Logic-Based Explainable Artificial Intelligence

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Lecture 03

Recapitulate second lecture

- Rigorous definitions of abductive and contrastive explanations

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- Example algorithm for finding one AXp/CXp

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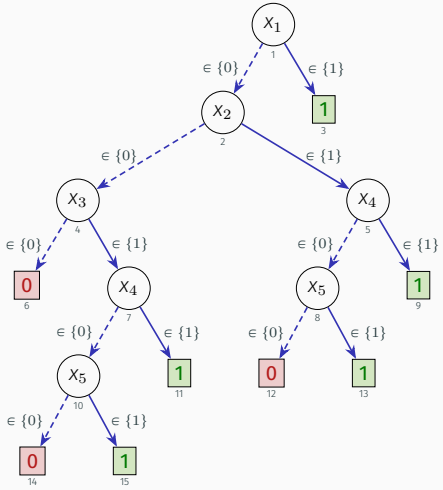
- Explanations for monotonic classifiers

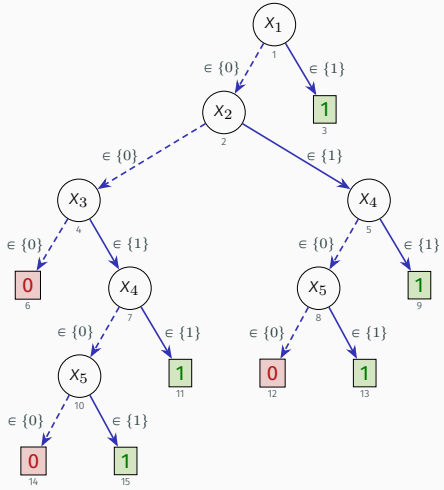
Recap AXps/CXps: DT example

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



Recap AXps/CXps: DT example

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



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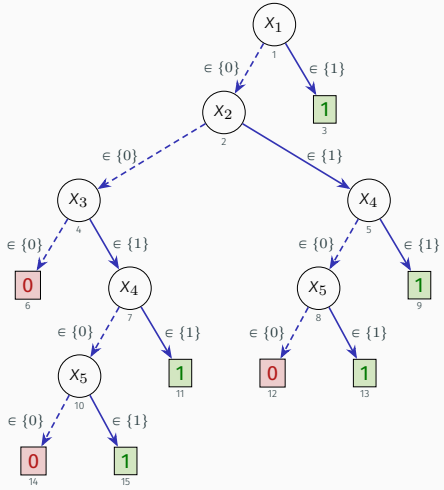

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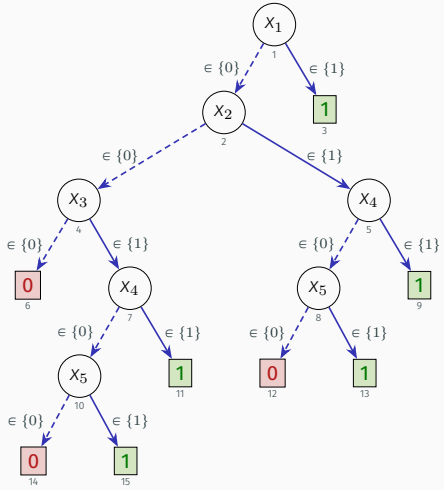

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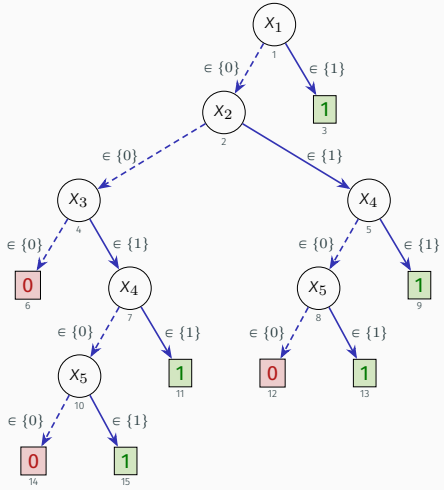

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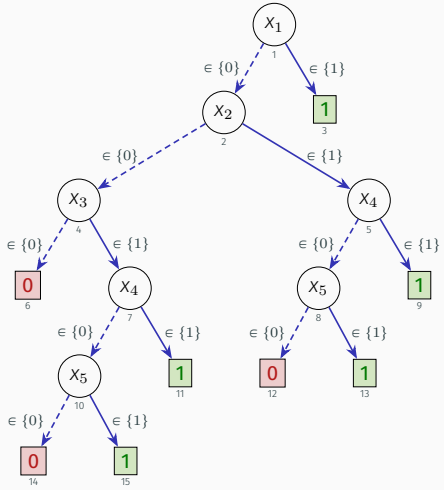

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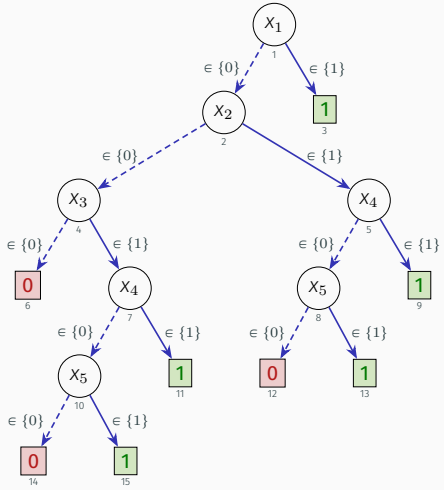

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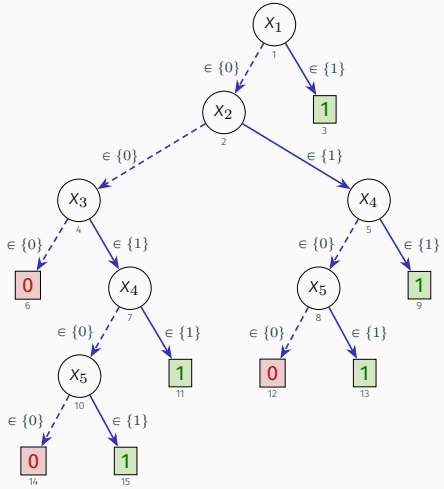
  - l_4: $\{2, 4\}$
  - l_5: $\{1\}$



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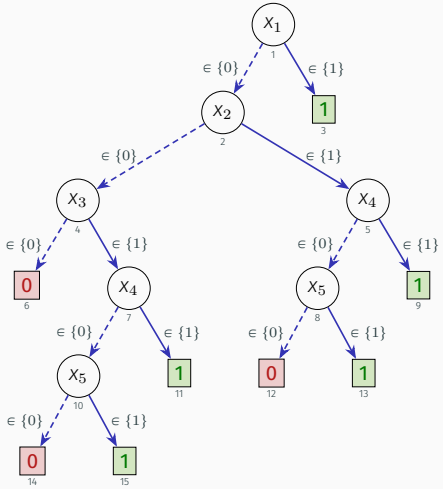
  - $\mathcal{L} = \{\{1\}, \{4\}, \{5\}\}$



Recap AXps/CXps: DL example

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

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

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

R_{DEF}: ELSE THEN 1

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

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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

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18	1	1	0	0	R_1	0
19	1	1	0	1	R_1	0
20	1	1	0	2	R_1	0
21	1	1	1	0	R_1	0
22	1	1	1	1	R_1	0
23	1	1	1	2	R_1	0

Plan for this course

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

Some comments...

