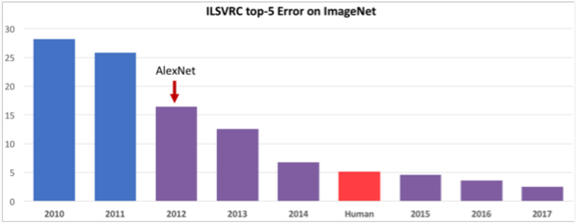
DeepMind

AlphaGo

AlphaGo Zero & **Alpha Zero**

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

Image & Speech Recognition

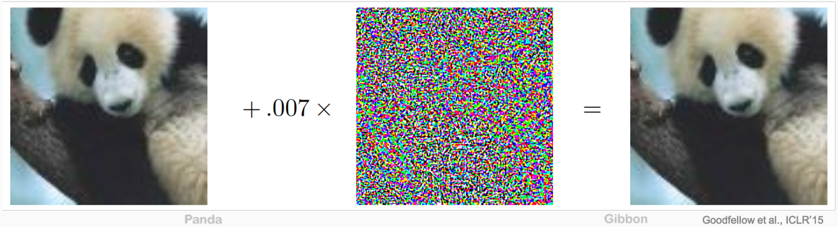


http://gradientscience.org/intro_adversarial/

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
- One **must** be able to validate operation of ML model, with rigor
  - Explanations; robustness; verification

ML models are brittle — adversarial examples



Goodfellow et al., ICLR'15

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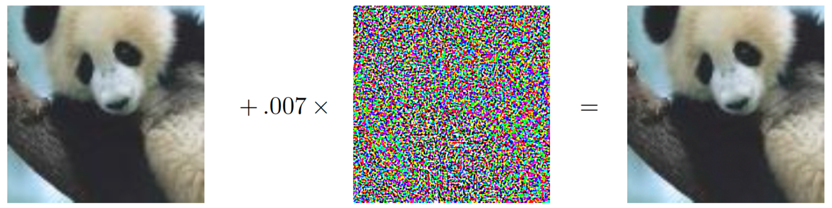
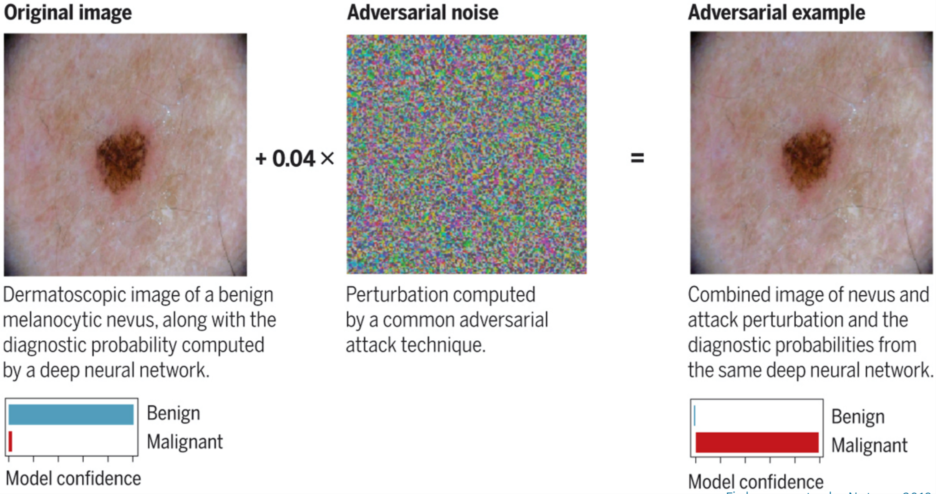


Panda Gibbon Goodfellow et al., ICLR'15

Eykholt et al'18 Aung et al'17

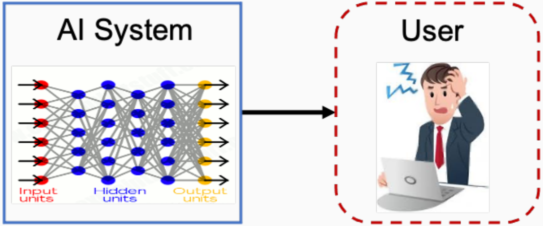
ML models are brittle — adversarial examples

Adversarial examples can be very problematic



Finlayson et al., Nature 2019

eXplainable AI (XAI)



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

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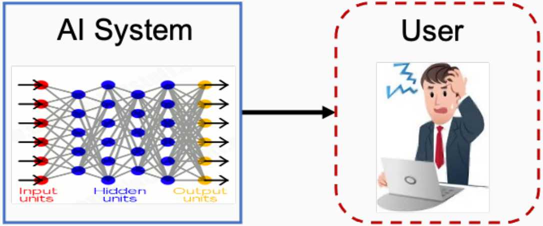

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    - How to be human understandable?
    - How to answer **Why?** questions? I.e. Why the prediction?
    - How to answer **Why Not?** questions? I.e. Why not some other prediction?
    - Which guarantees of rigor?

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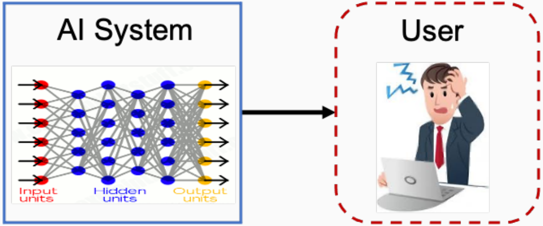

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    - Which guarantees of rigor?
  - Other queries: enumeration, membership, preferences, etc.
  - Links with robustness, fairness, model learning

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.

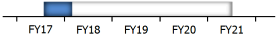
Proposal for a

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)

EXPLAINABLE ARTIFICIAL INTELLIGENCE



David Gunning
DARPA/I2O
Program Update November 2017

DARPA

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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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

Proposal for a

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...e (XAI)

...pdate November 2017

DARPA

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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

XAI & EU guidelines (AI HLEG)

Search

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

Digital Single Market

REPORT / STUDY | 8 April 2019

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

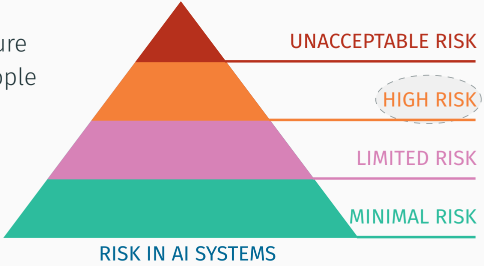
XAI & the principle of explicability

& thousands of recent papers!

XAI for high-risk & safety-critical applications

- High-risk (EU regulations, hopefully soon...):
  - Law enforcement
  - Management and operation of critical infrastructure
  - Biometric identification and categorization of people
  - ...

[EU21]



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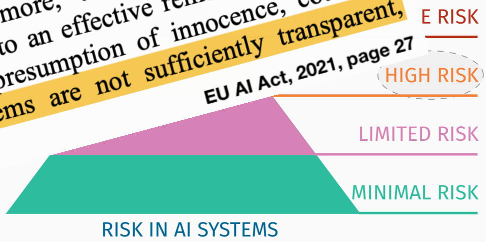
> otherwise incorrect or unjust manner. Furthermore, the exercise of important procedural fundamental rights, such as the right to an effective remedy and to a fair trial as well as the right of defence and the presumption of innocence, could be hampered, in particular, where such AI systems are not sufficiently transparent, explainable and documented.
>
> **EU AI Act, 2021, page 27**

[EU21]



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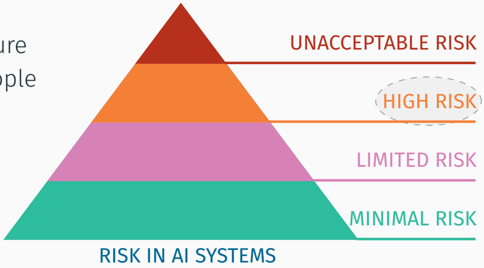

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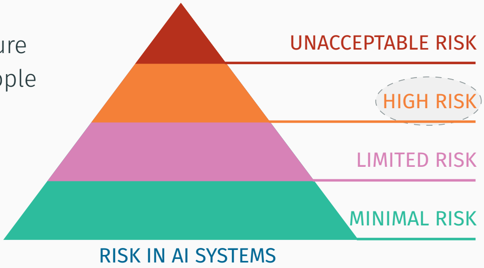


PERSPECTIVE
https://doi.org/10.1038/s42256-019-0048-x

nature machine intelligence

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

Cynthia Rudin

May 2019

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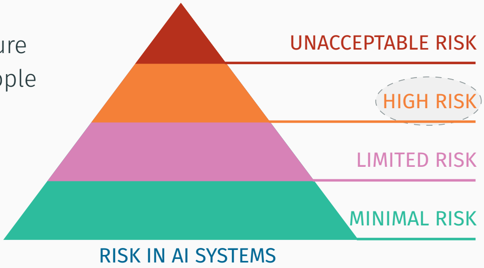


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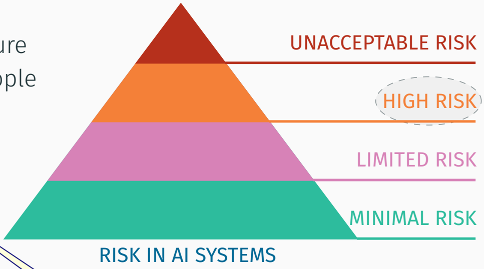

Main motivation for our work! (since 2019)

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

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- 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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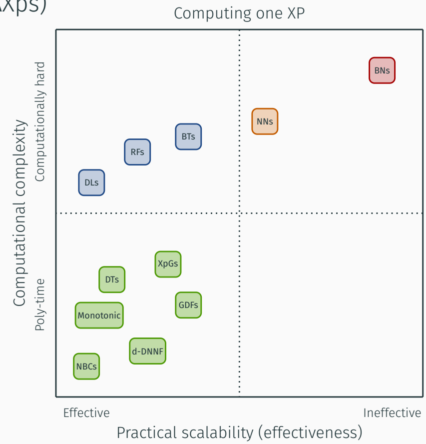
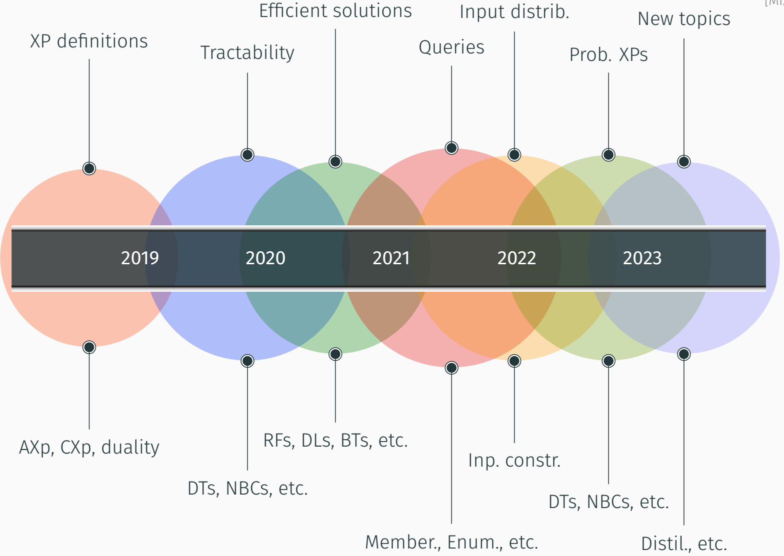


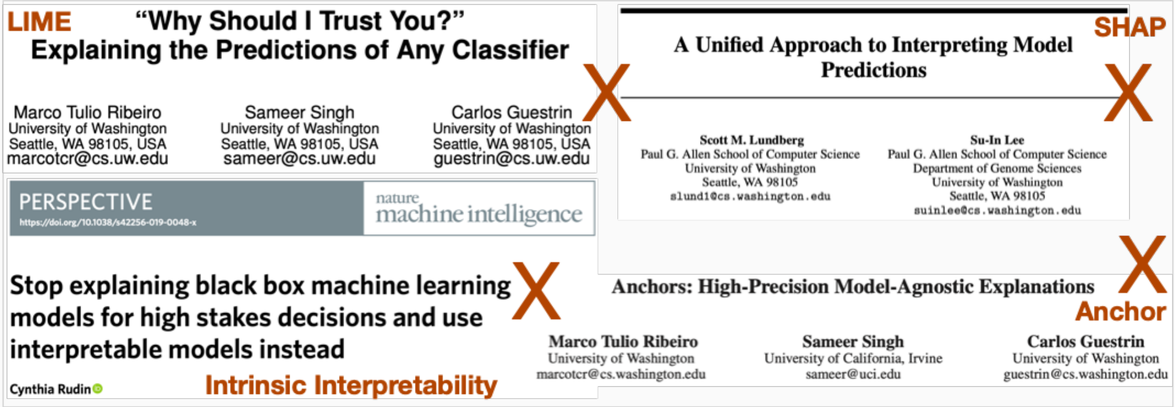
What have we been up to? 1. Created the field of symbolic (formal) XAI – II

[MI22, Mar22, MS23, Mar24]



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

[RSG16, LL17, RSG18, Rud19]



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

[MSH24, HMS24, HM23c]

research and advances

Check for updates

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

66 COMMUNICATIONS OF THE ACM | JULY 2024 | VOL. 67 | NO. 7

» 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 short course

- 1^{st} day:
  - Part #0a: Motivation
  - Part #1: Foundations
  - Part #2: Principles of symbolic XAI – feature selection (& myth of interpretability)
  - Part #3: Tractable symbolic XAI
  - Part #4: Intractable symbolic XAI (& myth of model-agnostic XAI)
  - Q&A
- 2^{nd} day:
  - Part #0b: Recapitulate
  - Part #5: Explainability queries
  - Part #6: Advanced topics
  - Part #7: Principles of symbolic XAI – feature attribution (& myth of Shapley values in XAI)
  - Part #8: Conclusions & research directions
  - Q&A

Part 1

Foundations

Classification problems

- Set of features $\mathcal{F} = \{1, 2, \ldots, m\}$, 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 $\mathcal{K} = \{c_1, \ldots, c_K\}$

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- ML model $\mathcal{M}_C$ computes a (non-constant) classification function $\kappa : \mathbb{F} \to \mathcal{K}$
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  - $\mathcal{M}_C$ is a tuple $(\mathcal{F}, \mathbb{F}, \mathcal{K}, \kappa)$
- Instance $(\mathbf{v}, c)$ for point $\mathbf{v} = (v_1, \ldots, v_m) \in \mathbb{F}$, 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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- General ML model:
  - $\mathbb{T}$: range of possible predictions
  - Non-constant function $\tau : \mathbb{F} \to \mathbb{T}$
  - ML model: $\mathcal{M}$ is a tuple $(\mathcal{F}, \mathbb{F}, \mathbb{T}, \tau)$

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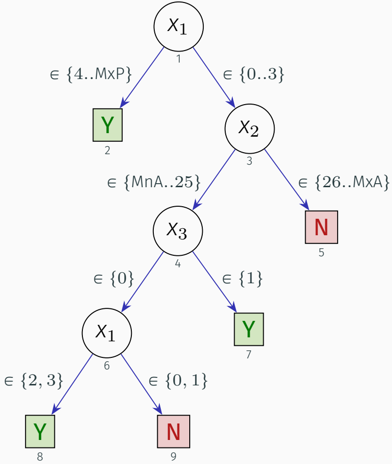
- Instance: $(\mathbf{v}, q)$, $q \in \mathbb{T}$

Example ML models – classification – decision trees (DTs)



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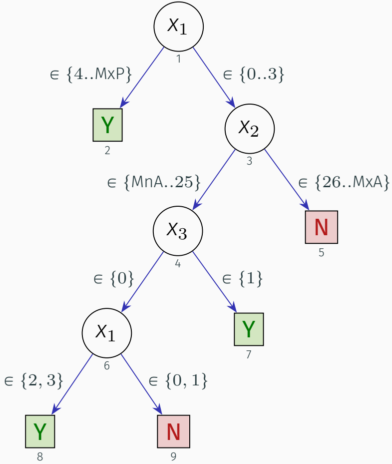
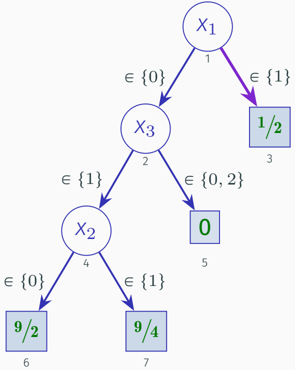


- Literals in DTs can use $=$ or $\in$

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

$\mathcal{F} = \{1, 2\}; \mathcal{D}_1 = \mathcal{D}_2 = \{0, 1\}; \mathcal{K} = \{\text{Y}, \text{N}\}$

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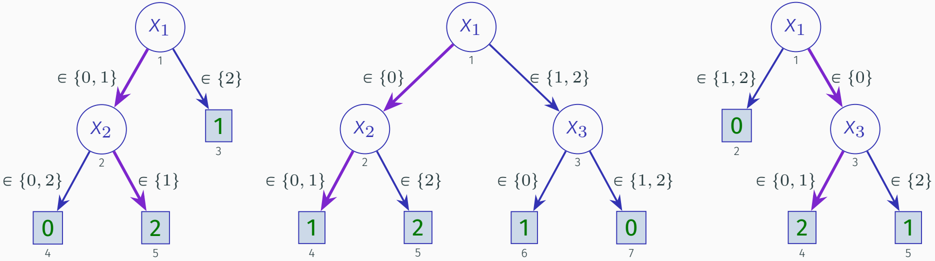
- Unordered rules – decision sets (DSs):

$$\begin{array}{llll} \text{IF} & x_1 + x_2 \geqslant 0 & \text{THEN} & \text{predict } \boxplus \\ \text{IF} & x_1 + x_2 < 0 & \text{THEN} & \text{predict } \boxminus \end{array}$$

$$\mathcal{F} = \{1,2\}; \mathcal{D}_1 = \mathcal{D}_2 = \mathbb{R}; \mathcal{K} = \{\boxplus, \boxminus\}$$

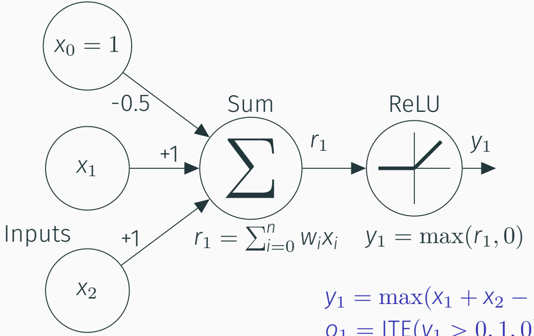
  - Issues of DSs: overlap; incomplete coverage

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)



$$y_1 = \max(x_1 + x_2 - 0.5, 0)$$
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Outline – Part 1

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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- MILP: decision/optimization problems defined on conjunctions of linear inequalities over integer & real-valued variables
- CP: constraint programming
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Basic knowledge on SAT & SMT assumed. See links below.

