LOGIC-BASED EXPLAINABLE ARTIFICIAL INTELLIGENCE

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ESSAI, Athens, Greece, July 2024

My team's recent & not so recent work...



New area of research, since circa 2018...



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Lecture 01

Recent & ongoing ML successes



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







AlphaGo Zero & Alpha Zero

Image & Speech Recognition







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

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- Accuracy in training/test data
- Complex ML models are brittle
 - Extensive work on finding adversarial examples
 - Extensive work on learning robust ML models
- More recently, complex ML models hallucinate
- One **must** be able to validate operation of ML model, with rigor
 - Explanations; robustness; verification

ML models are brittle — adversarial examples



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ML models are brittle — adversarial examples



Goodfellow et al., ICLR'15



Aung et al'17

ML models are brittle — adversarial examples



Adversarial examples can be very problematic

Original image



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



Malignant

Model confidence

Adversarial noise



Perturbation computed by a common adversarial attack technique.

Adversarial example



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



Benign Malignant

Model confidence Finlayson et al., Nature 2019

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eXplainable AI (XAI)



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

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- Many questions to address:
 - Properties of explanations
 - How to be human understandable?
 - How to answer Why? questions? I.e. Why the prediction?
 - · How to answer Why Not? questions? I.e. Why not some other prediction?
 - Which guarantees of rigor?

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- Goal of XAI: to help humans understand ML models
- Many questions to address:
 - Properties of explanations
 - How to be human understandable?
 - How to answer Why? questions? I.e. Why the prediction?
 - · How to answer Why Not? questions? I.e. Why not some other prediction?
 - Which guarantees of rigor?
 - Other queries: enumeration, membership, preferences, etc.
 - · Links with robustness, fairness, model learning

Importance of XAI

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

of 27 April 2016

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

(Text with EEA relevance)

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

Bryce Goodman,1* Seth Flaxman,2

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



Importance of XAI



XAI & EU guidelines (AI HLEG)



XAI & the principle of explicability



& thousands of recent papers!

- **High-risk** (EU regulations):
 - \cdot Law enforcement

• ...

- Management and operation of critical infrastructure
- Biometric identification and categorization of people





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- Management and operation of critical infrastructure
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- ...

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- And **safety-critical**:
 - Self-driving cars
 - Autonomous vehicles
 - Autonomous aereal devices



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- Management and operation of critical infrastructure
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- ...

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

Cynthia Rudin

May 2019

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- Management and operation of critical infrastructure
- · Biometric identification and categorization of people
- ...
- And **safety-critical**:
 - Self-driving cars
 - Autonomous vehicles
 - Autonomous aereal devices
 - ...

• ...

Correctness of explanations is paramount!

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





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May 2019

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

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

- \cdot Q: Can heuristic XAI be trusted in high-risk and/or safety-critical domains?
- Q: Can we validate results of heuristic XAI?

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

[MI22, Mar22, MS23, Mar24]

- Relationship with abduction abductive explanations (AXps)
- Contrastive explanations (CXps) [Mil19]
- Duality between AXps & CXps
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- Intractability results
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What have we been up to? 1. Created the field of symbolic (formal) XAI - II



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

[RSG16, LL17, RSG18, Rud19]



[MSH24, HMS24, HM23c]

research and advances

DOI:10.1145/3635301

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

BY JOAO MARQUES-SILVA AND XUANXIANG HUANG

Explainability Is *Not* a Game

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

key insights

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

Check for updates

- Lecture 01 units:
 - #01: Foundations
- Lecture 02 units:
 - #02: Principles of symbolic XAI feature selection
 - #03: Tractability in symbolic XAI (& myth of interpretability)
- Lecture 03 units:
 - #04: Intractability in symbolic XAI (& myth of model-agnostic XAI)
 - #05: Explainability queries
- Lecture 04 units:
 - #06: Advanced topics
- Lecture 05 units:
 - #07: Principles of symbolic XAI feature attribution (& myth of Shapley values in XAI)
 - #08: Conclusions & research directions

Unit #01

Foundations
Classification problems

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

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

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- ML model $\mathcal{M}_{\mathcal{C}}$ computes a (non-constant) classification function $\kappa : \mathbb{F} \to \mathcal{K}$
 - \mathcal{M}_{c} is a tuple $(\mathcal{F}, \mathbb{F}, \mathcal{K}, \kappa)$
- Instance (\mathbf{v}, c) for point $\mathbf{v} = (v_1, \dots, v_m) \in \mathbb{F}$, with prediction $c = \kappa(\mathbf{v})$, $c \in \mathcal{K}$
 - Goal: to compute explanations for (\mathbf{v}, c)

• For regression problems:

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

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- General ML model:
 - $\cdot \ensuremath{\ensuremath{\mathbb{T}}}$: range of possible predictions
 - + Non-constant function $\tau:\mathbb{F}\to\mathbb{T}$
 - ML model: \mathcal{M} is a tuple $(\mathcal{F}, \mathbb{F}, \mathbb{T}, \tau)$

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

Example ML models – classification – decision trees (DTs)



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• Literals in DTs can use = or \in

Example ML models - regression - regression trees (RTs)



• Literals in RTs can use = or ∈

• Ordered rules – decision lists (DLs):

IF $x_1 \wedge x_2$ THEN predict Y ELSE IF $\neg x_2 \lor x_3$ THEN predict N ELSE THEN predict Y $\mathcal{F} = \{1, 2, 3\}; \mathcal{D}_1 = \mathcal{D}_2 = \mathcal{D}_3 = \{0, 1\}; \mathcal{K} = \{Y, N\}$ • Ordered rules – decision lists (DLs):

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

• Unordered rules – decision sets (DSs):

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

Issues of DSs: overlap; incomplete coverage

Example ML models - classification - random forests (RFs)



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

Example ML models - classification - neural networks (NNs)



ML Models: Classification & Regression Problems

Basics of (non-symbolic) XAI

Motivation for Explanations

Brief Glimpse of Logic

Reasoning About ML Models

Understanding Intrinsic Interpretability

• Feature attribution:

•	LIME	[RSG16]
	SHAP	[117]

• ...

• Feature attribution: assign relative importance to features

۰LI	IME	[RSG16]
• SH	SHAP	[LL17]

• ...

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• LIME	[RSG16]
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Feature selection:	
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• LIME	[RSG16]
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Hybrid approaches:	
• Saliency maps	[BBM ⁺ 15]

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Intrinsic interpretability:	[Mol20, Rud19]
• DTs. DLs	

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Feature selection: select set of features	
Anchors	[RSG18]
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Hybrid approaches:	
• Saliency maps	[BBM+15]
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Intrinsic interpretability: the (interpretable) model is the explanation	[Mol20, Rud19]
• DTs, DLs,	

.

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Some examples

• Anchors:

[RSG18]

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

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- Obs: rules are used in tools like Anchors
 - · An anchor is a "high-precision rule"

[RSG16]

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- We seek a rigorous definition of rules for answering Why? questions such that,

[RSG16]

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- Obs: rules are used in tools like Anchors
 - · An anchor is a "high-precision rule"
- We seek a rigorous definition of rules for answering Why? questions such that,
 - <COND> is sufficient for the prediction
 - <COND> is irreducible
- We also seek the algorithms for the rigorous computation of such rules

[RSG16]

IF	$\neg X_1 \land X_2$	THEN	predict Y
ELSE IF	$\neg X_1 \land X_3$	THEN	predict Y
ELSE IF	$X_4 \wedge X_5$	THEN	predict N
ELSE		THEN	predict Y

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ELSE		THEN	predict Y

• Explanation for why $\kappa(1, 1, 1, 1, 1) = \mathbb{N}$?

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• Given
$$\mathbf{x} = (x_1, x_2, x_3, x_4, x_5)$$
,
IF $(x_1 = 1) \land (x_4 = 1) \land (x_5 = 1)$ THEN $\kappa(\mathbf{x}) = \mathbf{N}$

• I.e. $\{x_1 = 1, x_4 = 1, x_5 = 1\}$ suffice for DL to predict N

- Explanation for why $\kappa(1, 1, 1, 1, 1) = \mathbb{N}$?
 - Given $\mathbf{x} = (x_1, x_2, x_3, x_4, x_5)$, IF $(x_1 = 1) \land (x_4 = 1) \land (x_5 = 1)$ THEN $\kappa(\mathbf{x}) = \mathbf{N}$
 - I.e. $\{x_1 = 1, x_4 = 1, x_5 = 1\}$ suffice for DL to predict N
- Explanation for why $\kappa(1, 0, 0, 0, 0) = \mathbf{Y}$?

- Explanation for why $\kappa(1, 1, 1, 1, 1) = \mathbb{N}$?
 - Given $\mathbf{x} = (x_1, x_2, x_3, x_4, x_5)$, IF $(x_1 = 1) \land (x_4 = 1) \land (x_5 = 1)$ THEN $\kappa(\mathbf{x}) = \mathbf{N}$
 - I.e. $\{x_1 = 1, x_4 = 1, x_5 = 1\}$ suffice for DL to predict N
- Explanation for why $\kappa(1, 0, 0, 0, 0) = \mathbf{Y}$?
 - Given $\mathbf{x} = (x_1, x_2, x_3, x_4, x_5)$, IF $(x_4 = 0)$ THEN $\kappa(\mathbf{x}) = \mathbf{Y}$
 - I.e. $\{x_4 = 0\}$ suffices for DL to predict **Y**
A decision list example

- Explanation for why $\kappa(1, 1, 1, 1, 1) = \mathbb{N}$?
 - Given $\mathbf{x} = (x_1, x_2, x_3, x_4, x_5)$, IF $(x_1 = 1) \land (x_4 = 1) \land (x_5 = 1)$ THEN $\kappa(\mathbf{x}) = \mathbf{N}$
 - I.e. $\{x_1 = 1, x_4 = 1, x_5 = 1\}$ suffice for DL to predict N
- Explanation for why $\kappa(1, 0, 0, 0, 0) = \mathbf{Y}$?
 - Given $\mathbf{x} = (X_1, X_2, X_3, X_4, X_5)$, IF $(X_4 = 0)$ THEN $\kappa(\mathbf{x}) = \mathbf{Y}$
 - · I.e. $\{x_4 = 0\}$ suffices for DL to predict **Y**
 - Given $\mathbf{x} = (x_1, x_2, x_3, x_4, x_5)$,

IF $(x_5 = 0)$ THEN $\kappa(\mathbf{x}) = \mathbf{Y}$

• I.e. $\{x_5 = 0\}$ also suffices for DL to predict **Y**



X_1	X_2	X_3	X_4	$\kappa(\mathbf{x})$
0	0	0	0	1
0	0	0	1	1
0	0	1	0	1
0	0	1	1	1
0	1	0	0	0
0	1	0	1	1
0	1	1	0	1
0	1	1	1	1
1	0	0	0	0
1	0	0	1	0
1	0	1	0	0
1	0	1	1	0
1	1	0	0	0
1	1	0	1	0
1	1	1	0	0
1	1	1	1	0



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

$\langle 1 \rangle$	X_2	X_3	X_4	$\kappa(\mathbf{x})$
0	0	0	0	1
0	0	0	1	1
0	0	1	0	1
0	0	1	1	1
0	1	0	0	0
0	1	0	1	1
0	1	1	0	1
0	1	1	1	1
1	0	0	0	0
1	0	0	1	0
1	0	1	0	0
1	0	1	1	0
1	1	0	0	0
1	1	0	1	0
1	1	1	0	0
1	1	1	1	0



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

X_1	X_2	X_3	X_4	$\kappa(\mathbf{x})$
0	0	0	0	1
0	0	0	1	1
0	0	1	0	1
0	0	1	1	1
0	1	0	0	0
0	1	0	1	1
0	1	1	0	1
0	1	1	1	1
1	0	0	0	0
1	0	0	1	0
1	0	1	0	0
1	0	1	1	0
1	1	0	0	0
1	1	0	1	0
1	1	1	0	0
1	1	1	1	0



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 - Given $\mathbf{x} = (X_1, X_2, X_3, X_4)$,
 - IF $(x_1 = 0) \land (x_2 = 0)$ THEN $\kappa(\mathbf{x}) = \mathbf{1}$
 - I.e. $\{x_1 = 0, x_2 = 0\}$ suffice for DT to predict 1
- Explanation for why $\kappa(1, 1, 1, 1) = 0$?

<i>X</i> ₁	X_2	X_3	X_4	$\kappa(\mathbf{x})$
0	0	0	0	1
0	0	0	1	1
0	0	1	0	1
0	0	1	1	1
0	1	0	0	0
0	1	0	1	1
0	1	1	0	1
0	1	1	1	1
1	0	0	0	0
1	0	0	1	0
1	0	1	0	0
1	0	1	1	0
1	1	0	0	0
1	1	0	1	0
1	1	1	0	0
1	1	1	1	0



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

X_1	X_2	X_3	X_4	$\kappa(\mathbf{x})$
0	0	0	0	1
0	0	0	1	1
0	0	1	0	1
0	0	1	1	1
0	1	0	0	0
0	1	0	1	1
0	1	1	0	1
0	1	1	1	1
1	0	0	0	0
1	0	0	1	0
1	0	1	0	0
1	0	1	1	0
1	1	0	0	0
1	1	0	1	0
1	1	1	0	0
1	1	1	1	0



X_1	X_2	X_3	X_4	T_1	T_2	T_3	$\kappa(\mathbf{x})$
0	0	0	0	Ν	Ν	Ν	Ν
0	0	0	1	Ν	Υ	Ν	Ν
0	0	1	0	Ν	Ν	Ν	Ν
0	0	1	1	Ν	Ν	Ν	Ν
0	1	0	0	Ν	Ν	Υ	Ν
0	1	0	1	Ν	Υ	Υ	Υ
0	1	1	0	Ν	Ν	Ν	Ν
0	1	1	1	Ν	Ν	Ν	Ν
1	0	0	0	Ν	Ν	Ν	Ν
1	0	0	1	Ν	Υ	Ν	Ν
1	0	1	0	Ν	Ν	Υ	Ν
1	0	1	1	Ν	Ν	Υ	Ν
1	1	0	0	Υ	Ν	Υ	Υ
1	1	0	1	Υ	Υ	Υ	Υ
1	1	1	0	Υ	Ν	Υ	Υ
1	1	1	1	Υ	Ν	Υ	Υ



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

<i>x</i> ₁	X_2	<i>X</i> 3	X_4	T_1	T_2	T_3	$\kappa(\mathbf{x})$
0	0	0	0	Ν	Ν	Ν	N
0	0	0	1	Ν	Υ	Ν	Ν
0	0	1	0	Ν	Ν	Ν	Ν
0	0	1	1	Ν	Ν	Ν	Ν
0	1	0	0	Ν	Ν	Υ	Ν
0	1	0	1	Ν	Υ	Υ	Υ
0	1	1	0	Ν	Ν	Ν	Ν
0	1	1	1	Ν	Ν	Ν	Ν
1	0	0	0	Ν	Ν	Ν	Ν
1	0	0	1	Ν	Υ	Ν	Ν
1	0	1	0	Ν	Ν	Υ	Ν
1	0	1	1	Ν	Ν	Υ	Ν
1	1	0	0	Υ	Ν	Υ	Υ
1	1	0	1	Υ	Υ	Υ	Υ
1	1	1	0	Υ	Ν	Υ	Υ
1	1	1	1	Υ	Ν	Υ	Υ



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

X_1	X_2	X_3	X_4	T_1	T_2	T_3	$\kappa(\mathbf{x})$
0	0	0	0	Ν	Ν	Ν	Ν
0	0	0	1	Ν	Υ	Ν	Ν
0	0	1	0	Ν	Ν	Ν	Ν
0	0	1	1	Ν	Ν	Ν	Ν
0	1	0	0	Ν	Ν	Υ	Ν
0	1	0	1	Ν	Y	Υ	Υ
0	1	1	0	Ν	Ν	Ν	Ν
0	1	1	1	Ν	Ν	Ν	Ν
1	0	0	0	Ν	Ν	Ν	Ν
1	0	0	1	Ν	Υ	Ν	Ν
1	0	1	0	Ν	Ν	Υ	Ν
1	0	1	1	Ν	Ν	Υ	Ν
1	1	0	0	Υ	Ν	Υ	Υ
1	1	0	1	Υ	Υ	Υ	Υ
1	1	1	0	Υ	Ν	Υ	Υ
1	1	1	1	Υ	Ν	Υ	Y



- Explanation for why $\kappa(1, 0, 0, 1) = \mathbb{N}$?
 - Given $\mathbf{x} = (x_1, x_2, x_3, x_4)$, IF $(x_2 = 0)$ THEN $\kappa(\mathbf{x}) = \mathbf{N}$
 - · I.e. $\{x_2 = 0\}$ suffices for DT to predict N
- Explanation for why $\kappa(1, 1, 1, 1) = \mathbf{Y}$?