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

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- For high-risk and safety-critical domains:
  - Would you use an ML model that you cannot explain with rigor, and whose heuristic explanations can be incorrect, and so debugging/understanding with rigor is all but impossible?

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- What is the bottom line?
  - For high-risk and safety-critical domains, one **ought** to deploy models that can be explained with rigor
  - If that means using a fairly unexciting NN with up to 100K neurons, that is the cost of trust; **for anything else, one is trying his/her luck, in situations that could become catastrophic!**

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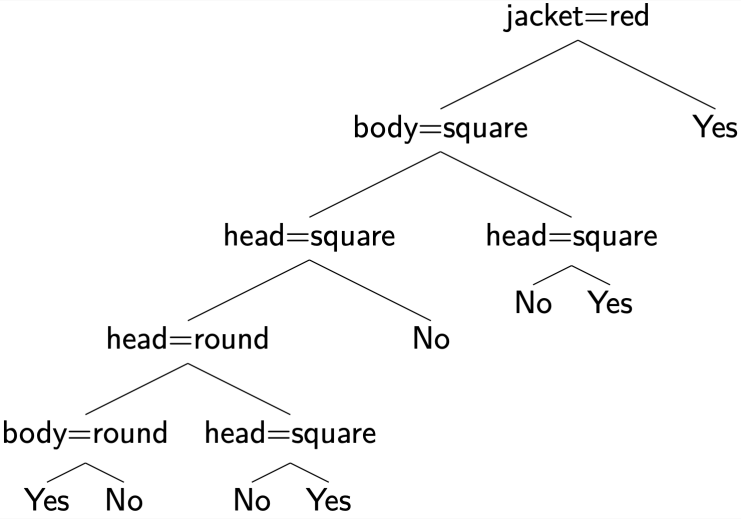
  - More examples next...

Priceless optimal sparse decision trees (OSDT) – & non-optimality!... [HRS19]



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

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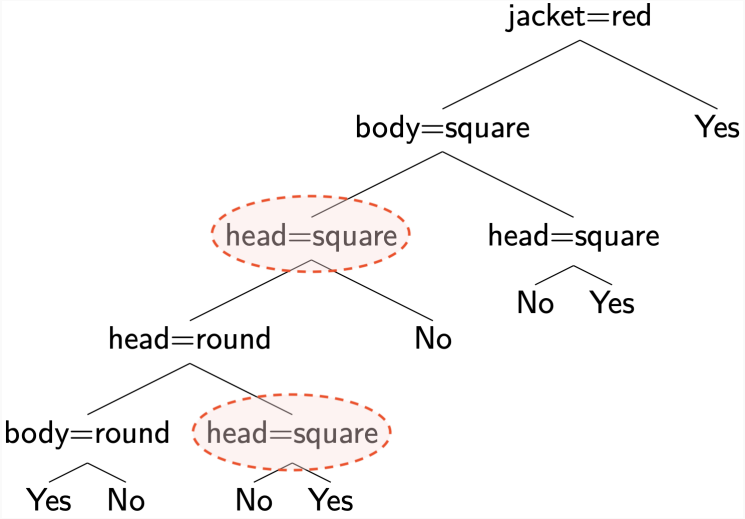

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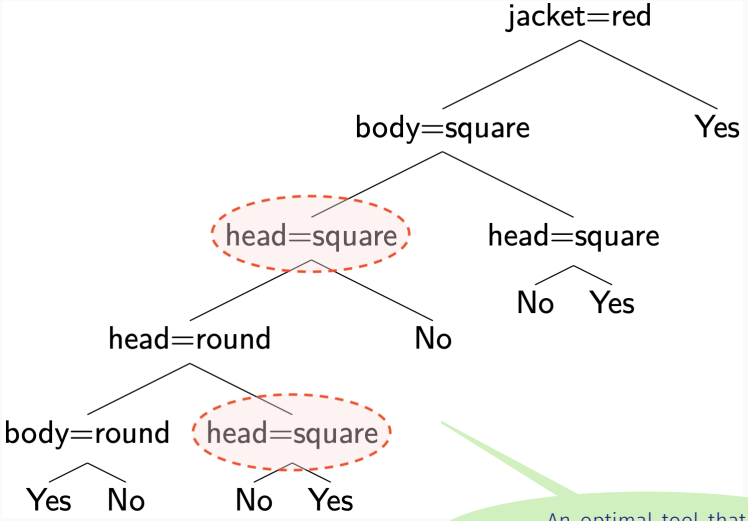

An optimal tool that produces **non-optimal** DTs...!?

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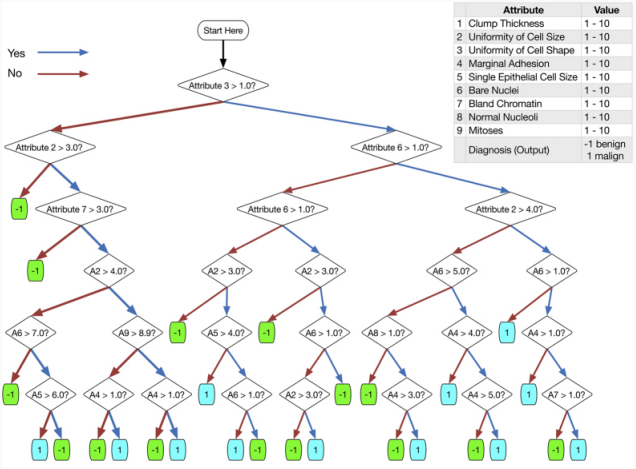
BTW, highly problematic decision trees also in precision medicine...



	Attribute	Value
1	Clump Thickness	1 - 10
2	Uniformity of Cell Size	1 - 10
3	Uniformity of Cell Shape	1 - 10
4	Marginal Adhesion	1 - 10
5	Single Epithelial Cell Size	1 - 10
6	Bare Nuclei	1 - 10
7	Bland Chromatin	1 - 10
8	Normal Nucleoli	1 - 10
9	Mitoses	1 - 10
	Diagnosis (Output)	-1 benign 1 malign

Example Interpretable Rules Induced by MediBoost:

A3 Uniformity of Cell Shape ≤ 1.0 $\wedge$ A2 Uniformity of Cell Size > 3.0 $\wedge$ A7 Bland Chromatin ≤ 3.0 $\Rightarrow$ predict benign

A3 Uniformity of Cell Shape > 1.0 $\wedge$ A6 Bare Nuclei ≤ 1.0 $\wedge$ A2 Uniformity of Cell Size ≤ 3.0 $\Rightarrow$ predict benign

Source: G. Valdes, J.M. Luna, E. Eaton, C.B. Simone, L.H. Ungar, & T.D. Solberg.