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- CP: constraint programming
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- Background on SAT/SMT: [BHvMW09]
  - `https://alexeyignatiev.github.io/ssa-school-2019/`
  - `https://alexeyignatiev.github.io/ijcai19tut/`

Basic definitions in propositional logic

- Variables ($\{x, x_1, \ldots\}$) & literals (x_1, $\neg x_1$)
- Well-formed formulas using $\neg$, $\wedge$, $\vee$, ...
- Clause: disjunction of literals
- Term: conjunction of literals
- Conjunctive normal form (CNF): conjunction of clauses
- Disjunctive normal form (DNF): disjunction of terms
- Simple to generalize to more expressive domains

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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    - $\mathbb{F} = \{0, 1\}^2$
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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 $x_1 \wedge x_3 \vDash \varphi$

Prime implicants & implicates

- 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. $\pi \models \varphi$
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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. $\varphi \models \eta$
  2. For any $\eta' \subsetneq \eta$, $\varphi \not\models \eta'$

Reasoning about inconsistency

- Formula $\mathcal{T} = \mathcal{B} \cup \mathcal{S}$, with
  - $\mathcal{B}$: background knowledge (base), i.e. hard constraints
  - $\mathcal{S}$: additional (inconsistent) knowledge, i.e. soft constraints
  - And, $\mathcal{T} \vDash \bot$
  - E.g. $\mathcal{B} = \{(x_1 \vee x_2), (x_1 \vee \neg x_3)\}$, $\mathcal{S} = \{(\neg x_1), (\neg x_2), (x_3)\}$

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- Minimal correction subset (MCS):
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- Duality:
  - MUSes are minimal-hitting sets (MHSes) of the MCSes, and vice-versa [Rei87]

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- Duality:
  - MUSes are minimal-hitting sets (MHSes) of the MCSes, and vice-versa [Rei87]
- Variants:
  - Smallest(-cost) MCS, i.e. complement of maximum(-cost) satisfiability (MaxSAT)
  - Smallest(-cost) MUS

SAT/SMT/MILP/CP solvers used as oracles

- 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]

Outline – Part 1

Decision sets with boolean features

- Example ML model:

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

  Rules:

$$
\begin{array}{llll}
\text{IF} & x_1 \wedge \neg x_2 \wedge x_3 & \text{THEN} & \text{predict } \boxplus \\
\text{IF} & x_1 \wedge \neg x_3 \wedge x_4 & \text{THEN} & \text{predict } \boxminus \\
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  - Yes, certainly: pick $(x_1, x_2, x_3, x_4) = (1, 0, 1, 1)$

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  IF $x_1 \wedge \neg x_2 \wedge x_3$ THEN predict ⊞

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

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

  ... and solve with SAT solver (after clausification) [Tse68, PG86]

  Or use PySAT [IMM18]

  ∴ 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)

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  $$\text{IF} \quad 2x_1 + x_2 > 0 \quad \text{THEN} \quad \text{predict } \boxplus$$
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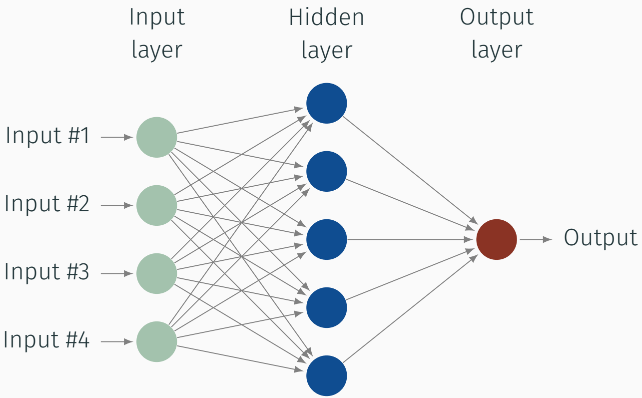
$$y_p \leftrightarrow (2x_1 + x_2 > 0) \ \wedge \ y_n \leftrightarrow (2x_1 - x_2 \leqslant 0) \ \wedge \ (y_p) \ \wedge \ (y_n)$$

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

$\therefore$ 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
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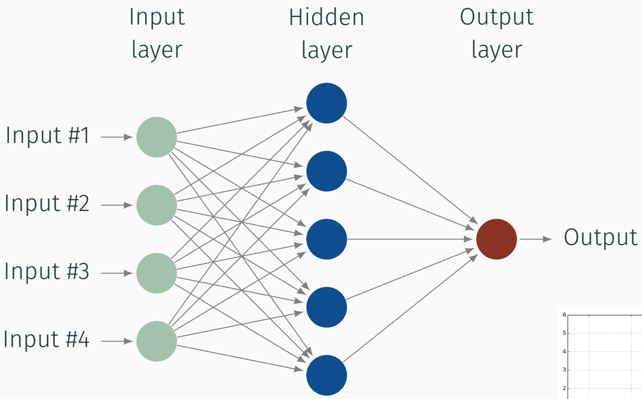

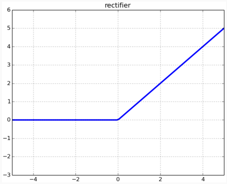

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- Each unit uses a **ReLU** activation function

[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]

$$\sum_{j=1}^{n} a_{i,j} x_j + b_i = y_i - s_i$$
$$z_i = 1 \rightarrow y_i \leqslant 0$$
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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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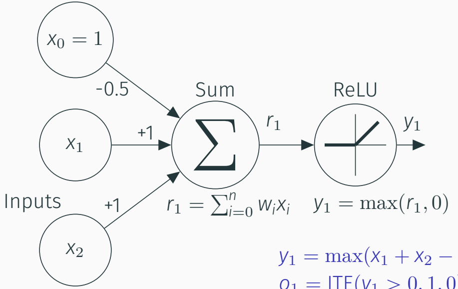

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x_1	x_2	r_1	y_1	o_1
0	0	-0.5	0	0
1	0	0.5	0.5	1
0	1	0.5	0.5	1
1	1	1.5	1.5	1

MILP encoding:

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$$y_1, s_1 \geqslant 0$$

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

$$1 + 0 - 0.5 = 0.5 - 0$$
$$1 \vee 0.5 \leqslant 0$$
$$0 \vee 0 \leqslant 0$$
$$1 = (0.5 > 0)$$
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Checking: $\mathbf{x} = (0, 0)$

$$0 + 0 - 0.5 = 0 - 0.5$$
$$0 \vee 0 \leqslant 0$$
$$1 \vee 0.5 \leqslant 0$$
$$0 = (0 > 0)$$
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$$y_1 = 0, s_1 = 0.5$$

Outline – Part 1

Basics of (non-symbolic) XAI – more detail later

- Feature attribution:
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  - SHAP [LL17]
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What is intrinsic interpretability?

- Goal is to deploy *interpretable* ML models [Rud19, Mol20, RCC+22, Rud22]
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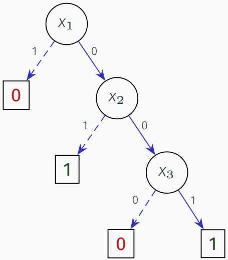

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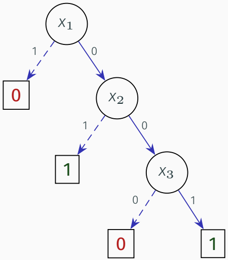

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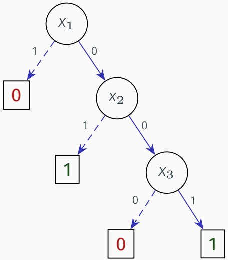

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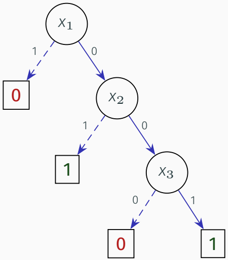

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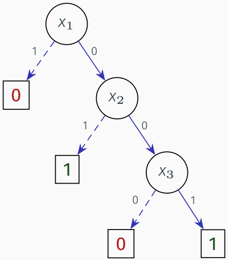

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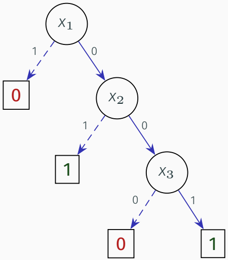

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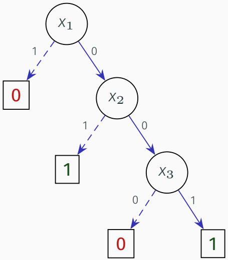

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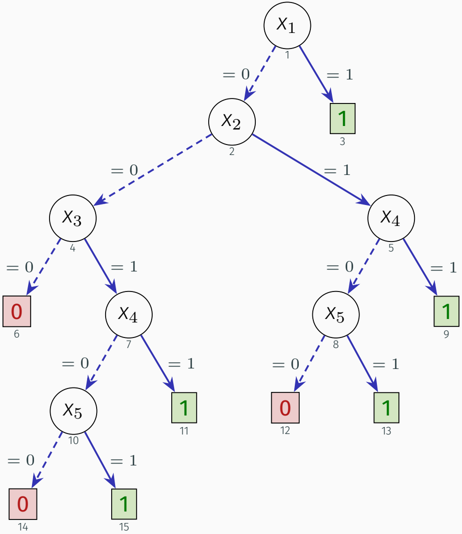
  - $\{1,3\}$ is easier to grasp; also, it is irreducible

Are *interpretable* models really interpretable? – DTs



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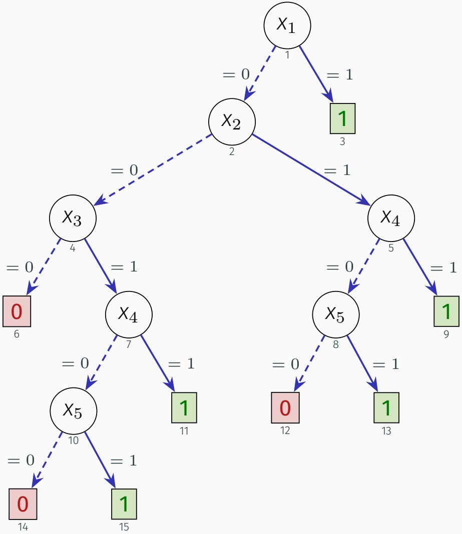

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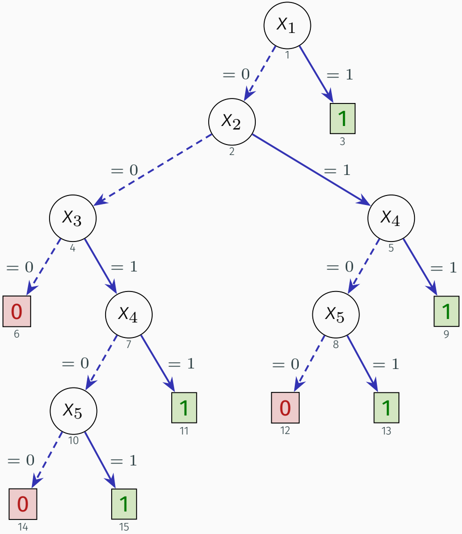

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x_3	x_5	x_1	x_2	x_4	$\kappa(\mathbf{x})$
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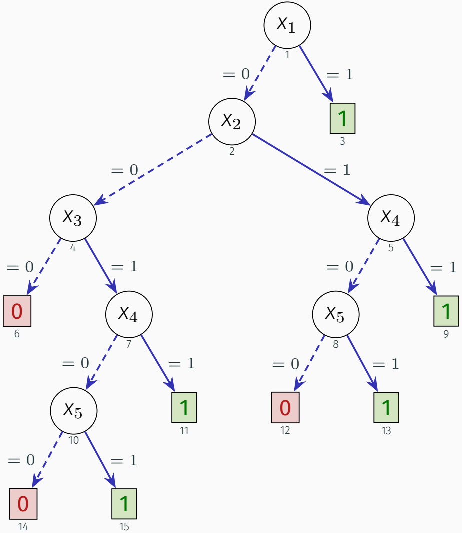

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$\therefore$ fixing $\{3, 5\}$ suffices for the prediction
Compare with $\{1, 2, 3, 4, 5\}$...

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[MSI23]

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    - Would he/she be able to compute the set $\{3, 4, 6\}$, by manual inspection?

Part 2

Principles of Symbolic XAI – Feature Selection

Outline – Part 2

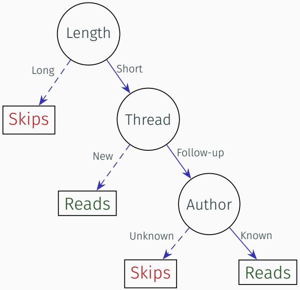
Definitions of Explanations

Duality Properties

Computational Problems

- Notation:

Original DT [PM17]



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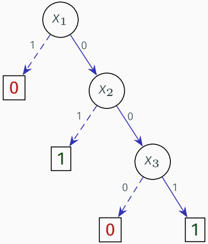

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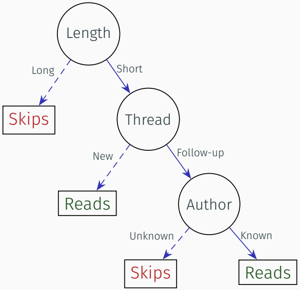

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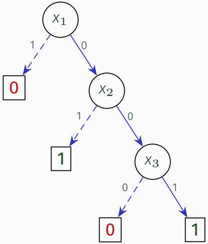

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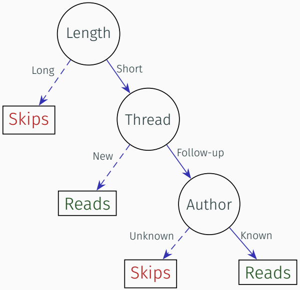

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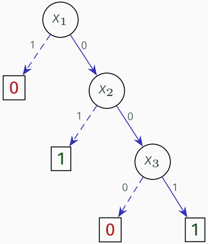

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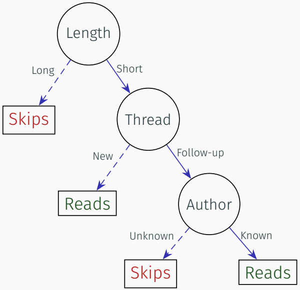

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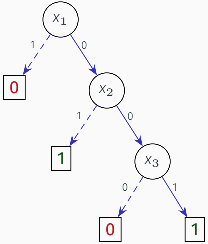

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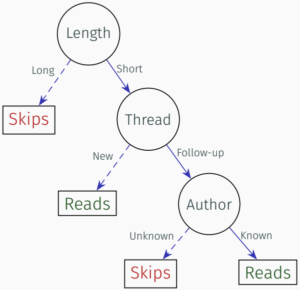

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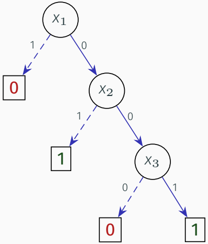

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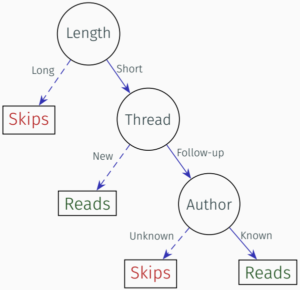

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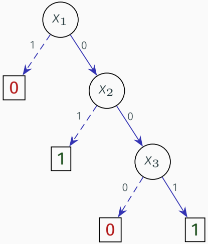

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    - One possible explanation is $\{\neg x_1, \neg x_2, x_3\}$ or simply $\{1, 2, 3\}$

The similarity predicate

[Mar24]

- Recall ML models for classification & regression:
  - Classification: $\mathcal{M}_C = (\mathcal{F}, \mathbb{F}, \mathcal{K}, \kappa)$
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- Bottom line:
  Reason about symbolic explainability by abstracting away type of ML model

Abductive explanations – answering Why? questions

- Instance $(\mathbf{v}, q)$, i.e. $c = \tau(\mathbf{v})$

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- Abductive explanation (AXp, PI-explanation): [SCD18, INM19a]
    - Subset-minimal set of features $\mathcal{X} \subseteq \mathcal{F}$ sufficient for ensuring prediction

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

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  - **Obs:** for some classes of classifiers, poly-time algorithms exist

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

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- Using probabilities, non-real-valued features: [WMHK21, IHI+22, ABOS22, IHI+23]

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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:

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

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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
  - I.e. can be viewed as attempt at formalizing local explanations [RSG16, LL17, RSG18]
- One can define explanations without picking a given point in feature space
  - Let $q \in \mathbb{T}$, and refefine the similarity predicate:
    - Classification: $\sigma(\mathbf{x}) = [\kappa(\mathbf{x}) = q]$
    - Regression: $\sigma(\mathbf{x}) = [|\kappa(\mathbf{x}) - q| \leqslant \delta]$, δ is user-specified
  - Let $\mathbb{L} = \{(x_i = v_i) \,|\, i \in \mathcal{F} \wedge v_i \in \mathbb{V}\}$
  - 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,

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

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

Outline – Part 2

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 (MHS) of the set of CXps

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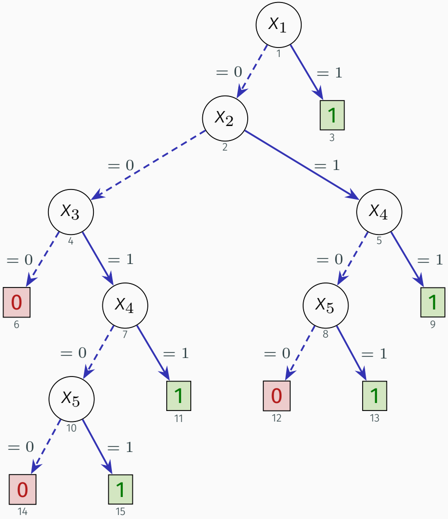
- An example



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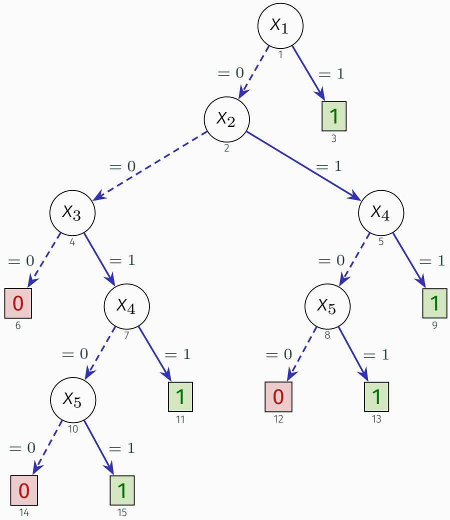

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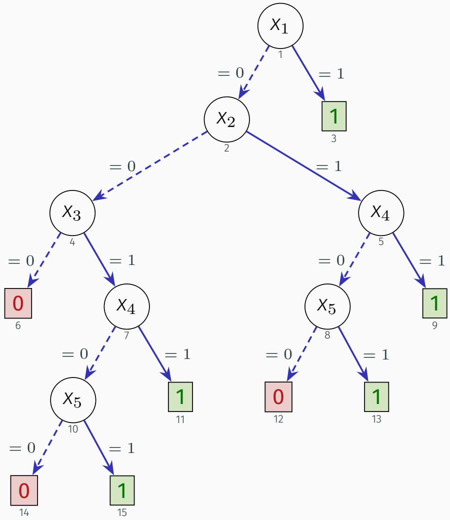

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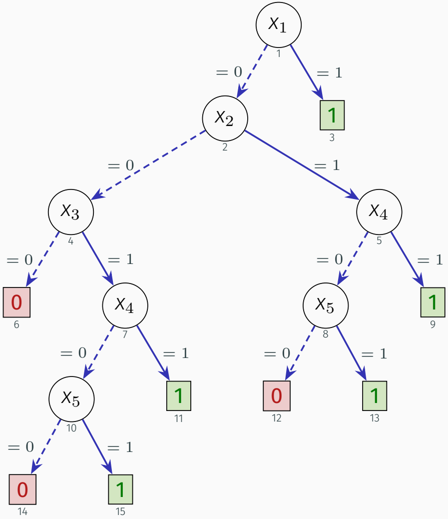

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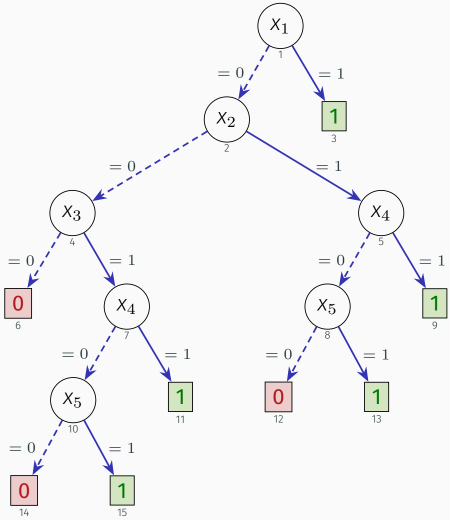

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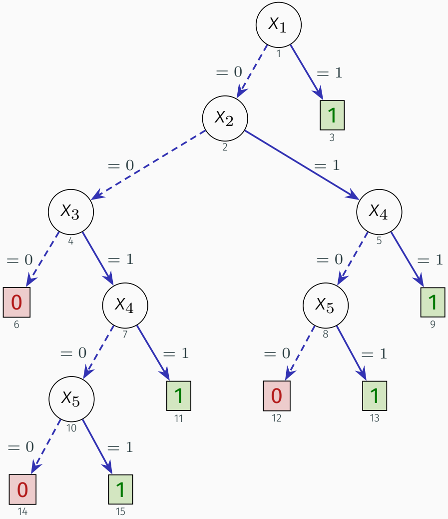

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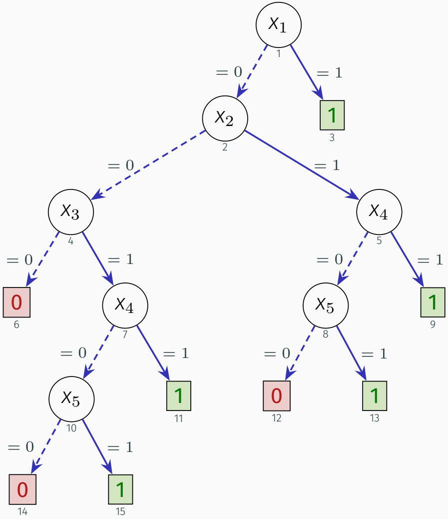
  - BTW,
    - $\{2, 5\}$ is not a CXp
    - $\{1, 2, 3, 4, 5\}$, $\{1, 2, 3, 5\}$ and $\{1, 3, 5\}$ are not AXps



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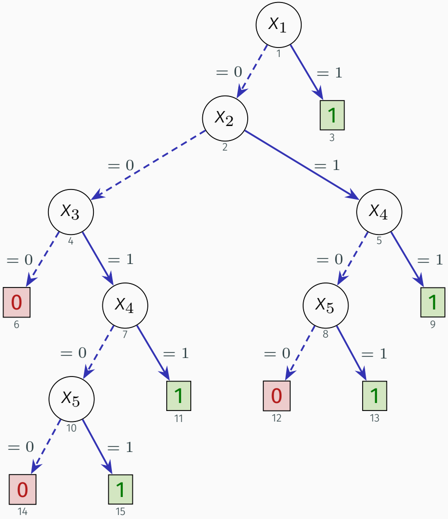
    - Why?



