Logic-Based Explainability in Machine Learning

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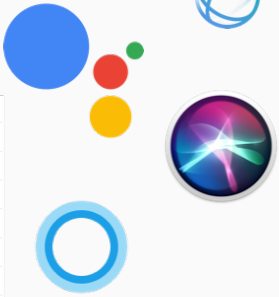
Recent & ongoing ML successes

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

DeepMind

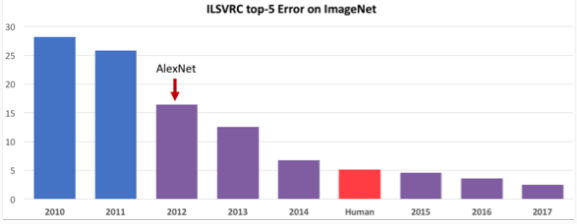
AlphaGo

AlphaGo Zero & **Alpha Zero**



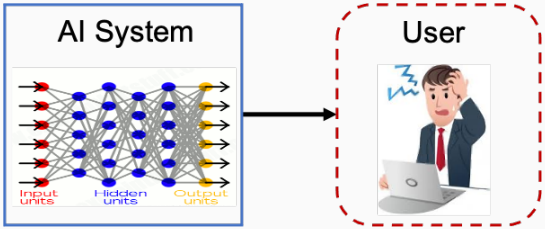
https://fr.wikipedia.org/wiki/Pepper_(robot)

Image & Speech Recognition



http://gradientscience.org/intro_adversarial/

eXplainable AI (XAI)



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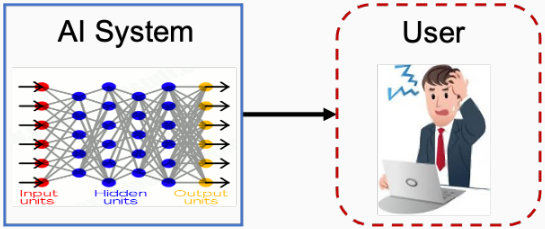

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    - How to be human understandable?
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    - Which guarantees of rigor?

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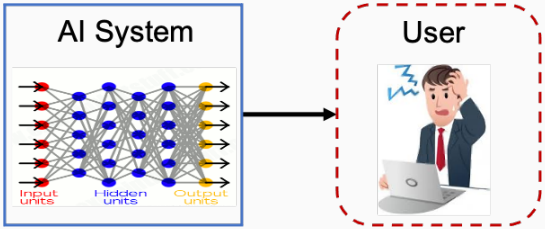

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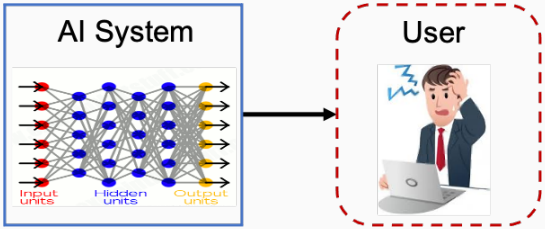

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  - Other queries: enumeration, membership, preferences, etc.
  - Links with robustness, fairness, learning

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]

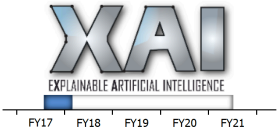
■ *We summarize the potential impact that the European Union's new General Data Protection Regulation will have on the routine use of machine-learning algorithms. Slated to take effect as law across the European Union in 2018, it will place restrictions on automated individual decision making (that is, 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)



David Gunning
DARPA/I2O
Program Update November 2017

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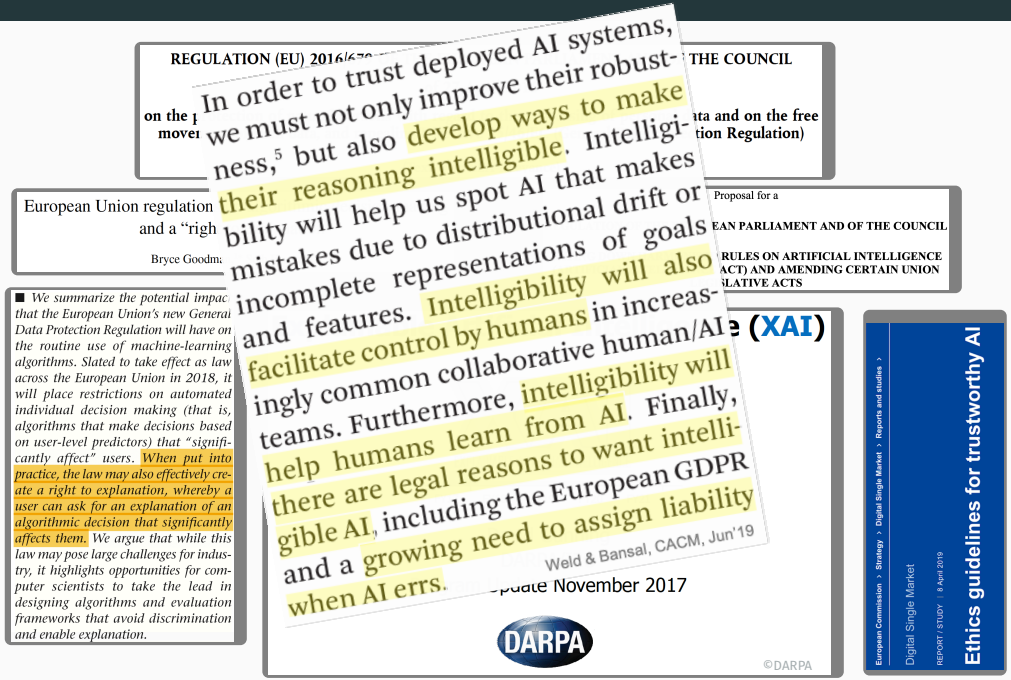
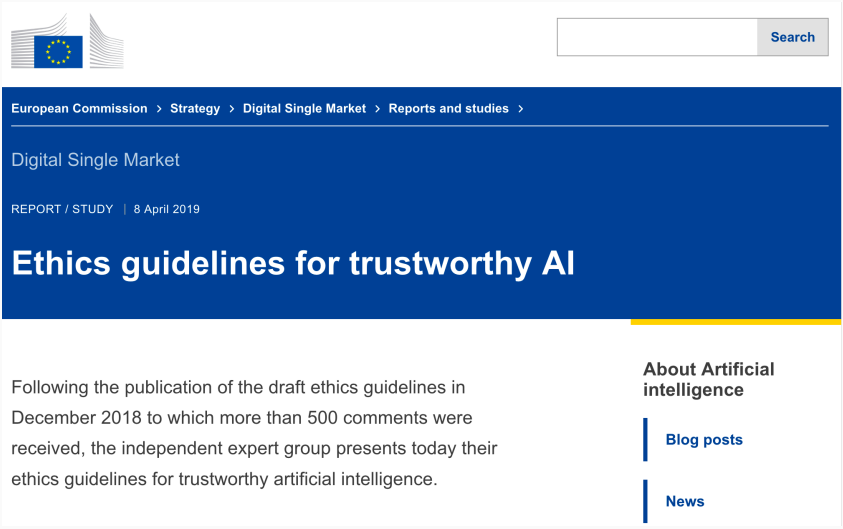


XAI & EU guidelines (AI HLEG)



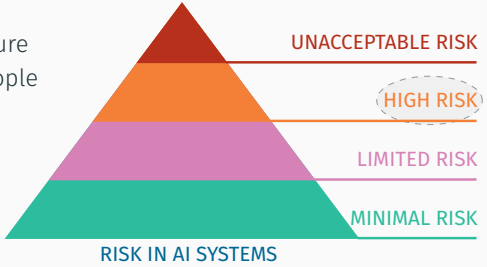
XAI & the principle of explicability

& thousands of recent papers!

XAI for high-risk & safety-critical applications

- High-risk (EU regulations):
  - Law enforcement
  - Management and operation of critical infrastructure
  - Biometric identification and categorization of people
  - ...
- Safety-critical:
  - Self-driving cars
  - Autonomous vehicles
  - Autonomous aereal devices
  - ...

[EU21]



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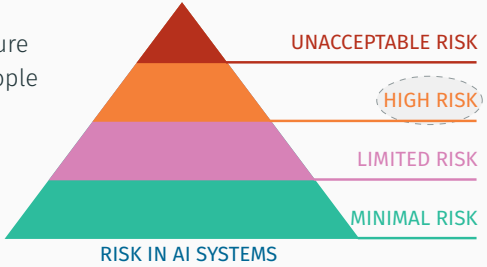

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- **Correctness of explanations is paramount!**
  - To build trust
  - To help debug AI systems
  - To prevent accidents
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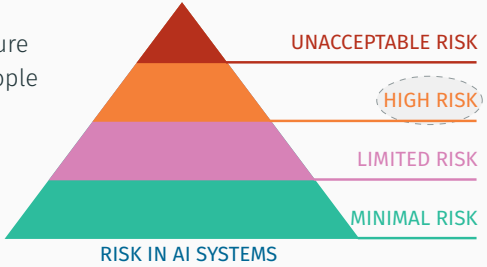

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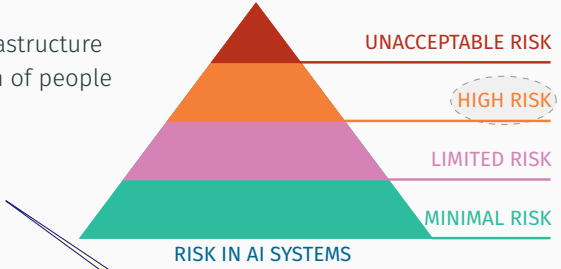
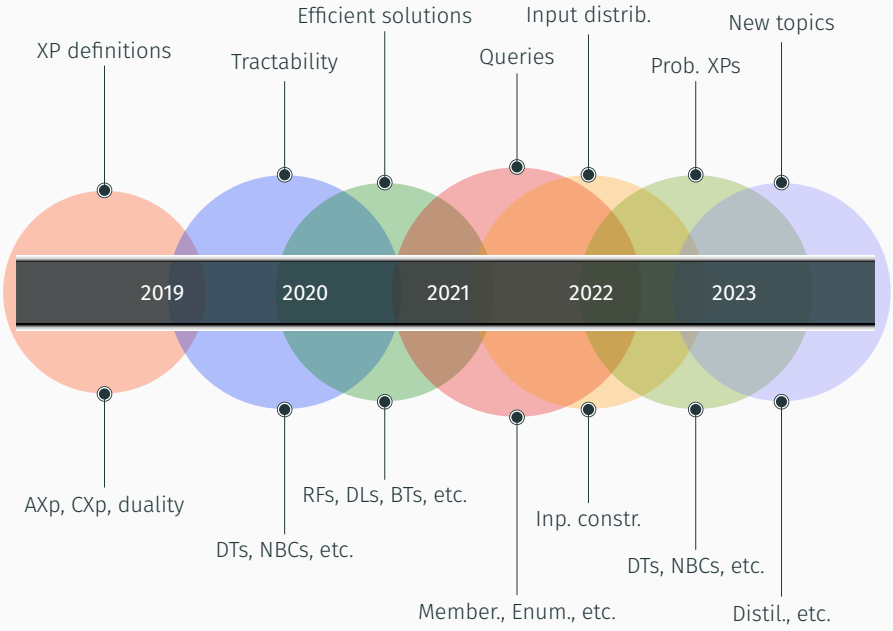


Main motivation for our work!