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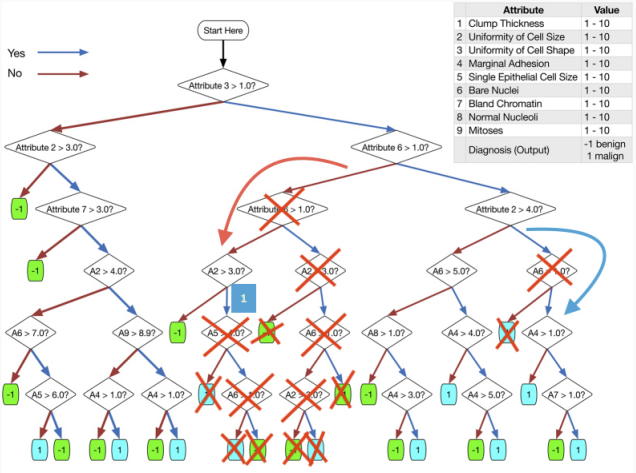

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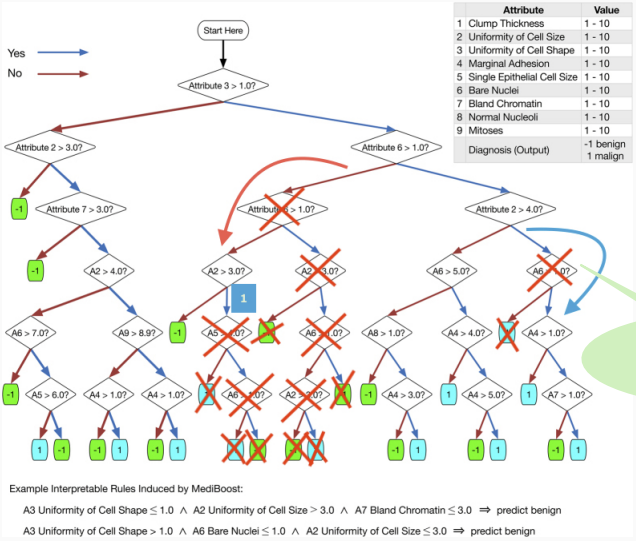

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And **massive** path redundancy**!**

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- And how to debug complex ML models if heuristic explanations are also incorrect (more later)?

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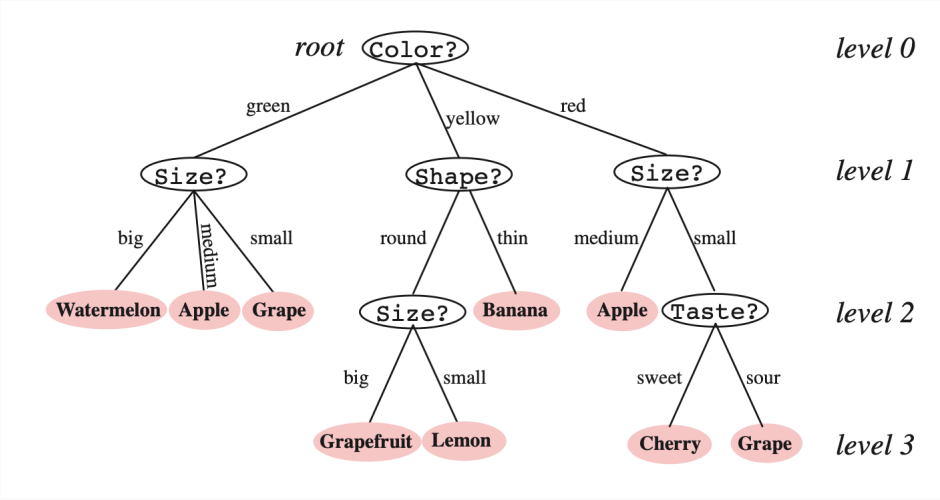
- Previous slides: two examples of obviously buggy DTs
- However, it is relatively simple to implement tree learners
- Can one really trust the operation of more complex ML models, even those subject to extensive testing?
- And how to debug complex ML models if heuristic explanations are also incorrect (more later)?
- For trustworthy AI, there exists no alternative to rigorous logic-based explanations!

BTW, problematic DTs even in books...

[dud01]



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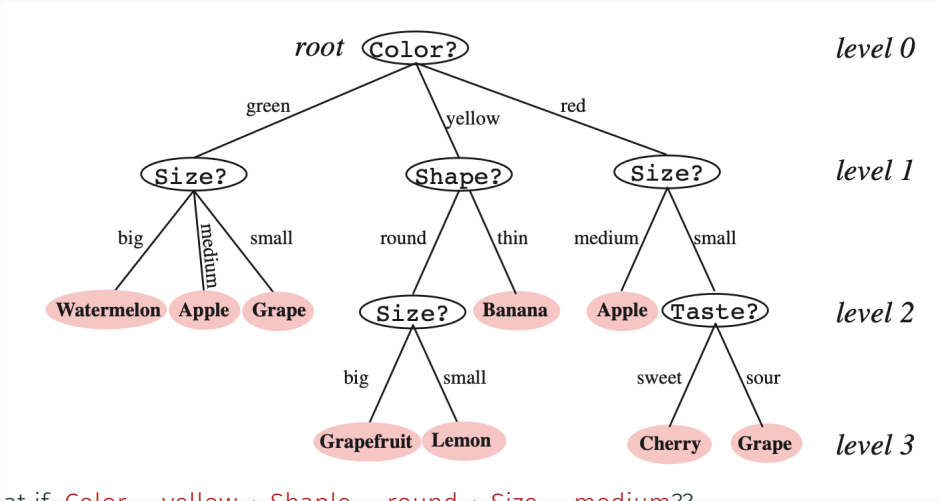

- What if $\text{Color} = \text{yellow} \wedge \text{Shaple} = \text{round} \wedge \text{Size} = \text{medium}$??

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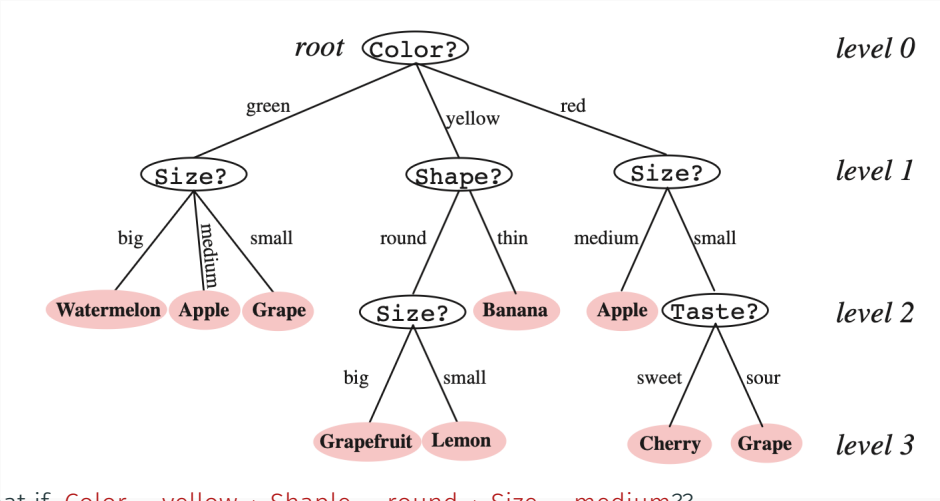