Outline – Part 2

Computational problems in (formal) explainability

- Compute one abductive/contrastive explanation

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Input: Predicate $\mathbb{P}$, parameterized by $\mathcal{T}$, $\mathcal{M}$
Output: One XP $\mathcal{S}$

```
procedure oneXP(ℙ)
    S ← F                      ▷ Initialization: ℙ(S) holds
    for i ∈ F do               ▷ Loop invariant: ℙ(S) holds
        if ℙ(S\{i}) then
            S ← S\{i}          ▷ Update S only if ℙ(S\{i}) holds
    return S                   ▷ Returned set S: ℙ(S) holds
```

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Exploiting MSMP, i.e. basic algorithm used for different problems.

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

- Recap:

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

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- Let,
  - Hard constraints, $\mathcal{B}$:

$$\mathcal{B} := \text{Encode}_{\mathcal{T}}(\neg\sigma(\mathbf{x})) \land_{i\in\mathcal{F}} (s_i \rightarrow (x_i = v_i))$$

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  - Soft constraints: $\mathcal{S} = \{s_i \mid i \in \mathcal{F}\}$

- **Claim**: Each MUS of $(\mathcal{B}, \mathcal{S})$ is an AXp & each MCS of $(\mathcal{B}, \mathcal{S})$ is a CXp

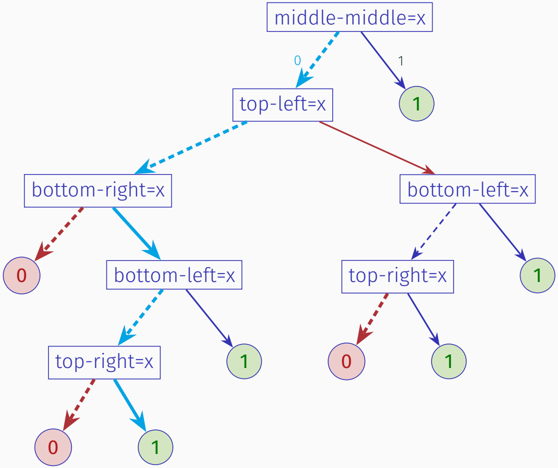
Part 3

Tractability in Symbolic XAI

Outline – Part 3

DT explanations

[IIM20]



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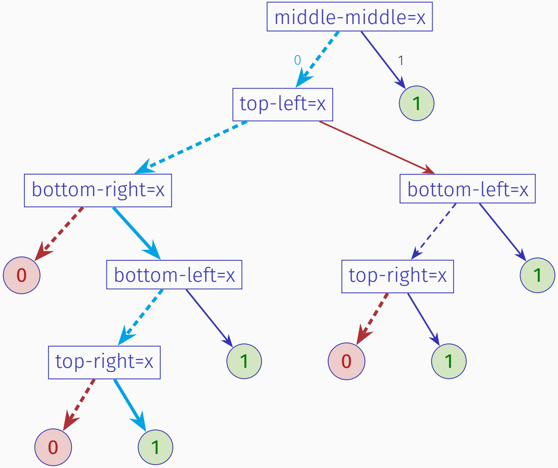
[IIM20]



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

DT explanations

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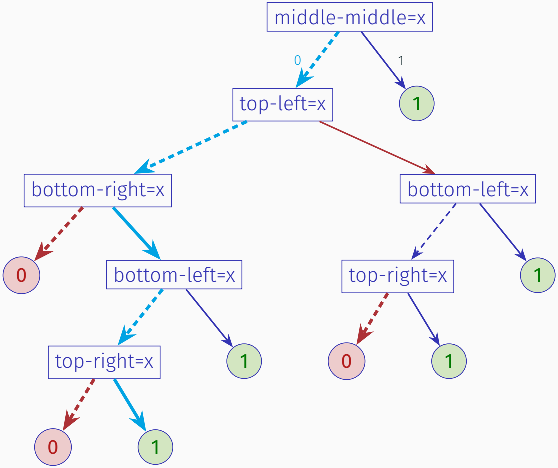

- Run PI-explanation algorithm based on NP-oracles
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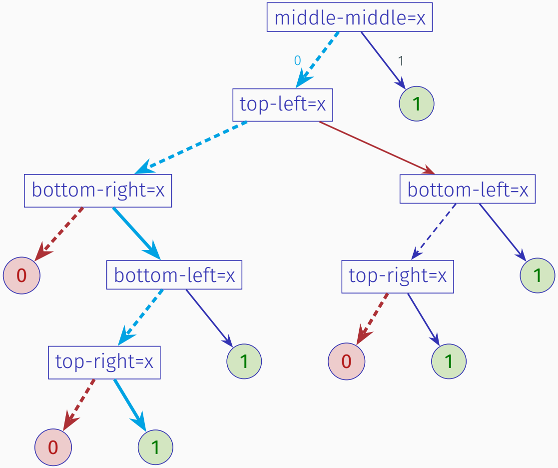
- For prediction 1, it suffices to ensure all paths with prediction 0 remain inconsistent

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 – Part 3

Explanations for Decision Trees

XAI Queries for DTs

Myth #01: Intrinsic Interpretability

Detour: From Decision Trees to Explained Decision Sets

Explanations for Monotonic Classifiers

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

Answering queries in DTs

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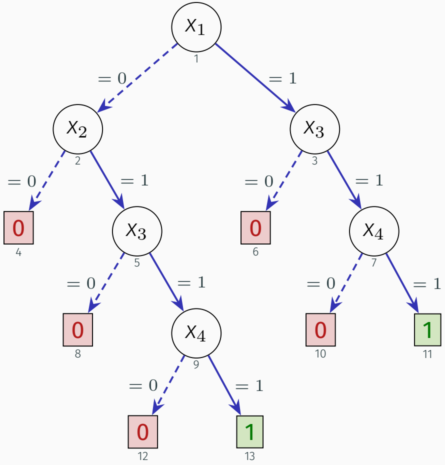
- Finding all CXps in polynomial-time; hence, finding one also in polynomial-time

Answering queries in DTs

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

Finding all CXps in polynomial-time

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



Finding all CXps in polynomial-time

- Basic algorithm:
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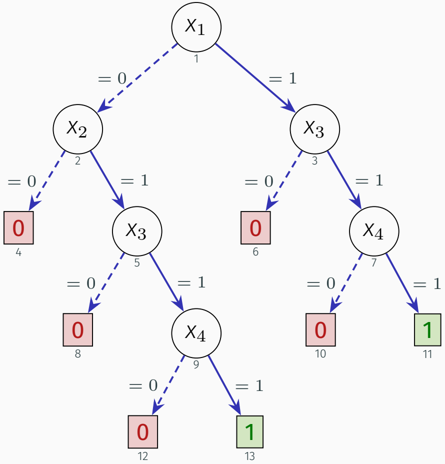
  - For each leaf node not predicting q:



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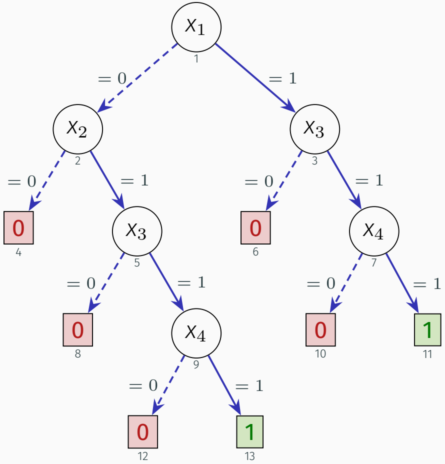

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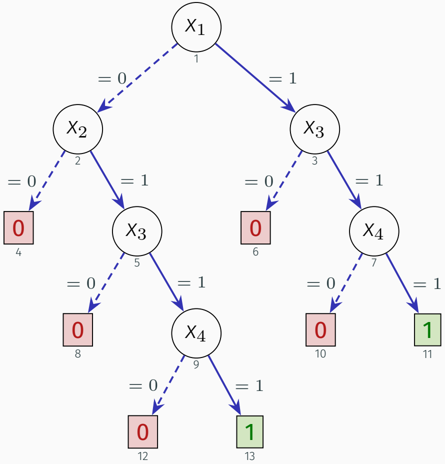

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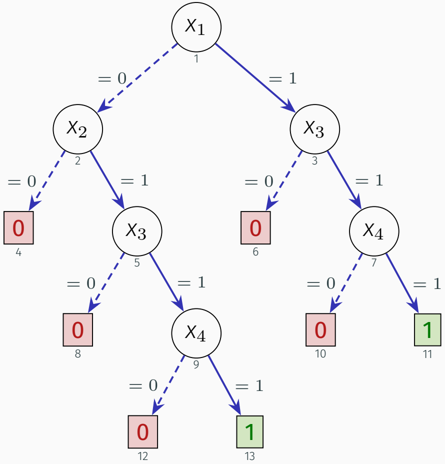

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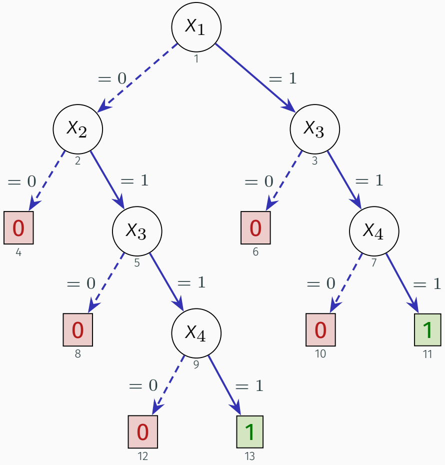

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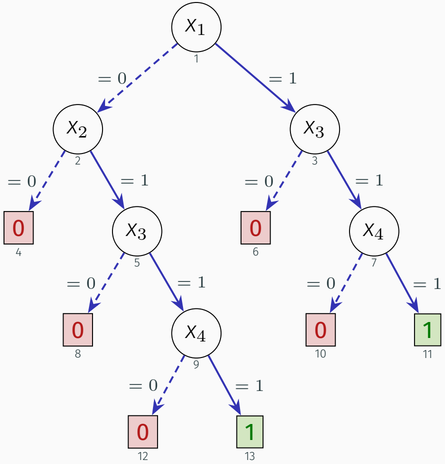

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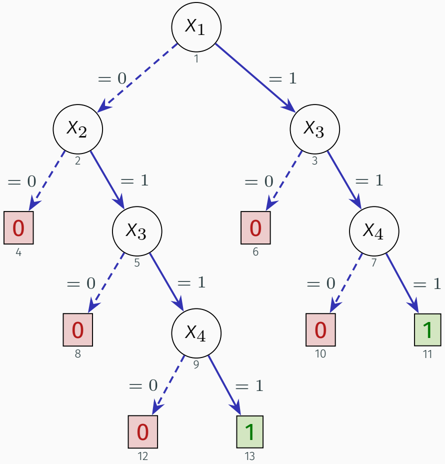
  - Add $\{1, 2\}$ to $\mathcal{L}$



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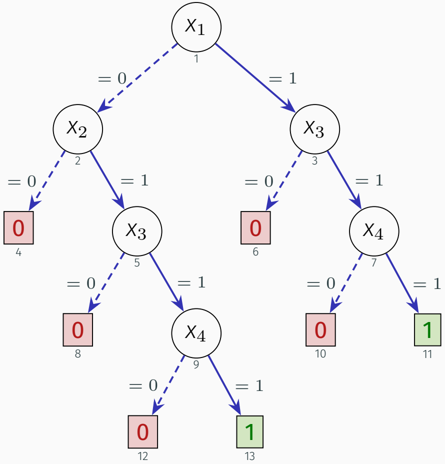

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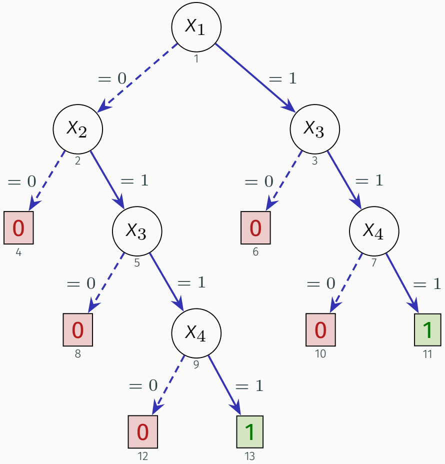

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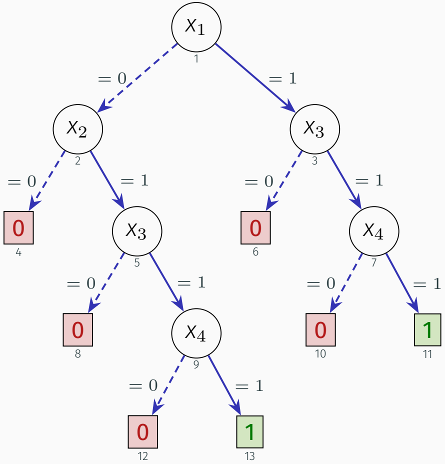
  - Add $\{3\}$ to $\mathcal{L}$



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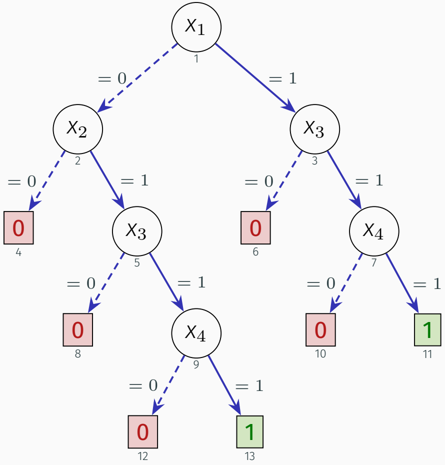

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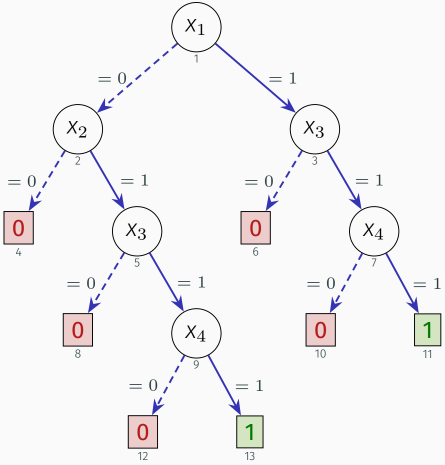
  - Remove from $\mathcal{L}$: $\{1, 3\}$ and $\{1, 4\}$



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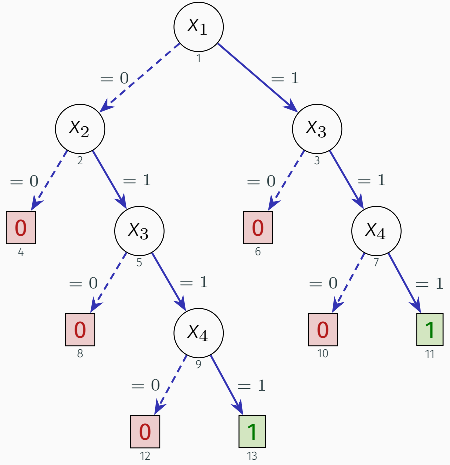
  - CXps: $\{\{1, 2\}, \{3\}, \{4\}\}$



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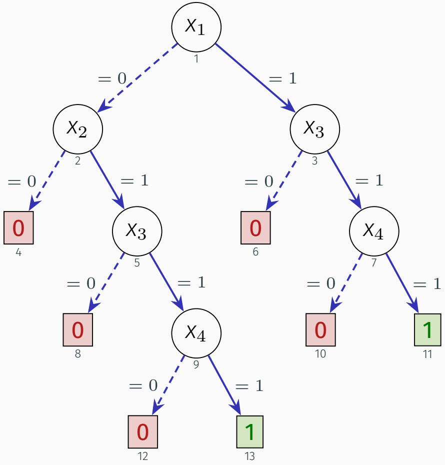
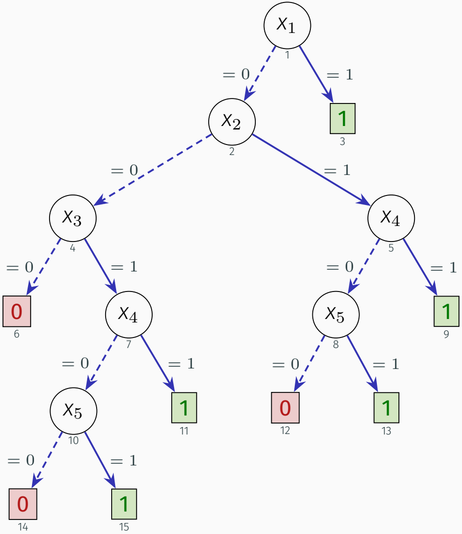
  - CXps: $\{\{1,2\},\{3\},\{4\}\}$
  - AXps: $\{\{1,3,4\},\{2,3,4\}\}$, by computing all MHSes

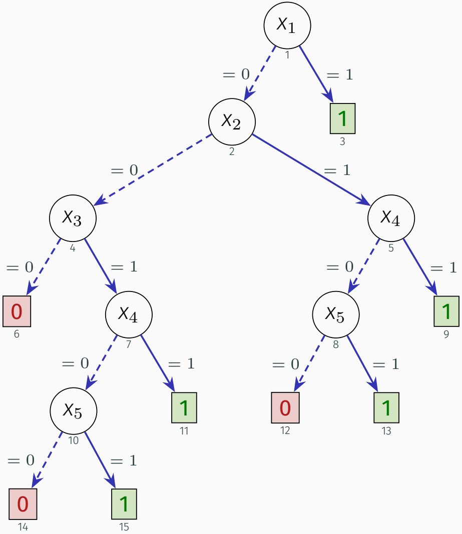


Outline – Part 3



- Case of optimal decision tree (DT) [HRS19]
- Explanation for $(0, 0, 1, 0, 1)$, with prediction 1?

Are *interpretable* models really interpretable? – DTs



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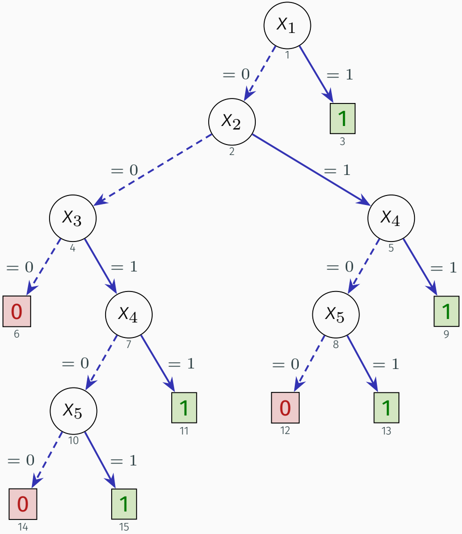
  - Clearly, IF $\neg x_1 \wedge \neg x_2 \wedge x_3 \wedge \neg x_4 \wedge x_5$ THEN $\kappa(\mathbf{x}) = 1$



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  - 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
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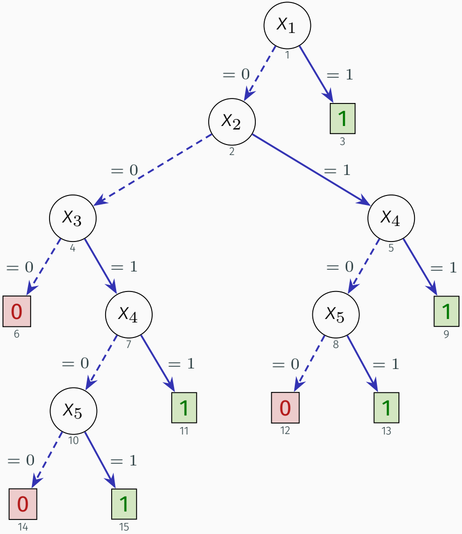

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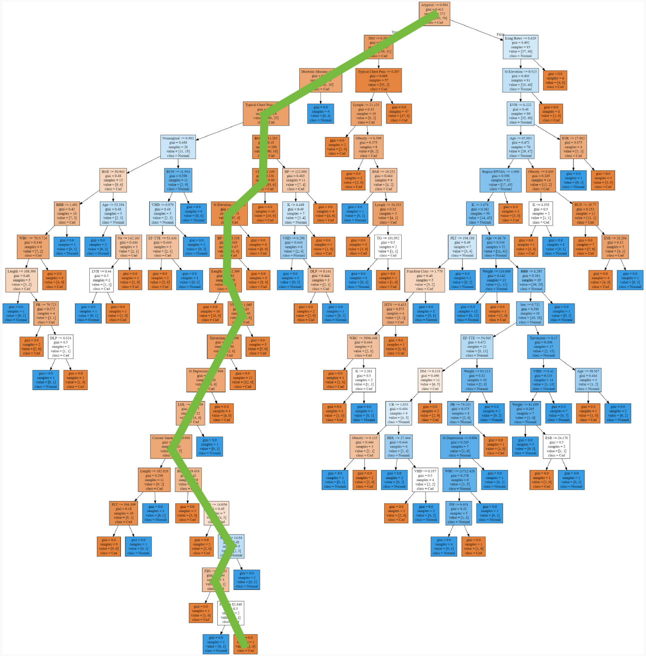
$\therefore$ one AXp is $\{3, 5\}$
Compare with $\{1, 2, 3, 4, 5\}$...