X_1	X_2	χ_3	X_4	T_1	T_2	T_3	$\kappa(\mathbf{x})$
0	0	0	0	Ν	Ν	Ν	Ν
0	0	0	1	Ν	Υ	Ν	Ν
0	0	1	0	Ν	Ν	Ν	Ν
0	0	1	1	Ν	Ν	Ν	Ν
0	1	0	0	Ν	Ν	Υ	Ν
0	1	0	1	Ν	Υ	Υ	Υ
0	1	1	0	Ν	Ν	Ν	Ν
0	1	1	1	Ν	Ν	Ν	Ν
1	0	0	0	Ν	Ν	Ν	Ν
1	0	0	1	Ν	Υ	Ν	Ν
1	0	1	0	Ν	Ν	Υ	Ν
1	0	1	1	Ν	Ν	Υ	Ν
1	1	0	0	Υ	Ν	Υ	Υ
1	1	0	1	Υ	Υ	Υ	Υ
1	1	1	0	Υ	Ν	Υ	Υ
1	1	1	1	Υ	Ν	Υ	Y



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

-							
X_1	X_2	χ_3	X_4	T_1	T_2	T_3	$\kappa(\mathbf{x})$
0	0	0	0	Ν	Ν	Ν	Ν
0	0	0	1	Ν	Υ	Ν	Ν
0	0	1	0	Ν	Ν	Ν	Ν
0	0	1	1	Ν	Ν	Ν	Ν
0	1	0	0	Ν	Ν	Υ	Ν
0	1	0	1	Ν	Υ	Υ	Υ
0	1	1	0	Ν	Ν	Ν	Ν
0	1	1	1	Ν	Ν	Ν	Ν
1	0	0	0	Ν	Ν	Ν	Ν
1	0	0	1	Ν	Υ	Ν	Ν
1	0	1	0	Ν	Ν	Υ	Ν
1	0	1	1	Ν	Ν	Υ	Ν
1	1	0	0	Υ	Ν	Υ	Y
1	1	0	1	Υ	Υ	Υ	Y
1	1	1	0	Υ	Ν	Υ	Y
1	1	1	1	Y	Ν	Y	Y



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

X_1	X_2	χ_3	X_4	T_1	T_2	T_3	$\kappa(\mathbf{x})$
0	0	0	0	Ν	Ν	Ν	Ν
0	0	0	1	Ν	Υ	Ν	Ν
0	0	1	0	Ν	Ν	Ν	Ν
0	0	1	1	Ν	Ν	Ν	Ν
0	1	0	0	Ν	Ν	Υ	Ν
0	1	0	1	Ν	Υ	Υ	Υ
0	1	1	0	Ν	Ν	Ν	Ν
0	1	1	1	Ν	Ν	Ν	Ν
1	0	0	0	Ν	Ν	Ν	Ν
1	0	0	1	Ν	Υ	Ν	Ν
1	0	1	0	Ν	Ν	Υ	Ν
1	0	1	1	Ν	Ν	Υ	Ν
1	1	0	0	Υ	Ν	Υ	Y
1	1	0	1	Υ	Y	Υ	Υ
1	1	1	0	Υ	Ν	Υ	Y
1	1	1	1	Υ	Ν	Υ	Υ



- Explanation for why $\kappa(1, 0, 0, 1) = \mathbb{N}$?
 - Given $\mathbf{x} = (x_1, x_2, x_3, x_4)$, IF $(x_2 = 0)$ THEN $\kappa(\mathbf{x}) = \mathbf{N}$
 - I.e. $\{x_2 = 0\}$ suffices for DT to predict N
- Explanation for why $\kappa(1, 1, 1, 1) = \mathbf{Y}$?
 - + Given $\mathbf{x} = (x_1, x_2, x_3, x_4)$, IF $(x_1 = 1) \land (x_2 = 1)$ THEN $\kappa(\mathbf{x}) = \mathbf{Y}$
 - · I.e. $\{x_1 = 1, x_2 = 1\}$ suffice for DT to predict **Y**
- Explanation for why $\kappa(0, 1, 1, 1) = \mathbb{N}$?

• Given $\mathbf{x} = (x_1, x_2, x_3, x_4)$, IF $(x_1 = 0) \land (x_2 = 1) \land (x_3 = 1)$ THEN $\kappa(\mathbf{x}) = \mathbf{N}$

• I.e. $\{x_1 = 0, x_2 = 1, x_3 = 1\}$ suffices for DT to predict N

X_1	X_2	χ_3	X_4	T_1	T_2	T_3	$\kappa(\mathbf{x})$
0	0	0	0	Ν	Ν	Ν	Ν
0	0	0	1	Ν	Υ	Ν	Ν
0	0	1	0	Ν	Ν	Ν	Ν
0	0	1	1	Ν	Ν	Ν	Ν
0	1	0	0	Ν	Ν	Υ	Ν
0	1	0	1	Ν	Υ	Υ	Y
0	1	1	0	Ν	Ν	Ν	Ν
0	1	1	1	Ν	Ν	Ν	Ν
1	0	0	0	Ν	Ν	Ν	Ν
1	0	0	1	Ν	Υ	Ν	Ν
1	0	1	0	Ν	Ν	Υ	Ν
1	0	1	1	Ν	Ν	Υ	Ν
1	1	0	0	Υ	Ν	Υ	Y
1	1	0	1	Υ	Υ	Υ	Y
1	1	1	0	Υ	Ν	Υ	Y
1	1	1	1	V	N	V	V



X_1	X_2	r_1	y_1	$\kappa(\mathbf{x})$
0	0	-0.5	0	0
0	1	0.5	0.5	1
1	0	0.5	0.5	1
1	1	1.5	1.5	1



<i>X</i> ₁	X_2	r_1	<i>y</i> ₁	$\kappa(\mathbf{x})$
0	0	-0.5	0	0
0	1	0.5	0.5	1
1	0	0.5	0.5	1
1	1	1.5	1.5	1

• Explanation for why $\kappa(1,1) = 1$?



X_1	X_2	r_1	y_1	$\kappa(\mathbf{x})$
0	0	-0.5	0	0
0	1	0.5	0.5	1
1	0	0.5	0.5	1
1	1	1.5	1.5	1

- Explanation for why $\kappa(1,1) = 1$?
 - Given $\mathbf{x} = (x_1, x_2)$, IF $(x_1 = 1)$ THEN $\kappa(\mathbf{x}) = \mathbf{1}$
 - I.e. $\{x_1 = 1\}$ suffices for NN to predict **1**



<i>X</i> ₁	X_2	r_1	y_1	$\kappa(\mathbf{x})$
0	0	-0.5	0	0
0	1	0.5	0.5	1
1	0	0.5	0.5	1
1	1	1.5	1.5	1

- Explanation for why $\kappa(1,1) = 1$?
 - Given $\mathbf{x} = (x_1, x_2)$, IF $(x_1 = 1)$ THEN $\kappa(\mathbf{x}) = \mathbf{1}$
 - I.e. $\{x_1 = 1\}$ suffices for NN to predict **1**
 - Given $\mathbf{x} = (x_1, x_2)$, IF $(x_2 = 1)$ THEN $\kappa(\mathbf{x}) = \mathbf{1}$
 - I.e. $\{x_2 = 1\}$ suffices for NN to predict **Y**

• Classification function:

$$\kappa(\mathsf{X}_1,\mathsf{X}_2,\mathsf{X}_3,\mathsf{X}_4) = \neg\mathsf{X}_1 \land \neg\mathsf{X}_2 \lor \mathsf{X}_1 \land \mathsf{X}_2 \land \mathsf{X}_4 \lor \neg\mathsf{X}_1 \land \mathsf{X}_2 \land \neg\mathsf{X}_3 \lor \neg\mathsf{X}_2 \land \mathsf{X}_3 \land \mathsf{X}_4$$

• Classification function:

$$\kappa(\mathsf{X}_1,\mathsf{X}_2,\mathsf{X}_3,\mathsf{X}_4) = \neg \mathsf{X}_1 \land \neg \mathsf{X}_2 \lor \mathsf{X}_1 \land \mathsf{X}_2 \land \mathsf{X}_4 \lor \neg \mathsf{X}_1 \land \mathsf{X}_2 \land \neg \mathsf{X}_3 \lor \neg \mathsf{X}_2 \land \mathsf{X}_3 \land \mathsf{X}_4$$

• Instance: ((0, 0, 0, 0), 1)

x_1	X_2	X_3	X_4	$\kappa(\mathbf{x})$
0	0	0	0	1
0	0	0	1	1
0	0	1	0	1
0	0	1	1	1
0	1	0	0	1
0	1	0	1	1
0	1	1	0	0
0	1	1	1	0
1	0	0	0	0
1	0	0	1	0
1	0	1	0	0
1	0	1	1	1
1	1	0	0	0
1	1	0	1	1
1	1	1	0	0
1	1	1	1	1

Classification function:

$$\kappa(\mathsf{X}_1,\mathsf{X}_2,\mathsf{X}_3,\mathsf{X}_4) = \neg\mathsf{X}_1 \land \neg\mathsf{X}_2 \lor \mathsf{X}_1 \land \mathsf{X}_2 \land \mathsf{X}_4 \lor \neg\mathsf{X}_1 \land \mathsf{X}_2 \land \neg\mathsf{X}_3 \lor \neg\mathsf{X}_2 \land \mathsf{X}_3 \land \mathsf{X}_4$$

- Instance: ((0, 0, 0, 0), 1)
- Given $\mathbf{x} = (x_1, x_2, x_3, x_4)$, IF $(x_1 = 0) \land (x_3 = 0)$ THEN $\kappa(\mathbf{x}) = \mathbf{1}$
- I.e. $\{x_1 = 0, x_3 = 0\}$ suffices for DT to predict **1**

X_1	X_2	X_3	X_4	$\kappa(\mathbf{x})$
0	0	0	0	1
0	0	0	1	1
0	0	1	0	1
0	0	1	1	1
0	1	0	0	1
0	1	0	1	1
0	1	1	0	0
0	1	1	1	0
1	0	0	0	0
1	0	0	1	0
1	0	1	0	0
1	0	1	1	1
1	1	0	0	0
1	1	0	1	1
1	1	1	0	0
1	1	1	1	1

ML Models: Classification & Regression Problems

Basics of (non-symbolic) XAI

Motivation for Explanations

Brief Glimpse of Logic

Reasoning About ML Models

Understanding Intrinsic Interpretability

Standard tools of the trade

- SAT: decision problem for propositional logic
 - Formulas most often represented in CNF
 - There are optimization variants: MaxSAT, PBO, MinSAT, etc.
 - There are quantified variants: QBF, QMaxSAT, etc.
- SMT: decision problem for (decidable) fragments of first-order logic (FOL)
 - There are optimization variants: MaxSMT, etc.
 - There are quantified variants
- MILP: decision/optimization problems defined on conjunctions of linear inequalities over integer & real-valued variables
- CP: constraint programming
 - \cdot There are optimization/quantified variants

Standard tools of the trade

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 - There are quantified variants
- MILP: decision/optimization problems defined on conjunctions of linear inequalities over integer & real-valued variables
- CP: constraint programming
 - \cdot There are optimization/quantified variants
- Background on SAT/SMT:
 - https://alexeyignatiev.github.io/ssa-school-2019/
 - https://alexeyignatiev.github.io/ijcai19tut/

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[BHvMW09]

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

• Deciding satisfiability, entailment

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

Basic definitions in propositional logic

- Atoms $(\{x, x_1, ...\})$ & literals $(x_1, \neg x_1)$
- Well-formed formulas using \neg , \land , \lor , ...
- 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

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- Well-formed formulas using \neg , \land , \lor , ...
- 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
- $CO(\psi(\mathbf{x}))$ decides whether $\psi(\mathbf{x})$ is satisfiable (i.e. whether it is consistent), using an oracle for SAT/SMT/MILP/CP/etc.