- What if $\text{Color} = \text{yellow} \wedge \text{Shaple} = \text{round} \wedge \text{Size} = \text{medium}$??
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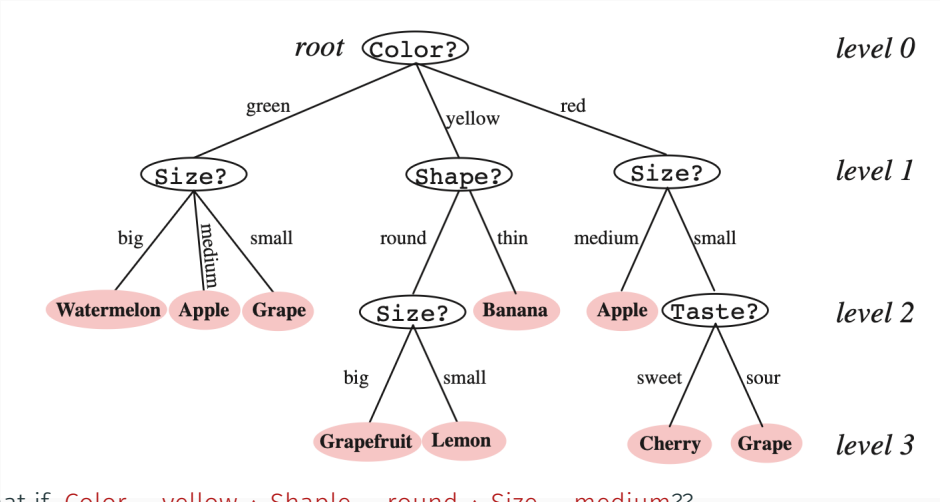

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- Or, what if $\text{Color} = \text{red} \wedge \text{Size} = \text{big}$??
- Easy to envision more serious use-cases...

Unit #04

(Efficient) Intractability in Symbolic XAI

An encoding for DLs – components

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

An encoding for DLs – components

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 & & \dots & & \\
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 & & \dots & & \\
\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}
\end{array}
$$

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

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

An encoding for DLs – components

$$
\begin{array}{llllll}
\mathrm{R}_1\text{:} & \text{IF} & (\tau_1) & \text{THEN} & d_1 \\
\mathrm{R}_2\text{:} & \text{ELSE IF} & (\tau_2) & \text{THEN} & d_2 \\
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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):

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

An encoding for DLs – components

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

- 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:

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

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

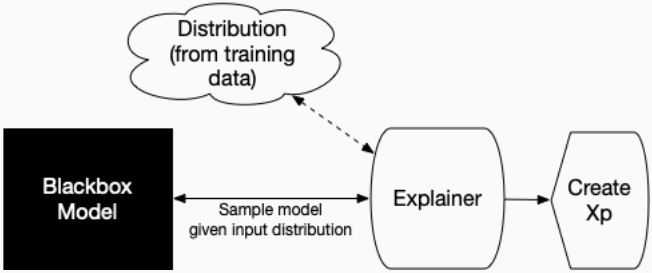
Outline – Unit #04

Explaining Decision Lists

Myth #02: Model-Agnostic Explainability

Progress Report on Symbolic XAI

What is model-agnostic explainability?



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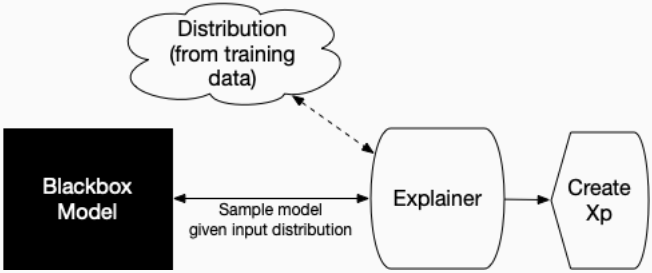

- Wildly popular XAI approach [RSG16, LL17, RSG18]
  - **Feature attribution**: LIME, SHAP, ... [RSG16, LL17]
  - **Feature selection**: Anchors, ... [RSG18]

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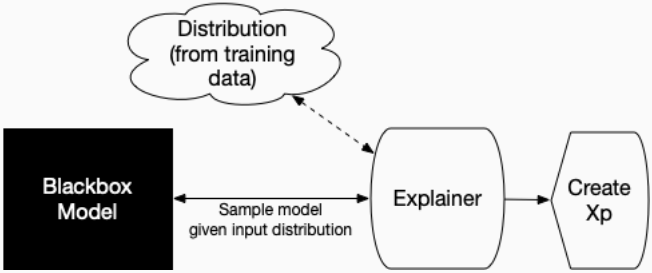

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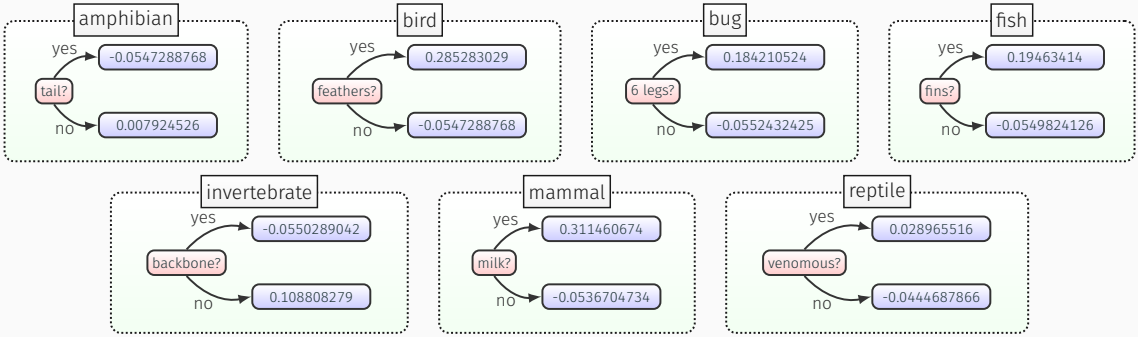
- **Q:** Are model-agnostic explanations rigorous?