Are *interpretable* models really interpretable? – large DTs



[GZM20]

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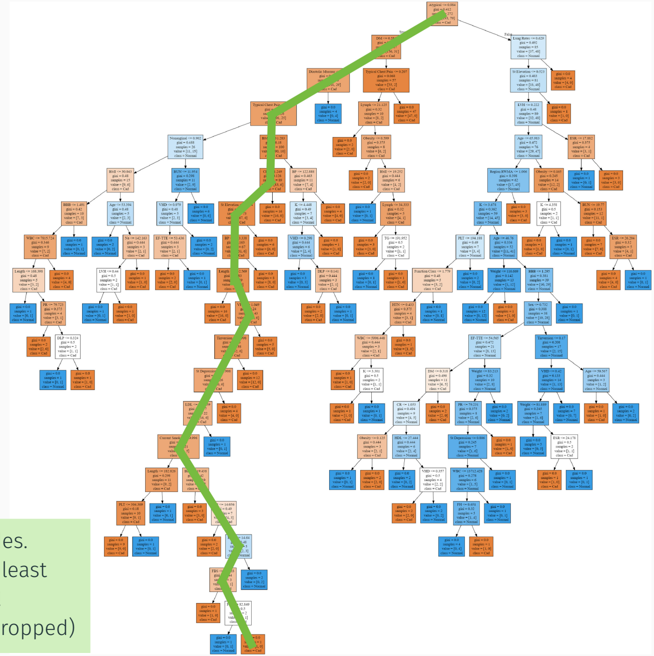

Path with 19 internal nodes.
By manual inspection, at least 10 literals are redundant!
(And at least 9 features dropped)

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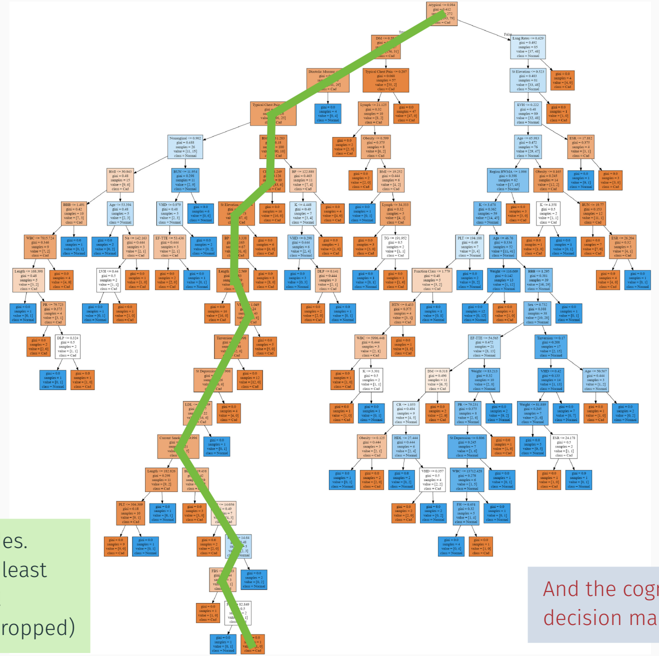

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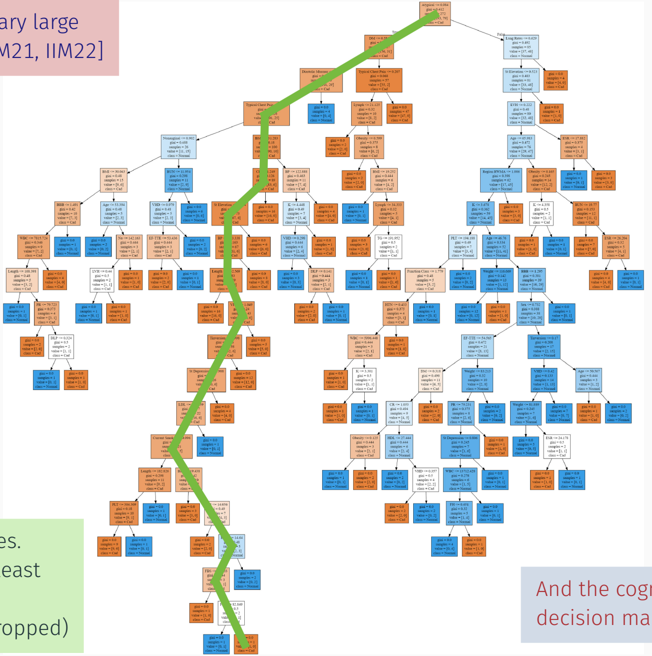
And the cognitive limits of human decision makers are well-known [Mil56]

Are *interpretable* models really interpretable? – large DTs

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

[GZM20]



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

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

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

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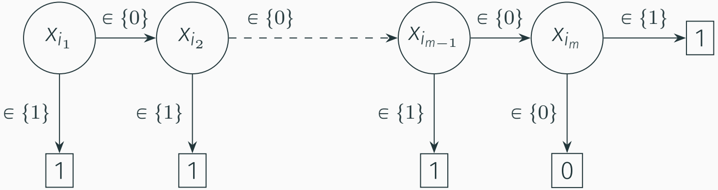

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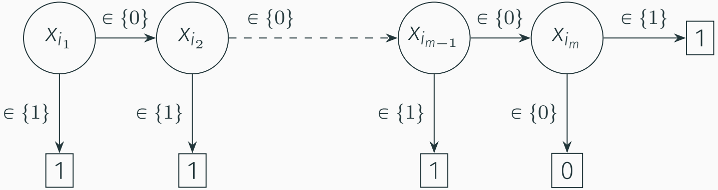

- Point: $(x_{i_1}, x_{i_2}, \ldots, x_{i_{m-1}}, x_{i_m}) = (0, 0, \ldots, 0, 1)$, and prediction 1

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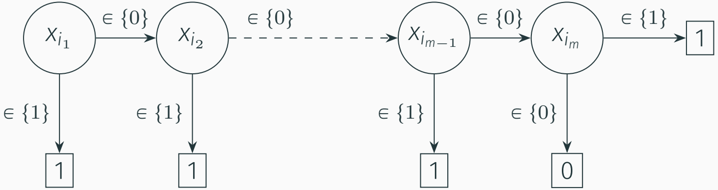

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- Explanation using path in DT: $\{i_1, i_2, \ldots, i_m\}$, i.e.

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

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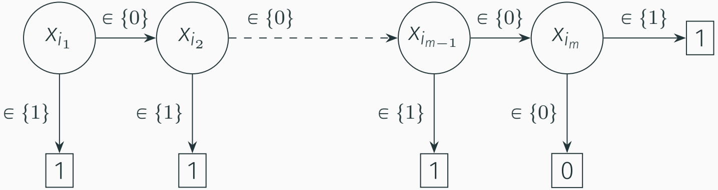

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- **But $\{i_m\}$ suffices for prediction, i.e.** $\forall(\mathbf{x} \in \{0, 1\}^m).(x_{i_m}) \rightarrow \kappa(\mathbf{x})$

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

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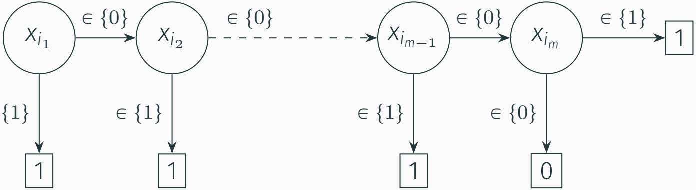


- Point: $(x_{i_1}, x_{i_2}, \ldots, x_{i_{m-1}}, x_{i_m}) = (0, 0, \ldots, 0, 1)$, and prediction 1
- Explanation using path in DT: $\{i_1, i_2, \ldots, i_m\}$, i.e.

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

- 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]

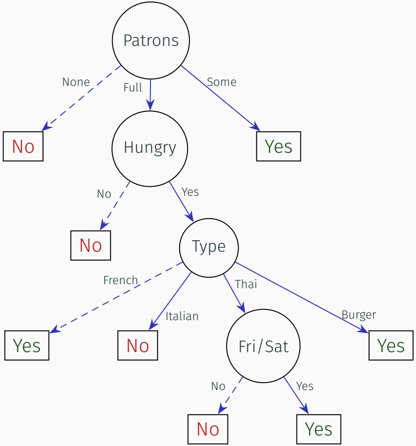
Explanation redundancy in DTs is ubiquitous – published DT examples

[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

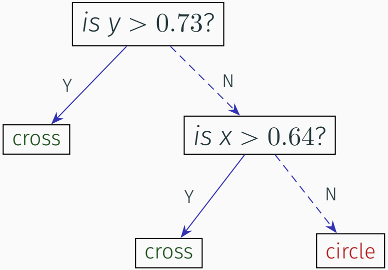
[RN10]



- 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]

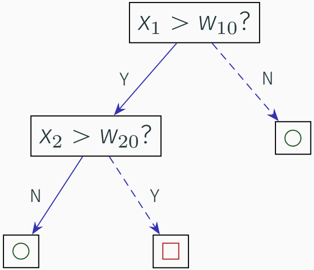


- Explanation for $(x, y) = (1.25, -1.13)$?

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]

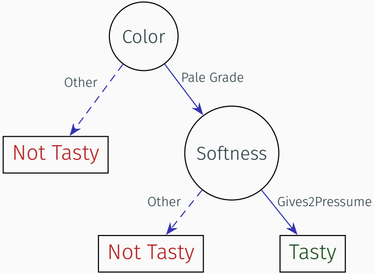


- Explanation for $(x_1, x_2) = (\alpha, \beta)$, with $\alpha > w_{10}$ and $\beta \leqslant w_{20}$?

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

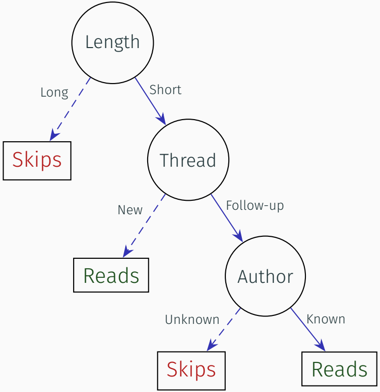
[SB14]



- Explanation for (color, softness) = (Pale Grade, Other)?

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

[PM17]



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

Explanation redundancy in DTs is ubiquitous – DTs from datasets

[IIM20, HIIM21, IIM22]

Dataset	(#F	#S)	IAI D	IAI #N	IAI %A	IAI #P	IAI %R	IAI %C	IAI %m	IAI %M	IAI %avg	ITI D	ITI #N	ITI %A	ITI #P	ITI %R	ITI %C	ITI %m	ITI %M	ITI %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	—	—	—

Are *interpretable* models really interpretable? – DLs

[MSI23]

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

Are *interpretable* models really interpretable? – DLs

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$\mathrm{R}_{\mathrm{DEF}}$:	ELSE			$\kappa(\mathbf{x}) = 1$

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- Recall: one AXp is $\{3, 4, 6\}$

Are *interpretable* models really interpretable? – DLs

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- What is the abductive explanation?
- Recall: one AXp is $\{3, 4, 6\}$
  - Why?
    - We need 3 (or 1) so that R_1 cannot fire
    - 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?

Are *interpretable* models really interpretable? – DLs

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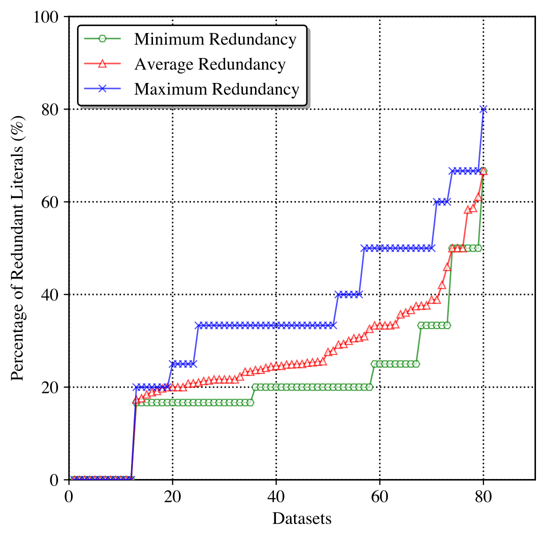
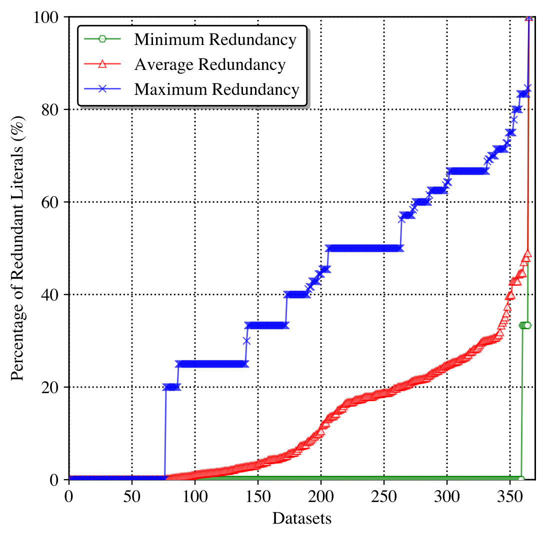
      (BTW, **we have proved that computing one AXp for DLs is computationally hard...**)

[IM21, MSI23]

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



DTs learned with Interpretable AI, max depth 6



DLs learned with CN2

Outline – Part 3

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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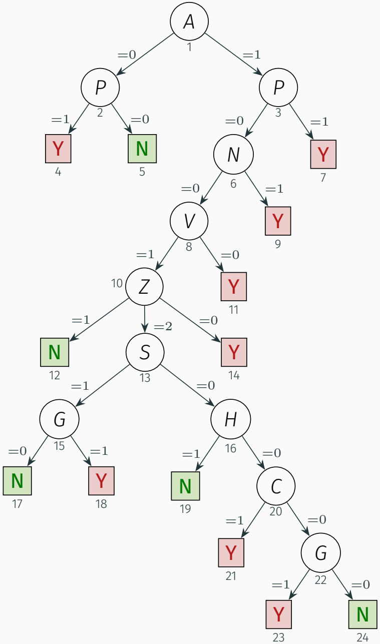
  - A DS without overlap and complete coverage computes a classification function
- And explaining DSs is computationally hard...

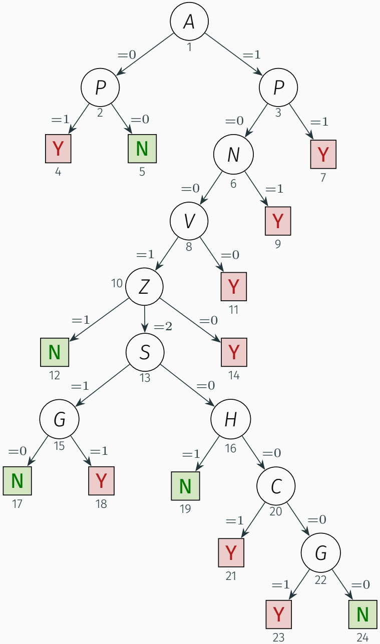
- One can extract explained DSs from DTs
  - Extract one AXp (viewed as a logic rule) from each path in DT
  - Resulting rules are non-overlapping, and cover feature space

Example



A
1
=0
=1
P
2
P
3
=1
=0
=0
=1
Y
4
N
5
N
6
Y
7
=0
=1
V
8
Y
9
=1
=0
10
Z
Y
11
=1
=2
=0
N
12
S
13
Y
14
=1
=0
G
15
H
16
=0
=1
=1
=0
N
17
Y
18
N
19
C
20
=1
=0
Y
21
G
22
=1
=0
Y
23
N
24

Example



R_{01}: IF $[P]$ THEN $\kappa(\cdot) = \mathbf{Y}$

R_{02}: IF $[\overline{A} \wedge \overline{P}]$THEN $\kappa(\cdot) = \mathbf{N}$

R_{03}: IF $[\overline{P} \wedge \overline{N} \wedge V \wedge Z = 1]$ THEN $\kappa(\cdot) = \mathbf{N}$

R_{04}: IF $[\overline{P} \wedge \overline{N} \wedge V \wedge Z = 2 \wedge S \wedge \overline{G}]$ THEN $\kappa(\cdot) = \mathbf{N}$

R_{05}: IF $[A \wedge Z = 2 \wedge S \wedge G]$ THEN $\kappa(\cdot) = \mathbf{Y}$

R_{06}: IF $[\overline{P} \wedge \overline{N} \wedge V \wedge Z = 2 \wedge \overline{S} \wedge H]$ THEN $\kappa(\cdot) = \mathbf{N}$

R_{07}: IF $[A \wedge Z = 2 \wedge \overline{S} \wedge \overline{H} \wedge C]$ THEN $\kappa(\cdot) = \mathbf{Y}$

R_{08}: IF $[A \wedge Z = 2 \wedge \overline{H} \wedge G]$ THEN $\kappa(\cdot) = \mathbf{Y}$

R_{09}: IF $[\overline{P} \wedge \overline{N} \wedge V \wedge Z = 2 \wedge \overline{C} \wedge \overline{G}]$ THEN $\kappa(\cdot) = \mathbf{N}$

R_{10}: IF $[A \wedge Z = 0]$ THEN $\kappa(\cdot) = \mathbf{Y}$

R_{11}: IF $[A \wedge \overline{V}]$ THEN $\kappa(\cdot) = \mathbf{Y}$

R_{12}: IF $[A \wedge N]$ THEN $\kappa(\cdot) = \mathbf{Y}$

Outline – Part 3

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		$\in \{0, \ldots, 10\}$
Feat. id	Feat. var.	Feat. name	Domain
1	Q	Quiz	$\{0, \ldots, 10\}$
2	X	Exam	$\{0, \ldots, 10\}$
3	H	Homework	$\{0, \ldots, 10\}$
4	R	Project	$\{0, \ldots, 10\}$

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

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

Also, $F \preccurlyeq E \preccurlyeq D \preccurlyeq C \preccurlyeq B \preccurlyeq A$

And, $\kappa(\mathbf{x_1}) \preccurlyeq \kappa(\mathbf{x_2})$ if $\mathbf{x}_1 \leqslant \mathbf{x}_2$

Explaining monotonic classifiers

- Instance $(\mathbf{v}, c)$
- Domain for $i \in \mathcal{F}$: $\lambda(i) \leqslant x_i \leqslant \mu(i)$
- Idea: refine lower and upper bounds on the prediction
  - $\mathbf{v}_\mathsf{L}$ and $\mathbf{v}_\mathsf{U}$
- Utilities:
  - FixAttr(i):

$$\begin{aligned}
&\mathbf{v}_\mathsf{L} \leftarrow (v_{\mathsf{L}_1}, \ldots, v_i, \ldots, v_{\mathsf{L}_N})\\
&\mathbf{v}_\mathsf{U} \leftarrow (v_{\mathsf{U}_1}, \ldots, v_i, \ldots, v_{\mathsf{U}_N})\\
&(\mathcal{A}, \mathcal{B}) \leftarrow (\mathcal{A} \backslash \{i\}, \mathcal{B} \cup \{i\})\\
&\textbf{return } (\mathbf{v}_\mathsf{L}, \mathbf{v}_\mathsf{U}, \mathcal{A}, \mathcal{B})
\end{aligned}$$

  - FreeAttr(i):

$$\begin{aligned}
&\mathbf{v}_\mathsf{L} \leftarrow (v_{\mathsf{L}_1}, \ldots, \lambda(i), \ldots, v_{\mathsf{L}_N})\\
&\mathbf{v}_\mathsf{U} \leftarrow (v_{\mathsf{U}_1}, \ldots, \mu(i), \ldots, v_{\mathsf{U}_N})\\
&(\mathcal{A}, \mathcal{B}) \leftarrow (\mathcal{A} \backslash \{i\}, \mathcal{B} \cup \{i\})\\
&\textbf{return } (\mathbf{v}_\mathsf{L}, \mathbf{v}_\mathsf{U}, \mathcal{A}, \mathcal{B})
\end{aligned}$$