The emergence of formal explainability – timeline



Today's short course – main topics

- Part #0: Motivation
- Part #1: Preliminaries & issues with XAI
- Part #2: Formal explainability
- Part #3: Computing explanations – basics
- Q&A and Break
- Part #4: Computing explanations – encodings
- Part #5: Tractable explanations
- Part #6: Explainability queries
- Part #7: Probabilistic explanations
- Part #8: Additional topics & wrap-up
- Q&A and Conclude

Part 1

Preliminaries & XAI Issues

Definitions – 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: $\mathbb{F} = \Pi_{i=1}^{m} D_i$

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- Set of classes $\mathcal{K} = \{c_1, \ldots, c_K\}$
- ML model $\mathbb{M}$ computes a (non-constant) classification function $\kappa : \mathbb{F} \to \mathcal{K}$
- 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 $(\mathbf{v}, c)$

Simple examples – (unordered) rules

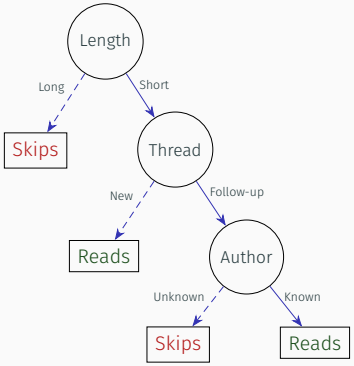
IF $x_1 + x_2 \geq 0$ THEN predict ⊞

IF $x_1 + x_2 < 0$ THEN predict ⊟

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

Simple examples – (unordered) rules & decision tree

IF $x_1 + x_2 \geq 0$ THEN predict $\boxplus$
IF $x_1 + x_2 < 0$ THEN predict $\boxminus$
$\mathcal{F} = \{1, 2\}; \mathcal{D}_1 = \mathcal{D}_2 = \mathbb{R}; \mathcal{K} = \{\boxplus, \boxminus\}$



Features: Length, Thread, Author
$\mathcal{F} = \{1, 2, 3\}$
$\mathcal{K} = \{\text{Skips}, \text{Reads}\}$
$\mathcal{D}_1 = \{\text{Long}, \text{Short}\}$
$\mathcal{D}_2 = \{\text{New}, \text{Follow-up}\}$
$\mathcal{D}_3 = \{\text{Unknown}, \text{Known}\}$

Outline

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 $\neg$, $\wedge$,$\vee$, $\ldots$
- 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 $\varphi : \mathbb{F} \to \{0, 1\}$
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- For non-boolean feature spaces, we let φ_c denote the predicate $\varphi(\mathbf{x}) = c$, i.e. $\varphi_c(\mathbf{x}) \in \{0, 1\}$

Prime implicants & implicates

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- A disjunction of literals ρ (also viewed as a set of literals where convenient) is a prime implicate of some function φ if
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  2. For any $\rho' \subsetneq \rho$, $\varphi \nvDash \rho'$

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, $\mathcal{T} \models \bot$
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- Minimal correction subset (MCS):
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- Duality:
  - MUSes are minimal-hitting sets (MHSes) of MCSes, and vice-versa [Rei87]

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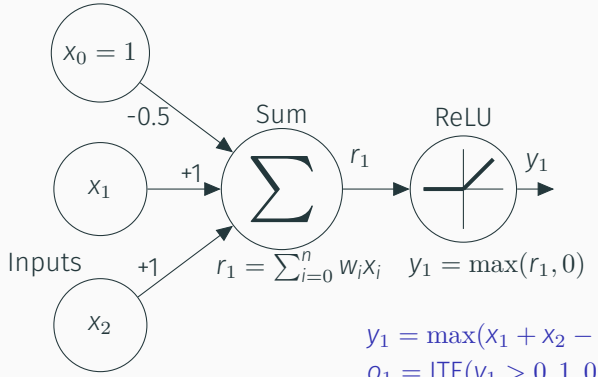
- Duality:
  - MUSes are minimal-hitting sets (MHSes) of MCSes, and vice-versa [Rei87]
- Variants:
  - Smallest(-cost) MCS, i.e. complement of maximum(-cost) satisfiability (MaxSAT)
  - Smallest(-cost) MUS

Outline

Neural networks (NNs) – $(\mathbf{v}, c) = ((1, 0), 1)$



$$y_1 = \max(x_1 + x_2 - 0.5, 0)$$
$$o_1 = \mathsf{ITE}(y_1 > 0, 1, 0)$$

Decision lists (DLs) – ordered rules – $(\mathbf{v}, c) = ((0, 0, 1, 2), 1)$

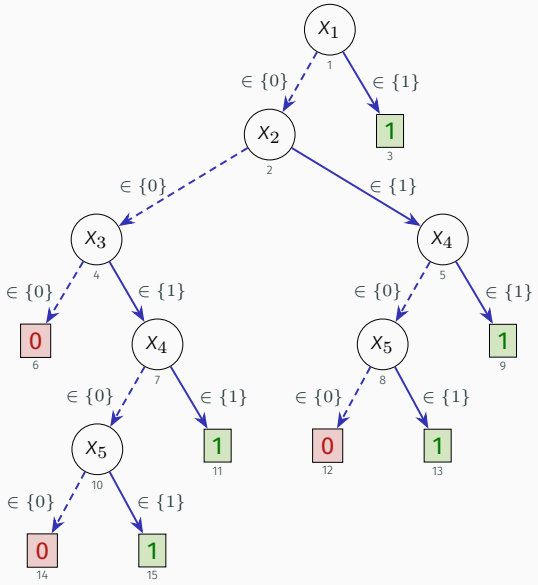
[Fla12]

Item	Definition
$\mathcal{F}_1$	$\{1, 2, 3, 4\}$
$\mathcal{D}_{1i}, i = 1, 2, 3$	$\{0, 1\}$
$\mathcal{D}_{14}$	$\{0, 1, 2\}$
$\mathcal{K}_1$	$\{0, 1\}$
κ_1	see below

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

Decision trees (DTs) – $(\mathbf{v}, c) = ((0, 0, 1, 0, 1), 1)$

[HRS19]



Monotonic classifiers – $(\mathbf{v}, c) = ((10, 10, 5, 0), A)$

[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	$\{0, \ldots, 10\}$

$$
\begin{aligned}
M &= \mathsf{ITE}(S \geq 9, A, \mathsf{ITE}(S \geq 7, B, \mathsf{ITE}(S \geq 5, C, \mathsf{ITE}(S \geq 4, D, \mathsf{ite}(S \geq 2, E, F))))) \\
S &= \max\left[0.3 \times Q + 0.6 \times X + 0.1 \times H, R\right]
\end{aligned}
$$

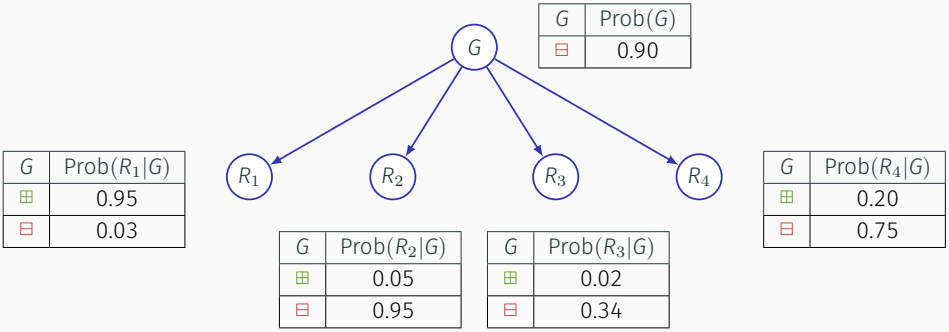
Also, $F \preccurlyeq E \preccurlyeq D \preccurlyeq C \preccurlyeq B \preccurlyeq A$

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

Other classifiers

- Naive-Bayes Classifier (NBC)

[Fla12, MGC+20]



G	Prob(G)
⊟	0.90

G	Prob(R_1|G)
⊞	0.95
⊟	0.03

G	Prob(R_2|G)
⊞	0.05
⊟	0.95

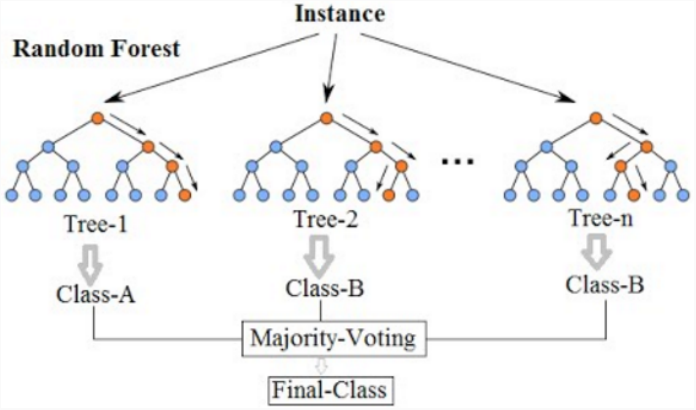
G	Prob(R_3|G)
⊞	0.02
⊟	0.34

G	Prob(R_4|G)
⊞	0.20
⊟	0.75

$$\text{Prob}(G, R_1, R_2, R_3, R_4) = \text{Prob}(G) \times \text{Prob}(R_1|G) \times \text{Prob}(R_2|G) \times \text{Prob}(R_3|G) \times \text{Prob}(R_4|G)$$

Other classifiers

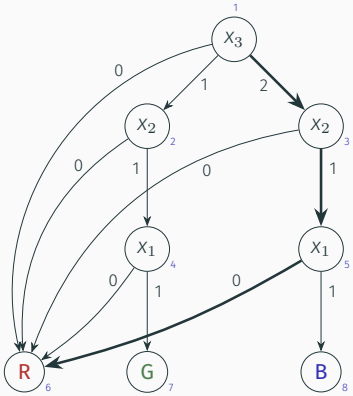
- Naive-Bayes Classifier (NBC)
- Random forests (RFs) & other tree ensembles (TEs), e.g. boosted trees (BTs)



Other classifiers

- Naive-Bayes Classifier (NBC)
- Random forests (RFs) & other tree ensembles (TEs), e.g. boosted trees (BTs)
- Decision graphs, decision diagrams, etc.

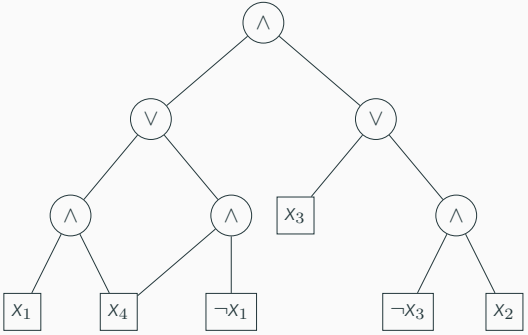
[HIIM21]



Other classifiers

- Naive-Bayes Classifier (NBC)
- Random forests (RFs) & other tree ensembles (TEs), e.g. boosted trees (BTs)
- Decision graphs, decision diagrams, etc.
- Propositional languages

[HII+22]



Outline

Non-formal XAI approaches – among best known

- Model-agnostic (MA) explainers:
  - LIME & SHAP [RSG16, LL17]
    - Goal: learn a simple interpretable ML model, e.g. linear classifier, decision tree, etc.
    - Approach: train classifier, sample-based vs. game theory
  - Anchor: [RSG18]
    - Goal: learn features deemed more relevant for prediction
    - Anchor is sample-based
  - No formal guarantees of rigor in computed explanations
- Intrinsic interpretability (II) [Rud19, Mol20]
  - (Interpretable) model is the explanation
  - E.g., DTs, DLs, DSs, etc.