Easy to spot problems – BT for zoo dataset

[INM19b, Ign20]



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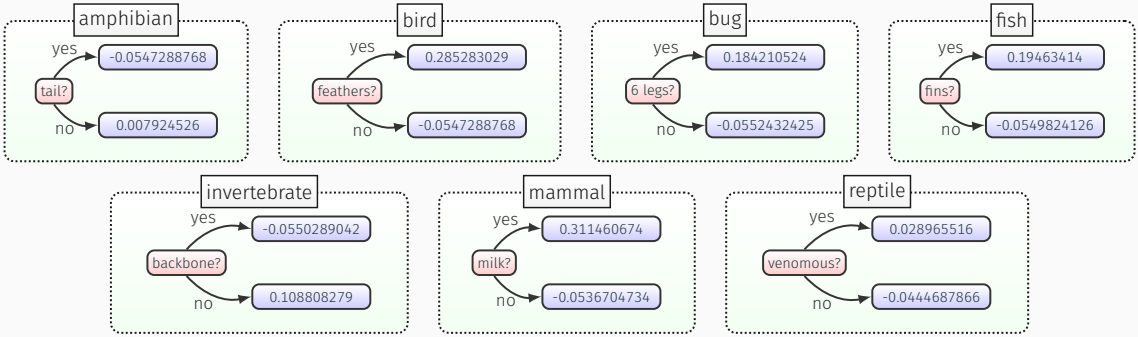


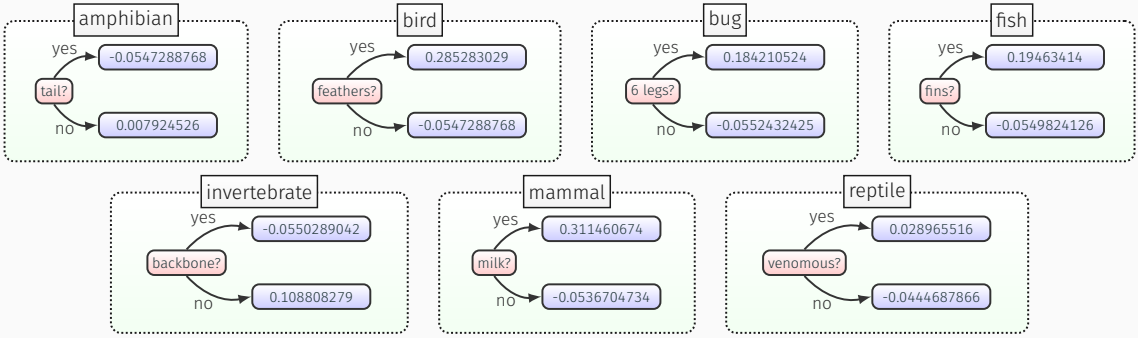
- Example instance:

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

THEN (class = reptile)

Easy to spot problems – BT for zoo dataset & Anchor

[INM19b, 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

THEN (class = reptile)

Easy to spot problems – BT for zoo dataset & Anchor

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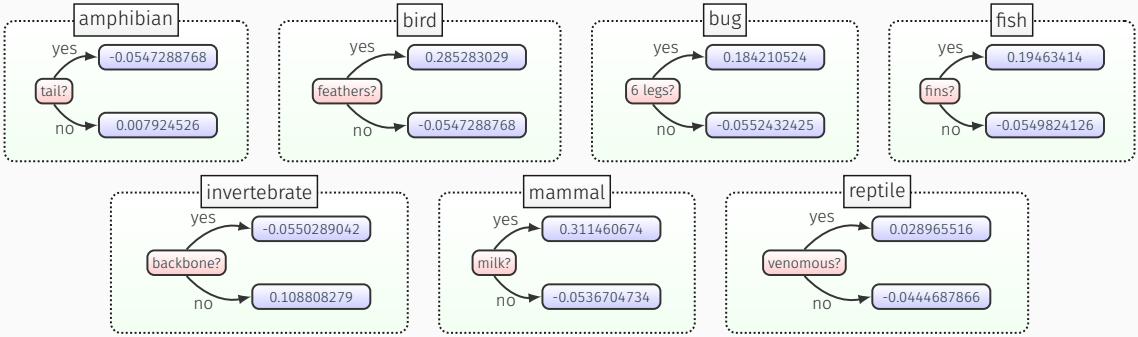


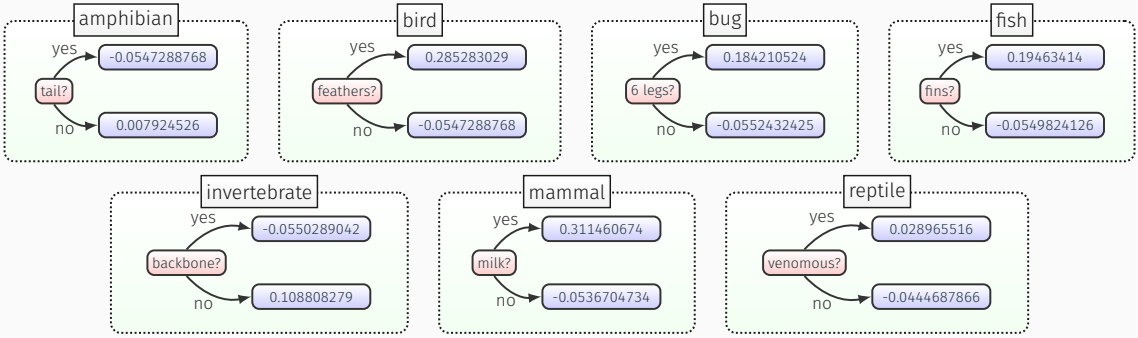
- Explanation obtained with Anchor: [RSG18]

IF $\neg hair \wedge \neg milk \wedge \neg toothed \wedge \neg fins$

THEN (class = reptile)

Easy to spot problems – BT for zoo dataset & Anchor

[INM19b, Ign20]



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

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

THEN (class = amphibian)

Model-agnostic explainers cannot be trusted

[INM19b]

Incorrect explanations:

Classifier for deciding bank loans

Model-agnostic explainers cannot be trusted

[INM19b]

Incorrect explanations:

Classifier for deciding bank loans

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

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 $= 50\text{K}$

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

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

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

$\therefore$ different outcomes & same explanation !?

How to validate model-agnostic explanations

- For feature selection, checking rigor is *easy*

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- Check whether $\mathcal{X}$ is a (rigorous) (W)AXp:
  1. $\mathcal{X}$ is sufficient for prediction:

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

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

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

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

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

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Dataset	% Incorrect	% Redundant	% Correct
adult	80.5%	1.6%	17.9%
lending	3.0%	0.0%	97.0%
rcdv	99.4%	0.4%	0.2%
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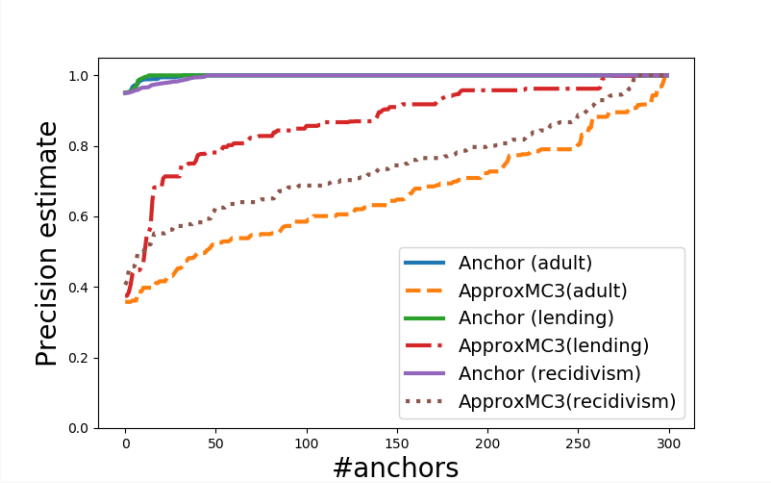
  - In this case, BNNs were used, to allow for model counting...
- For feature attribution we proposed different ways of assessing rigor [INM19b, NSM+19, Ign20, YIS+23]

Incorrect explanations are ubiquitous & likely...