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

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- Let τ represent some other formula, also defined on \mathbb{F} , and with $\tau : \mathbb{F} \to \{0, 1\}$
 - We say that τ entails φ , written as $\tau \models \varphi$, if:

 $\forall (\mathbf{x} \in \mathbb{F}).[\tau(\mathbf{x}) \rightarrow \varphi(\mathbf{x})]$

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 - We say that τ entails φ , written as $\tau \models \varphi$, if:

 $\forall (\mathbf{x} \in \mathbb{F}).[\tau(\mathbf{x}) \mathop{\rightarrow} \varphi(\mathbf{x})]$

- We say that $\tau(\mathbf{x})$ is **sufficient** for $\varphi(\mathbf{x})$
- To decide entailment:
 - $\tau \models \varphi$ if $\tau(\mathbf{x}) \land \neg \varphi(\mathbf{x})$ is **not** consistent, i.e. $CO(\tau(\mathbf{x}) \land \neg \varphi(\mathbf{x}))$ does not hold

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- We say that $\tau(\mathbf{x})$ is sufficient for $\varphi(\mathbf{x})$
- To decide entailment:
 - $\tau \models \varphi$ if $\tau(\mathbf{x}) \land \neg \varphi(\mathbf{x})$ is **not** consistent, i.e. $CO(\tau(\mathbf{x}) \land \neg \varphi(\mathbf{x}))$ does not hold
- An example:
 - $\cdot \ \mathbb{F} = \{0,1\}^2$
 - $\varphi(X_1, X_2) = X_1 \vee \neg X_2$
 - Clearly, $x_1 \models \varphi$ and $\neg x_2 \models \varphi$
 - Also, $CO(x_1 \land (\neg x_1 \land x_2))$ does not hold

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- Let τ represent some other formula, also defined on \mathbb{F} , and with $\tau:\mathbb{F}\to\{0,1\}$
 - We say that τ entails φ , written as $\tau \models \varphi$, if:

 $\forall (\mathbf{x} \in \mathbb{F}).[\tau(\mathbf{x}) \rightarrow \varphi(\mathbf{x})]$

- We say that $au(\mathbf{x})$ is sufficient for $arphi(\mathbf{x})$
- To decide entailment:
 - $\tau \models \varphi$ if $\tau(\mathbf{x}) \land \neg \varphi(\mathbf{x})$ is **not** consistent, i.e. $CO(\tau(\mathbf{x}) \land \neg \varphi(\mathbf{x}))$ does not hold
- An example:
 - $\boldsymbol{\cdot} \ \mathbb{F} = \{0,1\}^2$
 - $\varphi(x_1, x_2) = x_1 \vee \neg x_2$
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 - Also, $CO(x_1 \land (\neg x_1 \land x_2))$ does not hold

- Another example:
 - $\boldsymbol{\cdot} \ \mathbb{F} = \{0,1\}^3$
 - $\varphi(X_1, X_2, X_3) = X_1 \wedge X_2 \vee X_1 \wedge X_3$
 - Clearly, $x_1 \land x_2 \models \varphi$ and $x_1 \land x_3 \models \varphi$
 - Also, $CO(x_1 \land x_2 \land ((\neg x_1 \lor \neg x_2) \land (\neg x_1 \lor \neg x_3)))$ does not hold

• Classification function:

$$\kappa(\mathsf{X}_1,\mathsf{X}_2,\mathsf{X}_3,\mathsf{X}_4) = \neg\mathsf{X}_1 \land \neg\mathsf{X}_2 \lor \mathsf{X}_1 \land \mathsf{X}_2 \land \mathsf{X}_4 \lor \neg\mathsf{X}_1 \land \mathsf{X}_2 \land \neg\mathsf{X}_3 \lor \neg\mathsf{X}_2 \land \mathsf{X}_3 \land \mathsf{X}_4$$

• Instance: ((0, 1, 0, 0), 1)

$\langle 1 \rangle$	X_2	X_3	X_4	$\kappa(\mathbf{x})$
0	0	0	0	1
0	0	0	1	1
0	0	1	0	1
0	0	1	1	1
0	1	0	0	1
0	1	0	1	1
0	1	1	0	0
0	1	1	1	0
1	0	0	0	0
1	0	0	1	0
1	0	1	0	0
1	0	1	1	1
1	1	0	0	0
1	1	0	1	1
1	1	1	0	0
1	1	1	1	1

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 $\kappa(\mathsf{X}_1,\mathsf{X}_2,\mathsf{X}_3,\mathsf{X}_4) = \neg\mathsf{X}_1 \land \neg\mathsf{X}_2 \lor \mathsf{X}_1 \land \mathsf{X}_2 \land \mathsf{X}_4 \lor \neg\mathsf{X}_1 \land \mathsf{X}_2 \land \neg\mathsf{X}_3 \lor \neg\mathsf{X}_2 \land \mathsf{X}_3 \land \mathsf{X}_4$

- Instance: ((0, 1, 0, 0), 1)
- Localized explanation: any irreducible conjunction of literals, consistent with v, and that entails the prediction

$\langle 1 \rangle$	X_2	χ_3	X_4	$\kappa(\mathbf{x})$
0	0	0	0	1
0	0	0	1	1
0	0	1	0	1
0	0	1	1	1
0	1	0	0	1
0	1	0	1	1
0	1	1	0	0
0	1	1	1	0
1	0	0	0	0
1	0	0	1	0
1	0	1	0	0
1	0	1	1	1
1	1	0	0	0
1	1	0	1	1
1	1	1	0	0
1	1	1	1	1

Classification function:

 $\kappa(\mathsf{X}_1,\mathsf{X}_2,\mathsf{X}_3,\mathsf{X}_4) = \neg\mathsf{X}_1 \land \neg\mathsf{X}_2 \lor \mathsf{X}_1 \land \mathsf{X}_2 \land \mathsf{X}_4 \lor \neg\mathsf{X}_1 \land \mathsf{X}_2 \land \neg\mathsf{X}_3 \lor \neg\mathsf{X}_2 \land \mathsf{X}_3 \land \mathsf{X}_4$

- Instance: ((0, 1, 0, 0), 1)
- Localized explanation: any irreducible conjunction of literals, consistent with v, and that entails the prediction

• Given
$$\mathbf{x} = (x_1, x_2, x_3, x_4)$$
,

IF $(x_1 = 0) \land (x_3 = 0)$ THEN $\kappa(\mathbf{x}) = 1$

X_1	X_2	X_3	X_4	$\kappa(\mathbf{x})$
0	0	0	0	1
0	0	0	1	1
0	0	1	0	1
0	0	1	1	1
0	1	0	0	1
0	1	0	1	1
0	1	1	0	0
0	1	1	1	0
1	0	0	0	0
1	0	0	1	0
1	0	1	0	0
1	0	1	1	1
1	1	0	0	0
1	1	0	1	1
1	1	1	0	0
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,
IF $(x_1 = 0) \land (x_3 = 0)$ THEN $\kappa(\mathbf{x}) =$

• Global explanation: any irreducible conjunction of literals, that is consistent, and that entails the prediction

x_1	X_2	X_3	X_4	$\kappa(\mathbf{x})$
0	0	0	0	1
0	0	0	1	1
0	0	1	0	1
0	0	1	1	1
0	1	0	0	1
0	1	0	1	1
0	1	1	0	0
0	1	1	1	0
1	0	0	0	0
1	0	0	1	0
1	0	1	0	0
1	0	1	1	1
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ML Models: Classification & Regression Problems

Basics of (non-symbolic) XAI

Motivation for Explanations

Brief Glimpse of Logic

Reasoning About ML Models

Understanding Intrinsic Interpretability

Decision sets with boolean features

• Example ML model:

```
Features: x_1, x_2, x_3, x_4 \in \{0, 1\} (boolean)
Rules:
\begin{array}{c} |\mathsf{F} \quad x_1 \land \neg x_2 \land x_3 \quad \mathsf{THEN} \\ |\mathsf{F} \quad x_1 \land \neg x_3 \land x_4 \quad \mathsf{THEN} \end{array}
```