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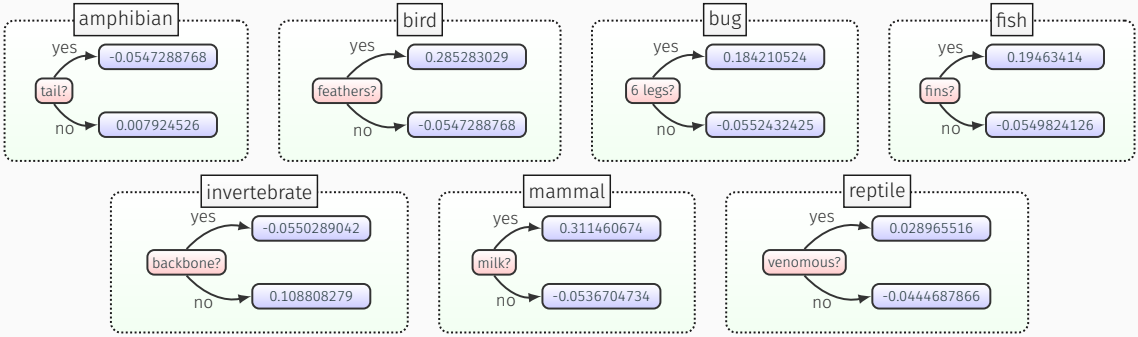
Can MA explainers be trusted?
Is II indeed *interpretable*?

An example – BT for zoo dataset

[INM19c, Ign20]



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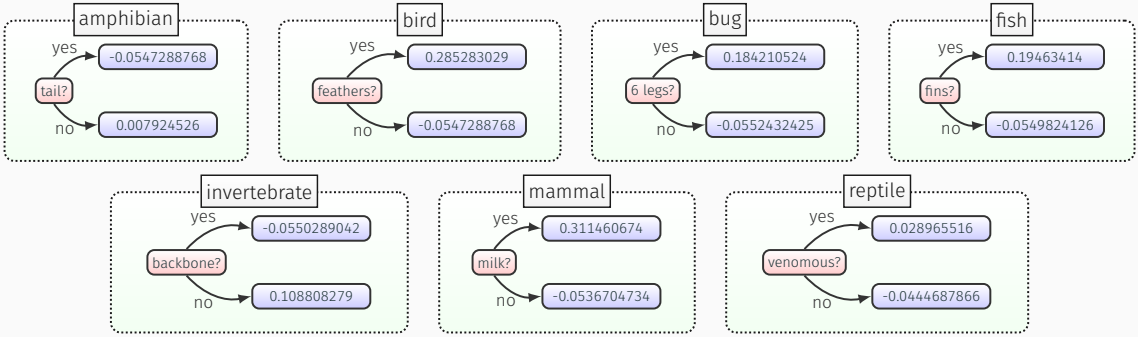


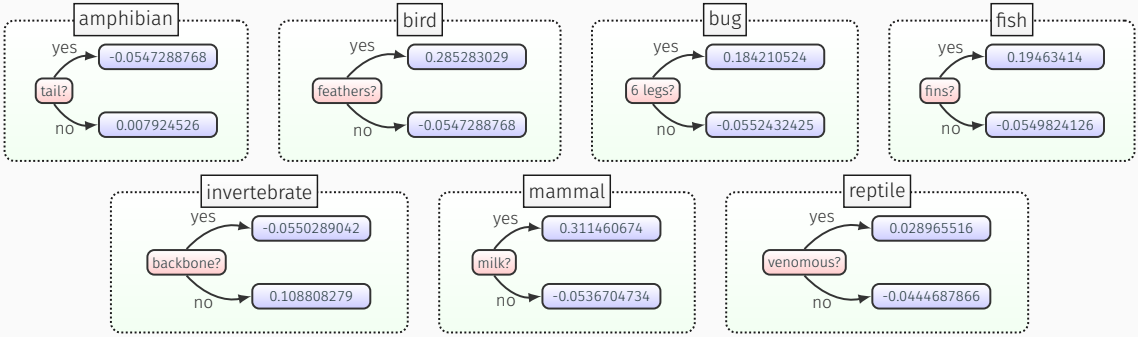
- Example instance:

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

THEN (class = reptile)

An example – BT for zoo dataset & Anchor

[INM19c, Ign20]



- Example instance (& Anchor picks):

[RSG18]

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

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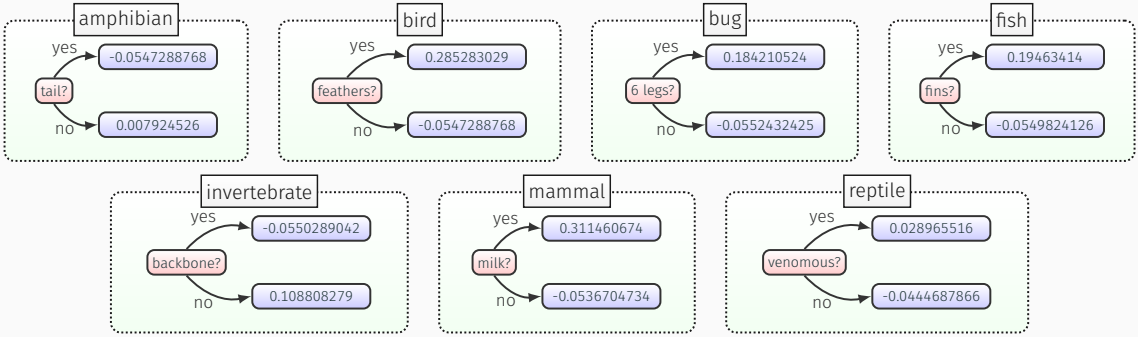
An example – BT for zoo dataset & Anchor

[INM19c, Ign20]

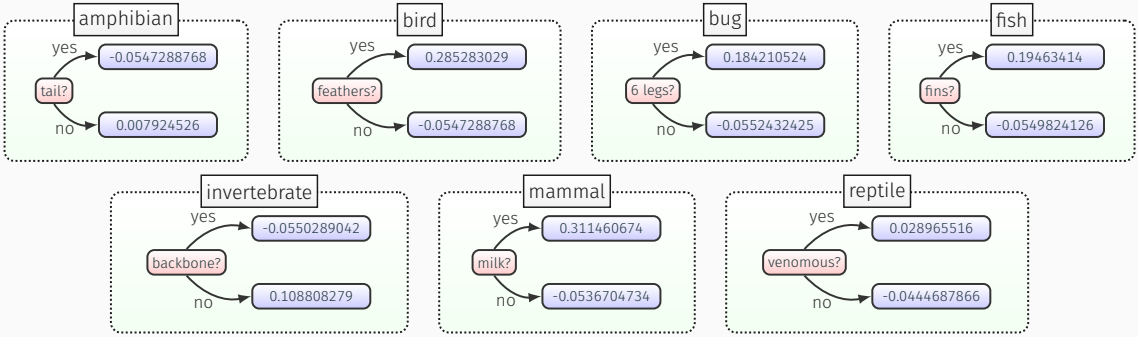


- Explanation obtained with Anchor: [RSG18]

IF	$\neg$*hair* $\wedge$ $\neg$*milk* $\wedge$ $\neg$*toothed* $\wedge$ $\neg$*fins*
THEN	(class = reptile)

An example – BT for zoo dataset & Anchor

[INM19c, Ign20]



- **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

Model-agnostic explainers cannot be trusted

[INM19c]

Incorrect explanations:

Classifier for deciding bank loans

Two samples: Bessie :– (v_1, Y) and Clive :– (v_2, N)

Model-agnostic explainers cannot be trusted

[INM19c]

Incorrect explanations:

Classifier for deciding bank loans

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

Explanation X: age $= 45$, salary $= 50\text{K}$

Model-agnostic explainers cannot be trusted

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Classifier for deciding bank loans

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

Explanation X: age $= 45$, salary $= 50\text{K}$

And,

- X is consistent with Bessie $:-(\mathbf{v}_1, \mathsf{Y})$
- X is consistent with Clive $:-(\mathbf{v}_2, \mathsf{N})$

Model-agnostic explainers cannot be trusted

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Classifier for deciding bank loans

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

Explanation X: age $= 45$, salary $= 50\text{K}$

And,

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

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

$\therefore$ different outcomes & same explanation !?

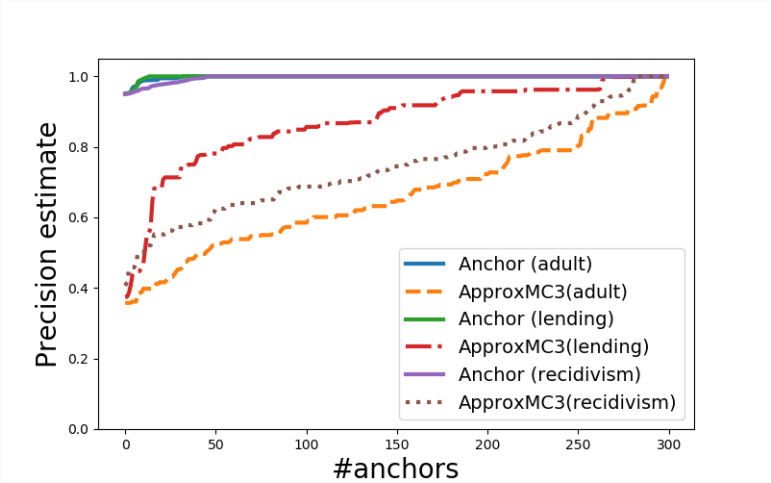
Incorrect explanations are ubiquitous...

[INM19c, Ign20]

Dataset	(# unique)	Explanations								
		incorrect			redundant			correct		
		LIME	Anchor	SHAP	LIME	Anchor	SHAP	LIME	Anchor	SHAP
adult	(5579)	61.3%	80.5%	70.7%	7.9%	1.6%	10.2%	30.8%	17.9%	19.1 %
lending	(4414)	24.0%	3.0%	17.0%	0.4%	0.0%	2.5%	75.6%	97.0%	80.5%
rcdv	(3696)	94.1%	99.4%	85.9%	4.6%	0.4%	7.9%	1.3%	0.2%	6.2%
compas	(778)	71.9%	84.4%	60.4%	20.6%	1.7%	27.8%	7.5%	13.9%	11.8%
german	(1000)	85.3%	99.7%	63.0%	14.6%	0.2%	37.0%	0.1 %	0.1 %	0.0%

Incorrect explanations are ubiquitous & likely...

[NSM+19]



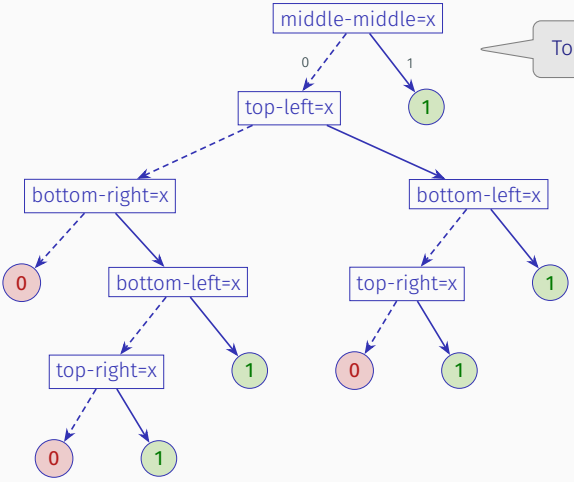
Decision trees are interpretable...