Computing one AXp

$\mathbf{v}_\mathsf{L} \leftarrow (v_1, \ldots, v_N)$
$\mathbf{v}_\mathsf{U} \leftarrow (v_1, \ldots, v_N)$ ▻ Ensures: $\kappa(\mathbf{v}_\mathsf{L}) = \kappa(\mathbf{v}_\mathsf{U})$
$(\mathcal{C}, \mathcal{D}, \mathcal{P}) \leftarrow (\mathcal{F}, \emptyset, \emptyset)$ ▻ $\mathcal{S}$: Some possible seed
for all $i \in \mathcal{S}$ **do**
  $(\mathbf{v}_\mathsf{L}, \mathbf{v}_\mathsf{U}, \mathcal{C}, \mathcal{D}) \leftarrow \mathsf{FreeAttr}(i, \mathbf{v}, \mathbf{v}_\mathsf{L}, \mathbf{v}_\mathsf{U}, \mathcal{C}, \mathcal{D})$ ▻ Require: $\kappa(\mathbf{v}_\mathsf{L}) = \kappa(\mathbf{v}_\mathsf{U})$, given $\mathcal{S}$
for all $i \in \mathcal{F} \setminus \mathcal{S}$ **do** ▻ Loop inv.: $\kappa(\mathbf{v}_\mathsf{L}) = \kappa(\mathbf{v}_\mathsf{U})$
  $(\mathbf{v}_\mathsf{L}, \mathbf{v}_\mathsf{U}, \mathcal{C}, \mathcal{D}) \leftarrow \mathsf{FreeAttr}(i, \mathbf{v}, \mathbf{v}_\mathsf{L}, \mathbf{v}_\mathsf{U}, \mathcal{C}, \mathcal{D})$
  if $\kappa(\mathbf{v}_\mathsf{L}) \neq \kappa(\mathbf{v}_\mathsf{U})$ **then** ▻ If invariant broken, fix it
    $(\mathbf{v}_\mathsf{L}, \mathbf{v}_\mathsf{U}, \mathcal{D}, \mathcal{P}) \leftarrow \mathsf{FixAttr}(i, \mathbf{v}, \mathbf{v}_\mathsf{L}, \mathbf{v}_\mathsf{U}, \mathcal{D}, \mathcal{P})$
return $\mathcal{P}$

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)

Part 4

(Efficient) Intractability in Symbolic XAI

Outline – Part 4

An encoding for DLs – components

R_1:	IF	(τ_1)	THEN	d_1
R_2:	ELSE IF	(τ_2)	THEN	d_2
		$\ldots$		
R_j:	ELSE IF	(τ_j)	THEN	d_j
		$\ldots$		
R_n:	ELSE IF	(τ_n)	THEN	d_n
$\mathrm{R}_{\mathrm{DEF}}$:	ELSE		THEN	d_{n+1}

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

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

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		$\ldots$		
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- Let $e_j = 1$ iff d_j matches c
- Require that at least one f_j, with $e_j = 0$ and $1 \leqslant j \leqslant n$, to be consistent (i.e. some rule up to j with prediction other than c to fire):

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

An encoding for DLs – components

R_1:	IF	(τ_1)	THEN	d_1
R_2:	ELSE IF	(τ_2)	THEN	d_2
		$\ldots$		
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		$\ldots$		
R_n:	ELSE IF	(τ_n)	THEN	d_n
R_{DEF}:	ELSE		THEN	d_{n+1}

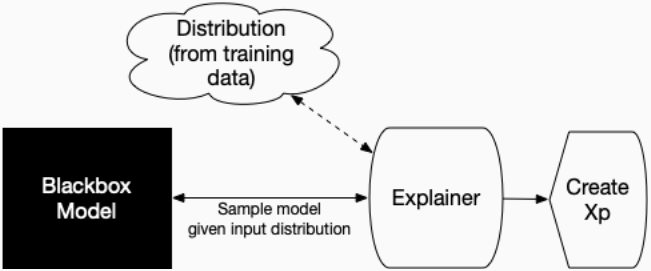
- The set of soft clauses is given by: $\mathcal{S} \triangleq \{(l_i), i = 1, \ldots, m\}$
- The set of hard clauses is given by:

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

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

Outline – Part 4

What is model-agnostic explainability?



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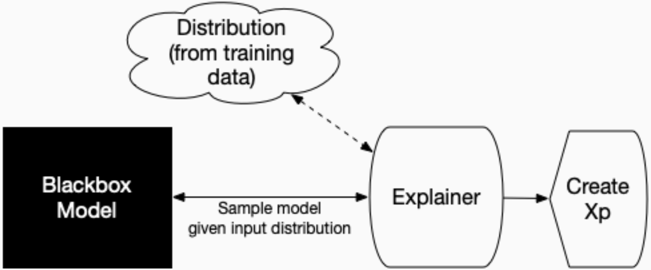

- Wildly popular XAI approach [RSG16, LL17, RSG18]
  - **Feature attribution**: LIME, SHAP, ... [RSG16, LL17]
  - **Feature selection**: Anchors, ... [RSG18]

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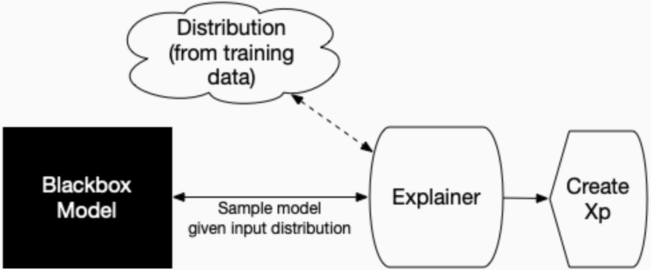

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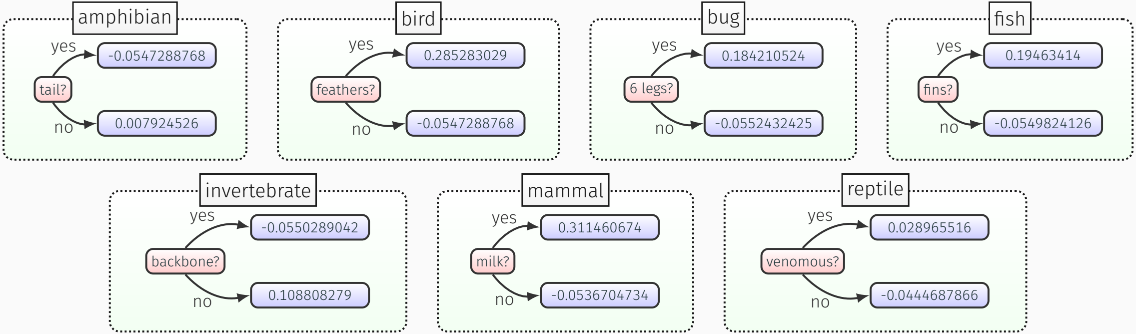
- **Q:** Are model-agnostic explanations rigorous?

Easy to spot problems – BT for zoo dataset

[INM19c, Ign20]



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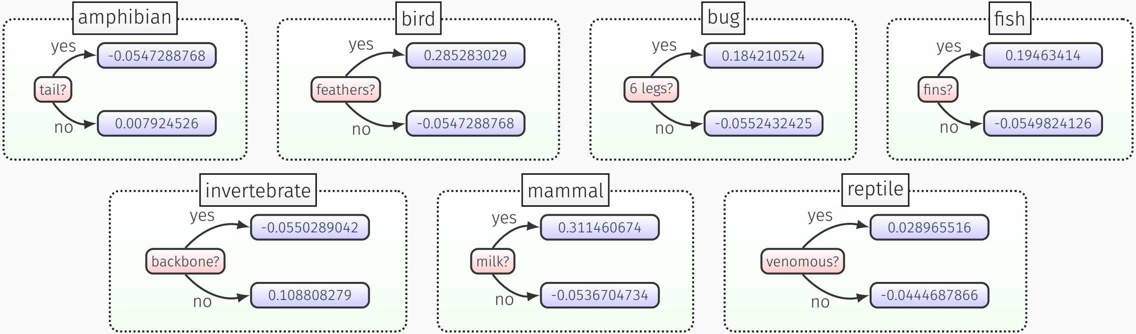
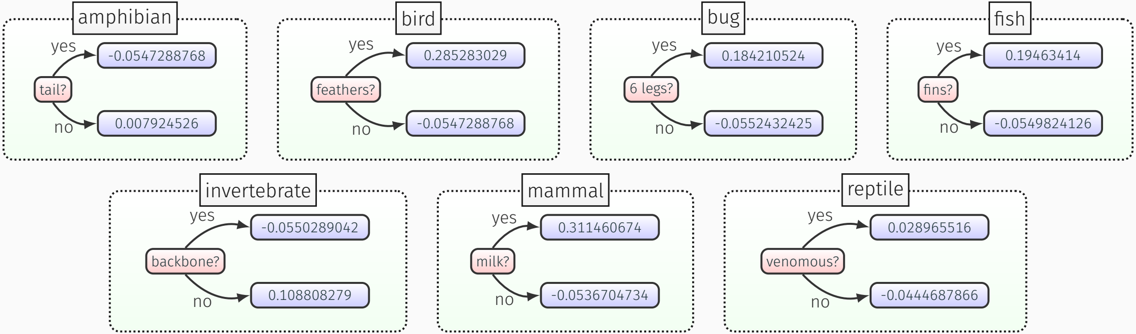


- Example instance:

IF (animal_name = pitviper) ∧ ¬hair ∧ ¬feathers ∧ eggs ∧ ¬milk ∧ ¬airborne ∧ ¬aquatic ∧ predator ∧ ¬toothed ∧ backbone ∧ breathes ∧ venomous ∧ ¬fins ∧ (legs = 0) ∧ tail ∧ ¬domestic ∧ ¬catsize

THEN (class = reptile)



- Example instance (& Anchor picks): [RSG18]

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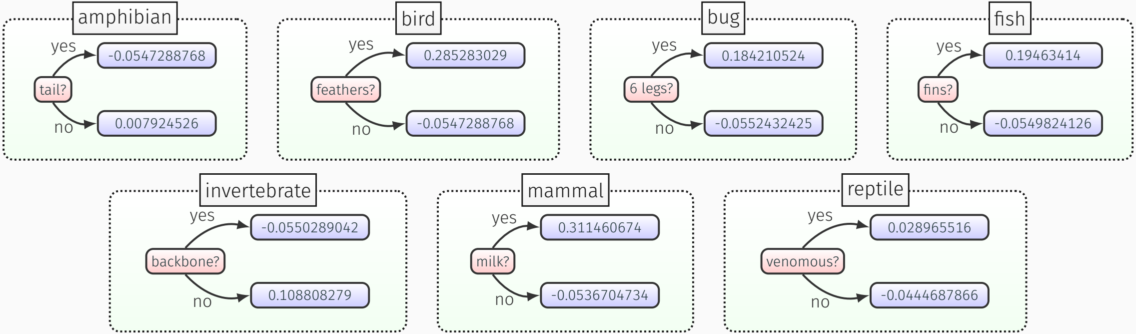

- Explanation obtained with Anchor: [RSG18]

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

Easy to spot problems – BT for zoo dataset & Anchor

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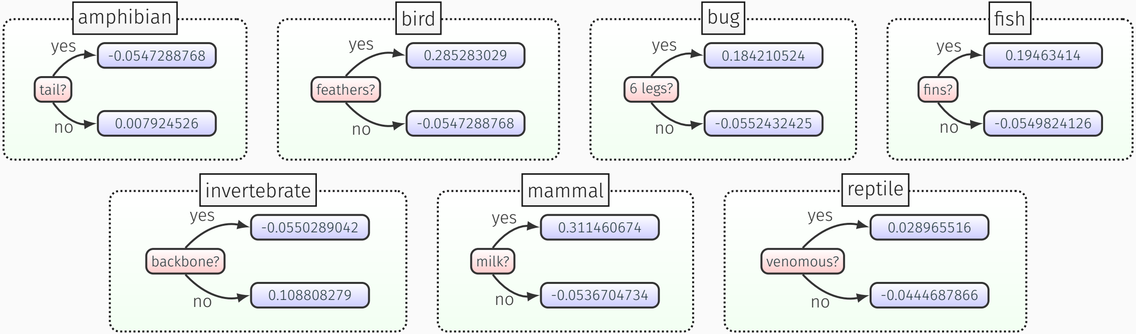

- **But**, explanation **incorrectly "explains"** another instance (from training data!)

IF	(animal_name = toad) ∧ ¬***hair*** ∧ ¬feathers ∧ eggs ∧ ¬***milk*** ∧ ¬airborne ∧ ¬aquatic ∧ ¬predator ∧ ¬***toothed*** ∧ backbone ∧ breathes ∧ ¬venomous ∧ ¬***fins*** ∧ (legs = 4) ∧ ¬tail ∧ ¬domestic ∧ ¬catsize
THEN	(class = amphibian)

Model-agnostic explainers cannot be trusted

[INM19c]

Incorrect explanations:

Classifier for deciding bank loans

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Two samples: Bessie $:= (v_1, \mathsf{Y})$ and Clive $:= (v_2, \mathsf{N})$

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X is consistent with Bessie $:= (\mathbf{v}_1, \text{Y})$

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X is consistent with Clive $:= (\mathbf{v}_2, \mathsf{N})$

$\therefore$ different outcomes & same explanation !?

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

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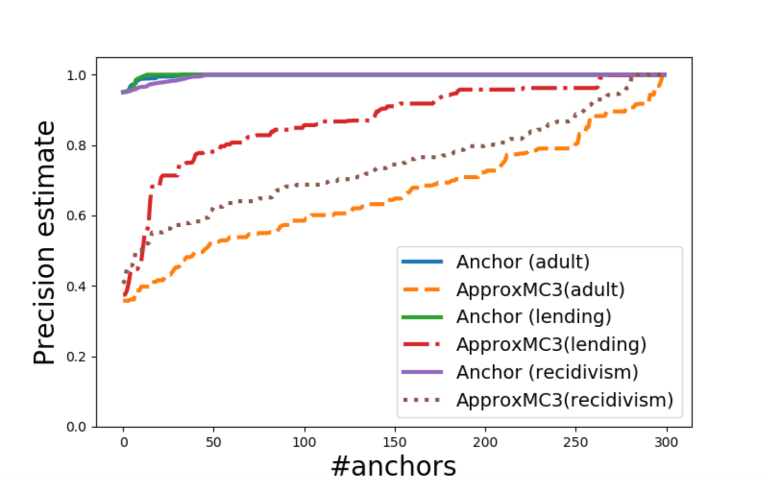
- For feature attribution we proposed different ways of assessing rigor [INM19c, NSM+19, Ign20, YIS+23]

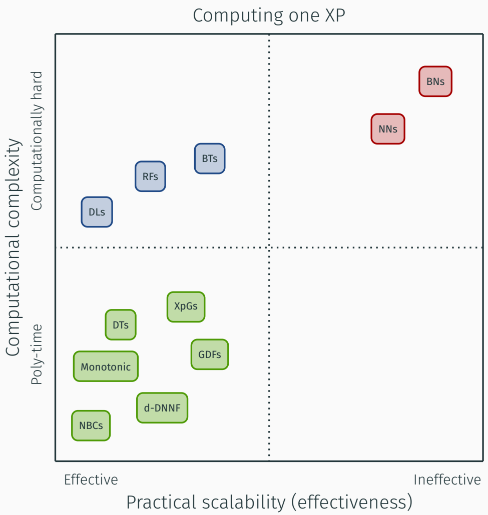
Incorrect explanations are ubiquitous & likely...

[NSM+19]



Outline – Part 4

[MI22, Mar22, MS23]



[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]
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    - Additional results [CM21, HII+22]
  - Comp. hard, but effective (efficient in practice):
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  - Comp. hard, and ineffective (hard in practice):
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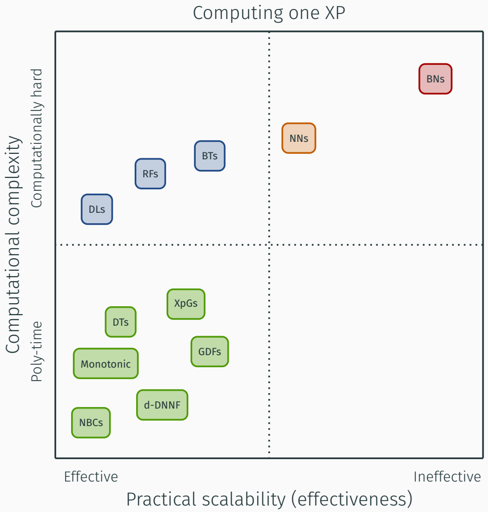
    - Bayesian networks (BNs) [SCD18]

Efficacy map – recent progress

[HM23b]



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Results for RFs in 2021 (with SAT)

[IMS21]

Dataset	(#F	#C	#I)	RF			CNF		SAT oracle				AXp (**RFxpl**)				Anchor	
				D	#N	%A	#var	#cl	MxS	MxU	#S	#U	Mx	m	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	0.03
		a	5.15	0.65	0.20	4.86	2.18	0.41
		M	9	6.11	0.41	9	24.80	1.81
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	0.01	0.04
		a	11.42	0.07	0.06	9.39	4.07	2.89
		M	19	0.26	0.20	19	27.05	22.23
voting	(16)	m	3	0.01	0.02	3	0.01	0.02
		a	4.56	0.04	0.13	3.46	0.3	0.25
		M	11	0.10	0.37	11	1.25	1.77
spect	(22)	m	3	0.02	0.02	3	0.02	0.04
		a	7.31	0.13	0.07	6.44	1.61	0.67
		M	20	0.88	0.29	20	8.97	10.73

Results for NNs in 2019 (with SMT/MILP)

[INM19a]

First rigorous approach for **explaining** NNs !

			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	0.03
		a	5.15	0.65	0.20	4.86	2.18	0.41
		M	9	6.11	0.41	9	24.80	1.81
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	0.01	0.04
		a	11.42	0.07	0.06	9.39	4.07	2.89
		M	19	0.26	0.20	19	27.05	22.23
voting	(16)	m	3	0.01	0.02	3	0.01	0.02
		a	4.56	0.04	0.13	3.46	0.3	0.25
		M	11	0.10	0.37	11	1.25	1.77
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Scales to (a few) **tens** of neurons...

Recent results for NNs (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
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Scales to a few **hundred** neurons

Questions?

Recap last lecture

- Symbolic XAI by feature selection:

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  - (W)AXps/(W)CXps & duality
    - Quantifier-based, probability-based, expected value-based

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    - For DTs: all CXps in polynomial-time
  - Intractability of XPs: DLs, RFs/BTs/TEs, NNs
  - And myths of non-symbolic XAI:
    - Intrinsic interpretability
    - Model-agnostic explainability

(W)AXps/(W)CXps

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

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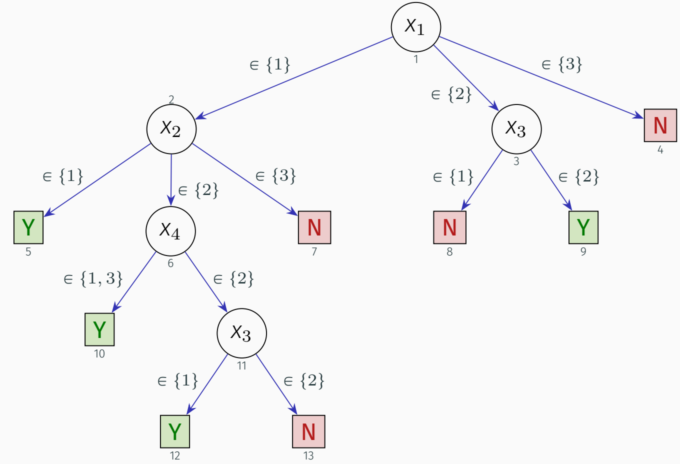
Input: Predicate $\mathbb{P}$, parameterized by $\mathcal{T}$, $\mathcal{M}$
Output: One XP $\mathcal{S}$

```
procedure oneXP(ℙ)
    𝒮 ← ℱ                          ▷ Initialization: ℙ(𝒮) holds
    for i ∈ ℱ do                   ▷ Loop invariant: ℙ(𝒮) holds
        if ℙ(𝒮\{i}) then
            𝒮 ← 𝒮\{i}              ▷ Update 𝒮 only if ℙ(𝒮\{i}) holds
    return 𝒮                       ▷ Returned set 𝒮: ℙ(𝒮) holds
```

Warm-up exercise – one AXp for example DT

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



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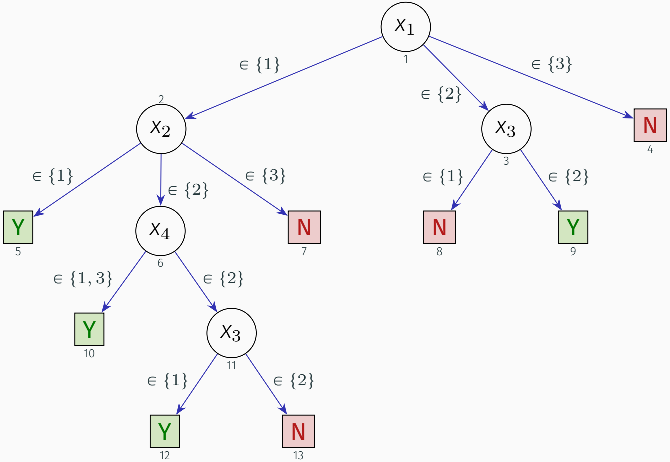

- AXp: $\{1, 2, 3\}$

Another warm-up exercise – one AXp for example DL

- DL:

$$
\begin{array}{llccl}
\mathrm{R}_1: & \mathrm{IF} & (x_1 \land x_3) & \mathrm{THEN} & \kappa(\mathbf{x}) = 0 \\
\mathrm{R}_2: & \mathrm{ELSE\ IF} & (x_1 \land x_5) & \mathrm{THEN} & \kappa(\mathbf{x}) = 0 \\
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  - The prediction is 1, due to R_3