IF

 $X_3 \wedge X_4$ THEN

predict 🖽

predict 🖯

predict 🖯

© J. Marques-Silva

Decision sets with boolean features

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```
Features:x_1, x_2, x_3, x_4 \in \{0, 1\} (boolean)Rules:IFx_1 \land \neg x_2 \land x_3THENTHENpredict \blacksquareIFx_1 \land \neg x_3 \land x_4THENpredict \boxdotIFx_3 \land x_4THENpredict \boxdot
```

• Q: Can the model predict both \boxplus and \boxminus for some instance, i.e. is there overlap?

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

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

 $\begin{array}{l} y_{p,1} \leftrightarrow (X_1 \wedge \neg X_2 \wedge X_3) \wedge \\ y_{n,1} \leftrightarrow (X_1 \wedge \neg X_3 \wedge X_4) \wedge \\ y_{n,2} \leftrightarrow (X_3 \wedge X_4) \wedge (y_p \leftrightarrow y_{p,1}) \wedge \\ (y_n \leftrightarrow (y_{n,1} \vee y_{n,2})) \wedge (y_p) \wedge (y_n) \end{array}$

... and solve with SAT solver (after clausification) Or use PySAT

[Tse68, PG86]

[IMM18]

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

• Example ML model:

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

IF $2x_1 + x_2 > 0$ THENpredict \boxplus IF $2x_1 - x_2 \leqslant 0$ THENpredict \blacksquare

• Example ML model:

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

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

$$y_p \leftrightarrow (2X_1 + X_2 > 0) \land y_n \leftrightarrow (2X_1 - X_2 \leq 0) \land (y_p) \land (y_n)$$

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

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

Neural networks



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

Neural networks



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- + 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
- $\cdot\,$ Each unit uses a ReLU activation function

[NH10]

Encoding NNs using MILP

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

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

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Encoding each **block**:

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

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

[KBD+17]

[FJ18]

Encoding NNs using MILP



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

[KBD+17]

Example - encoding a simple NN in MILP



<i>X</i> ₁	X_2	<i>r</i> ₁	<i>y</i> ₁	01
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:

$$\begin{aligned} x_1 + x_2 - 0.5 &= y_1 - s \\ z_1 &= 1 \rightarrow y_1 \leqslant 0 \\ z_1 &= 0 \rightarrow s_1 \leqslant 0 \\ o_1 &= (y_1 > 0) \\ x_1, x_2, z_1, o_1 \in \{0, 1\} \\ y_1, s_1 &\ge 0 \end{aligned}$$

Instance: $(\mathbf{x}, c) = ((1, 0), 1)$ 1 + 0 - 0.5 = 0.5 - 0 $1 \lor 0.5 \le 0$ $0 \lor 0 \le 0$ 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 $0 \lor 0 \le 0$ $1 \lor 0.5 \le 0$ 0 = (0 > 0) $x_1 = 0, x_2 = 0, z_1 = 1, o_1 = 0$ $y_1 = 0, s_1 = 0.5$ ML Models: Classification & Regression Problems

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Understanding Intrinsic Interpretability

- Goal is to deploy *interpretable* ML models
 - E.g. Decision trees, decision lists, decision sets, etc.
- The explanation is the model itself, because it is *interpretable*

[Rud19, Mol20, RCC+22, Rud22]

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[Lip18]



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

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[Lip18]

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 - $\{\neg x_1, \neg x_2, x_3\}$ or $\{1, 2, 3\}$ is a weak explanation!
- It is the case that: IF $\neg x_1 \land x_3$ THEN $\kappa(\mathbf{x}) = 1$
 - \therefore {1,3} is also **sufficient** for the prediction!

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

[Rud19, Mol20, RCC+22, Rud22]



Case of optimal decision tree (DT)

[HRS19]

• Explanation for (0, 0, 1, 0, 1), with prediction 1?



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



• Case of **optimal** decision tree (DT)

- [HRS19]
- Explanation for (0, 0, 1, 0, 1), with prediction 1?
 - + Clearly, IF $\neg x_1 \land \neg x_2 \land x_3 \land \neg x_4 \land x_5$ THEN $\kappa(\mathbf{x}) = 1$
 - But, x_1 , x_2 , x_4 are irrelevant for the prediction:

X ₃	X_5	X_1	X_2	x_4	$\kappa(\mathbf{x})$
1	1	0	0	0	1
1	1	0	0	1	1
1	1	0	1	0	1
1	1	0	1	1	1
1	1	1	0	0	1
1	1	1	0	1	1
1	1	1	1	0	1
1	1	1	1	1	1



• Case of **optimal** decision tree (DT)

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- Explanation for (0, 0, 1, 0, 1), with prediction 1?
 - + Clearly, IF $\neg x_1 \land \neg x_2 \land x_3 \land \neg x_4 \land x_5$ THEN $\kappa(\mathbf{x}) = 1$
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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

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

R_1 :	IF	$(X_1 \wedge X_3)$	THEN	$\kappa(\mathbf{x}) = 1$
R_2 :	ELSE IF	$(X_2 \land X_4 \land X_6)$	THEN	$\kappa(\mathbf{x}) = 0$
R_3 :	ELSE IF	$(\neg x_1 \land x_3)$	THEN	$\kappa(\mathbf{x}) = 1$
R_4 :	ELSE IF	$(X_4 \wedge X_6)$	THEN	$\kappa(\mathbf{x}) = 0$
R_5 :	ELSE IF	$(\neg x_1 \land \neg x_3)$	THEN	$\kappa(\mathbf{x}) = 1$
R_6 :	ELSE IF	(x_6)	THEN	$\kappa(\mathbf{x}) = 0$
R _{DEF} :	ELSE			$\kappa(\mathbf{x}) = 1$

• Instance: ((0, 1, 0, 1, 0, 1), 0), i.e. rule R₂ fires

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- Instance: ((0, 1, 0, 1, 0, 1), 0), i.e. rule R_2 fires
- What is an explanation for the prediction?

R_1 :	IF	$(X_1 \wedge X_3)$	THEN	$\kappa(\mathbf{x}) = 1$
R_2 :	ELSE IF	$(X_2 \wedge X_4 \wedge X_6)$	THEN	$\kappa(\mathbf{x}) = 0$
R_3 :	ELSE IF	$(\neg x_1 \land x_3)$	THEN	$\kappa(\mathbf{x}) = 1$
R_4 :	ELSE IF	$(X_4 \wedge X_6)$	THEN	$\kappa(\mathbf{x}) = 0$
R_5 :	ELSE IF	$(\neg x_1 \land \neg x_3)$	THEN	$\kappa(\mathbf{x}) = 1$
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R_4 :	ELSE IF	$(X_4 \wedge X_6)$	THEN	$\kappa(\mathbf{x}) = 0$
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- Instance: ((0, 1, 0, 1, 0, 1), 0), i.e. rule R₂ fires
- What is an explanation for the prediction?
- Fixing $\{3,4,6\}$ suffices for the prediction
 - · Why?
 - $\cdot\,$ We need 3 (or 1) so that R1 cannot fire
 - $\cdot\,$ With 3, we do not need 2, since with 4 and 6 fixed, then R_4 is guaranteed to fire

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 - Some questions:
 - Would average human decision maker be able to understand the irreducible set $\{3, 4, 6\}$?

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 - Some questions:
 - Would average human decision maker be able to understand the irreducible set $\{3, 4, 6\}$?
 - $\cdot \,$ Would he/she be able to compute the set $\{3,4,6\}$, by manual inspection?
Questions?

Lecture 02

• ML models: classification & regression

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

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- Answers to Why? questions as logic rules

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- Apparent difficulties with explaining interpretable models

- Lecture 01 units:
 - #01: Foundations
- Lecture 02 units:
 - #02: Principles of symbolic XAI feature selection
 - #03: Tractability in symbolic XAI (& myth of interpretability)
- Lecture 03 units:
 - #04: Intractability in symbolic XAI (& myth of model-agnostic XAI)
 - #05: Explainability queries
- Lecture 04 units:
 - #06: Advanced topics
- Lecture 05 units:
 - #07: Principles of symbolic XAI feature attribution (& myth of Shapley values in XAI)
 - #08: Conclusions & research directions

Unit #02

Principles of Symbolic XAI – Feature Selection

Definitions of Explanations

Duality Properties

Computational Problems

• Notation:



• What is an explanation?



Mapping
$x_1 = 1$ iff Length = Long
$x_2 = 1$ iff Thread = New
$x_3=1$ iff Author = Known
$\kappa(\cdot) = 1$ iff $\kappa'(\cdots) = \text{Reads}$
$\kappa(\cdot)=0$ iff $\kappa'(\cdots)=$ Skips

• Notation:



Rewritten DT 0 1 0

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- What is an explanation?
 - Answer to question "Why (the prediction)?" is a rule: IF <COND> THEN $\kappa(\mathbf{x}) = c$

Notation:





Mapping
$x_1 = 1$ iff Length = Long $x_2 = 1$ iff Throad = Now
$x_2 = 1$ in thread = New $x_3 = 1$ iff Author = Known
$\kappa(\cdot) = 1$ iff $\kappa'(\cdots) = \text{Reads}$ $\kappa(\cdot) = 0$ iff $\kappa'(\cdots) = \text{Skips}$

- What is an explanation?
 - Answer to question "Why (the prediction)?" is a rule: IF <COND> THEN $\kappa(\mathbf{x}) = c$

Explanation: set of literals (or just features) in <COND>; irreducibility matters! .

Notation:





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Rewritten DT 0 1 0

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 - It is the case that, IF $\neg x_1 \land \neg x_2 \land x_3$ THEN $\kappa(\mathbf{x}) = 1$
 - One possible explanation is $\{\neg x_1, \neg x_2, x_3\}$ or simply $\{1, 2, 3\}$

The similarity predicate

[Mar24]

- Recall ML models for classification & regression:
 - Classification: $\mathcal{M}_{C} = (\mathcal{F}, \mathbb{F}, \mathcal{K}, \kappa)$
 - Regression: $\mathcal{M}_{R} = (\mathcal{F}, \mathbb{F}, \mathbb{V}, \rho)$
 - General: $\mathcal{M} = (\mathcal{F}, \mathbb{F}, \mathbb{T}, \tau)$

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• Similarity predicate: $\sigma : \mathbb{F} \to \{\top, \bot\}$

- Classification: $\sigma(\mathbf{x}) \coloneqq [\kappa(\mathbf{x}) = \kappa(\mathbf{v})]$
 - + Obs: For boolean classifiers, no need for σ
- Regression: $\sigma(\mathbf{x}) \coloneqq [|\rho(\mathbf{x}) \rho(\mathbf{v})| \le \delta]$, where δ is user-specified

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- Bottom line:

Reason about symbolic explainability by abstracting away type of ML model

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[SCD18, INM19a]

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

[MM20]

$$\kappa(\mathsf{X}_1,\mathsf{X}_2,\mathsf{X}_3,\mathsf{X}_4) = \bigvee_{i=1}^4 \mathsf{X}_i$$

• Classifier:

$$\kappa(\mathsf{x}_1,\mathsf{x}_2,\mathsf{x}_3,\mathsf{x}_4) = \bigvee_{i=1}^4 \mathsf{x}_i$$

• Point $\mathbf{v} = (0, 0, 0, 1)$ with prediction $\kappa(\mathbf{v}) = 1$. AXp?

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- AXp $\mathcal{X} = \{4\}$

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- AXp $\mathcal{X} = \{4\}$
- In general, validity/consistency checked with SAT/SMT/MILP/CP reasoners

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- In general, validity/consistency checked with SAT/SMT/MILP/CP reasoners
 - Obs: for some classes of classifiers, poly-time algorithms exist

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

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

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

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• Definition of $\Upsilon(\mathcal{S})$:

$$\Upsilon(\mathcal{S}) \quad \coloneqq \quad \{ x \in \mathbb{F} \, | \, x_{\mathcal{S}} = v_{\mathcal{S}} \}$$

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$$\mathbf{E}[\tau(\mathbf{x}) \,|\, \mathbf{x}_{\mathcal{S}} = \mathbf{v}_{\mathcal{S}}] \quad \coloneqq \quad \frac{1}{|\Upsilon(\mathcal{S}; \mathbf{v})|} \sum_{\mathbf{x} \in \Upsilon(\mathcal{S}; \mathbf{v})} \tau(\mathbf{x})$$

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• Expected value, real-valued features:

$$\mathbf{E}[\tau(\mathbf{x}) \mid \mathbf{x}_{\mathcal{S}} = \mathbf{v}_{\mathcal{S}}] \quad \coloneqq \quad \frac{1}{|\Upsilon(\mathcal{S}; \mathbf{v})|} \int_{\Upsilon(\mathcal{S}; \mathbf{v})} \tau(\mathbf{x}) d\mathbf{x}$$

[WMHK21, IHI+22, ABOS22, IHI+23]

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

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- Definition of AXp remains unchanged
 - This is true when comparing against 1

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[Mil19, INAM20]

- Subset-minimal set of features $\mathcal{Y} \subseteq \mathcal{F}$ sufficient for changing prediction

$$\exists (\mathbf{x} \in \mathbb{F}). \bigwedge_{j \notin \mathcal{Y}} (x_j = v_j) \land (\neg \sigma(\mathbf{x}))$$

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$$\mathsf{WCXp}(\mathcal{Y}) := \exists (\mathbf{x} \in \mathbb{F}). \bigwedge_{j \notin \mathcal{Y}} (X_j = V_j) \land (\neg \sigma(\mathbf{x}))$$

• Defining CXp:

 $\mathsf{CXp}(\mathcal{Y}) \coloneqq \mathsf{WCXp}(\mathcal{Y}) \land \forall (\mathcal{Y}' \subsetneq \mathcal{Y}). \neg \mathsf{WCXp}(\mathcal{Y}')$

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$$\mathsf{NCXp}(\mathcal{Y}) \quad \coloneqq \quad \exists (\mathbf{x} \in \mathbb{F}). \bigwedge_{j \notin \mathcal{Y}} (\mathsf{x}_j = \mathsf{v}_j) \land (\neg \sigma(\mathbf{x}))$$

• Defining CXp:

$$\mathsf{CXp}(\mathcal{Y}) \coloneqq \mathsf{WCXp}(\mathcal{Y}) \land \forall (\mathcal{Y}' \subsetneq \mathcal{Y}). \neg \mathsf{WCXp}(\mathcal{Y}')$$

• But, WCXp is also monotone; hence,

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[Mil19, INAM20]

- Subset-minimal set of features $\mathcal{Y} \subseteq \mathcal{F}$ sufficient for changing prediction

$$\mathsf{NCXp}(\mathcal{Y}) \quad \coloneqq \quad \exists (\mathbf{x} \in \mathbb{F}). \bigwedge_{j \notin \mathcal{Y}} (x_j = v_j) \land (\neg \sigma(\mathbf{x}))$$

• Defining CXp:

 $\mathsf{CXp}(\mathcal{Y}) \coloneqq \mathsf{WCXp}(\mathcal{Y}) \land \forall (\mathcal{Y}' \subsetneq \mathcal{Y}). \neg \mathsf{WCXp}(\mathcal{Y}')$

• But, WCXp is also monotone; hence,

 $\mathsf{CXp}(\mathcal{Y}) \coloneqq \mathsf{WCXp}(\mathcal{Y}) \land \forall (t \in \mathcal{Y}). \neg \mathsf{WCXp}(\mathcal{Y} \setminus \{t\})$

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

[MM20]

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

- Point $\mathbf{v} = (0, 0, 0, 1)$ with prediction $\kappa(\mathbf{v}) = 1$
- · Define $\mathcal{Y} = \{1,2,3,4\} = \mathcal{F}$

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- + 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. $\exists (\mathbf{x} \in \{0,1\}^4) . \neg x_1 \land \neg \kappa(x_1, x_2, x_3, x_4)$?

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

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• Classifier:

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

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

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

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