[NSM+19]



Outline – Unit #04

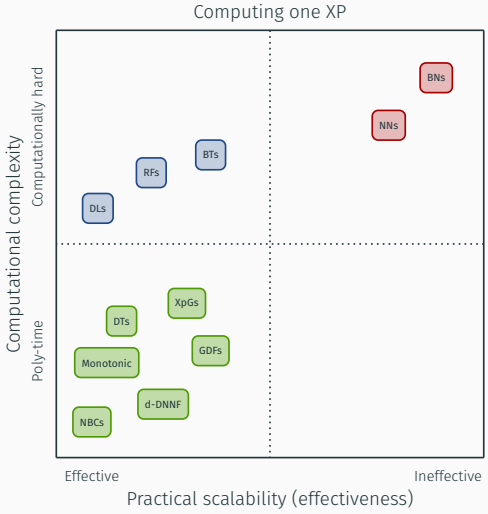
Explaining Decision Lists

Myth #02: Model-Agnostic Explainability

Progress Report on Symbolic XAI

Efficacy map – progress until 2022

[MI22, Mar22, MS23]



[INM19b, 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]
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    - Monotonic classifiers [MGC+21]
    - Propositional languages (e.g. d-DNNF, ...) [HII+22]
    - Additional results [CM21, HII+22]
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  - Comp. hard, and ineffective (hard in practice):
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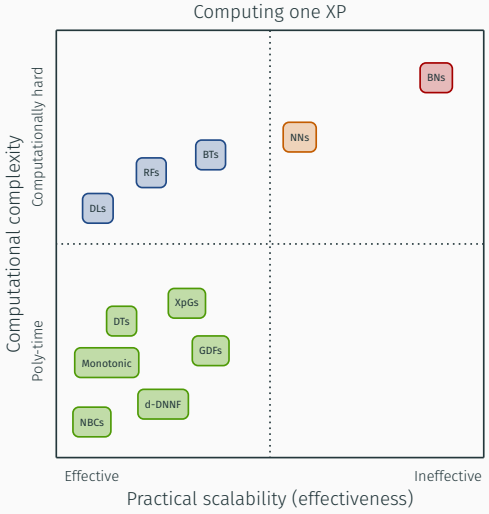
    - Bayesian networks (BNs) [SCD18]

Efficacy map – recent progress

[HM23]



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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 !

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

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

[HM23]

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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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 **tens of thousands** of neurons!

Largest for MNIST: **10142** neurons

Largest for GSTRB: **94308** neurons

Unit #05

Queries in Symbolic XAI

Outline – Unit #05

Enumeration of Explanations

Feature Necessity & Relevancy

How to navigate the space of XPs?

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

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

Recall computing one AXp/CXp – oneXP

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

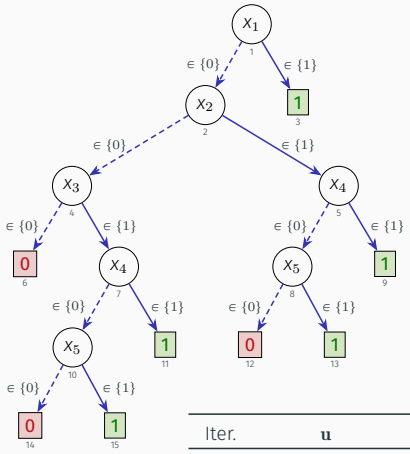
procedure oneXP($\mathbb{P}$)
  $\mathcal{S} \leftarrow \mathcal{F}$ ▷ Initialization: $\mathbb{P}(\mathcal{S})$ holds
  for $i \in \mathcal{F}$ **do** ▷ Loop invariant: $\mathbb{P}(\mathcal{S})$ holds
    if $\mathbb{P}(\mathcal{S}\backslash\{i\})$ **then**
      $\mathcal{S} \leftarrow \mathcal{S}\backslash\{i\}$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

Generic oracle-based enumeration algorithm

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

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

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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	Resulting $\mathcal{H}$
1	$(1, 1, 1, 1, 1)$	$\varnothing$	1	–	$\{3\}$	$(\neg u_3)$	$\{(\neg u_3)\}$
2	$(1, 1, 0, 1, 1)$	$\{3\}$	1	–	$\{5\}$	$(\neg u_5)$	$\{(\neg u_3), (\neg u_5)\}$
3	$(1, 1, 0, 1, 0)$	$\{3, 5\}$	0	$\{3, 5\}$	–	$(u_3 \vee u_5)$	$\{(\neg u_3), (\neg u_5), (u_3 \vee u_5)\}$
5	[outc = **false**]	–	–	–	–	–	$\{(\neg u_3), (\neg u_5), (u_3 \vee u_5)\}$

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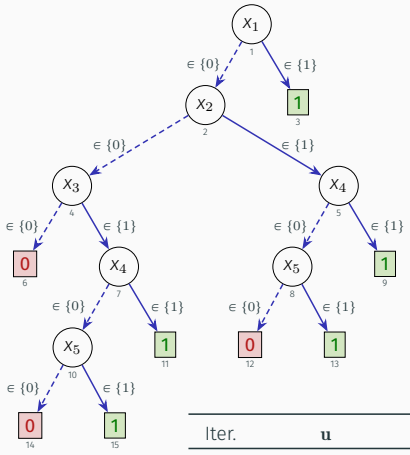

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Iter.	$\mathbf{u}$	$\mathcal{S}$	$\mathbb{P}_{\text{cxp}}(\cdot)$	AXp	CXp	Clause	Resulting $\mathcal{H}$
1	$(0,0,0,0,0)$	$\{1,2,3,4,5\}$	0	$\{3,5\}$	–	$(u_3 \vee u_5)$	$\{(u_3 \vee u_5)\}$
2	$(0,0,1,0,0)$	$\{1,2,4,5\}$	1	–	$\{3\}$	$(\neg u_3)$	$\{(u_3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

DTs admit more efficient algorithms

- Recall:
  - Given instance $(\mathbf{v}, c)$, create set $\mathcal{I}$
  - For each path P_k with prediction $d \neq c$:
    - Let I_k denote the features with literals inconsistent with $\mathbf{v}$
    - Add I_k to $\mathcal{I}$
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- $\mathcal{I}$ is the set of CXp's – algorithm runs in poly-time
- For AXp's: run std dualization algorithm [FK96]
  - Obs: starting hypergraph is poly-size!
  - And each MHS is an AXp