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    - The prediction is 1, due to R_3
- AXp: $\{1, 2\}$
- Quiz: write down the constraints and confirm AXp with SAT solver

Plan for this short course

- 1^{st} day:
  - Part #0a: Motivation
  - Part #1: Foundations
  - Part #2: Principles of symbolic XAI – feature selection (& myth of interpretability)
  - Part #3: Tractable symbolic XAI
  - Part #4: Intractable symbolic XAI (& myth of model-agnostic XAI)
  - Q&A
- 2^{nd} day:
  - Part #0b: Recapitulate
  - Part #5: Explainability queries
  - Part #6: Advanced topics
  - Part #7: Principles of symbolic XAI – feature attribution (& myth of Shapley values in XAI)
  - Part #8: Conclusions & research directions
  - Q&A

Part 5

Queries in Symbolic XAI

Outline – Part 5

Enumeration of Explanations

Feature Necessity & Relevancy

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- Best solution is a MARCO-like algorithm (for enumerating MUSes) [LPMM16]
  - On-demand enumeration of AXp's/CXp's

Generic oracle-based algorithm

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

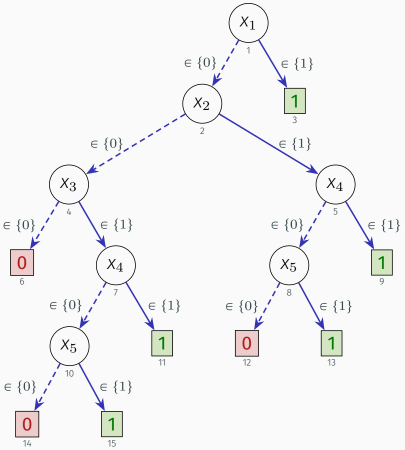
$\mathcal{H} \leftarrow \emptyset$ ▷ $\mathcal{H}$ defined on set $U = \{u_1, \ldots, u_m\}$
repeat
  $(\text{outc}, \mathbf{u}) \leftarrow \text{SAT}(\mathcal{H})$
  if $\text{outc} = \textbf{true}$ **then**
    $\mathcal{S} \leftarrow \{i \in \mathcal{F} \,|\, u_i = 0\}$ ▷ $\mathcal{S}$: *fixed* features
    $\mathcal{U} \leftarrow \{i \in \mathcal{F} \,|\, u_i = 1\}$ ▷ $\mathcal{U}$: *universal* features; $\mathcal{F} = \mathcal{S} \cup \mathcal{U}$
    if $\mathbb{P}_{\text{cxp}}(\mathcal{U}; \mathcal{T}, \mathcal{F}, \kappa, \mathbf{v})$ **then** ▷ $\mathcal{U} = \mathcal{F} \setminus \mathcal{S} \supseteq$ some CXp
      $\mathcal{P} \leftarrow \text{oneXP}(\mathcal{U}; \mathbb{P}_{\text{cxp}}, \mathcal{T}, \mathcal{F}, \kappa, \mathbf{v})$
      $\text{reportCXp}(\mathcal{P})$
      $\mathcal{H} \leftarrow \mathcal{H} \cup \{(\vee_{i \in \mathcal{P}} \neg u_i)\}$
    else ▷ $\mathcal{S} \supseteq$ some AXp
      $\mathcal{P} \leftarrow \text{oneXP}(\mathcal{S}; \mathbb{P}_{\text{axp}}, \mathcal{T}, \mathcal{F}, \kappa, \mathbf{v})$
      $\text{reportAXp}(\mathcal{P})$
      $\mathcal{H} \leftarrow \mathcal{H} \cup \{(\vee_{i \in \mathcal{P}} u_i)\}$
until $\text{outc} = \textbf{false}$

Recall oneXP

Input: Predicate $\mathbb{P}$, parameterized by $\mathcal{T}$, $\mathcal{M}$
Output: One XP $\mathcal{S}$

procedure oneXP($\mathbb{P}$)
  $\mathcal{S} \leftarrow \mathcal{F}$ ▷ Initialization: $\mathbb{P}(\mathcal{S})$ holds
  for $i \in \mathcal{F}$ **do** ▷ Loop invariant: $\mathbb{P}(\mathcal{S})$ holds
    if $\mathbb{P}(\mathcal{S} \backslash \{i\})$ **then**
      $\mathcal{S} \leftarrow \mathcal{S} \backslash \{i\}$ ▷ Update $\mathcal{S}$ only if $\mathbb{P}(\mathcal{S} \backslash \{i\})$ holds
  return $\mathcal{S}$ ▷ Returned set $\mathcal{S}$: $\mathbb{P}(\mathcal{S})$ holds

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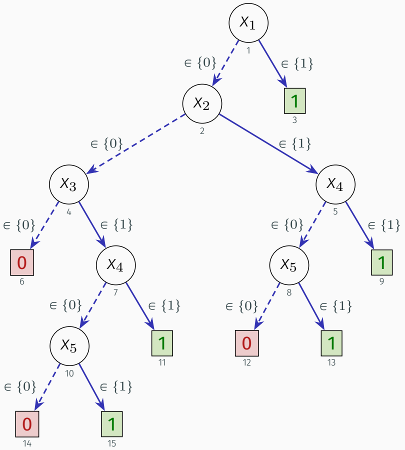
x_3	x_5	x_1	x_2	x_4	$\kappa_2(\mathbf{x})$
0	0	0	0	0	0
0	1	0	0	0	0
1	0	0	0	0	0
1	1	0	0	0	1

DT classifier – example run of enumerator



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

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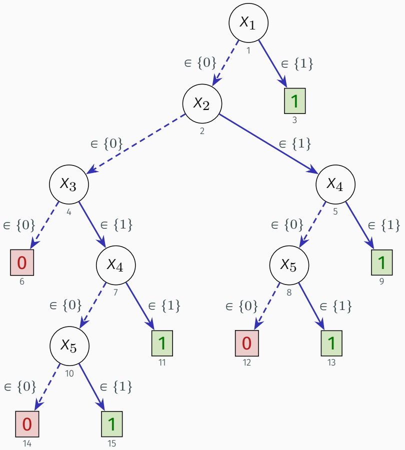
Iter.	$\mathbf{u}$	$\mathcal{S}$	$\mathbb{P}_{\text{cxp}}(\cdot)$	AXp	CXp	Clause
1	$(1,1,1,1,1)$	$\emptyset$	1	–	$\{3\}$	$(\neg u_3)$
2	$(1,1,0,1,1)$	$\{3\}$	1	–	$\{5\}$	$(\neg u_5)$
3	$(1,1,0,1,0)$	$\{3,5\}$	0	$\{3,5\}$	–	$(u_3 \vee u_5)$
5	[outc = **false**]	–	–	–	–	–

DT classifier – another example run of enumerator



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Iter.	$\mathbf{u}$	$\mathcal{S}$	$\mathbb{P}_{\text{cxp}}(\cdot)$	AXp	CXp	Clause
1	$(0,0,0,0,0)$	$\{1,2,3,4,5\}$	0	$\{3,5\}$	–	$(u_3 \vee u_5)$
2	$(0,0,1,0,0)$	$\{1,2,4,5\}$	1	–	$\{3\}$	$(\neg u_3)$
3	$(0,0,1,0,1)$	$\{1,2,4\}$	1	–	$\{5\}$	$(\neg u_5)$
5	[outc = **false**]	–	–	–	–	–

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 $\mathcal{I}$
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- $\mathcal{I}$ is the set of CXp's – algorithm runs in poly-time

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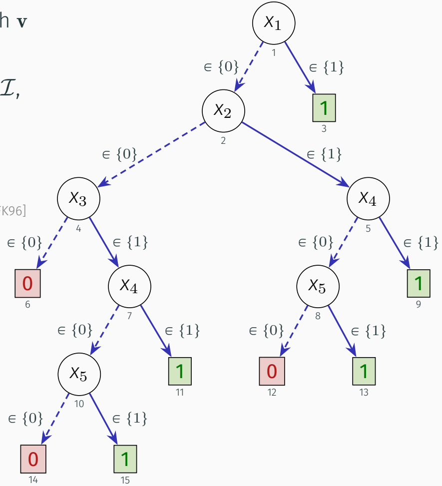
- Example:
  - $I_1 = \{3\}$
  - $I_2 = \{5\}$
  - $I_3 = \{2, 5\}$
  - $\therefore$ keep I_1 an I_2
  - AXp's: MHSes yield $\{\{3, 5\}\}$



Outline – Part 5

Feature necessity

- Consider instance $(\mathbf{v}, c)$
- Sets of all AXp's & CXp's:

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- A feature $i \in \mathcal{F}$ is **irrelevant** if $i \notin F_{\mathbb{A}}$ (and so, if $i \notin F_{\mathbb{C}}$)
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An example

- Consider the classifier:

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

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

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- 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**)

Abstraction refinement for feature relevancy

- **Claim**: $\mathcal{X} \subseteq \mathcal{F}$ and $t \in \mathcal{X}$. If WAXp($\mathcal{X}$) holds and 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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- Approach:
  - Guess weak AXp candidates: $t \in \mathcal{X} \wedge \text{WAXp}(\mathcal{X})$
  - Check weak AXp candidates: $\neg\text{WAXp}(\mathcal{X} \setminus \{t\})$

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  - Block counterexamples

A general abstraction refinement algorithm

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

function FRPCGR($\mathbf{v}, t; \mathcal{F}, \kappa$)
    $\mathcal{H} \leftarrow \emptyset$ ▷ $\mathcal{H}$ overapproximates the subsets of $\mathcal{F}$ that do not contain an AXp containing t
    repeat
        $(\text{outc}, \mathbf{s}) \leftarrow \text{SAT}(\mathcal{H}, s_t)$ ▷ **Use SAT oracle to pick candidate wAXp containing** t
        if outc = **true then**
            $\mathcal{P} \leftarrow \{i \in \mathcal{F} \mid s_i = 1\}$ ▷ Set $\mathcal{P}$ is the candidate wAXp, and $t \in \mathcal{P}$
            $\mathcal{D} \leftarrow \{i \in \mathcal{F} \mid s_i = 0\}$ ▷ Set $\mathcal{D}$ contains the features not included in $\mathcal{P}$
            if $\neg$WAXp($\mathcal{P}$) **then** ▷ Is $\mathcal{P}$ not a wAXp?
                $\mathcal{H} \leftarrow \mathcal{H} \cup \text{newPosCl}(\mathcal{D}; t, \kappa)$ ▷ Picked set is *not* a wAXp; block set
            else ▷ Picked set is a wAXp
                if $\neg$WAXp($\mathcal{P} \setminus \{t\}$) **then** ▷ $\mathcal{P}$ without t not a wAXp?
                    reportWeakAXp($\mathcal{P}$) ▷ Feature t is included in any AXp $\mathcal{X} \subseteq \mathcal{P}$
                    return true
                $\mathcal{H} \leftarrow \mathcal{H} \cup \text{newNegCl}(\mathcal{P}; t, \kappa)$ ▷ t unneeded for keeping prediction; block set
    until outc = **false**
    return false ▷ If $\mathcal{H}$ becomes inconsistent, then there is no AXp that contains t

Part 6

Advanced Topics

Outline – Part 6

Inflated Explanations

Probabilistic Explanations

Constrained Explanations

Distance-Restricted Explanations

Certified Explainability

Towards more expressive explanations – inflated explanations

[IISM24]

- Recall:

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

  - 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

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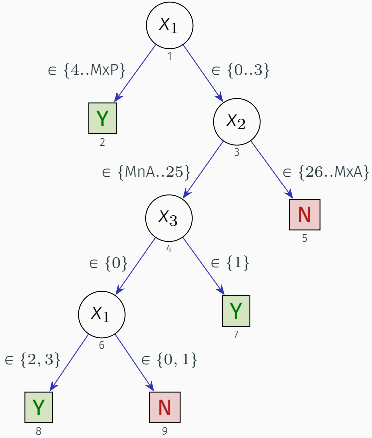
- Inflated explanations allow for more expressive literals, i.e. $=$ replaced with $\in$, and individual values replaced by ranges of values
  - Definition: Given an AXp, expand set of values of each feature, in some chosen order, such that the set of picked features remains unchanged

Inflated explanations – an example

[IIM22]



- Explanation for $((1, 10, 0, 2), \text{Y})$? (Obs: MnA $\leqslant 10$)

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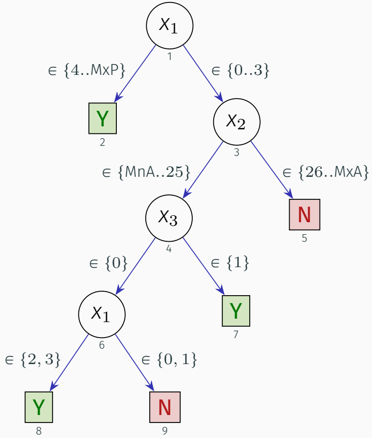

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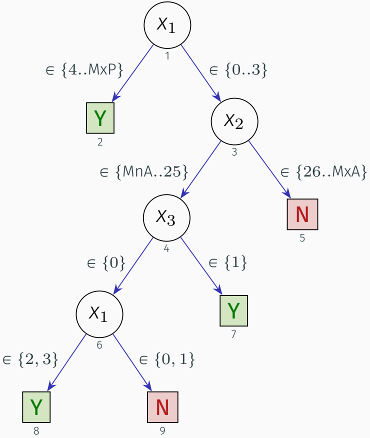
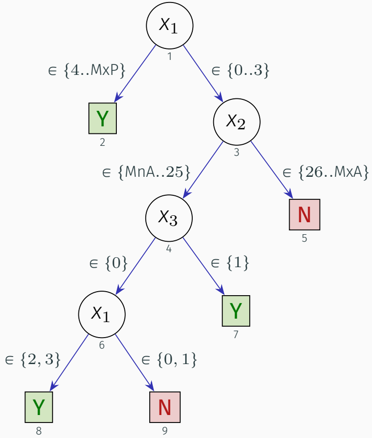


- Explanation for $((1, 10, 0, 2), \mathsf{Y})$? (Obs: $\mathsf{MnA} \leqslant 10$)
  - AXp: $\{1, 2\}$
  - Default interpretation: $\forall(\mathbf{x} \in \mathbb{F}).(x_1 = 2 \land x_2 = 10) \rightarrow (\kappa(\mathbf{x}) = \mathsf{Y})$

Inflated explanations – an example

[IIM22]



- Explanation for $((1,10,0,2),\mathsf{Y})$? (Obs: $\mathsf{MnA} \leqslant 10$)
  - AXp: $\{1,2\}$
  - Default interpretation: $\forall(\mathbf{x} \in \mathbb{F}).(x_1 = 2 \land x_2 = 10) \rightarrow (\kappa(\mathbf{x}) = \mathsf{Y})$
  - With inflated explanations: $\forall(\mathbf{x} \in \mathbb{F}).(x_1 \in \{2..\mathsf{MxP}\} \land x_2 \in \{\mathsf{MnA}..25\}) \rightarrow (\kappa(\mathbf{x}) = \mathsf{Y})$

Approach

- Compute 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 expanded domains simultaneously

Outline – Part 6

Probabilistic (formal) explanations

[WMHK21, IIN+22, IHI+22, ABOS22, IHI+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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- Probabilistic explanations provide smaller explanations, by trading off rigor of explanation by explanation size
- Definition of weak probabilistic AXp $\mathcal{X} \subseteq \mathcal{F}$:

$$\mathsf{WPAXp}(\mathcal{X}) \quad := \quad \mathbf{Pr}(\kappa(\mathbf{x}) = c) \,|\, \mathbf{x}_{\mathcal{X}} = \mathbf{v}_{\mathcal{X}}) \geqslant \delta$$

  - 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 $\mathcal{X}$
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  - Obs: for $\delta = 1$ we obtain a WAXp
- But definition of WPAXp is non-monotonic
  - Standard algorithms for finding one AXp cannot be used
  - Recent dedicated algorithms for simple ML models [IHI+23]
  - Recent approximate algorithms for simple ML models [IMM24]

Results for decision trees

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

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
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	1.49
					90	9	4	7.2	96	24.65	9	5	7.4	97.0	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	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	0.04
					90	8	2	5.3	95.9	0.23	8	2	5.4	96.6	94.6	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	0.38
					90	9	3	7.3	98.3	4.06	9	3	7.5	98.6	98.0	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	0.03
					90	9	3	3.3	94.8	0.10	9	3	3.4	94.6	100	0.03

Outline – Part 6

Not all inputs may be possible – input constraints

[GR22, YIS+23]

- Infer constraints on the inputs
  - Learn simple rules relating inputs
  - Represent rules as a constraint set, e.g. $\mathcal{C}(\mathbf{x})$
- Redefine WAXps/WCXps to account for input constraints:

$$\forall(\mathbf{x} \in \mathbb{F}).\left[\bigwedge\nolimits_{j\in\mathcal{X}}(x_j = v_j) \land \mathcal{C}(\mathbf{x})\right] \rightarrow (\kappa(\mathbf{x}) = c)$$

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

  - Compute AXps/CXps given new definitions

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

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

Outline – Part 6

How to tackle poor performance on NNs?

- For NNs, computation of AXps scales to a few tens of neurons [INM19a]

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  - Obs: we already proved some basic (duality) properties for global explanations [INM19b]
- Change definition of WAXp/WCXp to account for l_p distance to $\mathbf{v}$:

$$\forall(\mathbf{x} \in \mathbb{F}).\left[\bigwedge_{j\in\mathcal{X}}(x_j = v_j) \land \left(\|\mathbf{x}-\mathbf{v}\|_{l_p} \leqslant \epsilon\right)\right] \rightarrow (\sigma(\mathbf{x}))$$

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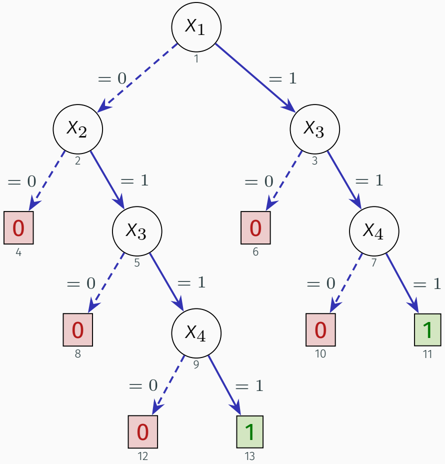
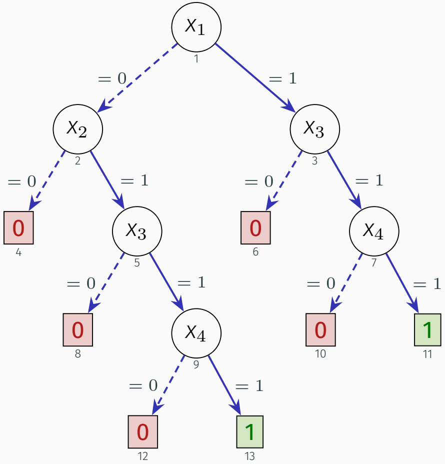
  - Norm l_p is arbitrary, e.g. Hamming, Manhattan, Euclidean, etc.
  - **Distance-restricted explanations**: $\mathfrak{d}$AXp/$\mathfrak{d}$CXp

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



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

- Plain AXps/CXps:



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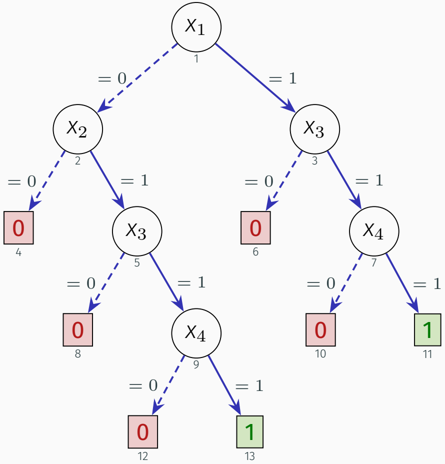
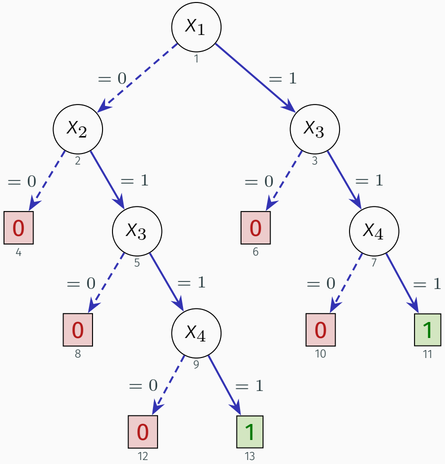
  - AXps?



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

- Plain AXps/CXps:
  - AXps? $\{\{1, 3, 4\}, \{2, 3, 4\}\}$
  - CXps?