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• Definition of CXp remains unchanged

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

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

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

[INM19b]

[RSG16, LL17, RSG18]

Definitions of Explanations

Duality Properties

Computational Problems

[INAM20, Mar22]

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· Claim:

 $\mathcal{S} \subseteq \mathcal{F}$ is an AXp iff it is a minimal hitting set (MHS) of the set of CXps

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



[INAM20, Mar22]

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 - AXps: $\{\{3,5\}\}$



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[INAM20, Mar22]

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[INAM20, Mar22]

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- An example, $(\mathbf{v}, c) = ((0, 0, 1, 0, 1), 1)$:
 - AXps: {{3,5}}
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 - Each CXp is an MHS of the set of AXps



[INAM20, Mar22]

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 - Each AXp is an MHS of the set of CXps
 - Each CXp is an MHS of the set of AXps
 - BTW,
 - + $\{2,5\}$ is not a CXp
 - + $\{1,2,3,4,5\}$, $\{1,2,3,5\}$ and $\{1,3,5\}$ are not AXps



[INAM20, Mar22]

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 - · Why?



Definitions of Explanations

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Computational Problems

Computational problems in (formal) explainability

Compute one abductive/contrastive explanation

- Compute one abductive/contrastive explanation
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• Monotone predicates for WAXp & WCXp:

 $\mathbb{P}_{\exp}(\mathcal{S}) \triangleq \neg \operatorname{\mathsf{CO}}\left(\left[\left(\bigwedge_{i \in \mathcal{S}} (\mathsf{X}_i = \mathsf{V}_i)\right) \land (\neg \sigma(\mathbf{x})\right)\right]\right) \qquad \mathbb{P}_{\exp}(\mathcal{S}) \triangleq \operatorname{\mathsf{CO}}\left(\left[\left(\bigwedge_{i \in \mathcal{F} \backslash \mathcal{S}} (\mathsf{X}_i = \mathsf{V}_i)\right) \land (\neg \sigma(\mathbf{x}))\right]\right)$

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

- 1: procedure $oneXP(\mathbb{P})$
- 2: $\mathcal{S} \leftarrow \mathcal{F}$
- 3: for $i \in \mathcal{F}$ do
- 4: if $\mathbb{P}(S \setminus \{i\})$ then
- 5: $\mathcal{S} \leftarrow \mathcal{S} \setminus \{i\}$
- 6: return S

 $\succ \text{Initialization: } \mathbb{P}(\mathcal{S}) \text{ holds}$ $\succ \text{Loop invariant: } \mathbb{P}(\mathcal{S}) \text{ holds}$

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Exploiting MSMP, i.e. basic algorithm used for different problems. $\succ \text{Initialization: } \mathbb{P}(\mathcal{S}) \text{ holds}$ $\succ \text{Loop invariant: } \mathbb{P}(\mathcal{S}) \text{ holds}$

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Detour: More Connections with Automated Reasoning

- A conjunction of literals π (which will be viewed as a set of literals where convenient) is a prime implicant of some function φ if,
 - 1. $\pi \models \varphi$
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Prime implicants & implicates

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 - Example:
 - $\cdot \ \mathbb{F} = \{0,1\}^3$
 - $\cdot \varphi(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3) = \mathbf{x}_1 \wedge \mathbf{x}_2 \vee \mathbf{x}_1 \wedge \mathbf{x}_3$
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 - Clearly, $x_1 \wedge x_2 \models \varphi$
 - Also, $x_1 \not\models \varphi$ and $x_2 \not\models \varphi$
- A disjunction of literals η (also viewed as a set of literals where convenient) is a prime implicate of some function φ if
 - 1. $\varphi \models \eta$
 - 2. For any $\eta' \subsetneq \eta$, $\varphi \not\models \eta'$

Reasoning about inconsistency

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

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- Minimal unsatisfiable subset (MUS):
 - $\cdot \;$ Subset-minimal set $\mathcal{U} \subseteq \mathcal{S}$, s.t. $\mathcal{B} \cup \mathcal{U} \vDash \bot$
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- Minimal correction subset (MCS):
 - $\cdot \ \, \text{Subset-minimal set} \ \, \mathcal{C} \subseteq \mathcal{S} \text{, s.t.} \ \, \mathcal{B} \cup (\mathcal{S} \backslash \mathcal{C}) \not \models \bot$
 - E.g. $C = \{(\neg x_1)\}$

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 - E.g. $\mathcal{B} = \{(x_1 \lor x_2), (x_1 \lor \neg x_3)\}, \mathcal{S} = \{(\neg x_1), (\neg x_2), (x_3)\}$
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 - $\cdot \;$ Subset-minimal set $\mathcal{U} \subseteq \mathcal{S}$, s.t. $\mathcal{B} \cup \mathcal{U} \models \bot$
 - E.g. $\mathcal{U} = \{(\neg x_1), (\neg x_2)\}$
- Minimal correction subset (MCS):
 - $\cdot \ \, \text{Subset-minimal set} \ \, \mathcal{C} \subseteq \mathcal{S} \text{, s.t.} \ \, \mathcal{B} \cup (\mathcal{S} \backslash \mathcal{C}) \not \models \bot$
 - E.g. $\mathcal{C} = \{(\neg x_1)\}$
- Duality:
 - MUSes are minimal-hitting sets (MHSes) of the MCSes, and vice-versa

[Rei87]

- + Formula $\mathcal{T} = \mathcal{B} \cup \mathcal{S}$, with
 - \cdot *B*: background knowledge (base), i.e. hard constraints
 - \cdot *S*: additional (inconsistent) knowledge, i.e. soft constraints
 - · And, $\mathcal{T} \vDash \bot$
 - E.g. $\mathcal{B} = \{(x_1 \lor x_2), (x_1 \lor \neg x_3)\}, \mathcal{S} = \{(\neg x_1), (\neg x_2), (x_3)\}$
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[Rei87]

[MM20]

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

• Recap:

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

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 - Hard constraints, B:

$$\mathcal{B} := \wedge_{i \in \mathcal{F}} (S_i \rightarrow (X_i = V_i)) \wedge \text{Encode}_{\mathcal{T}}(\neg \sigma(\mathbf{x}))$$

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

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- Soft constraints: $S = \{s_i \mid i \in F\}$
- + Claim: Each MUS of $(\mathcal{B}, \mathcal{S})$ is an AXp & each MCS of $(\mathcal{B}, \mathcal{S})$ is a CXp
 - Can use MUS/MCS algorithms for AXps/CXps

Unit #03

Tractability in Symbolic XAI

Explanations for Decision Trees

XAI Queries for DTs

Myth #01: Intrinsic Interpretability

Detour: From Decision Trees to Explained Decision Sets

Explanations for Decision Graphs

Explanations for Monotonic Classifiers

Review examples







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



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

DT explanations in polynomial time



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

Explanations for Decision Trees

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Explanations for Monotonic Classifiers

Review examples
- Finding one AXp in polynomial-time covered
- Finding one CXp in polynomial-time

- Finding one CXp in polynomial-time
- Finding all CXps in polynomial-time

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

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

• Basic algorithm:

$$\cdot \ \mathcal{L} = \varnothing$$



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



Explanations for Decision Trees

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Review examples



Case of optimal decision tree (DT)

[HRS19]

• Explanation for (0, 0, 1, 0, 1), with prediction 1?



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



• Case of **optimal** decision tree (DT)

- [HRS19]
- Explanation for (0, 0, 1, 0, 1), with prediction 1?
 - + Clearly, IF $\neg x_1 \land \neg x_2 \land x_3 \land \neg x_4 \land x_5$ THEN $\kappa(\mathbf{x}) = 1$
 - But, x_1 , x_2 , x_4 are irrelevant for the prediction:

X ₃	X_5	X_1	X_2	x_4	$\kappa(\mathbf{x})$		
1	1	0	0	0	1		
1	1	0	0	1	1		
1	1	0	1	0	1		
1	1	0	1	1	1		
1	1	1	0	0	1		
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1	1	1	1	1	1
_					

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



[GZM20]



Path with 19 internal nodes. By manual inspection, at least 10 literals are redundant! (And at least 9 features dropped) • J. Marques-Silva [GZM20]



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

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



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

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

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

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

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 $(\mathbf{X}_{i_1} = 0) \land (\mathbf{X}_{i_2} = 0) \land \ldots \land (\mathbf{X}_{i_{m-1}} = 0) \land (\mathbf{X}_{i_m} = 1) \rightarrow \kappa(\mathbf{X}_1, \ldots, \mathbf{X}_m)$

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

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- But $\{i_m\}$ suffices for prediction, i.e. $\forall (\mathbf{x} \in \{0, 1\}^m) . (X_{i_m}) \rightarrow \kappa(\mathbf{x})$
- AXp's can be arbitrarily smaller than paths in (optimal) DTs!

[IIM20, IIM22]

Explanation redundancy in DTs is ubiquitous – published DT examples

1111122	
1111/122	

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



• Explanation for (P, H, T, W) = (Full, Yes, Thai, No)?

[RN10]

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

 $x_1 > w_{10}?$ y $x_2 > w_{20}?$ N Y O

• 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 !

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



[SB14

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

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



- Explanation for (L, T, A) = (Short, Follow-Up, Unknown)?
- Explanation for (L, T, A) = (Short, Follow-Up, Known)?

[PM17]

Explanation redundancy in DTs is ubiquitous – DTs from datasets

Dataset	(#F	(#F #S)	IAI					ITI												
butubet	(110)	D	#N	%A	#P	%R	%C	%m	%M	%avg	D	#N	%A	#P	%R	%C	%m	%M	%avg
adult	(12	6061)	6	83	78	42	33	25	20	40	25	17	509	73	255	75	91	10	66	22
anneal	(38	886)	6	29	99	15	26	16	16	33	21	9	31	100	16	25	4	12	20	16
backache	(32	180)	4	17	72	9	33	39	25	33	30	3	9	91	5	80	87	50	66	54
bank	(19	36293)	6	113	88	57	5	12	16	20	18	19	1467	86	734	69	64	7	63	27
biodegradation	(41	1052)	5	19	65	10	30	1	25	50	33	8	71	76	36	50	8	14	40	21
cancer	(9	449)	6	37	87	19	36	9	20	25	21	5	21	84	11	54	10	25	50	37
car	(6	1728)	6	43	96	22	86	89	20	80	45	11	57	98	29	65	41	16	50	30
colic	(22	357)	6	55	81	28	46	6	16	33	20	4	17	80	9	33	27	25	25	25
compas	(11	1155)	6	77	34	39	17	8	16	20	17	15	183	37	92	66	43	12	60	27
contraceptive	(9	1425)	6	99	49	50	8	2	20	60	37	17	385	48	193	27	32	12	66	21
dermatology	(34	366)	6	- 33	90	17	23	3	16	33	21	7	17	95	9	22	0	14	20	17
divorce	(54	150)	5	15	90	8	50	19	20	33	24	2	5	96	3	33	16	50	50	50
german	(21	1000)	6	25	61	13	38	10	20	40	29	10	99	72	50	46	13	12	40	22
heart-c	(13	302)	6	43	65	22	36	18	20	33	22	4	15	75	8	87	81	25	50	34
heart-h	(13	293)	6	37	59	19	31	4	20	40	24	8	25	77	13	61	60	20	50	32
kr-vs-kp	(36	3196)	6	49	96	25	80	75	16	60	33	13	67	99	34	79	43	7	70	35
lending	(9	5082)	6	45	73	23	73	80	16	50	25	14	507	65	254	69	80	12	75	25
letter	(16	18668)	6	127	58	64	1	0	20	20	20	46	4857	68	2429	6	7	6	25	9
lymphography	(18	148)	6	61	76	31	35	25	16	33	21	6	21	86	11	9	0	16	16	16
mortality	(118	13442)	6	111	74	56	8	14	16	20	17	26	865	76	433	61	61	7	54	19
mushroom	(22	8124)	6	39	100	20	80	44	16	33	24	5	23	100	12	50	31	20	40	25
pendigits	(16	10992)	6	121	88	61	0	0	-	-	-	38	937	85	469	25	86	6	25	11
promoters	(58	106)	1	3	90	2	0	0	-	-	-	3	9	81	5	20	14	33	33	33
recidivism	(15	3998)	6	105	61	53	28	22	16	33	18	15	611	51	306	53	38	9	44	16
seismic_bumps	(18	2578)	6	37	89	19	42	19	20	33	24	8	39	93	20	60	79	20	60	42
shuttle	(9	58000)	6	63	99	32	28	7	20	33	23	23	159	99	80	33	9	14	50	30
soybean	(35	623)	6	63	88	32	9	5	25	25	25	16	71	89	36	22	1	9	12	10
spambase	(57	4210)	6	63	75	32	37	12	16	33	19	15	143	91	72	76	98	7	58	25
spect	(22	228)	6	45	82	23	60	51	20	50	35	6	15	86	8	87	98	50	83	65
splice	(2	3178)	3	7	50	4	0	0	-	-	-	88	177	55	89	0	0	_	-	_

Are interpretable models really interpretable? - DLs

R_1 :	IF	$(X_1 \wedge X_3)$	THEN	$\kappa(\mathbf{x}) = 1$
R_2 :	ELSE IF	$(X_2 \land X_4 \land X_6)$	THEN	$\kappa(\mathbf{x}) = 0$
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R_5 :	ELSE IF	$(\neg x_1 \land \neg x_3)$	THEN	$\kappa(\mathbf{x}) = 1$
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• Instance: ((0, 1, 0, 1, 0, 1), 0), i.e. rule R₂ fires

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[MSI23]

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 - · Why?
 - $\cdot\,$ We need 3 (or 1) so that R1 cannot fire
 - $\cdot\,$ With 3, we do not need 2, since with 4 and 6 fixed, then R_4 is guaranteed to fire
 - Some questions:
 - Would average human decision maker be able to understand the AXp?
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[IM21, MSI23]

[MSI23]



DTs learned with Interpretable AI, max depth 6

DLs learned with CN2

[MSI23]

Explanations for Decision Trees

XAI Queries for DTs

Myth #01: Intrinsic Interpretability

Detour: From Decision Trees to Explained Decision Sets

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Explanations for Monotonic Classifiers

Review examples

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

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- And explaining DSs is computationally hard...

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

Example



Example



 R_{01} : IF [P] THEN $\kappa(\cdot) = \mathbf{Y}$ R_{02} : IF $[\overline{A} \land \overline{P}]$ THEN $\kappa(\cdot) = \mathbf{N}$ R_{03} : IF $[\overline{P} \land \overline{N} \land V \land Z = 1]$ THEN $\kappa(\cdot) = \mathbf{N}$ R_{04} : IF $[\overline{P} \land \overline{N} \land V \land Z = 2 \land S \land \overline{G}]$ THEN $\kappa(\cdot) = \mathbf{N}$ R_{05} : IF $[\mathsf{A} \land \mathsf{Z} = 2 \land \mathsf{S} \land \mathsf{G}]$ THEN $\kappa(\cdot) = \mathbf{Y}$ R_{06} : IF $[\overline{P} \land \overline{N} \land V \land Z = 2 \land \overline{S} \land H]$ THEN $\kappa(\cdot) = \mathbf{N}$ R_{07} : IF $[\mathsf{A} \land \mathsf{Z} = 2 \land \overline{\mathsf{S}} \land \overline{\mathsf{H}} \land \mathsf{C}]$ THEN $\kappa(\cdot) = \mathbf{Y}$ R_{08} : IF $[A \land Z = 2 \land \overline{H} \land G]$ THEN $\kappa(\cdot) = \mathbf{Y}$ R_{09} : IF $[\overline{P} \land \overline{N} \land V \land Z = 2 \land \overline{C} \land \overline{G}]$ THEN $\kappa(\cdot) = \mathbf{N}$ R_{10} : IF $[A \land Z = 0]$ THEN $\kappa(\cdot) = \mathbf{Y}$ R_{11} : IF $[A \land \overline{V}]$ THEN $\kappa(\cdot) = \mathbf{Y}$ R_{12} : IF $[A \land N]$ THEN $\kappa(\cdot) = \mathbf{Y}$