[Bre01, Rud19, Mol20]

"On interpretability, trees rate an A+." [Bre01]

General agreement on interpretability of decision trees [Rud19, Mol20, ANS20, Int21]

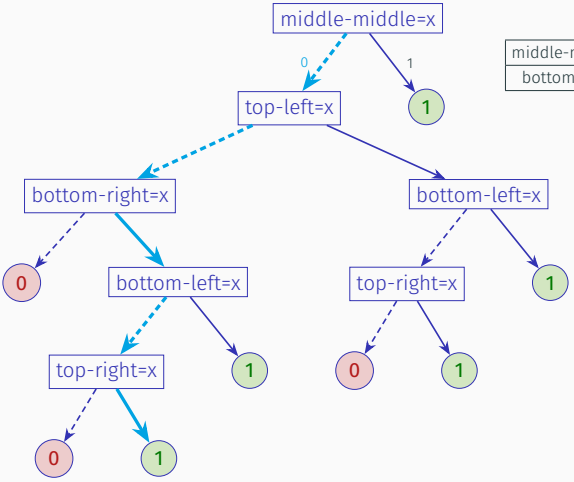
Decision tree explanations can be redundant



Tool: OSDT; train accuracy: 82.881%

Source: Xiyang Hu, Cynthia Rudin, Margo I. Seltzer: **Optimal Sparse Decision Trees**. **NeurIPS 2019**: 7265-7273

Decision tree explanations can be redundant



middle-middle $=$ x iff MM $=1$	top-left $=$ x iff TL $=1$	
bottom-right $=$ x iff BR $=1$	bottom-left $=$ x iff BL $=1$	top-right $=$ x iff TR $=1$

Q: What is explanation for

$(\text{MM} = 0) \wedge (\text{TL} = 0) \wedge (\text{BR} = 1) \wedge$

$(\text{BL} = 0) \wedge (\text{TR} = 1)$?

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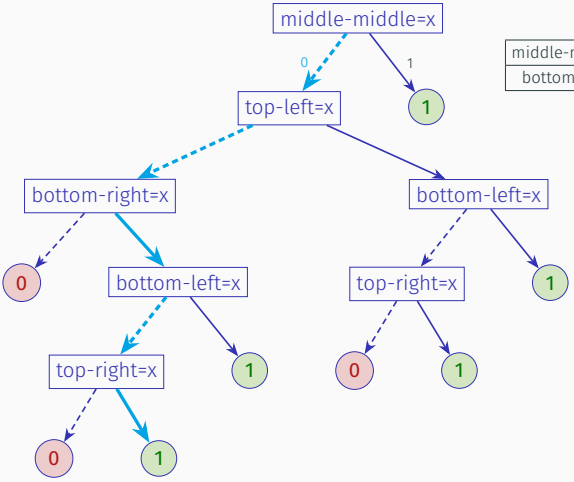

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Q: What is explanation for

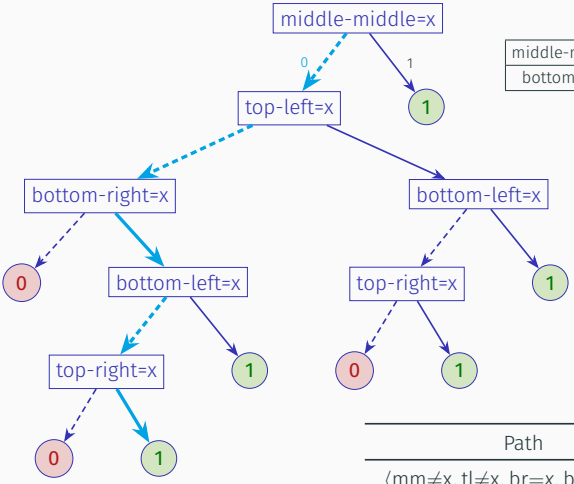
$(\text{MM}=0) \wedge (\text{TL}=0) \wedge (\text{BR}=1) \wedge$

$(\text{BL}=0) \wedge (\text{TR}=1)$?

IF $(\neg\text{MM} \wedge \neg\text{TL} \wedge \text{BR} \wedge \neg\text{BL} \wedge \text{TR})$ THEN $(\kappa(\cdot)=\mathbf{1})$?

Source: Xiyang Hu, Cynthia Rudin, Margo I. Seltzer: **Optimal Sparse Decision Trees**. **NeurIPS 2019**: 7265-7273

Decision tree explanations can be redundant



middle-middle = x iff MM = 1	top-left = x iff TL = 1	
bottom-right = x iff BR = 1	bottom-left = x iff BL = 1	top-right = x iff TR = 1

Q: What is explanation for

$(\text{MM} = 0) \land (\text{TL} = 0) \land (\text{BR} = 1) \land$

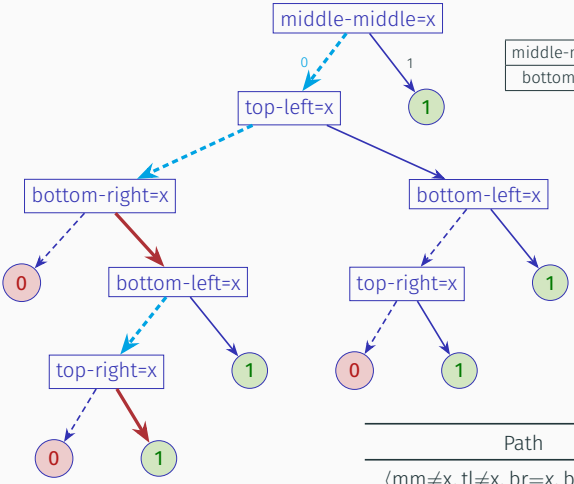
$(\text{BL} = 0) \land (\text{TR} = 1)$?

IF $(\neg\text{MM} \land \neg\text{TL} \land \text{BR} \land \neg\text{BL} \land \text{TR})$ THEN $(\kappa(\cdot) = \mathbf{1})$?

Path	Reduced XP	Dropped
⟨mm≠x, tl≠x, br=x, bl≠x, tr=x⟩		

Source: Xiyang Hu, Cynthia Rudin, Margo I. Seltzer: **Optimal Sparse Decision Trees**. **NeurIPS 2019**: 7265-7273

Decision tree explanations can be arbitrarily redundant



middle-middle = x iff MM = 1	top-left = x iff TL = 1	
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BR = 1, TR = 1			
MM	BL	TL	$\kappa(\cdot)$
0	0	0	1
0	0	1	1
0	1	0	1
0	1	1	1
1	0	0	1
1	0	1	1
1	1	0	1
1	1	1	1

Path	Reduced XP	Dropped
$\langle$mm≠x, tl≠x, br=x, bl≠x, tr=x$\rangle$	$\langle$br=x, tr=x$\rangle$	{mm≠x, tl≠x, bl≠x}

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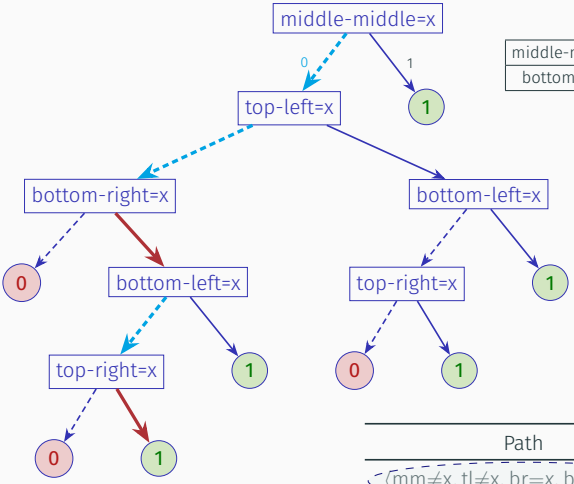

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MM	BL	TL	$\kappa(\cdot)$
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0	1	1	1
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1	0	1	1
1	1	0	1
1	1	1	1

Path	Reduced XP	Dropped
⟨mm≠x, tl≠x, br=x, bl≠x, tr=x⟩	⟨br=x, tr=x⟩	{mm≠x, tl≠x, bl≠x}

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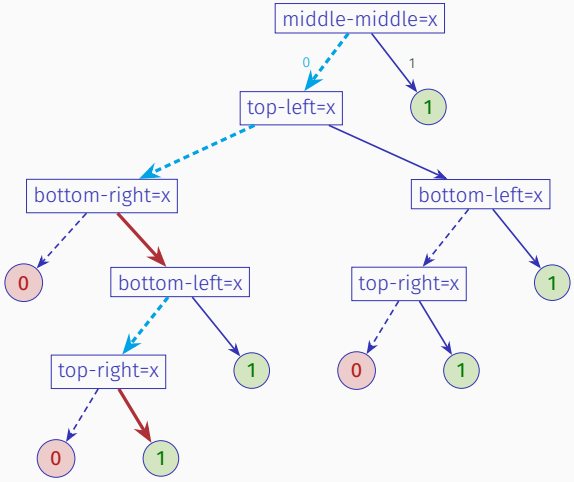
Decision tree explanations can be arbitrarily redundant



# tree paths	8
# red. paths	5
% red. paths	62.5%

Source: Xiyang Hu, Cynthia Rudin, Margo I. Seltzer: Optimal Sparse Decision Trees. NeurIPS 2019: 7265-7273

Decision trees are interpretable...

[Bre01, Rud19, Mol20]

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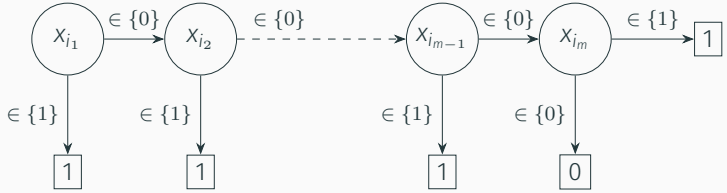
$$\kappa(x_1, x_2, \ldots, x_{m-1}, x_m) = \bigvee_{i=1}^{m} x_i$$

- Decision tree (DT), by picking variables in order $\langle i_1, i_2, \ldots, i_m \rangle$, permutation of $\langle 1, 2, \ldots, m \rangle$:



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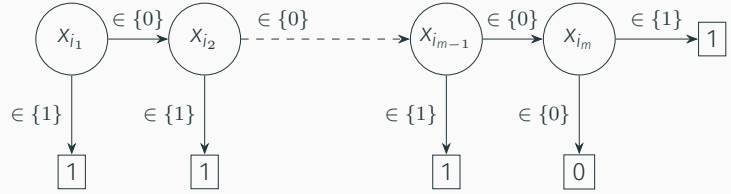

- Point: $(x_{i_1}, x_{i_2}, \ldots, x_{i_{m-1}}, x_{i_m}) = (0, 0, \ldots, 0, 1)$, and prediction 1

Decision trees are interpretable...

[Bre01, Rud19, Mol20]

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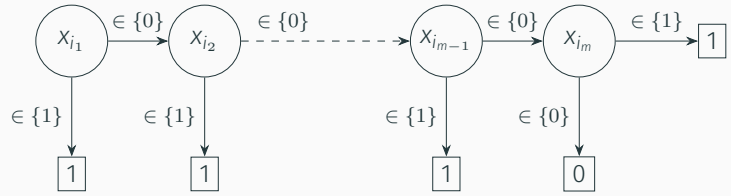


- Point: $(x_{i_1}, x_{i_2}, \ldots, x_{i_{m-1}}, x_{i_m}) = (0, 0, \ldots, 0, 1)$, and prediction 1
- Explanation using path in DT: $\{i_1, i_2, \ldots, i_m\}$, i.e.

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

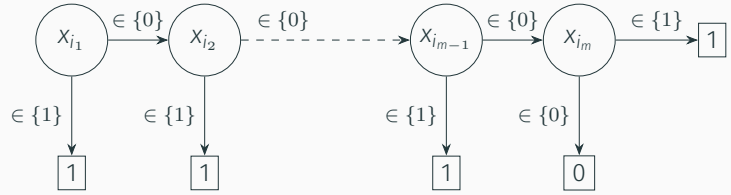
Decision trees are interpretable...