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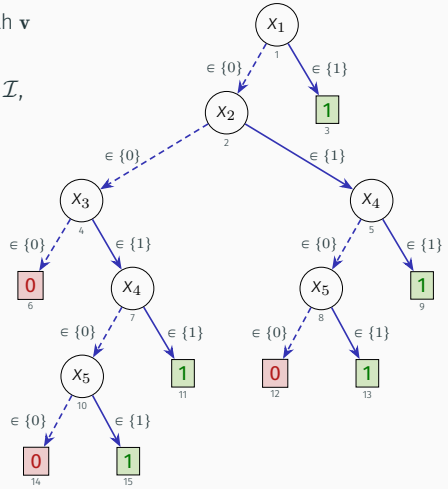
  - Remove from $\mathcal{I}$ the sets that have a proper subset in $\mathcal{I}$, and duplicates
- $\mathcal{I}$ is the set of CXp's – algorithm runs in poly-time
- For AXp's: run std dualization algorithm [FK96]
  - Obs: starting hypergraph is poly-size!
  - And each MHS is an AXp
- Example:
  - $I_1 = \{3\}$
  - $I_2 = \{5\}$
  - $I_3 = \{2, 5\}$
  - $\therefore$ keep I_1 an I_2
  - AXp's: MHSes yield $\{\{3, 5\}\}$



Outline – Unit #05

Enumeration of Explanations

Feature Necessity & Relevancy

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

[HCM+23]

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Feature necessity

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- Sets of all AXp's & CXp's:

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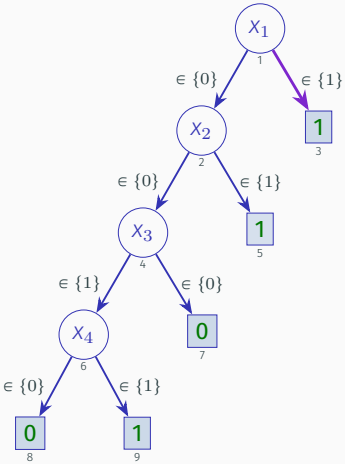
- **Claim #04:** AXp-necessity of $t \in \mathcal{F}$ is in P if t has a domain size which is polynomially-bounded on instance size
  - This holds for any classifier!
  - Let $\mathbf{u}$ be obtained from $\mathbf{v}$ by replacing the constant v_t by some variable $u_t \in \mathcal{D}_t$
  - Feature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

An example

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



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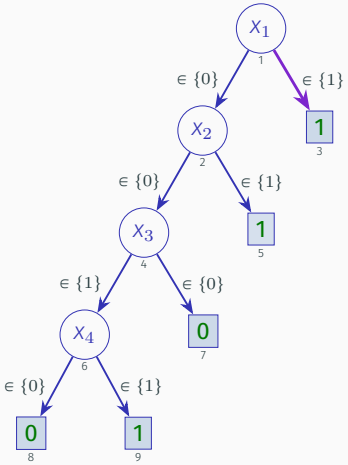

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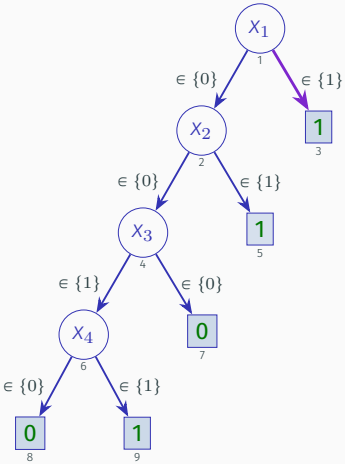

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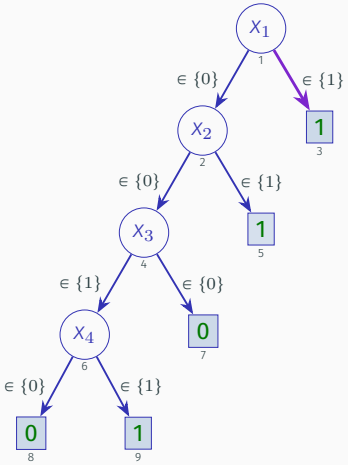

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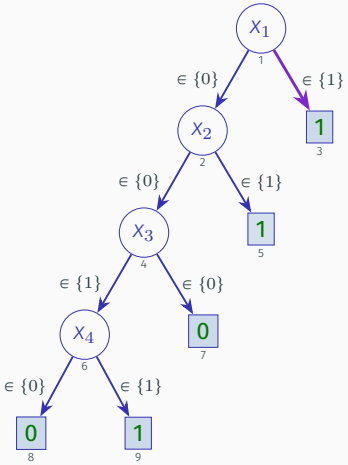

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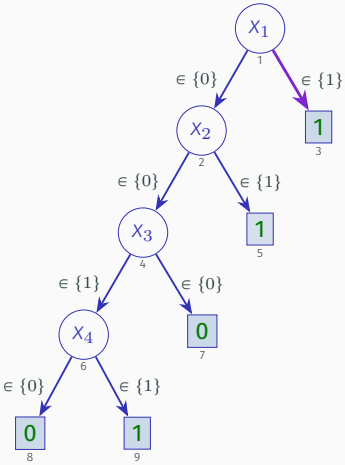

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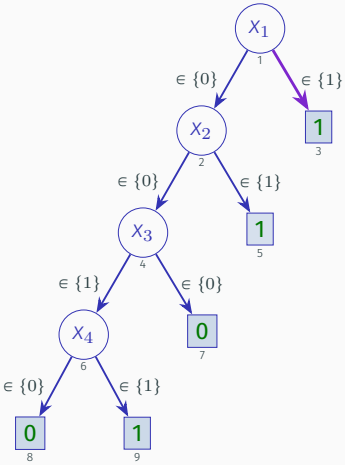

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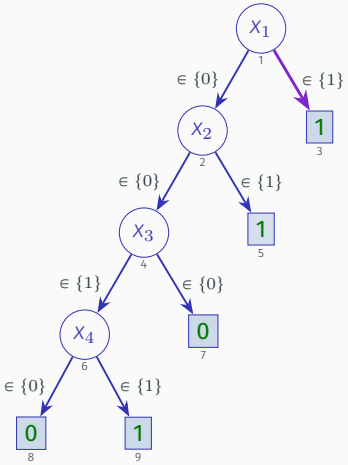

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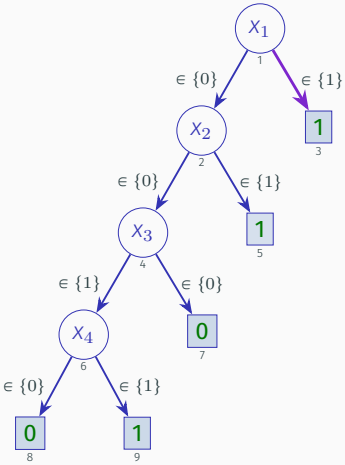

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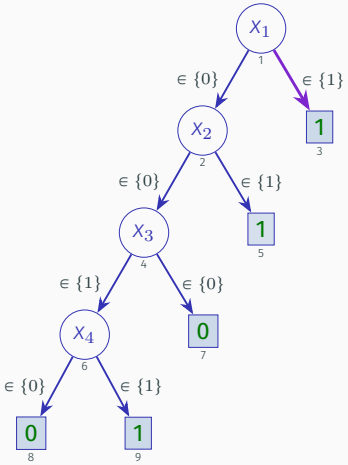

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- Features 1, 2, 3 are irrelevant, since there are not included in any AXp/CXp

  - Obs: irrelevant features are absolutely unimportant!