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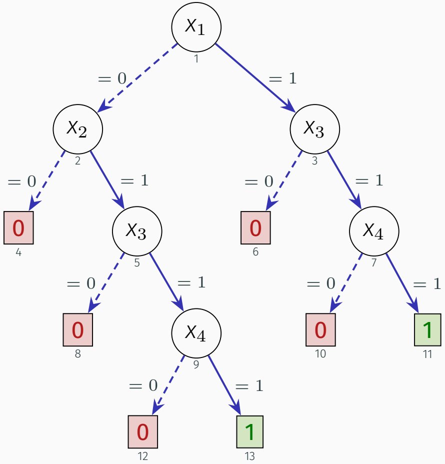

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    - AXps? $\{\{1,3,4\},\{2,3,4\}\}$
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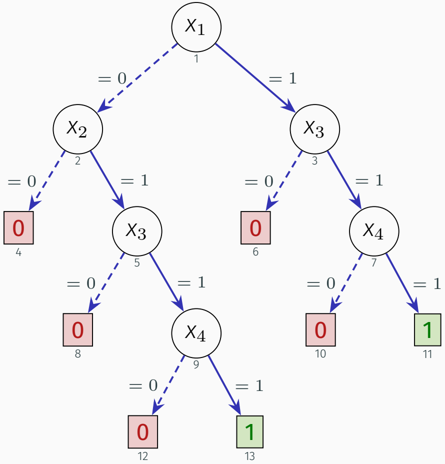
- Distance-restricted AXps/CXps, $\mathfrak{d}$AXp/$\mathfrak{d}$CXp, with Hamming distance (l_0) and $\epsilon = 1$:



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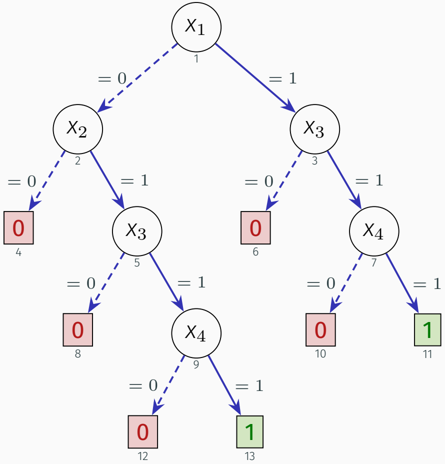
  - CXps? $\{\{1,2\},\{3\},\{4\}\}$
- Distance-restricted AXps/CXps, $\mathfrak{d}$AXp/$\mathfrak{d}$CXp, with Hamming distance (l_0) and $\epsilon = 1$:
  - $\mathfrak{d}$AXps?



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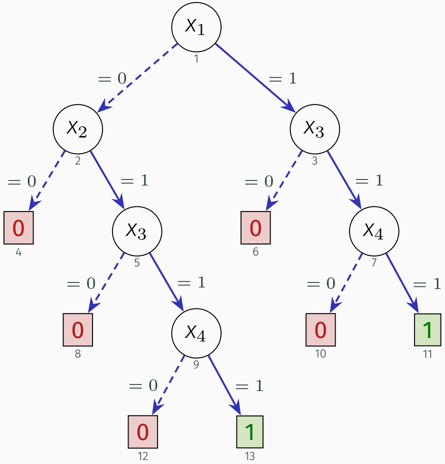

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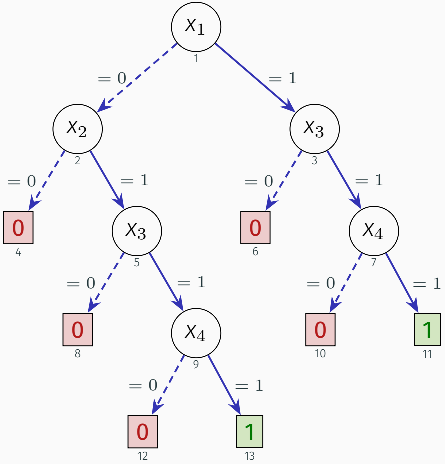

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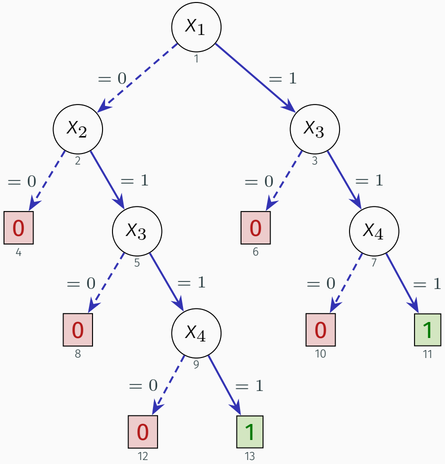
  - AXps? $\{\{1,3,4\},\{2,3,4\}\}$
  - CXps? $\{\{1,2\},\{3\},\{4\}\}$
- Distance-restricted AXps/CXps, $\mathfrak{d}$AXp/$\mathfrak{d}$CXp, with Hamming distance (l_0) and $\epsilon = 1$:
  - $\mathfrak{d}$AXps? $\{\{3,4\}\}$
  - $\mathfrak{d}$CXps? $\{\{3\},\{4\}\}$
- Given ϵ, larger adversarial examples are excluded



Relating explanations with adversarial examples

- Distance-restricted WAXps/WCXps:

$$\forall(\mathbf{x} \in \mathbb{F}). \left[\bigwedge\nolimits_{j \in \mathcal{X}} (x_j = v_j) \wedge \left(\|\mathbf{x} - \mathbf{v}\|_{l_p} \leqslant \epsilon\right)\right] \rightarrow (\sigma(\mathbf{x}))$$

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- Given norm l_p and distance ϵ, there exists a (distance-restricted) WCXp iff there exists an adversarial example
    - Use robustness tool to decide existence of WCXp
    - But, WAXp decided given non existence of CXp!

Relating explanations with adversarial examples

- Distance-restricted WAXps/WCXps:

$$\forall(\mathbf{x} \in \mathbb{F}). \left[\bigwedge_{j\in\mathcal{X}}(x_j = v_j) \land \left(\|\mathbf{x} - \mathbf{v}\|_{l_p} \leqslant \epsilon\right)\right] \rightarrow (\sigma(\mathbf{x}))$$

$$\exists(\mathbf{x} \in \mathbb{F}). \left[\bigwedge_{j\in\mathcal{X}}(x_j = v_j) \land \left(\|\mathbf{x} - \mathbf{v}\|_{l_p} \leqslant \epsilon\right)\right] \land (\neg\sigma(\mathbf{x}))$$

- Given norm l_p and distance ϵ, there exists a (distance-restricted) WCXp iff there exists an adversarial example
  - **Use robustness tool to decide existence of WCXp**
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- At present: clear scalability improvements for explaining NNs (see next) [HM23b, WWB23, IHM+24]

Basic algorithm

[HM23b]

Input: Arguments: ϵ; Parameters: $\mathcal{E}$, p
Output: One ∂AXp $\mathcal{S}$

function FindAXpDel(ϵ; $\mathcal{E}$, p)
  $\mathcal{S} \leftarrow \mathcal{F}$ ▷ Initially, no feature is allowed to change
  for $i \in \mathcal{F}$ **do** ▷ Invariant: ∂WAXp($\mathcal{S}$)
    $\mathcal{S} \leftarrow \mathcal{S} \setminus \{i\}$
    outc ← FindAdvEx($\epsilon, \mathcal{S}; \mathcal{E}, p$)
    if outc **then**
      $\mathcal{S} \leftarrow \mathcal{S} \cup \{i\}$
  return $\mathcal{S}$ ▷ ∂WAXp($\mathcal{S}$) ∧ minimal($\mathcal{S}$) → ∂AXp($\mathcal{S}$)

- Necessary to tackle number of features:
  - Exploiting parallelization [IHM+24]

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

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

More recent results (from 2024)... [IHM+24]

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

Outline – Part 6

Inflated Explanations

Probabilistic Explanations

Constrained Explanations

Distance-Restricted Explanations

Certified Explainability

Certified explainer (for monotonic classification)

[HM23f]

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  - Formalize algorithm, e.g. explanations for monotonic classifiers, e.g. using Coq
  - Prove that formalized algorithm is correct
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- Certification envisioned for **any** explainability algorithm

Part 7

Principles of Symbolic XAI – Feature Attribution

Outline – Part 7

What are Shapley values?

- First proposed in game theory in the early 50s [Sha53]
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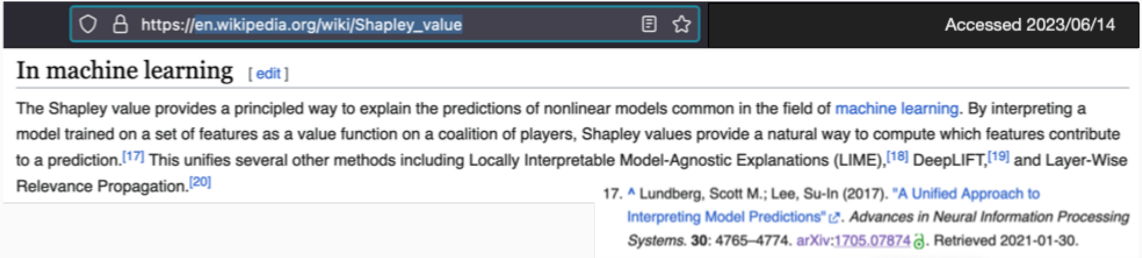
https://en.wikipedia.org/wiki/Shapley_value

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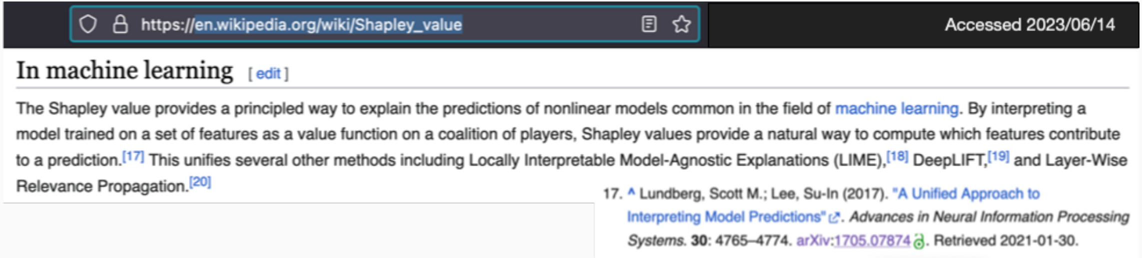
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- **Q:** Do Shapley values for XAI **really** provide a rigorous measure of feature importance?

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

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

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- Sc: $\mathcal{F} \rightarrow \mathbb{R}$ defined by,

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

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

- **Obs:** Uniform distribution assumed; it suffices for our purposes

How are Shapley values computed in practice?

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

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- 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****."*
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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, or relevant features with a Shapley of zero?
    - Recap: **relevant** features occur in **some** AXp/CXp; **irrelevant** features do **not** occur in **any** AXp/CXp

Outline – Part 7

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

[HM23c, HM23d, HM23e, MH23]

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

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

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  - Issue I3 occurs if,

$$\mathsf{Relevant}(i) \land (\mathsf{Sv}(i) = 0)$$

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

  - Issue I4 occurs if,

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

  - Issue I5 occurs if,

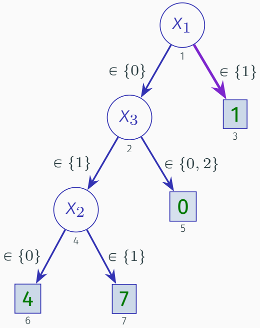
$$[\mathsf{Irrelevant}(i) \land \forall_{1 \leq j \leq m, j \neq i} (|\mathsf{Sv}(j)| < |\mathsf{Sv}(i)|)]$$

Some stats – all boolean functions with 4 variables

[HM23c, HM23d, HM23e, MH23]

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	$[\text{Irrelevant}(i) \land (\text{Sv}(i) \neq 0)]$
# of I2 issues	105184	
# of functions with I2 issues	40448	
% I2 issues / function	61.72	$[\text{Irrelevant}(i_1) \land \text{Relevant}(i_2) \land (\lvert\text{Sv}(i_1)\rvert > \lvert\text{Sv}(i_2)\rvert)]$
# of I3 issues	43008	
# of functions with I3 issues	7800	
% I3 issues / function	11.90	$[\text{Relevant}(i) \land (\text{Sv}(i) = 0)]$
# of I4 issues	5728	
# of functions with I4 issues	2592	
% I4 issues / function	3.96	$[\text{Irrelevant}(i_1) \land (\text{Sv}(i_1) \neq 0)] \land [\text{Relevant}(i_2) \land (\text{Sv}(i_2) = 0)]$
# of I5 issues	1664	
# of functions with I5 issues	1248	
% I5 issues / function	1.90	$[\text{Irrelevant}(i) \land \forall_{1 \leqslant j \leqslant m, j \neq i} (\lvert\text{Sv}(j)\rvert < \lvert\text{Sv}(i)\rvert)]$

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



DT1

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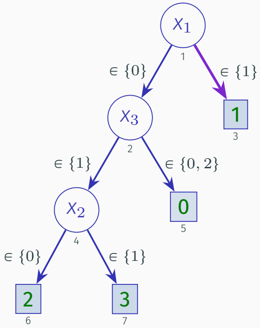
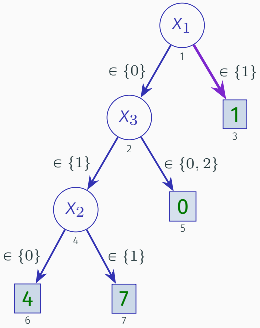
Tabular representations



DT2

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



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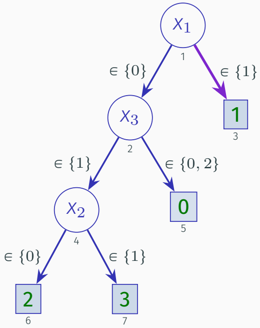
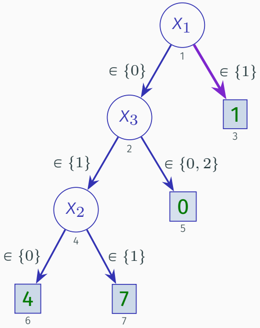


DT2

Computing XPs – make sense...



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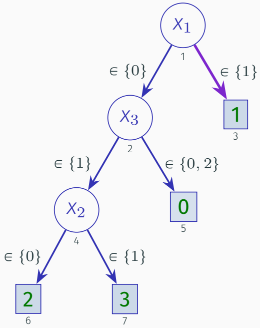

DT2

XPs: AXps/CXps		
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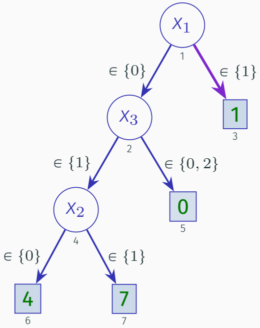
Computing XPs, AEs – also make sense...



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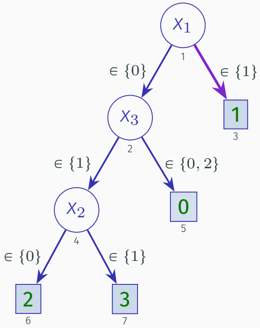

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Adversarial Examples	
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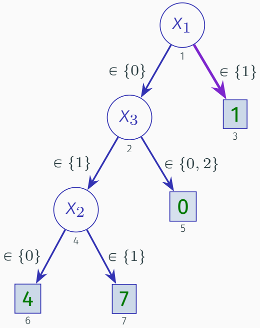

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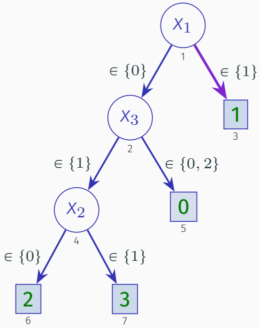

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Shapley values			
DT	Sc(1)	Sc(2)	Sc(3)
DT1	0.000	0.083	-0.500
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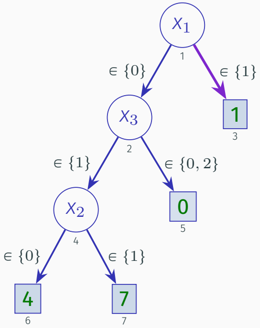
Computing XPs, AEs & Svs – what???



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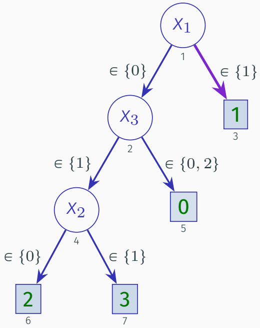

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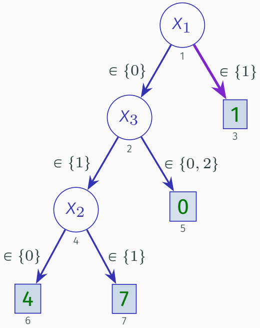

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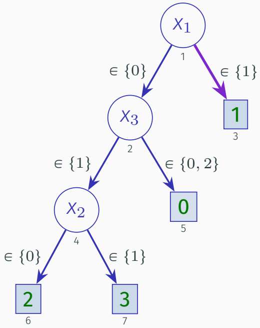

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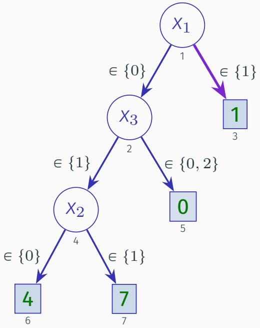

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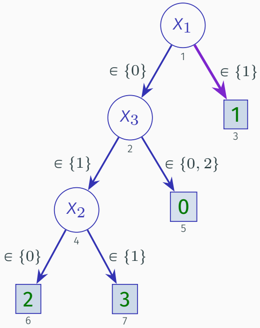

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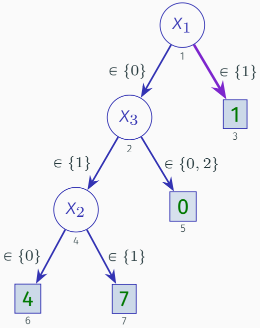

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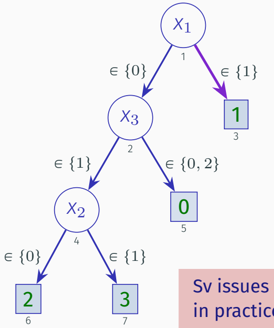

DT2

Sv issues also occur in practice [HM23e]

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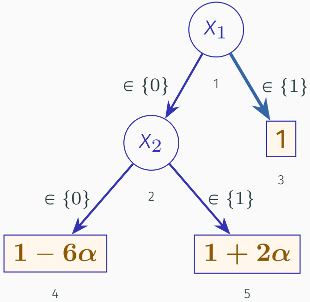

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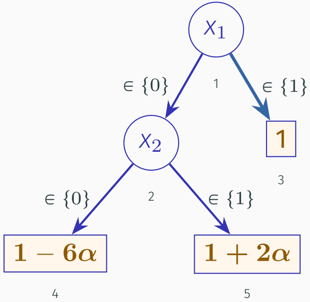

- Instance: $((1, 1), 1)$

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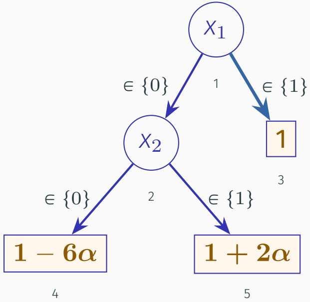
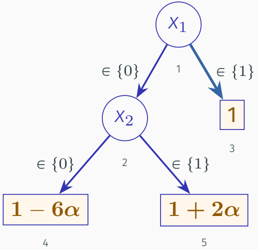


- Instance: $((1, 1), 1)$
- $\text{Sc}_E(1) = 0$
- $\text{Sc}_E(2) = \alpha$

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



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

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

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

Outline – Part 7

Exact Shapley Values for XAI

Myth #03: Shapley Values for XAI

Corrected SHAP Scores

Detour: 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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Corrected SHAP scores & feature importance scores

[LHMS24, LHAMS24]

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- Replace characteristic function based on expected values by new characteristic function based on AXps/WAXps [LHMS24]
  - Resulting scores are Shapley values, and identified issues no longer observed

Corrected SHAP scores & feature importance scores

[LHMS24, LHAMS24]

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- Observed tight connection between feature attribution and power indices from a priori voting power
- Feature importance scores [LHAMS24]
  - Generalize recent axiomatic aggregations [BIL+24]
  - Adapt best known power indices
  - Devise new scores for XAI

An initial compromise

- Replace the characteristic function used for SHAP scores:

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

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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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- Issues with non-boolean classifiers disappear; issues with boolean classifiers remain

Fixing the known issues of SHAP scores

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- Known issues of SHAP scores guaranteed not to occur

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

  - **Recall:** $\mathbf{E}[\sigma(\mathbf{x}) \,|\, \mathbf{x}_{\mathcal{S}} = \mathbf{v}_{\mathcal{S}}] = 1$ holds iff $\mathcal{S}$ is a WAXp
- 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

Outline – Part 7

Exact Shapley Values for XAI

Myth #03: Shapley Values for XAI

Corrected SHAP Scores

Detour: Power Indices

Feature Importance Scores

What is a priori voting power?