[Bre01, Rud19, Mol20]

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

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

- Decision tree (DT), by picking variables in order $\langle i_1, i_2, \ldots, i_m \rangle$, permutation of $\langle 1, 2, \ldots, m \rangle$:



- 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.** $\forall(\mathbf{x} \in \{0, 1\}^m).(x_{i_m}) \rightarrow \kappa(\mathbf{x})$

Minimal decision trees are not interpretable!

[IIM20, HIIM21, IIM22]

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

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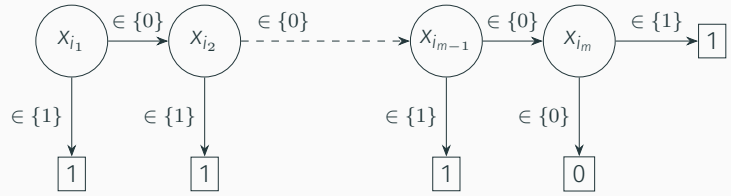

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  True explanations arbitrarily smaller than paths in DT; $\therefore$ **DTs are not interpretable***

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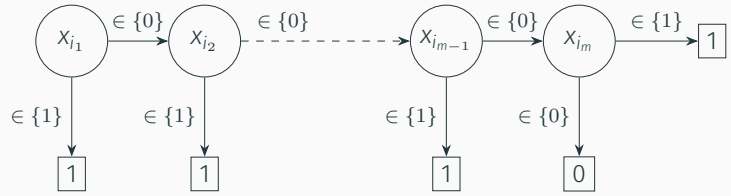

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True explanations arbitrarily smaller than paths in DT; **$\therefore$ DTs are not interpretable***

*Pick any definition of interpretability that correlates with succinctness ...

[Lip18]

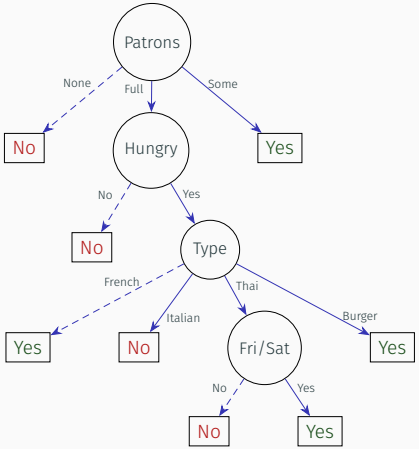
Explanation redundancy in DTs is ubiquitous – published DT examples

[IIM22]

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

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

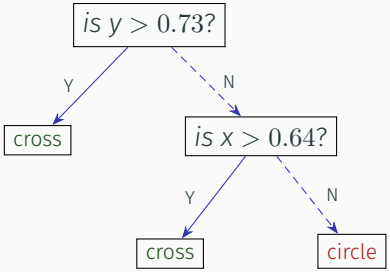
[RN10]



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

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

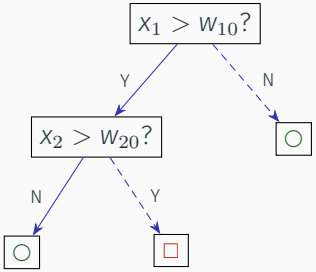
[Zho12]



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

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

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



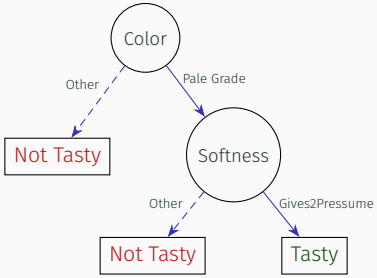
[Alp14]

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

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

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

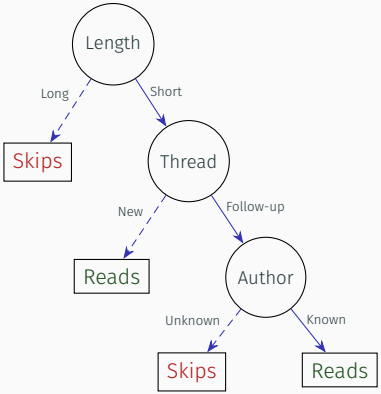
[SB14]



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

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

[PM17]



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

Explanation redundancy in DTs is ubiquitous – DTs from datasets

[IIM20, HIIM21, IIM22]

Dataset	(#F	#S)	IAI									ITI								
			D	#N	%A	#P	%R	%C	%m	%M	%avg	D	#N	%A	#P	%R	%C	%m	%M	%avg
adult	(12	6061)	6	83	78	42	33	25	20	40	25	17	509	73	255	75	91	10	66	22
anneal	(38	886)	6	29	99	15	26	16	16	33	21	9	31	100	16	25	4	12	20	16
backache	(32	180)	4	17	72	9	33	39	25	33	30	3	9	91	5	80	87	50	66	54
bank	(19	36 293)	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	18 668)	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	13 442)	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	10 992)	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	58 000)	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	—	—	—

Outline

Rules with ordinal features

- Example ML model:

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

  Rules:

  IF $2x_1 + x_2 > 0$ THEN predict ⊞

  IF $2x_1 - x_2 \leq 0$ THEN predict ⊟

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- **Q:** Can the model predict both ⊞ and ⊟ for some instance?
  - Yes, of course: pick $x_1 = 0$ and $x_2 = 1$
  - A formalization:

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

... and solve with SMT solver

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

Decision sets

- Example ML model:

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

  Rules:

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

  IF $x_1 \wedge \neg x_3 \wedge x_4$ THEN predict ⊟

  IF $x_3 \wedge x_4$ THEN predict ⊟

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- **Q:** Can the model predict both ⊞ and ⊟ for some instance?
  - Yes, certainly: pick $(x_1, x_2, x_3, x_4) = (1, 0, 1, 1)$

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  Rules:

  $$\begin{array}{llll} \text{IF} & x_1 \wedge \neg x_2 \wedge x_3 & \text{THEN} & \text{predict } \boxplus \\ \text{IF} & x_1 \wedge \neg x_3 \wedge x_4 & \text{THEN} & \text{predict } \boxminus \\ \text{IF} & x_3 \wedge x_4 & \text{THEN} & \text{predict } \boxminus \end{array}$$

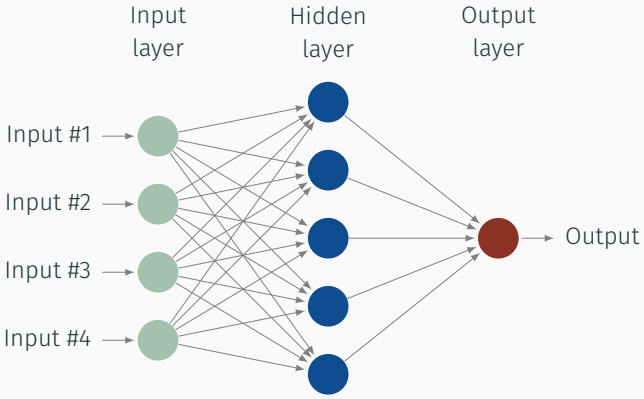
- **Q:** Can the model predict both $\boxplus$ and $\boxminus$ for some instance?
  - Yes, certainly: pick $(x_1, x_2, x_3, x_4) = (1, 0, 1, 1)$
  - A formalization:

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

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

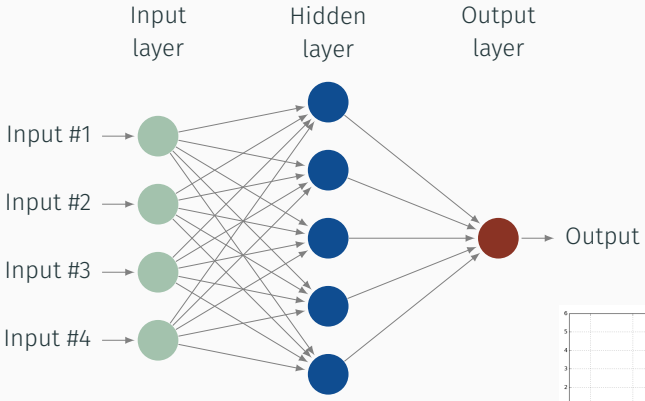
$\therefore$ There exists a model iff there exists a point in feature space yielding both predictions

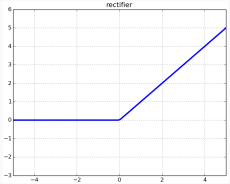
Neural networks



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

Neural networks





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

[NH10]

Encoding NNs using MILP

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

$$\mathbf{x}' = \mathbf{A} \cdot \mathbf{x} + \mathbf{b}$$
$$\mathbf{y} = \max(\mathbf{x}', \mathbf{0})$$

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Encoding each **block**: [FJ18]

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

Simpler encodings exist, but **not** as effective [KBD+17]

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

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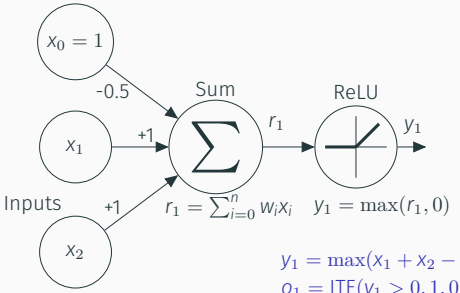
Encoding a simple NN in MILP



$y_1 = \max(x_1 + x_2 - 0.5, 0)$
$o_1 = \mathsf{ITE}(y_1 > 0, 1, 0)$

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

MILP encoding:

$x_1 + x_2 - 0.5 = y_1 - s_1$
$z_1 = 1 \rightarrow y_1 \leq 0$
$z_1 = 0 \rightarrow s_1 \leq 0$
$o_1 = (y_1 > 0)$
$x_1, x_2, z_1, o_1 \in \{0, 1\}$
$y_1, s_1 \geq 0$

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

$1 + 0 - 0.5 = 0.5 - 0$
$1 \vee 0.5 \leq 0$
$0 \vee 0 \leq 0$
$1 = (0.5 > 0)$
$x_1 = 1, x_2 = 0, z_1 = 0, o_1 = 1$
$y_1 = 0.5, s_1 = 0$

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

$0 + 0 - 0.5 = 0 - 0.5$
$0 \vee 0 \leq 0$
$1 \vee 0.5 \leq 0$
$0 = (0 > 0)$
$x_1 = 0, x_2 = 0, z_1 = 1, o_1 = 0$
$y_1 = 0, s_1 = 0.5$

Part 2

Formal Explainability

Outline

Abductive explanations – answering Why? questions

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

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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

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

Abductive explanations – answering Why? questions

- Instance $(\mathbf{v}, c)$, i.e. $c = \kappa(\mathbf{v})$
- **Abductive explanation** (AXp, PI-explanation): [SCD18, INM19a]
  - **Subset-minimal** set of features $\mathcal{X} \subseteq \mathcal{F}$ sufficient for **ensuring** prediction

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

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Recap weak CXp: $\exists(\mathbf{x} \in \mathbb{F}).\ \bigwedge_{j \notin \mathcal{Y}}(x_j = v_j) \land (\kappa(\mathbf{x}) \neq c)$

A simple example – CXp's

- Classifier:

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

- Point $\mathbf{v} = (0, 0, 0, 1)$ with prediction $\kappa(\mathbf{v}) = 1$
- Define $\mathcal{Y} = \{1, 2, 3, 4\} = \mathcal{F}$
- Can feature 1 be removed, i.e. $\exists(\mathbf{x} \in \{0, 1\}^4).\neg x_1 \land \neg\kappa(x_1, x_2, x_3, x_4)$? Yes
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- CXp $\mathcal{Y} = \{4\}$
- **Obs:** AXp is MHS of CXp and vice-versa...