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Review examples

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

Example of XpG – DTs





Example of XpG – OMDDs

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



· XpG:



• Algorithm (with no inconsistent paths):

 $\mathcal{S} \leftarrow \mathcal{F}$ For each feature *i* in \mathcal{F}



• Algorithm (with no inconsistent paths):

 $S \leftarrow F$ For each feature *i* in FDrop feature *i* from *S*, i.e. *i* is free



• Algorithm (with no inconsistent paths):

 $S \leftarrow \mathcal{F}$ For each feature *i* in \mathcal{F} Drop feature *i* from *S*, i.e. *i* is free If path to some **0** not blocked by 0-valued literals, then

Add feature i back to ${\cal S}$



• Algorithm (with no inconsistent paths):

 $S \leftarrow F$ For each feature *i* in FDrop feature *i* from S, i.e. *i* is free If path to some **0** not blocked by 0-valued literals, then Add feature *i* back to S

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• Example:

 $\cdot \ S = \{1, 2, 3\}$



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- Example:
 - $S = \{1, 2, 3\}$
 - Feature 1 cannot be dropped, e.g.

 $\mathsf{S}_3 \mathop{\rightarrow} \mathsf{S}_2 \mathop{\rightarrow} \mathsf{S}_1 \mathop{\rightarrow} 0$



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 - $\cdot \ S = \{1, 2, 3\}$
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- Example:
 - $S = \{1, 2, 3\}$
 - Feature 1 cannot be dropped, e.g.
 - $S_3 \rightarrow S_2 \rightarrow S_1 \rightarrow 0$
 - + Both features 2 and 3 dropped from ${\cal S}$
 - Return $\mathcal{S} = \{1\}$

· XpG:



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Review examples

[MGC+21]

Variable	Me	aning	Range		
$\kappa(\cdot) \triangleq M$	Stude	nt grade	$\in \{A, B, C, D, E, F\}$		
S	Fina	l score	$\in \{0, \dots, 10\}$		
Feat. id	Feat. var.	Feat. name	Domain		
1	Q	Quiz	$\{0, \dots, 10\}$		
2	Х	Exam	$\{0,\ldots,10\}$		
3	Н	Homework	$\{0,\ldots,10\}$		
4	R	Project	$\{0,\ldots,10\}$		

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

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

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

And,
$$\kappa(\mathbf{x_1}) \leqslant \kappa(\mathbf{x_2})$$
 if $\mathbf{x_1} \leqslant \mathbf{x_2}$

Explaining monotonic classifiers

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

$$\begin{split} \mathbf{v}_{L} \leftarrow (V_{L_{1}}, \dots, V_{i}, \dots, V_{L_{N}}) \\ \mathbf{v}_{U} \leftarrow (V_{U_{1}}, \dots, V_{i}, \dots, V_{U_{N}}) \\ (\mathcal{A}, \mathcal{B}) \leftarrow (\mathcal{A} \backslash \{i\}, \mathcal{B} \cup \{i\}) \\ \text{return} (\mathbf{v}_{L}, \mathbf{v}_{U}, \mathcal{A}, \mathcal{B}) \end{split}$$

• FreeAttr(*i*):

$$\begin{split} \mathbf{v}_{L} \leftarrow (v_{L_{1}}, \dots, \lambda(i), \dots, v_{L_{N}}) \\ \mathbf{v}_{U} \leftarrow (v_{U_{1}}, \dots, \mu(i), \dots, v_{U_{N}}) \\ (\mathcal{A}, \mathcal{B}) \leftarrow (\mathcal{A} \backslash \{i\}, \mathcal{B} \cup \{i\}) \\ \text{return } (\mathbf{v}_{L}, \mathbf{v}_{U}, \mathcal{A}, \mathcal{B}) \end{split}$$

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

▷ Ensures: $\kappa(\mathbf{v}_L) = \kappa(\mathbf{v}_U)$ ▷ S: Some possible seed

▷ Require: $\kappa(\mathbf{v}_{L}) = \kappa(\mathbf{v}_{U})$, given S▷ Loop inv.: $\kappa(\mathbf{v}_{L}) = \kappa(\mathbf{v}_{U})$

⊳ If invariant broken, fix it

+ Obs: $\mathcal{S} = \varnothing$ for computing a single AXp/CXp
Computing one AXp - example

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

Foat	Initial values		Changed values		Predictions		Doc	Resulting values	
Teat.	\mathbf{v}_{L}	\mathbf{v}_{\cup}	\mathbf{v}_{L}	\mathbf{v}_{\cup}	$\kappa(\mathbf{v}_{L})$	$\kappa(\mathbf{v}_{U})$	Dec.	\mathbf{v}_{L}	\mathbf{v}_{\cup}
1	(10,10,5,0)	(10, 10, 5, 0)	(0,10,5,0)	(10, 10, 5, 0)	С	А	\checkmark	(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	А	\checkmark	(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	А	×	(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	А	×	(10,10,0,0)	(10,10,10,10)

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

$$WAXp(\mathcal{X}) := \forall (\mathbf{x} \in \mathbb{F}). \bigwedge_{j \in \mathcal{X}} (x_j = v_j) \to (\sigma(\mathbf{x}))$$
$$WCXp(\mathcal{Y}) := \exists (\mathbf{x} \in \mathbb{F}). \bigwedge_{j \notin \mathcal{Y}} (x_j = v_j) \land (\neg \sigma(\mathbf{x}))$$

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

- 1: procedure oneXP(ℙ)
- 2: $\mathcal{S} \leftarrow \mathcal{F}$
- 3: for $i \in \mathcal{F}$ do
- 4: if $\mathbb{P}(S \setminus \{i\})$ then
- 5: $\mathcal{S} \leftarrow \mathcal{S} \setminus \{i\}$
- 6: return S

ightarrow Initialization: $\mathbb{P}(\mathcal{S})$ holds ightarrow Loop invariant: $\mathbb{P}(\mathcal{S})$ holds

 $\succ \text{ Update } S \text{ only if } \mathbb{P}(S \setminus \{i\}) \text{ holds}$ $\succ \text{ Returned set } S: \mathbb{P}(S) \text{ holds}$



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



• Finding on AXp:



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



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



- Finding on AXp:
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 - 4th path inconsistent: $H_4 = \{1\}$



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 - 1st path inconsistent: $H_1 = \{3\}$
 - 2nd path inconsistent: $H_2 = \{2\}$
 - 3rd path inconsistent: $H_3 = \{1\}$
 - 4th path inconsistent: $H_4 = \{1\}$
- AXp is MHS of H_j sets: $\{1, 2, 3\}$



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



• Finding CXps:



- Finding CXps:
 - 1st path: $I_1 = \{3\}$



- Finding CXps:
 - 1st path: $I_1 = \{3\}$
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 - $\cdot \mathcal{L} = \{\{1\}, \{2\}, \{3\}\} = \mathbb{C}$
- Finding AXps: (i.e. all MHSes of sets in C



- Finding CXps:
 - 1st path: $I_1 = \{3\}$
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 - 3rd path: $I_3 = \{1\}$
 - 4th path: $I_4 = \{1\}$
 - · $\mathcal{L} = \{\{1\}, \{2\}, \{3\}\} = \mathbb{C}$
- Finding AXps: (i.e. all MHSes of sets in \mathbb{C} • $\mathbb{A} = \{\{1, 2, 3\}\}$

R_1 :	IF	$(X_1 \wedge X_3)$	THEN	$\kappa(\mathbf{x}) = 0$
R_2 :	ELSE IF	$(X_1 \wedge X_5)$	THEN	$\kappa(\mathbf{x}) = 0$
R_3 :	ELSE IF	$(X_2 \wedge X_4)$	THEN	$\kappa(\mathbf{x}) = 1$
R_4 :	ELSE IF	$(X_1 \wedge X_7)$	THEN	$\kappa(\mathbf{x}) = 0$
R_5 :	ELSE IF	$(\neg X_4 \land X_6)$	THEN	$\kappa(\mathbf{x}) = 1$
R_6 :	ELSE IF	$(\neg X_4 \land \neg X_6)$	THEN	$\kappa(\mathbf{x}) = 1$
R ₇ :	ELSE IF	$(\neg x_2 \land x_6)$	THEN	$\kappa(\mathbf{x}) = 1$
R_{DEF} :	ELSE			$\kappa(\mathbf{x}) = 0$

• DL:

R_1 :	IF	$(X_1 \wedge X_3)$	THEN	$\kappa(\mathbf{x}) = 0$
R_2 :	ELSE IF	$(X_1 \wedge X_5)$	THEN	$\kappa(\mathbf{x}) = 0$
R_3 :	ELSE IF	$(X_2 \wedge X_4)$	THEN	$\kappa(\mathbf{x}) = 1$
R_4 :	ELSE IF	$(X_1 \wedge X_7)$	THEN	$\kappa(\mathbf{x}) = 0$
R_5 :	ELSE IF	$(\neg X_4 \land X_6)$	THEN	$\kappa(\mathbf{x}) = 1$
R_6 :	ELSE IF	$(\neg X_4 \land \neg X_6)$	THEN	$\kappa(\mathbf{x}) = 1$
R ₇ :	ELSE IF	$(\neg x_2 \land x_6)$	THEN	$\kappa(\mathbf{x}) = 1$
R_{DEF} :	ELSE			$\kappa(\mathbf{x}) = 0$

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

 $\cdot\,$ The prediction is 1, due to R_3

R_1 :	IF	$(X_1 \wedge X_3)$	THEN	$\kappa(\mathbf{x}) = 0$
R_2 :	ELSE IF	$(X_1 \wedge X_5)$	THEN	$\kappa(\mathbf{x}) = 0$
R_3 :	ELSE IF	$(X_2 \wedge X_4)$	THEN	$\kappa(\mathbf{x}) = 1$
R_4 :	ELSE IF	$(X_1 \wedge X_7)$	THEN	$\kappa(\mathbf{x}) = 0$
R_5 :	ELSE IF	$(\neg X_4 \land X_6)$	THEN	$\kappa(\mathbf{x}) = 1$
R_6 :	ELSE IF	$(\neg X_4 \land \neg X_6)$	THEN	$\kappa(\mathbf{x}) = 1$
R ₇ :	ELSE IF	$(\neg X_2 \land X_6)$	THEN	$\kappa(\mathbf{x}) = 1$
R_{DEF} :	ELSE			$\kappa(\mathbf{x}) = 0$

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

R_1 :	IF	$(X_1 \wedge X_3)$	THEN	$\kappa(\mathbf{x}) = 0$
R_2 :	ELSE IF	$(X_1 \wedge X_5)$	THEN	$\kappa(\mathbf{x}) = 0$
R_3 :	ELSE IF	$(X_2 \wedge X_4)$	THEN	$\kappa(\mathbf{x}) = 1$
R_4 :	ELSE IF	$(X_1 \wedge X_7)$	THEN	$\kappa(\mathbf{x}) = 0$
R_5 :	ELSE IF	$(\neg X_4 \land X_6)$	THEN	$\kappa(\mathbf{x}) = 1$
R_6 :	ELSE IF	$(\neg X_4 \land \neg X_6)$	THEN	$\kappa(\mathbf{x}) = 1$
R ₇ :	ELSE IF	$(\neg x_2 \land x_6)$	THEN	$\kappa(\mathbf{x}) = 1$
R_{DEF} :	ELSE			$\kappa(\mathbf{x}) = 0$

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

R_1 :	IF	$(X_1 \wedge X_3)$	THEN	$\kappa(\mathbf{x}) = 0$
R_2 :	ELSE IF	$(X_1 \wedge X_5)$	THEN	$\kappa(\mathbf{x}) = 0$
R_3 :	ELSE IF	$(X_2 \wedge X_4)$	THEN	$\kappa(\mathbf{x}) = 1$
R_4 :	ELSE IF	$(X_1 \wedge X_7)$	THEN	$\kappa(\mathbf{x}) = 0$
R_5 :	ELSE IF	$(\neg X_4 \land X_6)$	THEN	$\kappa(\mathbf{x}) = 1$
R_6 :	ELSE IF	$(\neg X_4 \land \neg X_6)$	THEN	$\kappa(\mathbf{x}) = 1$
R ₇ :	ELSE IF	$(\neg X_2 \land X_6)$	THEN	$\kappa(\mathbf{x}) = 1$
R_{DEF} :	ELSE			$\kappa(\mathbf{x}) = 0$

- Instance: $\mathbf{v} = (0, 1, 0, 1, 0, 1, 0)$
 - $\cdot\,$ The prediction is 1, due to ${\sf R}_3$
- AXp: {1,2}
- $\cdot\,$ Quiz: write down the constraints and confirm AXp with SAT solver

Questions?

Lecture 03

• Rigorous definitions of abductive and contrastive explanations

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

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

• Instance: ((0, 0, 1, 0, 0), 0)



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



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



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


- Instance: ((0, 0, 1, 0, 0), 0)
- One AXp: $\{1,4,5\}$
- All CXps:
 - $I_1: \{5\}$
 - l_2 : {4}



- Instance: ((0, 0, 1, 0, 0), 0)
- One AXp: $\{1,4,5\}$
- All CXps:
 - $I_1: \{5\}$
 - I_2 : {4}
 - I_3 : {2,5}



- Instance: ((0, 0, 1, 0, 0), 0)
- One AXp: $\{1,4,5\}$
- All CXps:
 - $I_1: \{5\}$
 - l_2 : {4}
 - I_3 : {2,5}
 - I_4 : $\{2, 4\}$



- Instance: ((0, 0, 1, 0, 0), 0)
- One AXp: $\{1,4,5\}$
- All CXps:
 - I_1 : {5}
 - l_2 : {4}
 - I_3 : {2,5}
 - I_4 : $\{2, 4\}$
 - 1₅: {1}



- Instance: ((0, 0, 1, 0, 0), 0)
- One AXp: $\{1,4,5\}$
- All CXps:
 - $I_1: \{5\}$
 - l_2 : {4}
 - I_3 : {2,5}
 - I_4 : $\{2, 4\}$
 - 1₅: {1}
 - $\mathcal{L} = \{\{1\}, \{4\}, \{5\}\}$



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	X1	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

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:
 - \cdot {1}, by flipping the value of feature 1
 - \cdot {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

- Lecture 01 units:
 - #01: Foundations
- Lecture 02 units:
 - #02: Principles of symbolic XAI feature selection
 - #03: Tractability in symbolic XAI (& myth of interpretability)
- Lecture 03 units:
 - #04: Intractability in symbolic XAI (& myth of model-agnostic XAI)
 - #05: Explainability queries
- Lecture 04 units:
 - #06: Advanced topics
- Lecture 05 units:
 - #07: Principles of symbolic XAI feature attribution (& myth of Shapley values in XAI)
 - #08: Conclusions & research directions

Some comments...

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

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 - Most likely answer: No!

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 - fly with a airliner whose planes crash in about 1% of its flights?

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 - undergo an optional surgery that might be life-threatening in about 5% of the cases?

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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 are likely to be wrong, 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!...



Source: Xiyang Hu, Cynthia Rudin, Margo I. Seltzer: Optimal Sparse Decision Trees. NeurIPS 2019: 7265-7273 [HRS19]

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[HRS19]

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



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

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- 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!

Unit #04

(Efficient) Intractability in Symbolic XAI

Explaining Decision Lists

Myth #02: Model-Agnostic Explainability

Progress Report on Symbolic XAI

R_1 :	IF	(au_1)	THEN	d_1
R_2 :	ELSE IF	(au_2)	THEN	d_2
R_j :	ELSE IF	(au_j)	THEN	d_j
R _n :	ELSE IF	(τ_n)	THEN	dn
R _{def} :	ELSE		THEN	d_{n+1}



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

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



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

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

R_1 :	IF	(τ_1)	THEN	d_1
R_2 :	ELSE IF	(τ_2)	THEN	d_2
		•••		
R_j :	ELSE IF	(τ_j)	THEN	d_j
		•••		
R_n :	ELSE IF	(τ_n)	THEN	dn
R _{def} :	ELSE		THEN	d_{n+1}

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

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

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

Explaining Decision Lists

Myth #02: Model-Agnostic Explainability

Progress Report on Symbolic XAI
What is model-agnostic explainability?



What is model-agnostic explainability?



 Wildly pop 	ular XAI approach	[RSG16, LL17, RSG18]
• Feature	e attribution: LIME, SHAP,	[RSG16, LL17]
• Feature	e selection: Anchors,	[RSG18]

What is model-agnostic explainability?



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

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

Easy to spot problems - BT for zoo dataset



Easy to spot problems - BT for zoo dataset



- Example instance:

Easy to spot problems - BT for zoo dataset & Anchor



• 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



• Explanation obtained with Anchor:

[RSG18]

IF \neg hair $\land \neg$ milk $\land \neg$ toothed $\land \neg$ finsTHEN(class = reptile)

Easy to spot problems - BT for zoo dataset & Anchor



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

Incorrect explanations:

Classifier for deciding bank loans

Incorrect explanations:Classifier for deciding bank loansTwo samples:Bessie := (v_1, \mathbf{Y}) and Clive := (v_2, \mathbf{N})

Incorrect explanations:Classifier for deciding bank loansTwo samples:Bessie := (v_1, \mathbf{Y}) and Clive := (v_2, \mathbf{N}) Explanation X:age = 45, salary = 50K