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

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

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    - Thus, we can decide feature relevancy with $\exists\forall$ alternation

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  - Pick a set of features $\mathcal{P}$ containing t (i.e. existential quantification), such that,
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- General case: best solution is to exploit **abstraction refinement**

Abstraction refinement for feature relevancy

- **Claim**: $\mathcal{X} \subseteq \mathcal{F}$ and $t \in \mathcal{X}$. If 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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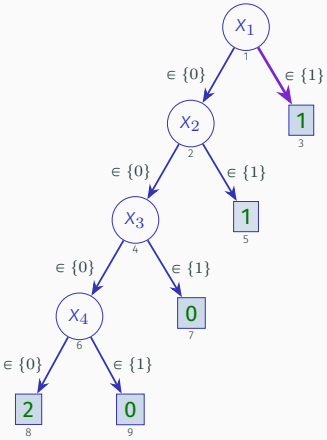
  - Block counterexamples in both cases

A general abstraction refinement algorithm

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

function FRPCGR($\mathbf{v}, t; \mathcal{F}, \kappa$)
  $\mathcal{H} \leftarrow \varnothing$ ▷ $\mathcal{H}$ overapproximates the subsets of $\mathcal{F}$ that do not contain an AXp containing t
  repeat
    $(\text{outc}, \mathbf{s}) \leftarrow \text{SAT}(\mathcal{H}, \mathsf{s}_t)$ ▷ **Use SAT oracle to pick candidate WAXp containing** t
    if outc $=$ **true then**
      $\mathcal{P} \leftarrow \{i \in \mathcal{F} \,|\, \mathsf{s}_i = 1\}$ ▷ Set $\mathcal{P}$ is the candidate WAXp, and $t \in \mathcal{P}$
      $\mathcal{D} \leftarrow \{i \in \mathcal{F} \,|\, \mathsf{s}_i = 0\}$ ▷ Set $\mathcal{D}$ contains the features not included in $\mathcal{P}$
      if $\neg$WAXp($\mathcal{P}$) **then** ▷ Is $\mathcal{P}$ not a WAXp?
        $\mathcal{H} \leftarrow \mathcal{H} \cup \text{newPosCl}(\mathcal{D}; t, \kappa)$ ▷ $\mathcal{P}$ is *not* a WAXp; must pick some non-picked feature
      else ▷ $\mathcal{P}$ is a WAXp
        if $\neg$WAXp($\mathcal{P}\backslash\{t\}$) **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
        $\mathcal{H} \leftarrow \mathcal{H} \cup \text{newNegCl}(\mathcal{P}; t, \kappa)$ ▷ WAXp($\mathcal{P}\backslash\{t\}$) holds; some feature in $\mathcal{P}$ must not be picked
  until outc $=$ **false**
  return false ▷ If $\mathcal{H}$ becomes inconsistent, then there is no AXp that contains t

An example: feature relevancy for DT, using abstraction refinement



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

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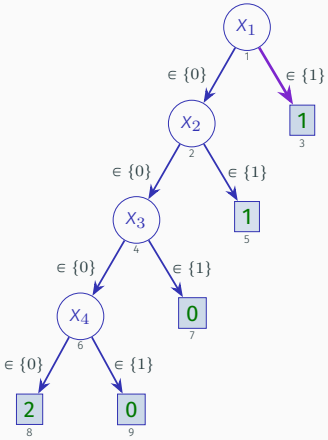
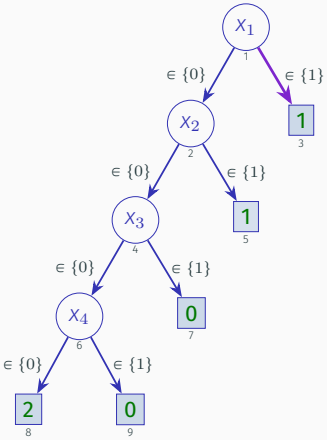


- Instance: $(\mathbf{v}, c) = ((1, 1, 1, 1), 1)$
- Is $t = 1$ relevant?

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

Another example



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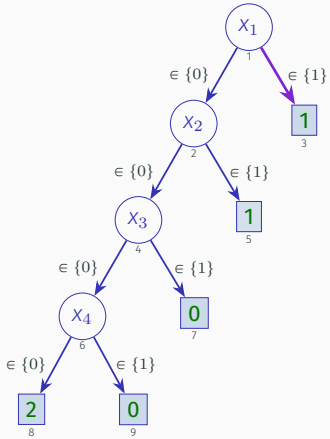
- Is $t = 4$ relevant?

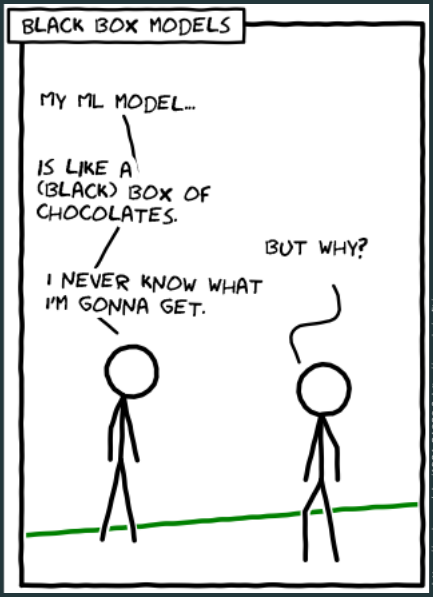
Another example



- Instance: $(\mathbf{v}, c) = ((1, 1, 1, 1), 1)$
- Is $t = 4$ relevant?

$t = 4$					
$\mathbf{s}$	$\mathcal{P}$	WAXp($\mathcal{P}$)	WAXp($\mathcal{P}\backslash\{t\}$)	Return?	Clause
$(1, 1, 1, 1)$	$\{1, 2, 3, 4\}$	✓	✓	$--$	$(\neg u_1 \vee \neg u_2 \vee \neg u_3)$
$(1, 1, 0, 1)$	$\{1, 2, 4\}$	✓	✓	$--$	$(\neg u_1 \vee \neg u_2)$
$(1, 0, 0, 1)$	$\{1, 4\}$	✓	✓	$--$	$(\neg u_1)$
$(0, 1, 0, 1)$	$\{2, 4\}$	✓	✓	$--$	$(\neg u_2)$
$(0, 0, 0, 1)$	$\{4\}$	✗	$-$	$--$	$(u_1 \vee u_2 \vee u_3)$
$(0, 0, 1, 1)$	$\{3, 4\}$	✗	$-$	$--$	$(u_1 \vee u_2)$
[outc = **false**]	$--$	$-$	$-$	**false**	$--$

Questions?


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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