Recap weak CXp: $\exists(\mathbf{x} \in \mathbb{F}).\ \bigwedge_{j \notin \mathcal{Y}}(x_j = v_j) \land (\kappa(\mathbf{x}) \neq c)$

Outline

More on AXp's and CXp's

- Duality: [INAM20, INM19b]
  - Instance $(\mathbf{v}, c)$, i.e. $c = \kappa(\mathbf{v})$
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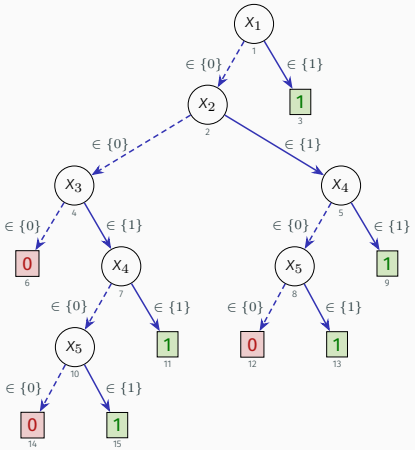
- Global AXp's defined wrt class [INM19b]
  - Counterexamples (CEx's): break (i.e. inconsistent with) prediction of class
  - MHS duality between global AXp's and CEx's
    - Also, connection with adversarial examples

Case study: DT running example



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

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

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

- AXp's: $\{3, 5\}$
  - Other features irrelevant for ensuring the prediction
- CXp's:
  - $\{3\}$, by flipping the value of feature 3
  - $\{5\}$, by flipping the value of feature 5
  - But also, $\{\{3\}, \{5\}\}$ by MHS duality

Case study: DL running example

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

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

Case study: DL running example

R_1: IF $(x_1 = 1)$ THEN 0

R_2: ELSE IF $(x_2 = 1)$ THEN 1

R_3: ELSE IF $(x_4 = 1)$ THEN 0

R_{DEF}: ELSE THEN 1

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

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

Part 3

Computing Explanations – Basics

Outline

How to compute XPs in general?

- Recall:
  - For (weak) AXp:

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

  - For (weak) CXp:

$$\mathsf{WeakCXp}(\mathcal{Y}) \quad := \quad \exists(\mathbf{x} \in \mathbb{F}).\ \bigwedge\nolimits_{j \notin \mathcal{Y}} (x_j = v_j) \land (\kappa(\mathbf{x}) \neq c)$$

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- Encode predicates for computing AXp/CXp
  - For AXp (double negate logic statement):

$$\mathbb{P}_{\text{axp}}(\mathcal{S}) \triangleq \neg \text{co}\left(\left[\!\left[\left(\bigwedge\nolimits_{i \in \mathcal{S}} (x_i = v_i)\right) \land (\kappa(\mathbf{x}) \neq c)\right]\!\right]\right)$$

  - For CXp (use logic statement):

$$\mathbb{P}_{\text{cxp}}(\mathcal{S}) \triangleq \text{co}\left(\left[\!\left[\left(\bigwedge\nolimits_{i \in \mathcal{F} \setminus \mathcal{S}} (x_i = v_i)\right) \land (\kappa(\mathbf{x}) \neq c)\right]\!\right]\right)$$

How to compute XPs in general?

- Recall:
  - For (weak) AXp:

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- And, find subset or cardinality minimal set

Computing one AXp/CXp

[MM20]

Input: Predicate $\mathbb{P}$, parameterized by $\mathcal{T}$, $\mathcal{F}$, κ, $\mathbf{v}$
Output: One XP $\mathcal{S}$

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

Computing smallest AXp/CXp – with hitting set dualization

[MM20]

Input: Predicate $\mathbb{P}_{\text{axp}}$, parameterized by $\mathcal{T}$, $\mathcal{F}$, κ, $\mathbf{v}$
Output: Smallest XP $\mathcal{M}$

1: **procedure** minXP($\mathbb{P}$)
2: $\quad\mathcal{H} \leftarrow \emptyset$
3: $\quad$**while true do**
4: $\quad\quad\mathcal{M} \leftarrow$ MinimumHS($\mathcal{H}$)
5: $\quad\quad$**if** $\mathbb{P}_{\text{axp}}(\mathcal{M})$ **then**
6: $\quad\quad\quad$**return** $\mathcal{M}$
7: $\quad\quad$**else**
8: $\quad\quad\quad\mu \leftarrow$ GetAssignment()
9: $\quad\quad\quad\mathcal{L} \leftarrow$ PickFalseLits($\mathcal{H} \setminus \mathcal{M}, \mu$)
10: $\quad\quad\quad\mathcal{H} \leftarrow \mathcal{H} \cup \mathcal{L}$

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[MM20]

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Output: Smallest XP $\mathcal{M}$

```
1:  procedure minXP(ℙ)
2:      ℋ ← ∅
3:      while true do
4:          ℳ ← MinimumHS(ℋ)
5:          if ℙ_axp(ℳ) then
6:              return ℳ
7:          else
8:              μ ← GetAssignment()
9:              ℒ ← PickFalseLits(ℋ \ ℳ, μ)
10:             ℋ ← ℋ ∪ ℒ
```

- Obs: computing smallest CXp akin to solving MaxSAT [INM19a]

Outline

Initial results for NNs (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

Initial results for NNs (with SMT/MILP)

[INM19a]

First rigorous approach for **explaining** NNs !

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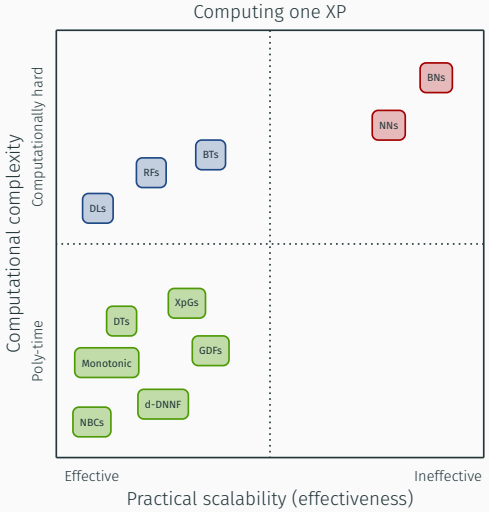
Scales to (a few) tens of neurons...

Efficacy map – current status



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

- **Formal explanations efficient for several families of classifiers**
  - Polynomial-time:
    - Naive-Bayes classifiers (NBCs) [MGC+20]
    - Decision trees (DTs) [IIM20, HIIM21]
    - XpG's: DTs, OBDDs, OMDDs, etc. [HIIM21]
    - Monotonic classifiers [MGC+21]
    - Propositional languages (e.g. d-DNNF, ...) [HII+22]
    - Additional results [CM21, HII+22]
  - Comp. hard, but effective (efficient in practice):
    - Random forests (RFs) [IMS21]
    - Decision lists (DLs) [IM21]
    - Boosted trees (BTs) [INM19c, Ign20, IISMS22]
  - Comp. hard, and ineffective (hard in practice):
    - Neural networks (NNs) [INM19a]
    - Bayesian networks (BNs) [SCD18]

Results for RFs (using SAT oracles)

[IMS21]

Dataset	(#F	#C	#I)	RF			CNF		SAT oracle				PI-expl (**RFxp1**)				Anchor	
				D	#N	%A	#var	#cl	MxS	MxU	#S	#U	Mx	m	avg	%w	avg	%w
ann-thyroid	(21	3	718)	4	2192	98	17 854	29 230	0.12	0.15	2	18	0.36	0.05	0.13	96	0.32	4
appendicitis	(7	2	43)	6	1920	90	5181	10 085	0.02	0.02	4	3	0.05	0.01	0.03	100	0.48	0
banknote	(4	2	138)	5	2772	97	8068	16 776	0.01	0.01	2	2	0.03	0.02	0.02	100	0.19	0
biodegradation	(41	2	106)	5	4420	88	11 007	23 842	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	11 963	0.04	0.02	6	7	0.07	0.01	0.04	100	0.85	0
ionosphere	(34	2	71)	5	2096	87	7174	14 406	0.02	0.02	22	11	0.11	0.02	0.03	100	12.43	0
karhunen	(64	10	200)	5	6198	91	36 708	70 224	1.06	1.41	35	29	14.64	0.65	2.78	100	28.15	0
letter	(16	26	398)	8	44 304	82	28 991	68 148	1.97	3.31	8	8	6.91	0.24	1.61	70	2.48	30
magic	(10	2	381)	6	9840	84	29 530	66 776	0.51	1.84	6	4	2.13	0.07	0.14	99	0.91	1
new-thyroid	(5	3	43)	5	1766	100	17 443	28 134	0.03	0.01	3	2	0.08	0.03	0.05	100	0.36	0
pendigits	(16	10	220)	6	12 004	95	30 522	59 922	2.40	1.32	10	6	4.11	0.14	0.94	96	3.68	4
ring	(20	2	740)	6	6188	89	19 114	42 362	0.27	0.44	11	9	1.25	0.05	0.25	92	7.25	8
segmentation	(19	7	42)	4	1966	90	21 288	35 381	0.11	0.17	8	10	0.53	0.11	0.31	100	4.13	0
shuttle	(9	7	1160)	3	1460	99	18 669	29 478	0.11	0.08	2	7	0.34	0.05	0.14	99	0.42	1
sonar	(60	2	42)	5	2614	88	9938	20 537	0.04	0.06	36	24	0.43	0.04	0.09	100	23.02	0
spectf	(44	2	54)	5	2306	88	6707	13 449	0.07	0.06	20	24	0.34	0.02	0.07	100	8.12	0
texture	(40	11	550)	5	5724	87	34 293	64 187	0.79	0.63	23	17	3.24	0.19	0.93	100	28.13	0
twonorm	(20	2	740)	5	6266	94	21 198	46 901	0.08	0.08	12	8	0.28	0.06	0.10	100	5.73	0
vowel	(13	11	198)	6	10 176	90	44 523	88 696	1.66	2.11	8	5	4.52	0.15	1.15	66	1.67	34
waveform-40	(40	3	500)	5	6232	83	30 438	58 380	0.50	0.86	15	25	7.07	0.11	0.88	100	11.93	0
wpbc	(33	2	78)	5	2432	76	9078	18 675	1.00	1.53	20	13	5.33	0.03	0.65	79	3.91	21

Part 4

Computing Explanations – Encodings

Outline

Computing XPs of DLs

An encoding for DLs – components

$$
\begin{array}{lllll}
\mathsf{R}_1\text{:} & \text{IF} & (\tau_1) & \text{THEN} & d_1 \\
\mathsf{R}_2\text{:} & \text{ELSE IF} & (\tau_2) & \text{THEN} & d_2 \\
 & & \cdots & & \\
\mathsf{R}_j\text{:} & \text{ELSE IF} & (\tau_j) & \text{THEN} & d_j \\
 & & \cdots & & \\
\mathsf{R}_n\text{:} & \text{ELSE IF} & (\tau_n) & \text{THEN} & d_n \\
\mathsf{R}_{\text{DEF}}\text{:} & \text{ELSE} & & \text{THEN} & d_{n+1}
\end{array}
$$

- 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 $\tau_j \nvDash \bot$ and $\tau_k \vDash \bot$, for $1 \leq k < j$, with $e_k = 1$:

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

An encoding for DLs – components

$$
\begin{array}{llllll}
\mathsf{R}_1\text{:} & \mathsf{IF} & (\tau_1) & \mathsf{THEN} & d_1 \\
\mathsf{R}_2\text{:} & \mathsf{ELSE\ IF} & (\tau_2) & \mathsf{THEN} & d_2 \\
 & & \cdots & & \\
\mathsf{R}_j\text{:} & \mathsf{ELSE\ IF} & (\tau_j) & \mathsf{THEN} & d_j \\
 & & \cdots & & \\
\mathsf{R}_n\text{:} & \mathsf{ELSE\ IF} & (\tau_n) & \mathsf{THEN} & d_n \\
\mathsf{R}_{\mathsf{DEF}}\text{:} & \mathsf{ELSE} & & \mathsf{THEN} & d_{n+1}
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- 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
- Require that at least one f_j, with $e_j = 0$ and $1 \leq j \leq n$, to be consistent (i.e. some rule up to j with prediction other than c to fire):

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

An encoding for DLs – components

$$
\begin{array}{lllll}
\mathsf{R}_1\colon & \text{IF} & (\tau_1) & \text{THEN} & d_1 \\
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 & & \cdots & & \\
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 & & \cdots & & \\
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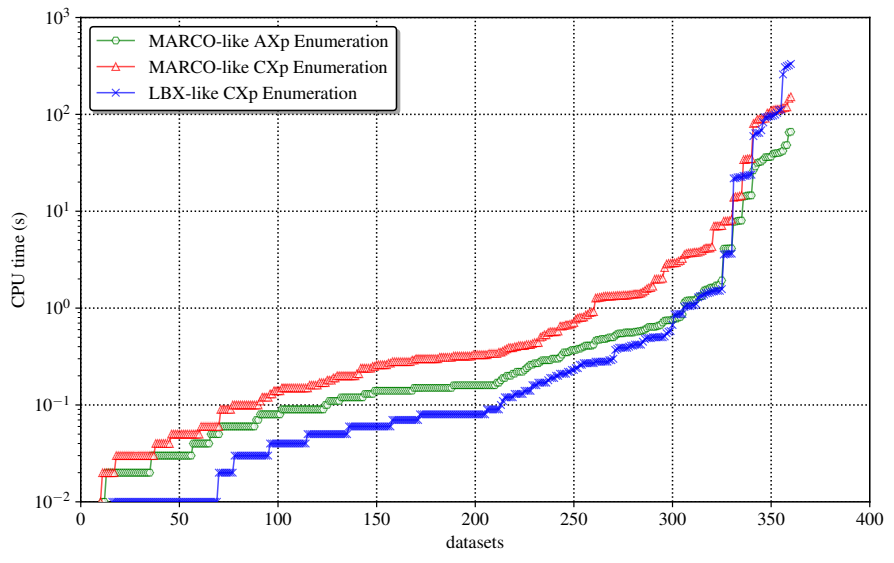
\mathsf{R}_{\mathsf{DEF}}\colon & \text{ELSE} & & \text{THEN} & d_{n+1}
\end{array}
$$

- 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:

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

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

Empirical Evidence



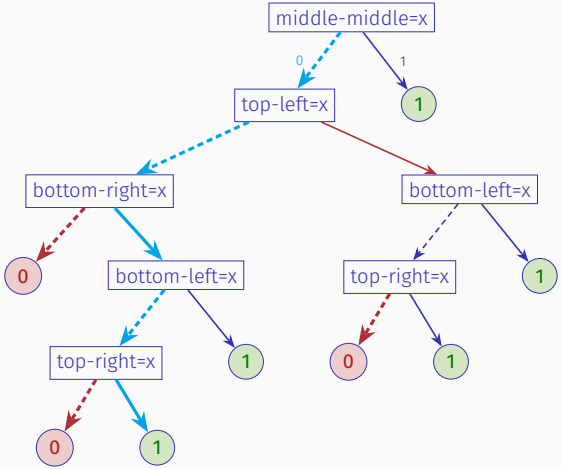
Part 5

Tractable Explanations

Outline

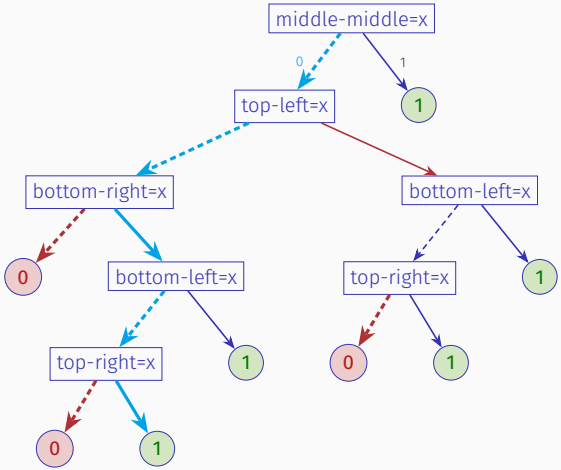
DT explanations

[IIM20, IIM22]



DT explanations

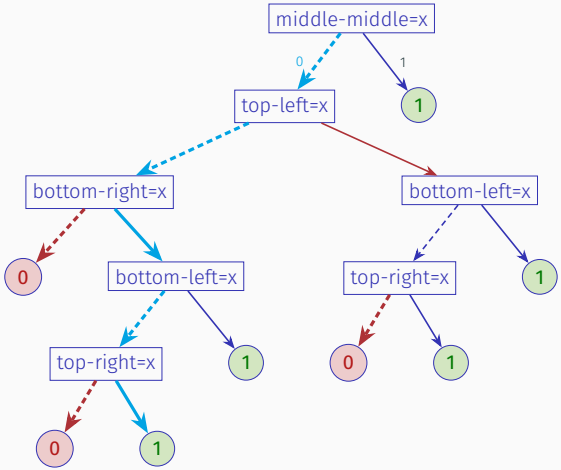
[IIM20, IIM22]



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

DT explanations

[IIM20, IIM22]



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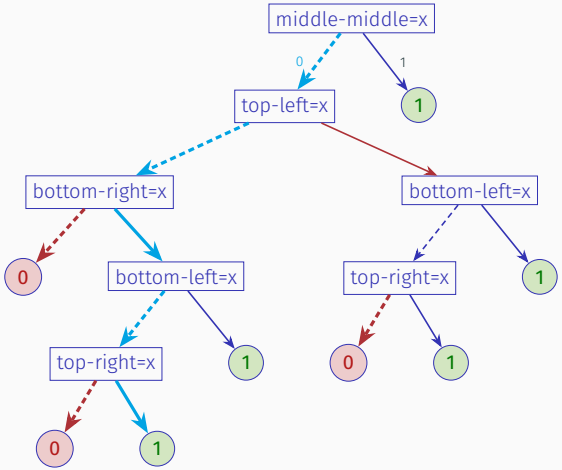
- For prediction 1, it suffices to ensure all paths with prediction 0 remain inconsistent

DT explanations in polynomial time

[IIM20, IIM22]



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- 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]

DT explanations in polynomial time

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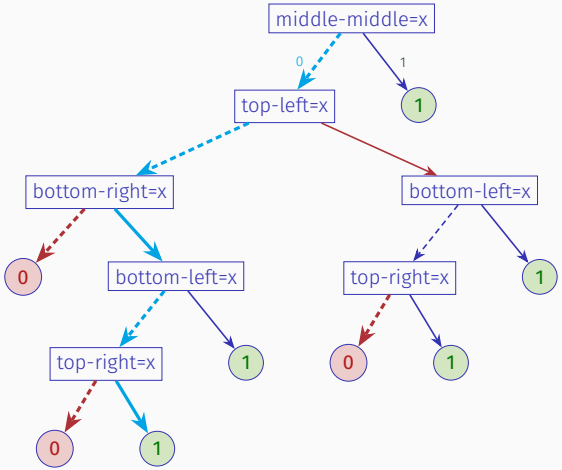

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    - E.g. BR and TR suffice for prediction
  - Well-known to be solvable in polynomial time [EG95]
- Alternative: use Horn encoding (see notes)

Preliminary results for DTs

[IIM20, HIIM21, IIM22]

Dataset	(#F	#S)	IAI									ITI								
			D	#N	%A	#P	%R	%C	%m	%M	%avg	D	#N	%A	#P	%R	%C	%m	%M	%avg
adult	(12	6061)	6	83	78	42	33	25	20	40	25	17	509	73	255	75	91	10	66	22
anneal	(38	886)	6	29	99	15	26	16	16	33	21	9	31	100	16	25	4	12	20	16
backache	(32	180)	4	17	72	9	33	39	25	33	30	3	9	91	5	80	87	50	66	54
bank	(19	36 293)	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	18 668)	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	13 442)	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	10 992)	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	58 000)	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	—	—	—

Outline

Explaining monotonic classifiers

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

    $\mathbf{v}_\mathsf{L} \leftarrow (v_{\mathsf{L}_1}, \ldots, v_i, \ldots, v_{\mathsf{L}_N})$
    $\mathbf{v}_\mathsf{U} \leftarrow (v_{\mathsf{U}_1}, \ldots, v_i, \ldots, v_{\mathsf{U}_N})$
    $(\mathcal{A}, \mathcal{B}) \leftarrow (\mathcal{A} \setminus \{i\}, \mathcal{B} \cup \{i\})$
    return $(\mathbf{v}_\mathsf{L}, \mathbf{v}_\mathsf{U}, \mathcal{A}, \mathcal{B})$
  - FreeAttr(i):

    $\mathbf{v}_\mathsf{L} \leftarrow (v_{\mathsf{L}_1}, \ldots, \lambda(i), \ldots, v_{\mathsf{L}_N})$
    $\mathbf{v}_\mathsf{U} \leftarrow (v_{\mathsf{U}_1}, \ldots, \mu(i), \ldots, v_{\mathsf{U}_N})$
    $(\mathcal{A}, \mathcal{B}) \leftarrow (\mathcal{A} \setminus \{i\}, \mathcal{B} \cup \{i\})$
    return $(\mathbf{v}_\mathsf{L}, \mathbf{v}_\mathsf{U}, \mathcal{A}, \mathcal{B})$

Computing one AXp

1: $\mathbf{v}_\mathsf{L} \leftarrow (v_1, \ldots, v_N)$
2: $\mathbf{v}_\mathsf{U} \leftarrow (v_1, \ldots, v_N)$ ▷ Ensures: $\kappa(\mathbf{v}_\mathsf{L}) = \kappa(\mathbf{v}_\mathsf{U})$
3: $(\mathcal{C}, \mathcal{D}, \mathcal{P}) \leftarrow (\mathcal{F}, \emptyset, \emptyset)$ ▷ $\mathcal{S}$: Some possible seed
4: **for all** $i \in \mathcal{S}$ **do**
5: $(\mathbf{v}_\mathsf{L}, \mathbf{v}_\mathsf{U}, \mathcal{C}, \mathcal{D}) \leftarrow \text{FreeAttr}(i, \mathbf{v}, \mathbf{v}_\mathsf{L}, \mathbf{v}_\mathsf{U}, \mathcal{C}, \mathcal{D})$ ▷ Require: $\kappa(\mathbf{v}_\mathsf{L}) = \kappa(\mathbf{v}_\mathsf{U})$, given $\mathcal{S}$
6: **for all** $i \in \mathcal{F} \setminus \mathcal{S}$ **do** ▷ Loop inv.: $\kappa(\mathbf{v}_\mathsf{L}) = \kappa(\mathbf{v}_\mathsf{U})$
7: $(\mathbf{v}_\mathsf{L}, \mathbf{v}_\mathsf{U}, \mathcal{C}, \mathcal{D}) \leftarrow \text{FreeAttr}(i, \mathbf{v}, \mathbf{v}_\mathsf{L}, \mathbf{v}_\mathsf{U}, \mathcal{C}, \mathcal{D})$
8: **if** $\kappa(\mathbf{v}_\mathsf{L}) \neq \kappa(\mathbf{v}_\mathsf{U})$ **then** ▷ If invariant broken, fix it
9: $(\mathbf{v}_\mathsf{L}, \mathbf{v}_\mathsf{U}, \mathcal{D}, \mathcal{P}) \leftarrow \text{FixAttr}(i, \mathbf{v}, \mathbf{v}_\mathsf{L}, \mathbf{v}_\mathsf{U}, \mathcal{D}, \mathcal{P})$
10: **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 6

Explainability Queries

Outline

How to navigate the space of XPs?