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    - 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

An example – EEC (EU) members voting power in 1958

Coutry	Acronym	# Votes
France	F	4
Germany	D	4
Italy	I	4
Belgium	B	2
Netherlands	N	2
Luxembourg	L	1
Quota:	12	

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- WVG: $[12; 4, 4, 4, 2, 2, 1]$
- **Q**: What should be the voting power of Luxembourg?
- Can Luxembourg (L) *matter* for some winning coalition?
- Perhaps surprisingly, answer is **No**!
  - In 1958, Luxembourg was a dummy voter/player

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- Many power indices proposed over the years:
  - Penrose [Pen46]
  - Shapley-Shubik [SS54]
  - Banzhaf [BI65]
  - Coleman [Col71]
  - Johnston [Joh78]
  - Deegan-Packel [DP78]
  - Holler-Packel [HP83]
  - Andjiga [ACL03]
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  - ...

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  - Responsability* [CH04, BIL+24]
  - ...
- 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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    - If the voter votes Yes, then we have a winning coalition; and
    - If the voter votes No, then we have a losing coalition.
- Understanding 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
- Obs: A subset-minimal winning coalition corresponds to an AXp
  - And a non-minimal winning coalition corresponds to a WAXp

Example power indices I

- Necessary definitions:

$$\mathbb{WA}_i(\mathcal{E}) = \{\mathcal{S} \subseteq \mathcal{F} \,|\, \text{WAXp}(\mathcal{S};\mathcal{E}) \land i \in \mathcal{S}\}$$
$$\mathbb{WC}_i(\mathcal{E}) = \{\mathcal{S} \subseteq \mathcal{F} \,|\, \text{WCXp}(\mathcal{S};\mathcal{E}) \land i \in \mathcal{S}\}$$
$$\mathbb{A}_i(\mathcal{E}) = \{\mathcal{S} \subseteq \mathcal{F} \,|\, \text{AXp}(\mathcal{S};\mathcal{E}) \land i \in \mathcal{S}\}$$
$$\mathbb{C}_i(\mathcal{E}) = \{\mathcal{S} \subseteq \mathcal{F} \,|\, \text{CXp}(\mathcal{S};\mathcal{E}) \land i \in \mathcal{S}\}$$

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- Power indices of Holler-Packel and Deegan-Packel: [HP83, DP78]

$$\mathrm{Sc}_H(i;\mathcal{E}) = \sum\nolimits_{\mathcal{S}\in\mathbb{A}_i(\mathcal{E})} \left({}^1/|\mathbb{A}(\mathcal{E})|\right)$$
$$\mathrm{Sc}_D(i;\mathcal{E}) = \sum\nolimits_{\mathcal{S}\in\mathbb{A}_i(\mathcal{E})} \left({}^1/(|\mathcal{S}| \times |\mathbb{A}(\mathcal{E})|)\right)$$

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

Example power indices II

- Additional definitions:

$$\mathsf{Crit}(i,\mathcal{S};\mathcal{E}) = \mathsf{WAXp}(\mathcal{S};\mathcal{E}) \land \neg\mathsf{WAXp}(\mathcal{S}\setminus\{i\};\mathcal{E})$$

Example power indices II

- Additional definitions:

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

- Power indices of Shapley-Shubik, Banzhaf and Johnston: [SS54, BI65, Joh78]

$$\begin{aligned}
\mathsf{Sc}_S(i; \mathcal{E}) &= \sum\nolimits_{\mathcal{S}\subseteq\mathcal{F} \wedge \mathsf{Crit}(i,\mathcal{S};\mathcal{E})} \left({}^1\!/\!\left(|\mathcal{F}| \times \binom{|\mathcal{F}|-1}{|\mathcal{S}|-1} \right) \right) \\
\mathsf{Sc}_B(i; \mathcal{E}) &= \sum\nolimits_{\mathcal{S}\subseteq\mathcal{F} \wedge \mathsf{Crit}(i,\mathcal{S};\mathcal{E})} \left({}^1\!/2^{|\mathcal{F}|-1} \right) \\
\mathsf{Sc}_J(i; \mathcal{E}) &= \sum\nolimits_{\mathcal{S}\subseteq\mathcal{F} \wedge \mathsf{Crit}(i,\mathcal{S};\mathcal{E})} \left({}^1\!/\Delta(\mathcal{S}) \right)
\end{aligned}$$

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

Example #01

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

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

- AXps:

$$\begin{array}{lllll} 1 & & & & \\ 2 & 3 & 4 & 5 & 6 \\ 2 & 3 & 4 & 5 & 7 \end{array}$$

Example #01

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

$$\begin{array}{ccccc} 1 & & & & \\ 2 & 3 & 4 & 5 & 6 \\ 2 & 3 & 4 & 5 & 7 \end{array}$$

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

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- AXps:

$$\begin{array}{ccc} 1 & 2 & \\ 1 & 3 & 4 \\ 1 & 3 & 5 \end{array}$$

Example #02

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

$$\begin{matrix} 1 & 2 & \\ 1 & 3 & 4 \\ 1 & 3 & 5 \end{matrix}$$

- 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

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- AXps:

$$\begin{array}{ccccc} 2 & 3 & 4 & 5 & 6 \\ 1 & 3 & 4 & & \\ 1 & 4 & 5 & & \\ 1 & 4 & 6 & & \\ 1 & 3 & 6 & & \\ 1 & 5 & 6 & & \\ 1 & 2 & & & \\ 1 & 3 & 5 & & \end{array}$$

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: $[21; 12, 9, 4, 4, 1, 1, 1]$

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

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Example #04

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

$$\begin{array}{cccc} 1 & 2 & & \\ 1 & 3 & 4 & 5 \\ 1 & 3 & 4 & 6 \\ 1 & 3 & 4 & 7 \end{array}$$

- 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 – Part 7

From power indices to feature importance scores

- A Feature Importance Score 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

Some examples

- More notation:

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

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

- Some templates:
    - Shapley-Shubik:

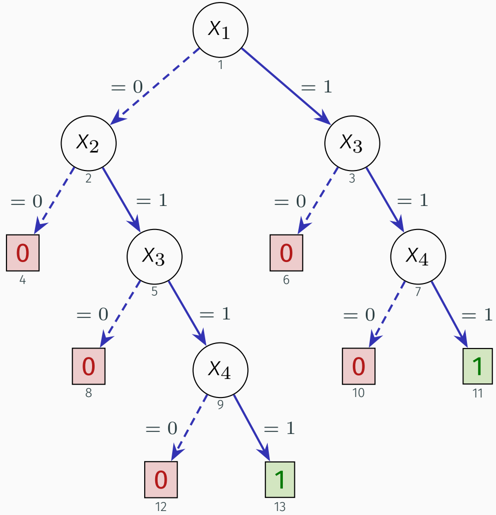
$$\mathrm{TSc}_S(i;\mathcal{E},v) := \sum_{\mathcal{S}\in\{\mathcal{T}\subseteq\mathcal{F} \mid i\in\mathcal{T}\}} \left(\frac{\Delta_i(\mathcal{S};\mathcal{E},v)}{|\mathcal{F}| \times \binom{|\mathcal{F}|-1}{|\mathcal{S}|-1}} \right)$$

    - Banzhaf:

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

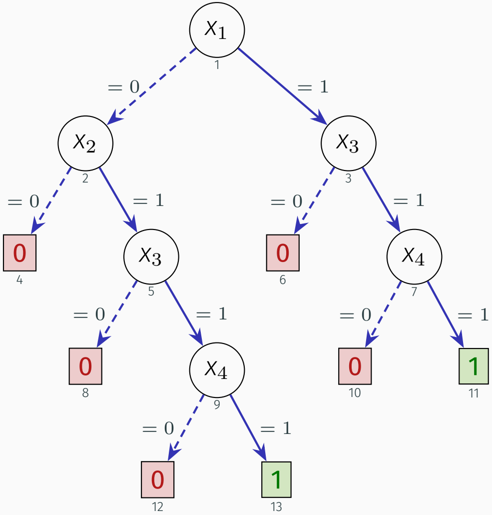
A concrete example

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



A concrete example

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



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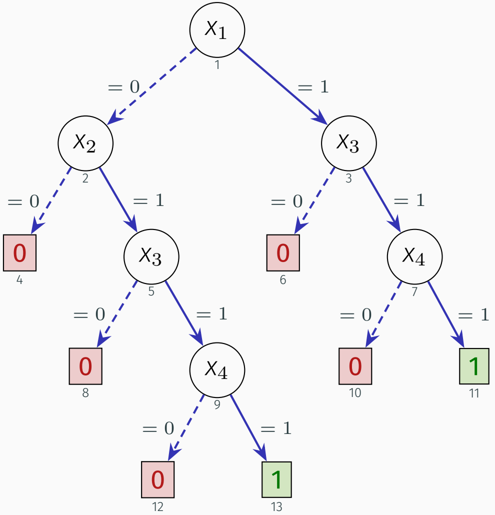
  - B (norm.): $\langle 0.125, 0.125, 0.375, 0.375 \rangle$



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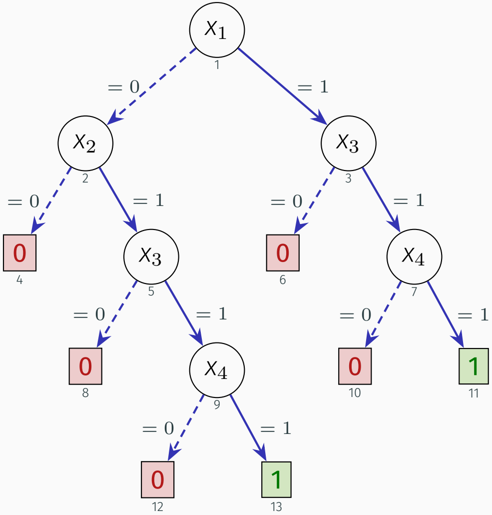

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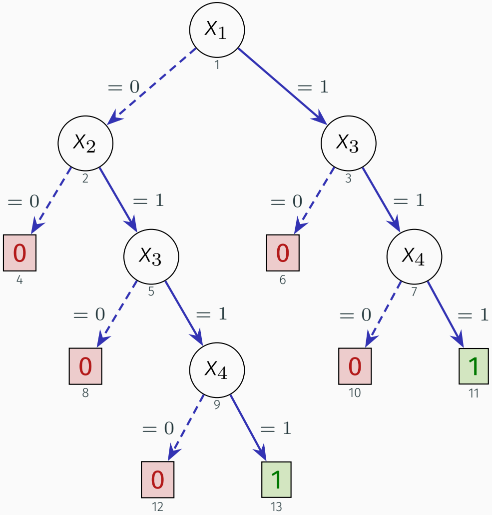
  - HP: $\langle 0.167, 0.167, 0.333, 0.333\rangle$



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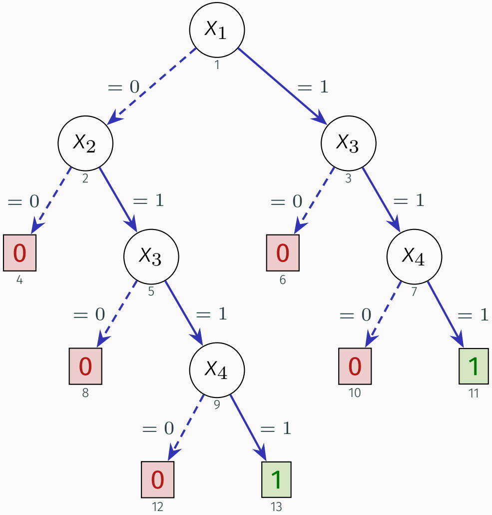
  - DP: $\langle 0.167, 0.167, 0.333, 0.333 \rangle$



Part 8

Conclusions & Research Directions

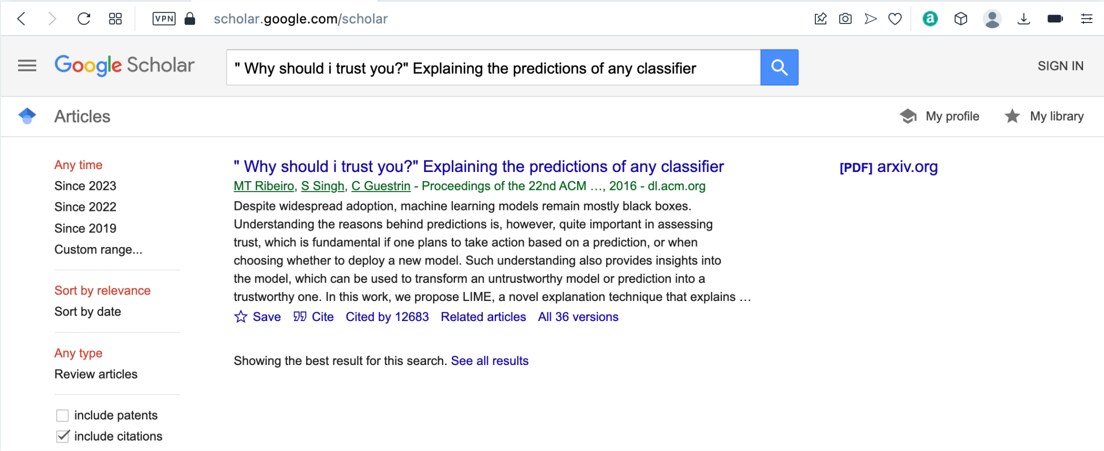
Outline – Part 8

Some Words of Concern

Conclusions & Research Directions

Can heuristic XAI's myths be stopped?

LIME on 2023/05/31:



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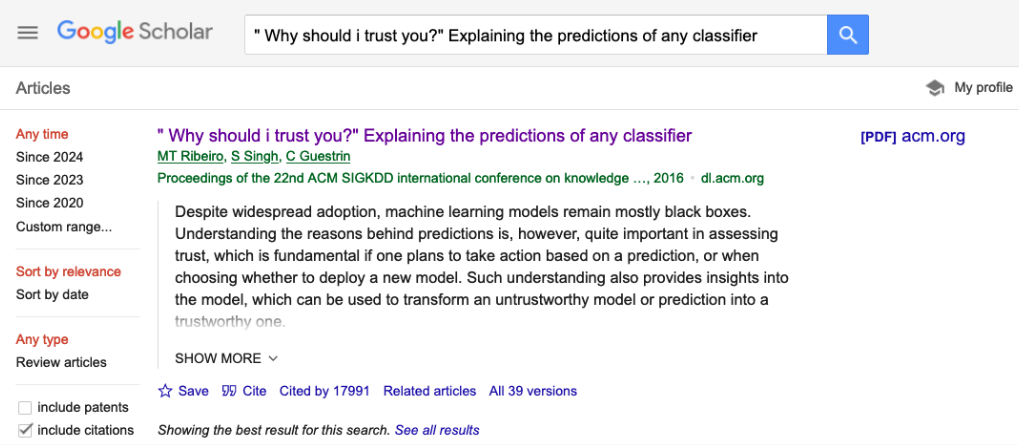
LIME on 2024/07/02:



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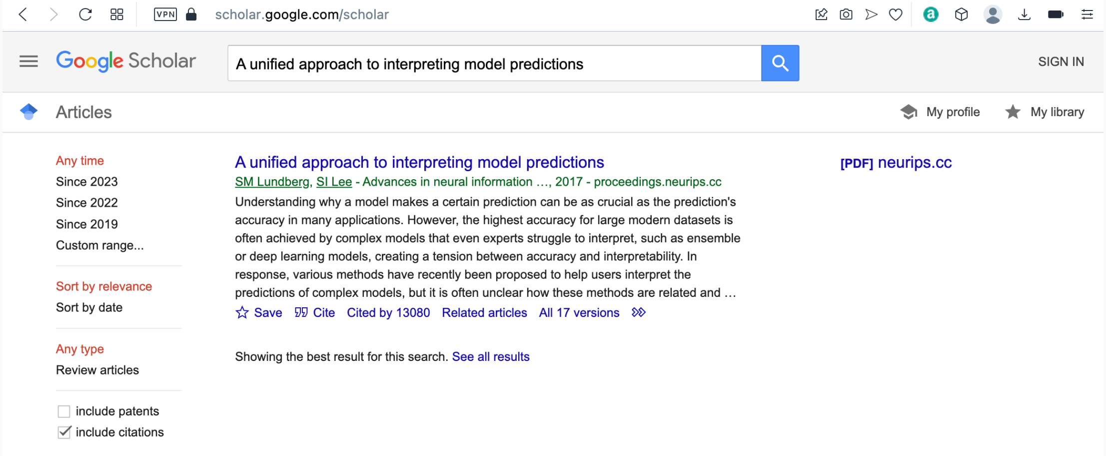
SHAP on 2023/05/31:



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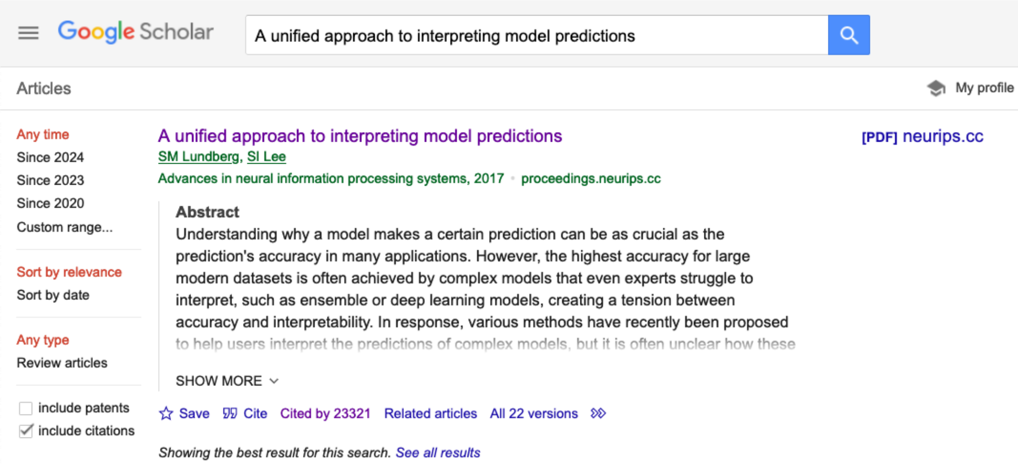

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- (Heuristic) XAI research experiences a persistent “*Don’t Look Up*” moment...

What's the bottom line?

- (Heuristic) 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]

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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...

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

doi:10.3233/FAIA240183

Exploring Large Language Models Capabilities to Explain Decision Trees

Some unsettling works...

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

ACM ISBN 979-8-4007-0450-5/24/06
https://doi.org/10.1145/3630106.3658953

Some unsettling works...

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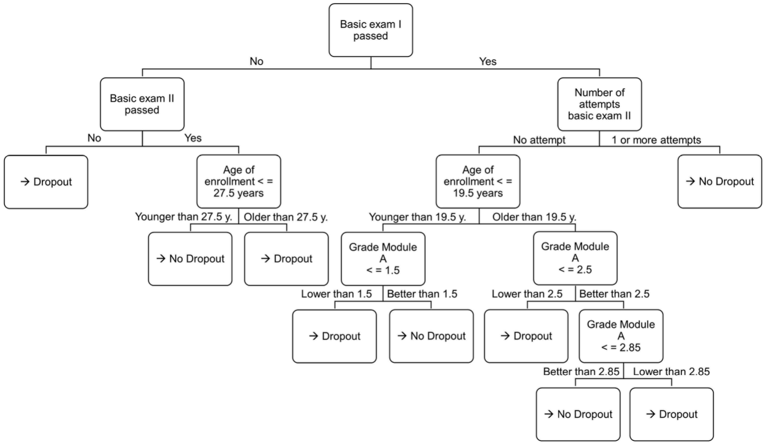
  - All CXps in polynomial-time [HIIM21, IIM22]



Outline – Part 8

Some Words of Concern

Conclusions & Research Directions

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- Brief overview of formal XAI & its recent progress:
  - Abductive & contrastive explanations
  - Skimmed through their computation in practice
  - Duality & enumeration
  - Other explainability queries – feature relevancy

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- Established tight connection between feature selection and feature attribution in XAI
- Symbolic XAI aggregates many fields of research:
  machine learning, formal methods, automated reasoning, optimization, computational social choice (& game theory), etc.

Research directions

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- Probabilitistic explanations

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- Certified XAI tools
- ... And trying to curb the massive momentum of (heuristic) XAI **myths**!

Q & A

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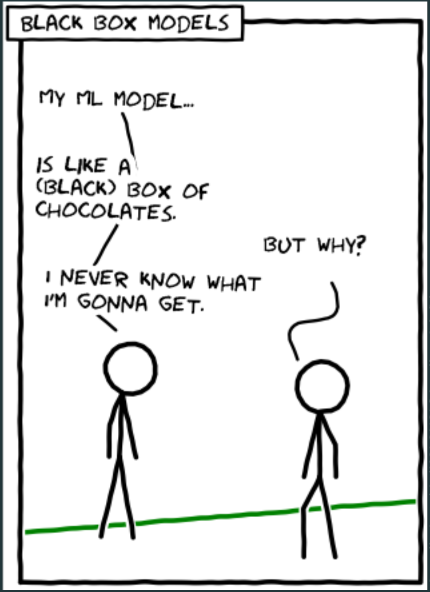

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