```
Incorrect explanations:
```

Classifier for deciding bank loans

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

Explanation X: age = 45, salary = 50K

And,

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

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

```
Incorrect explanations:
```

Classifier for deciding bank loans

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

Explanation X: age = 45, salary = 50K

And,

- X is consistent with Bessie \coloneqq (\mathbf{v}_1, \mathbf{Y})
- X is consistent with $Clive := (\mathbf{v}_2, \mathbf{N})$
- : different outcomes & same explanation !?

• For feature selection, checking rigor is *easy*

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- $\cdot\,$ Let ${\mathcal X}$ be the features reported by model-agnostic tool

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- $\cdot\,$ Let ${\mathcal X}$ be the features reported by model-agnostic tool
- Check whether \mathcal{X} is a (rigorous) (W)AXp:
 - 1. \mathcal{X} is sufficient for prediction:

$$\forall (\mathbf{x} \in \mathbb{F}). \bigwedge_{j \in \mathcal{X}} (X_j = V_j) \rightarrow (\kappa(\mathbf{x}) = C)$$

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

$$\forall (t \in \mathcal{X}). \exists (\mathbf{x} \in \mathbb{F}). \bigwedge_{j \in (\mathcal{X} \setminus \{t\})} (X_j = V_j) \rightarrow (\kappa(\mathbf{x}) \neq c)$$

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

- For feature selection, checking rigor is *easy*
- $\cdot\,$ Let ${\mathcal X}$ be the features reported by model-agnostic tool
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Depending on logic encoding used for classifier, different automated reasoners can be employed

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

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

[INM19c, Ign20, YIS+23]

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[INM19c, Ign20, YIS+23]

• Results for boosted trees, due to non-scalability with NNs

[CG16]

- Obs: Lack of rigor of model-agnostic explanations known since 2019
- Results for boosted trees, due to non-scalability with NNs
- Some results for Anchors

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%
compas	84.4%	1.7%	13.9%
german	99.7%	0.2%	0.1%

[INM19c, Ign20, YIS+23]

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[INM19c, Ign20, YIS+23]

[CG16]

[RSG18]

• **Obs:** Results are **not** positive even if we count how often prediction changes

[NSM+19]

• In this case, BNNs were used, to allow for model counting...

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- Results for boosted trees, due to non-scalability with NNs
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rcdv	99.4%	0.4%	0.2%
compas	84.4%	1.7%	13.9%
german	99.7%	0.2%	0.1%

[INM19c, Ign20, YIS+23]

[CG16]

[RSG18]

- **Obs:** Results are **not** positive even if we count how often prediction changes
- [NSM+19]

- $\cdot\,$ In this case, BNNs were used, to allow for model counting...
- For feature attribution we proposed different ways of assessing rigor

[INM19c, NSM+19, Ign20, YIS+23]

Incorrect explanations are ubiquitous & likely...



Explaining Decision Lists

Myth #02: Model-Agnostic Explainability

Progress Report on Symbolic XAI

Efficacy map – progress until 2022

	Computing one XP
Computational complexity Poly-time computationally hard	RFS GTS DIS CDFS GDFS G-DNNF
	Effective Ineffective
	Practical scalability (effectiveness)

[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-E 	DNNF,) [HII+22]
 Additional results 	[CM21, HII+22]
• Comp. hard, but effective (efficien	t 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)
 - Bayesian networks (BNs)

[INM19a]



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

• Formal explanations efficient for several families of classifiers

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	 Naive-Bayes classifiers (NBCs) 	[MGC+20]
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	 Additional results 	[CM21, HII+22]
•	Comp. hard, but effective (efficient in pra	actice):
	 Random forests (RFs) 	[IMS21]
	 Decision lists (DLs) 	[IM21]
	Boosted trees (BTs)	lgn20, IISMS22]
•	Comp. hard, but some practical scalabili	ty:
	 Neural networks (NNs) 	[HM23b]
•	Comp. hard, and ineffective (hard in practice)	ctice):
	 Bayesian networks (BNs) 	[SCD18]

Results for RFs in 2021 (with SAT)

Dataset	(#F	#C	#1)	RF		CNF SAT o		SAT ora	AT oracle		AXp (RFxpl)			Anch	ior		
Databet	\		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)

Dataset			Mini	mal expla	nation	Mini	mum expl	anation
			size	SMT (s)	MILP (s)	size	SMT (s)	MILP (s)
australian	(14)	m a M	$\begin{smallmatrix}&1\\8.79\\14\end{smallmatrix}$	$0.03 \\ 1.38 \\ 17.00$	$0.05 \\ 0.33 \\ 1.43$			
backache	(32)	m a M	$\begin{array}{r}13\\19.28\\26\end{array}$	$0.13 \\ 5.08 \\ 22.21$	$0.14 \\ 0.85 \\ 2.75$			_ _ _
breast-cancer	(9)	m a M	$3 \\ 5.15 \\ 9$	$0.02 \\ 0.65 \\ 6.11$	$0.04 \\ 0.20 \\ 0.41$	$\substack{\substack{3\\4.86\\9}}$	$0.02 \\ 2.18 \\ 24.80$	0.03 0.41 1.81
cleve	(13)	m a M	$\begin{smallmatrix}&4\\8.62\\13\end{smallmatrix}$	$0.05 \\ 3.32 \\ 60.74$	$0.07 \\ 0.32 \\ 0.60$	4 7.89 13		$0.07 \\ 5.14 \\ 39.06$
hepatitis	(19)	m a M	$\begin{array}{c} 6\\11.42\\19\end{array}$	$0.02 \\ 0.07 \\ 0.26$	$0.04 \\ 0.06 \\ 0.20$	$\begin{array}{c}4\\9.39\\19\end{array}$	$0.01 \\ 4.07 \\ 27.05$	0.04 2.89 22.23
voting	(16)	m a M	$\begin{array}{c}3\\4.56\\11\end{array}$	$0.01 \\ 0.04 \\ 0.10$	$0.02 \\ 0.13 \\ 0.37$	$\begin{array}{c}3\\3.46\\11\end{array}$	$0.01 \\ 0.3 \\ 1.25$	$0.02 \\ 0.25 \\ 1.77$
spect	(22)	m a M	$3 \\ 7.31 \\ 20$	$0.02 \\ 0.13 \\ 0.88$	$0.02 \\ 0.07 \\ 0.29$	$\begin{array}{c}3\\6.44\\20\end{array}$	$0.02 \\ 1.61 \\ 8.97$	$0.04 \\ 0.67 \\ 10.73$

Results for NNs in 2019 (with SMT/MILP)

First rigoro	ous approach			Mini	mal expla	nation	Mini	mum expl	anation
for expla	ining NNs !			size	SMT (s)	MILP (s)	size	SMT (s)	MILP (s)
	australian	(14)	m a M		$0.03 \\ 1.38 \\ 17.00$	$0.05 \\ 0.33 \\ 1.43$	_ _ _		
	backache	(32)	m a M	$ \begin{array}{r} 13 \\ 19.28 \\ 26 \end{array} $	$0.13 \\ 5.08 \\ 22.21$	$0.14 \\ 0.85 \\ 2.75$			
	breast-cancer	(9)	m a M	$3 \\ 5.15 \\ 9$	$0.02 \\ 0.65 \\ 6.11$	$0.04 \\ 0.20 \\ 0.41$	$\substack{\substack{3\\4.86\\9}}$	$0.02 \\ 2.18 \\ 24.80$	$0.03 \\ 0.41 \\ 1.81$
	cleve	(13)	m a M	$\begin{smallmatrix}&4\\8.62\\13\end{smallmatrix}$	$0.05 \\ 3.32 \\ 60.74$	$0.07 \\ 0.32 \\ 0.60$	4 7.89 13		$0.07 \\ 5.14 \\ 39.06$
	hepatitis	(19)	m a M		$0.02 \\ 0.07 \\ 0.26$	$0.04 \\ 0.06 \\ 0.20$	4 9.39 19	$0.01 \\ 4.07 \\ 27.05$	$0.04 \\ 2.89 \\ 22.23$
	voting	(16)	m a M	$\begin{array}{c}3\\4.56\\11\end{array}$	$0.01 \\ 0.04 \\ 0.10$	$0.02 \\ 0.13 \\ 0.37$	$3 \\ 3.46 \\ 11$	$0.01 \\ 0.3 \\ 1.25$	$0.02 \\ 0.25 \\ 1.77$
	spect	(22)	m a M	$3 \\ 7.31 \\ 20$	$0.02 \\ 0.13 \\ 0.88$	$0.02 \\ 0.07 \\ 0.29$	$\begin{array}{c}3\\6.44\\20\end{array}$	$0.02 \\ 1.61 \\ 8.97$	$0.04 \\ 0.67 \\ 10.73$

Results for NNs in 2019 (with SMT/MILP)

irst rigoro	us approach			Min	imal expla	nation	Mini	imum expl	anation
for expla i	ining NNs !			size	SMT (s)	MILP (s)	size	SMT (s)	MILP (s)
	australian	(14)	m a M	$\begin{array}{c}1\\8.79\\14\end{array}$	$0.03 \\ 1.38 \\ 17.00$	$0.05 \\ 0.33 \\ 1.43$	_ _ _		_ _ _
	backache	(32)	m a M	$\begin{smallmatrix}&13\\19.28\\&26\end{smallmatrix}$	$0.13 \\ 5.08 \\ 22.21$	$0.14 \\ 0.85 \\ 2.75$			
	breast-cancer	(9)	m a M	$3 \\ 5.15 \\ 9$	$0.02 \\ 0.65 \\ 6.11$	$0.04 \\ 0.20 \\ 0.41$	$\begin{smallmatrix}&3\\4.86\\&9\end{smallmatrix}$	0.02 2.18 24.80	$0.03 \\ 0.41 \\ 1.81$
	cleve	(13)	m a M	$\begin{smallmatrix}&4\\8.62\\13\end{smallmatrix}$	$0.05 \\ 3.32 \\ 60.74$	$0.07 \\ 0.32 \\ 0.60$	4 7.89 13		$0.07 \\ 5.14 \\ 39.06$
	hepatitis	(19)	m a M	$\begin{array}{c} 6\\11.42\\19\end{array}$	$0.02 \\ 0.07 \\ 0.26$	$0.04 \\ 0.06 \\ 0.20$	4 9.39 19	$0.01 \\ 4.07 \\ 27.05$	0.04 2.89 22.23
	voting	(16)	m a M	$3 \\ 4.56 \\ 11$	$0.01 \\ 0.04 \\ 0.10$	$0.02 \\ 0.13 \\ 0.37$	$3 \\ 3.46 \\ 11$	$0.01 \\ 0.3 \\ 1.25$	$0.02 \\ 0.25 \\ 1.77$
	spect	(22)	m a M	$3 \\ 7.31 \\ 20$	$0.02 \\ 0.13 \\ 0.88$	$0.02 \\ 0.07 \\ 0.29$	$\begin{array}{c}3\\6.44\\20\end{array}$	$0.02 \\ 1.61 \\ 8.97$	0.04 0.67 10.73

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

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

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

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

Scales to a few hundred neurons

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Model			D	eletior	ı			SwiftXplain							
	avgC	nCalls	Len	Mn	Mx	avg	то	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	

Model			D	eletior	ı			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	



Model			D	eletion	1			SwiftXplain							
	avgC	nCalls	Len	Mn	Mx	avg	то	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	



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

Unit #05

Queries in Symbolic XAI
Enumeration of Explanations

Feature Necessity & Relevancy

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

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• Complexity results:

•	For NBCs: enumeration with polynomial delay	[MGC+20]
•	For monotonic classifiers: enumeration is computationally hard	[MGC+21]
•	Recall: for DTs, enumeration of CXp's is in P	[HIIM21, IIM22]

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- $\cdot\,$ There are algorithms for direct enumeration of CXp's
 - Akin to enumerating MCSes

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• Recall: for DTs, enumeration of CXp's is in P	[HIIM21, IIM22]
There are algorithms for direct enumeration of CXp's	
Akin to enumerating MCSes	
No known algorithms for direct enumeration of AXp's	[MM20]
 Akin to enumerating MUSes 	

.

.

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Complexity results:	
 For NBCs: enumeration with polynomial delay 	[MGC+20]
\cdot For monotonic classifiers: enumeration is computationally hard	[MGC+21]
• Recall: for DTs, enumeration of CXp's is in P	[HIIM21, IIM22]
• There are algorithms for direct enumeration of CXp's	
Akin to enumerating MCSes	
 No known algorithms for direct enumeration of AXp's 	[MM20]
Akin to enumerating MUSes	
\cdot Enumeration of MCSes $+$ dualization often not realistic	[LS08, FK96]
 There can be too many CXp's 	

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• Recall: for DTs, enumeration of CXp's is in P	[HIIM21, IIM22]
\cdot There are algorithms for direct enumeration of CXp's	
Akin to enumerating MCSes	
 No known algorithms for direct enumeration of AXp's 	[MM20]
Akin to enumerating MUSes	
\cdot Enumeration of MCSes $+$ dualization often not realistic	[LS08, FK96]
• There can be too many CXp's	
\cdot Best solution is a MARCO-like algorithm (for enumerating MUSes)	[LPMM16]
 On-demand enumeration of AXp's/CXp's 	

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

- 1: procedure $oneXP(\mathbb{P})$
- 2: $\mathcal{S} \leftarrow \mathcal{F}$
- 3: for $i \in \mathcal{F}$ do
- 4: if $\mathbb{P}(S \setminus \{i\})$ then
- 5: $\mathcal{S} \leftarrow \mathcal{S} \setminus \{i\}$
- 6: return S

 $\succ \text{Initialization: } \mathbb{P}(\mathcal{S}) \text{ holds}$ $\succ \text{Loop invariant: } \mathbb{P}(\mathcal{S}) \text{ holds}$

 $\succ \text{ Update } S \text{ only if } \mathbb{P}(S \setminus \{i\}) \text{ holds}$ $\succ \text{ Returned set } S: \mathbb{P}(S) \text{ holds}$

Generic oracle-based enumeration algorithm

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

DT classifier – example run of enumerator



DT classifier - another example run of enumerator



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 ${f v}$
 - + Add I_k to $\mathcal I$
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- Example:
 - $l_1 = \{3\}$
 - $l_2 = \{5\}$
 - $I_3 = \{2, 5\}$
 - · \therefore keep I_1 an I_2
 - AXp's: MHSes yield $\{\{3,5\}\}$



Enumeration of Explanations

Feature Necessity & Relevancy

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

[HCM+23]

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- Claim: (C)CDP is in polynomial-time for DTs, decision graphs, monotonic classifiers, among others
- Claim: (C)CDP is in NP-complete for DLs, RFs, BTs, boolean NNs and BNNs

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More on feature necessity

[HCM+23]

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[HCM+23]

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 - This holds for any classifier!
 - Let **u** be obtained from **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 $u_t \in \mathcal{D}_t$

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

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

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

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- General case: best solution is to exploit abstraction refinement

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- But then, by monotonicity, WAXp($\mathcal{X} \setminus \{t\}$) must hold (i.e. any superset of \mathcal{Z} is a weak AXp); hence a contradiction.

Abstraction refinement for feature relevancy

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

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• Approach:

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- Let $\mathcal{Z} \subseteq \mathcal{X} \subseteq \mathcal{F}$ be an AXp such that $t \notin \mathcal{Z}$.
- Then $\mathcal{Z} \subseteq \mathcal{X} \setminus \{t\}$.
- But then, by monotonicity, WAXp($\mathcal{X} \setminus \{t\}$) must hold (i.e. any superset of \mathcal{Z} is a weak AXp); hence a contradiction.
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 - Repeatedly guess weak WAXp candidates \mathcal{X} , with $t \in \mathcal{X}$

[e.g. use SAT oracle]

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 - \cdot Block counterexamples in both cases

[e.g. use SAT oracle] [e.g. use WAXp oracle] [e.g. use WAXp oracle] Input: Instance v, Target Feature t; Feature Set \mathcal{F} , Classifier κ

```
1: function FRPCGR(\mathbf{v}, t; \mathcal{F}, \kappa)
                                                               \triangleright \mathcal{H} overapproximates the subsets of \mathcal{F} that do not contain an AXp containing t
  2:
           \mathcal{H} \leftarrow \emptyset
 3:
           repeat
 4.
                 (OUTC, s) \leftarrow SAT(\mathcal{H}, s_t)
                                                                                                           \triangleright Use SAT oracle to pick candidate WAXp containing t
  5:
                if outc = true then
                                                                                                                                \triangleright Set \mathcal{P} is the candidate WAXp, and t \in \mathcal{P}
 6:
                      \mathcal{P} \leftarrow \{i \in \mathcal{F} \mid s_i = 1\}
 7:
                      \mathcal{D} \leftarrow \{i \in \mathcal{F} \mid s_i = 0\}
                                                                                                                     \triangleright Set \mathcal{D} contains the features not included in \mathcal{P}
 8:
                      if \neg WAXp(\mathcal{P}) then
                                                                                                                                                                     \triangleright Is \mathcal{P} not a WAXp?
 9:
                            \mathcal{H} \leftarrow \mathcal{H} \cup \mathsf{newPosCl}(\mathcal{D}; t, \kappa)
                                                                                                         \triangleright \mathcal{P} is not a WAXp; must pick some non-picked feature
10.
                       else
                                                                                                                                                                              \triangleright \mathcal{P} is a WAXp
11:
                            if \neg WAXp(\mathcal{P} \setminus \{t\}) then
                                                                                                                                                         \triangleright \mathcal{P} without t not a WAXp?
                                  reportWeakAXp(\mathcal{P})
                                                                                                                                \triangleright Feature t is included in any AXp \mathcal{X} \subseteq \mathcal{P}
12.
13:
                                   return true