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

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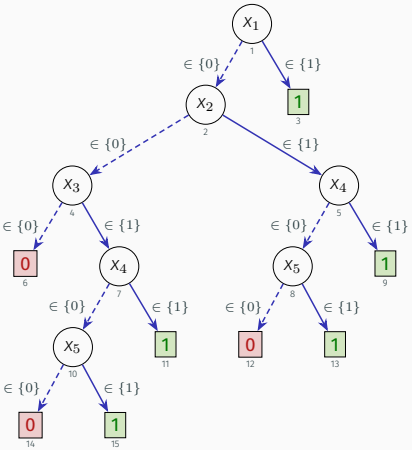
- Best solution is a MARCO-like algorithm (for enumerating MUSes) [LPMM16]
  - On-demand enumeration of AXp's/CXp's

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

DT classifier – example run of enumerator

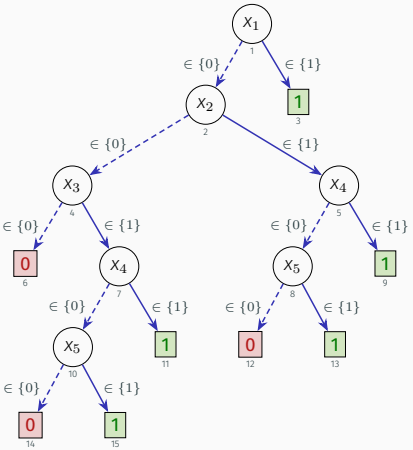


- Instance: $(\mathbf{v}, c) = ((0, 0, 1, 0, 1), 1)$

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

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

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
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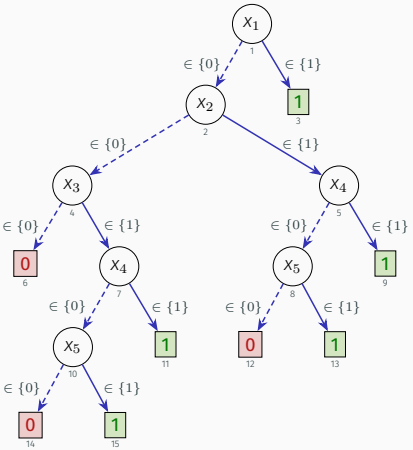
1	1	1	1	1	1

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

Iter.	$\mathbf{u}$	$\mathcal{S}$	$\mathbb{P}_{\text{cxp}}(\cdot)$	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	$[\text{outc} = \textbf{false}]$	–	–	–	–	–

DT classifier – another example run of enumerator



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1	1	1	0	1	1
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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

- 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 $\mathbf{v}$
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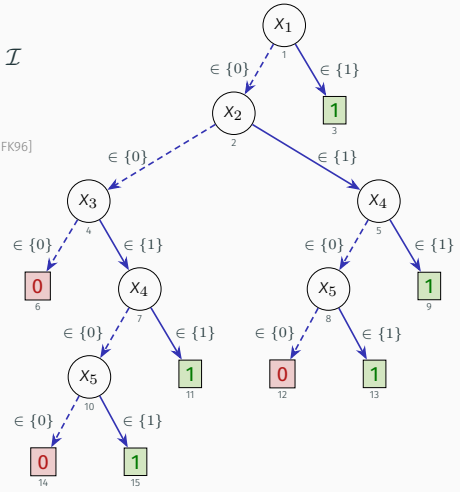
  - And each MHS is an AXp
- Example:
  - $I_1 = \{3\}$
  - $I_2 = \{5\}$
  - $I_3 = \{2, 5\}$
  - $\therefore$ keep I_1 an I_2
  - AXp's: MHSes yield $\{\{3, 5\}\}$

[FK96]



Outline

What is feature membership?

- The feature membership problem (FMP):
  - Given an instance $(\mathbf{v}, c)$ and a (sensitive) target feature $t \in \mathcal{F}$
  - Q: Does there exist an AXp/CXp that includes t?

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  - For 3 and 5, the answer to FMP is **true**
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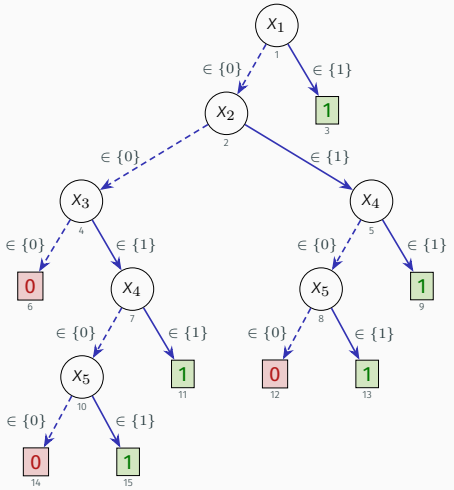

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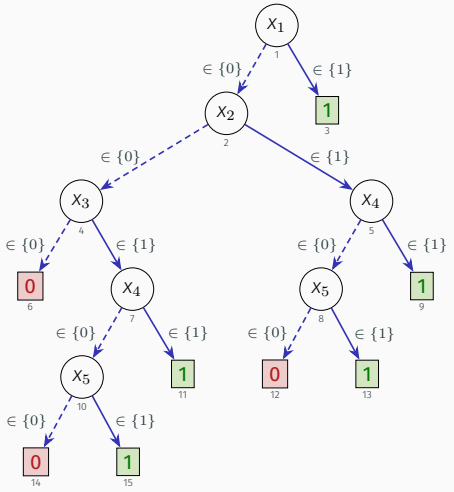
  - For 1, 2, 4, the answer to FMP is **false**
- Some results:
  - Σ_2^{P}-hard for DNF classifiers [HIIM21]
    - Hence, Σ_2^{P}-hard for NNs, RFs, BTs, etc.
  - In P for decision trees [HIIM21]
  - In NP when computing AXp/CXp is in P [HM22]



Additional observations

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- FMP in NP if computing one AXp is in P:
  - Guess a set $\mathcal{X}$, that contains t
  - Check (in poly-time) that $\mathcal{X}$ is weak AXp
  - For each feature $j \in \mathcal{X}$, check (in poly-time) that $\mathcal{X} \setminus \{j\}$ is not a weak AXp
  - Overall algorithm runs in poly-time

Outline

Additional explicability queries

- Class queries [AKM20, ABB+21]
  - Mandatory/forbidden features for class
  - Necessary features for class
  - ...
- Explanation queries:
  - Smallest AXp's
  - Finding one AXp
  - Finding on CXp
- Complexity: [ABB+21]
  - Poly-time for DTs
  - Computationally hard for other classifiers: DLs, RFs, BTs, boolean NNs, BNNs

Part 7

Probabilistic Explanations

Outline

Defining Probabilistic Explanations

Why probabilistic XPs?

- Explanation size can exceed cognitive limits of human decision makers
- Smallest explanations are rarely significantly smaller than irreducible explanations
- Goal of probabilistic explanations is to trade off smaller size for less rigor
  - I.e. find set $\mathcal{X}$ such that

$$\Pr_{\mathbf{x}}(\kappa(\mathbf{x}) = c \,|\, \mathbf{x}_{\mathcal{X}} = \mathbf{v}_{\mathcal{X}}) \geq \delta$$

  Obs: for $\delta = 1$, set $\mathcal{X}$ is a (weak) AXp
- Weak probabilistic abductive explanation:

$$\text{WeakPAXp}(\mathcal{X}; \mathbb{F}, \kappa, \mathbf{v}, c, \delta) \quad := \quad \Pr_{\mathbf{x}}(\kappa(\mathbf{x}) = c \,|\, \mathbf{x}_{\mathcal{X}} = \mathbf{v}_{\mathcal{X}}) \geq \delta$$

- Probabilistic abductive explanation:
  - Subset-minimal (PAXp) vs. cardinality minimal (minPAXp)

Overview of main results

- For boolean circuit classifiers, computing one minPAXp is NP^{PP}-hard [WMHK21]
- For DTs, finding one minPAXp/PAXp is NP-hard [IIN+22, ABRS22]
  - Approximate Weak PAXp's can be computed in linear time (see notes)
- For NBCs, dynamic programming approach [IM22]
- Recent hardness results [ABRS22]
- General approach?

Part 8

Additional Topics & Conclusions

Outline

Additional Topics

Beyond ML Explanations

Links with fairness, robustness & model learning

- Robustness: [INM19b]
  - Link with adversarial examples
- Model learning: [NIPM18]
  - Efforts on learning *interpretable* models
- Fairness: [ICS+20]
  - Criterion: Fairness Through Unawareness (FTU)
  - Assess bias on dataset/classifier
  - Bias on classifier related with XPs

Some additional topics

- Input constraints [GR22, YIS+22]
- Surrogate models [BAMT21]
- Generalized explanation literals [IIM22]
- Localized explanations
  - Require sufficiency close to reference point
- Certification of explainability
  - Certify results generated with implemented algorithms

Outline

Explainability beyond ML explanations

- Model-based diagnosis & abduction
- AI planning
- Optimization
- Problem solving
- ...
- XPs relevant for any sort of algorithmic decision making

Conclusions

- Critical limitations of widely used XAI approaches:
  - Model-agnostic methods can compute **incorrect** explanations
    - Similar limitations for methods based on saliency maps for NNs
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    - Initial theoretical insights, e.g. duality between AXp's and CXp's (and so between "Why?" and "Why not?" explanations)
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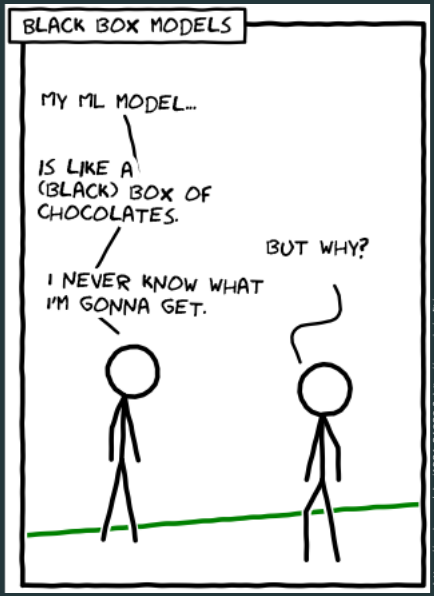
    - Initial theoretical insights, e.g. duality between AXp's and CXp's (and so between "Why?" and "Why not?" explanations)
  - Other problems of crucial importance: enumeration, membership, etc.
- Ongoing research related with:
  - Computation of AXp's & CXp's
  - Enumeration of explanations
  - Deciding membership of features in explanations
  - Probabilistic rigorous explanations
  - Surrogate models, input constraints, etc.
  - Also, complexity of explainability

Q & A

Acknowledgment: joint work with A. Ignatiev, Y. Izza, X. Huang, M. Cooper, N. Asher, N. Narodytska, E. Hebrard, M. Siala, et al.


BLACK BOX MODELS
MY ML MODEL...
IS LIKE A (BLACK) BOX OF CHOCOLATES.
I NEVER KNOW WHAT I'M GONNA GET.
BUT WHY?
https://arxiv.org/abs/1901.01686 & http://cmx.io/edit/

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