ightarrow WAXp(\mathcal{P} \setminus \{t\}) holds; some feature in \mathcal{P} must not be picked
14.
                            \mathcal{H} \leftarrow \mathcal{H} \cup \mathsf{newNegCl}(\mathcal{P}; t, \kappa)
15:
            until outc = false
16.
            return false
                                                                                        \triangleright If \mathcal{H} becomes inconsistent, then there is no AXp that contains t
```
An example: feature relevancy for DT, using abstraction refinement



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

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			t = 1		
s	\mathcal{P}	$WAXp(\mathcal{P})$	$WAXp(\mathcal{P} \setminus \{t\})$	Return?	Clause
(1, 1, 1, 1)	$\{1, 2, 3, 4\}$	\checkmark	\checkmark		$(\neg u_2 \lor \neg u_3 \lor \neg u_4)$
(1, 1, 0, 1)	$\{1, 2, 4\}$	\checkmark	\checkmark		$(\neg u_2 \lor \neg u_4)$
(1, 1, 0, 0)	$\{1, 2\}$	\checkmark	\checkmark		$(\neg u_2)$
(1, 0, 0, 0)	$\{1\}$	\checkmark	×	true	

Another example



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

Another example



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			t = 4		
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(1, 1, 1, 1)	$\{1, 2, 3, 4\}$	\checkmark	\checkmark		$(\neg u_1 \lor \neg u_2 \lor \neg u_3)$
(1, 1, 0, 1)	$\{1, 2, 4\}$	\checkmark	\checkmark		$(\neg u_1 \lor \neg u_2)$
(1, 0, 0, 1)	$\{1, 4\}$	\checkmark	\checkmark		$(\neg u_1)$
(0, 1, 0, 1)	$\{2, 4\}$	\checkmark	\checkmark		$(\neg u_2)$
(0, 0, 0, 1)	$\{4\}$	×	_		$(u_1 \lor u_2 \lor u_3)$
(0, 0, 1, 1)	$\{3, 4\}$	×	—		$(u_1 \lor u_2)$
outc = false]		_	-	false	

Questions?

Lecture 04

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

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



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



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 - Yes! Thus, feature 1 is AXp-necessary (i.e. singleton CXp)



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



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- Are there CXp-necessary features?
 - No! There are no singleton AXps



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- Confirmation:



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 - Does there exist u_1 , such that $\kappa(u_1, 0, 0, 0) \neq \kappa(0, 0, 0, 0)$?
 - Yes! Thus, feature 1 is AXp-necessary (i.e. singleton CXp)
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 - Does there exist u_3 , such that $\kappa(0, 0, u_3, 0) \neq \kappa(0, 0, 0, 0)$?
 - No! Thus, feature 3 is not AXp-necessary
- Are there CXp-necessary features?
 - No! There are no singleton AXps
- Confirmation:
 - + CXps: $\{\{1\},\{2\},\{3,4\}\}$ (2 is also AXp-necessary)
 - AXps: $\{\{1,2,3\},\{1,2,4\}\}$



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



- Instance $(\mathbf{v}, c) = ((1, 1, 1, 1), 1)$
- Are there CXp-necessary features?



- Instance $(\mathbf{v}, c) = ((1, 1, 1, 1), 1)$
- Are there CXp-necessary features?
 - Yes! Features 1 and 2 (i.e. singleton AXps)



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 - Yes! Features 1 and 2 (i.e. singleton AXps)
- Are there AXp-necessary features?



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 - Yes! Features 1 and 2 (i.e. singleton AXps)
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- Confirmation:
 - AXps: $\{\{1\}, \{2\}, \{3, 4\}\}$
 - CXps: $\{\{1,2,3\},\{1,2,4\}\}$



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

$$\kappa(\mathbf{X}_1, \mathbf{X}_2, \mathbf{X}_3, \mathbf{X}_4, \mathbf{X}_5) \quad \coloneqq \quad \begin{cases} 1 \\ 0 \end{cases}$$

IF $(10x_1 + 5x_2 + 5x_3 + 2x_4 + x_5 \ge 15)$ otherwise

• Instance: ((1, 1, 1, 1, 1), 1)

$$\kappa(x_1, x_2, x_3, x_4, x_5) := \begin{cases} 1 & \text{IF} (10x_1 + 5x_2 + 5x_3 + 2x_4 + x_5 \ge 15) \\ 0 & \text{otherwise} \end{cases}$$

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- All AXps: $\{\{1,2\},\{1,3\}\}$
- All CXps: $\{\{1\}, \{2, 3\}\}$
- AXp-necessary: {1} (singleton CXp)
- CXp-necessary:

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- All CXps: $\{\{1\}, \{2, 3\}\}$
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- CXp-necessary: Ø
- Relevant:

$$\kappa(x_1, x_2, x_3, x_4, x_5) := \begin{cases} 1 & \text{IF} (10x_1 + 5x_2 + 5x_3 + 2x_4 + x_5 \ge 15) \\ 0 & \text{otherwise} \end{cases}$$

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- Relevant: $\{1, 2, 3\}$
- Irrelevant:

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- · CXp-necessary: Ø
- Relevant: $\{1,2,3\}$
- Irrelevant: $\{4, 5\}$

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

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IF $(10x_1 + 5x_2 + 5x_3 + 2x_4 + x_5 \ge 10)$ otherwise

• Instance: ((1, 1, 1, 1, 1), 1)

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- Instance: ((1, 1, 1, 1, 1), 1)
- Obs: If $x_1 = 0$ and $x_2 = x_3 = 0$, then $\kappa(\mathbf{x}) = 0$; i.e. must either set $x_1 = 1$ or $x_2 = x_3 = 1$
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- All AXps: $\{\{1\},\{2,3\}\}$
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- All AXps: $\{\{1\},\{2,3\}\}$
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- All AXps: $\{\{1\},\{2,3\}\}$
- All CXps: $\{\{1,2\},\{1,3\}\}$
- · AXp-necessary: \varnothing
- CXp-necessary:

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- Relevant: $\{1,2,3\}$
- Irrelevant:

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

$$\kappa(x_1, x_2, x_3, x_4, x_5) := \begin{cases} 1 & \text{IF } (10x_1 + 5x_2 + 5x_3 + 2x_4 + x_5 \ge 10) \\ 0 & \text{otherwise} \end{cases}$$

- Instance: ((1, 1, 1, 1, 1), 1)
- Obs: If $x_1 = 0$ and $x_2 = x_3 = 0$, then $\kappa(\mathbf{x}) = 0$; i.e. must either set $x_1 = 1$ or $x_2 = x_3 = 1$

- All AXps: $\{\{1\},\{2,3\}\}$
- All CXps: $\{\{1,2\},\{1,3\}\}$
- · AXp-necessary: \varnothing
- CXp-necessary: {1} (singleton AXp)
- Relevant: $\{1, 2, 3\}$
- Irrelevant: $\{4, 5\}$

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• Partially enumerate AXps/CXps, exploiting bias in enumeration

- Lecture 01 units:
 - #01: Foundations
- Lecture 02 units:
 - #02: Principles of symbolic XAI feature selection
 - #03: Tractability in symbolic XAI (& myth of interpretability)
- Lecture 03 units:
 - #04: Intractability in symbolic XAI (& myth of model-agnostic XAI)
 - #05: Explainability queries
- Lecture 04 units:
 - #06: Advanced topics
- Lecture 05 units:
 - #07: Principles of symbolic XAI feature attribution (& myth of Shapley values in XAI)
 - #08: Conclusions & research directions

Detour: Monotonic Classification & Voting Power

- Monotonic classifier $\mathcal{M} = (\mathcal{F}, \mathbb{F}, \mathcal{K}, \kappa)$, such that each $\mathcal{D}_i = \{0, 1\}$ and $\mathcal{K} = \{0, 1\}$ are ordered (i.e. 0 < 1), and
 - · $\kappa(\mathbf{1})=1$;
 - · Non-constant classifier, i.e. $\kappa(\mathbf{0})=0$; and
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- Let $\mathbf{v}_1, \mathbf{v}_2 \in \mathbb{F}$ be such that $\kappa(\mathbf{v}_1) = \kappa(\mathbf{v}_2) = 1$, and $\mathbf{v}_1 \leq \mathbf{v}_2$ Define the explanation problems:
 - $\cdot \ \mathcal{E}_1 = (\mathcal{M}, (\mathbf{v}_1, 1))$
 - $\cdot \ \mathcal{E}_2 = (\mathcal{M}, (\mathbf{v}_2, 1))$
 - $\cdot \ \mathcal{E}_{\mathbb{1}} = (\mathcal{M}, ((1, \dots, 1), 1)) = (\mathcal{M}, (\mathbb{1}, 1))$

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

- ML model $\mathcal{M} = (\mathcal{F}, \mathbb{F}, \mathcal{K}, \kappa)$:
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 - With classification function:

$$\kappa(x_1, x_2, x_3, x_4, x_5, x_6) \quad \coloneqq \quad \begin{cases} 1 & \qquad \mathsf{IF} \left(4x_1 + 4x_2 + 4x_3 + 2x_4 + 2x_5 + x_6 \geqslant 12 \right) \\ 0 & \qquad \mathsf{otherwise} \end{cases}$$

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 - AXp: $\{2, 3, 4, 5\}$; Q: Is feature 6 relevant?

$$\kappa(\mathbf{X}_1, \mathbf{X}_2, \mathbf{X}_3, \mathbf{X}_4, \mathbf{X}_5, \mathbf{X}_6) \quad \coloneqq \quad \begin{cases} 1 \\ 0 \end{cases}$$

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 - Example: [12; 4, 4, 4, 2, 2, 1]
 - Problem: find a measure of importance of each voter !
 - · I.e. measure the a priori voting power of each voter

Coutry	Acronym	# Votes
France	F	4
Germany	D	4
Italy	I	4
Belgium	В	2
Netherlands	Ν	2
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- Perhaps surprisingly, answer is **No**!
 - In 1958, Luxembourg was a **dummy** voter/player

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• The corresponding classifier is:

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

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$$\mathbb{A} = \{\{1, 2\}, \{1, 3, 4, 5\}, \{1, 3, 4, 6\}, \{1, 3, 4, 7\}\}$$

$$\mathbb{C} = \{\{1\}, \{2,3\}, \{2,4\}, \{2,5,6,7\}\}$$

- WVG: [21; 12, 9, 4, 4, 1, 1, 1]
- Computing the AXps:
 - Must include feature 1; sum of weights of others equals 20...
 - Either include feature 2, or features 3 and 4, plus any one of features 5, 6, 7
- AXps:

$$\mathbb{A} = \{\{1, 2\}, \{1, 3, 4, 5\}, \{1, 3, 4, 6\}, \{1, 3, 4, 7\}\}$$

• CXps:

$$\mathbb{C} = \{\{1\}, \{2,3\}, \{2,4\}, \{2,5,6,7\}\}$$

• Q: How should features be ranked in terms of importance?

• WVG: [16; 9, 9, 7, 3, 1, 1]

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SHAP scores, i.e. the use of Shapley values for XAI, exhibit critical theoretical flaws (more tomorrow) [MSH24, HM524, HM524]

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- SHAP scores, i.e. the use of Shapley values for XAI, exhibit critical theoretical flaws (more tomorrow) [MSH24, HMS24, HMS24,
- $\cdot\,$ Recently, we have devised ways of correcting SHAP scores
- In turn, this revealed novel connections between logic-based XAI and a priori voting power
- Homework:
 - Create your own weighted voting games;
 - $\cdot\,$ Compute the sets of AXps and CXps; and
 - · Assess the importance of features and how they compare to each other

[LHMS24]

Unit #06

Advanced Topics

Changing Assumptions

Inflated Explanations

Probabilistic Explanations

Constrained Explanations

Distance-Restricted Explanations

Additional Topics

General definition of prediction sufficiency

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

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

• $S \subseteq F$ suffices for prediction *c* if:

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

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

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

• And one can also envision generalizations of σ !
Changing Assumptions

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Additional Topics

[IISM24]

• Recall:

$$\mathsf{WAXp}(\mathcal{X}) \quad \coloneqq \quad \forall (\mathbf{x} \in \mathbb{F}). \bigwedge_{j \in \mathcal{X}} (\mathbf{X}_j = \mathbf{V}_j) \to (\kappa(\mathbf{x}) = c)$$

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

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

[IIM22]

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



[IIM22]



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$$\forall (\mathbf{x} \in \mathbb{F}) . (X_1 = 2 \land X_2 = 20) \rightarrow (\kappa(\mathbf{x}) = \mathsf{Y})$$

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

Changing Assumptions

Inflated Explanations

Probabilistic Explanations

Constrained Explanations

Distance-Restricted Explanations

Additional Topics

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

• Explanation size is critical for human understanding

[Mil56]

• Probabilistic explanations provide smaller explanations, by trading off rigor of explanation by explanation size

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• Explanation size is critical for human understanding

[Mil56]

- Probabilistic explanations provide smaller explanations, by trading off rigor of explanation by explanation size
- Definition of weak probabilistic AXp $\mathcal{X} \subseteq \mathcal{F}$:

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

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

• Weak probabilistic AXp (WPAXp):

$$\begin{aligned} \mathsf{N}\mathsf{eakPAXp}(\mathcal{X}; \mathbb{F}, \kappa, \mathbf{v}, c, \delta) &:= \\ \mathsf{Pr}_{\mathbf{x}}(\kappa(\mathbf{x}) = c \,|\, \mathbf{x}_{\mathcal{X}} = \mathbf{v}_{\mathcal{X}}) \geqslant \delta \ := \ \frac{|\{\mathbf{x} \in \mathbb{F} : \kappa(\mathbf{x}) = c \land (\mathbf{x}_{\mathcal{X}} = \mathbf{v}_{\mathcal{X}})\}|}{|\{\mathbf{x} \in \mathbb{F} : (\mathbf{x}_{\mathcal{X}} = \mathbf{v}_{\mathcal{X}})\}|} \geqslant \delta \end{aligned}$$

• Weak probabilistic AXp (WPAXp):

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• Probabilistic AXp (PAXp):

$$\begin{split} \mathsf{PAXp}(\mathcal{X};\mathbb{F},\kappa,\mathbf{v},c,\delta) &:= \\ \mathsf{WeakPAXp}(\mathcal{X};\mathbb{F},\kappa,\mathbf{v},c,\delta) \land \forall (\mathcal{X}' \subsetneq \mathcal{X}).\neg \mathsf{WeakPAXp}(\mathcal{X}';\mathbb{F},\kappa,\mathbf{v},c,\delta) \end{split}$$

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• Locally-minimal PAXp (LmPAXp):

 $\mathsf{LmPAXp}(\mathcal{X}; \mathbb{F}, \kappa, \mathbf{v}, c, \delta) := \\ \mathsf{WeakPAXp}(\mathcal{X}; \mathbb{F}, \kappa, \mathbf{v}, c, \delta) \land \forall (j \in \mathcal{X}). \neg \mathsf{WeakPAXp}(\mathcal{X} \setminus \{j\}; \mathbb{F}, \kappa, \mathbf{v}, c, \delta)$

• Weak probabilistic AXp (WPAXp):

- definition is non-monotonic

$$\begin{split} \mathsf{WeakPAXp}(\mathcal{X};\mathbb{F},\kappa,\mathbf{v},c,\delta) &:= \\ \mathsf{Pr}_{\mathbf{x}}(\kappa(\mathbf{x}) = c \,|\, \mathbf{x}_{\mathcal{X}} = \mathbf{v}_{\mathcal{X}}) \geqslant \delta \,:=\, \frac{|\{\mathbf{x} \in \mathbb{F} : \kappa(\mathbf{x}) = c \land (\mathbf{x}_{\mathcal{X}} = \mathbf{v}_{\mathcal{X}})\}|}{|\{\mathbf{x} \in \mathbb{F} : (\mathbf{x}_{\mathcal{X}} = \mathbf{v}_{\mathcal{X}})\}|} \geqslant \delta \end{split}$$

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• Locally-minimal PAXp (LmPAXp): – may differ from PAXp due to non-monotonicity

$$\mathsf{LmPAXp}(\mathcal{X}; \mathbb{F}, \kappa, \mathbf{v}, c, \delta) :=$$

WeakPAXp $(\mathcal{X}; \mathbb{F}, \kappa, \mathbf{v}, c, \delta) \land \forall (j \in \mathcal{X}). \neg \mathsf{WeakPAXp}(\mathcal{X} \setminus \{j\}; \mathbb{F}, \kappa, \mathbf{v}, c, \delta)$

• **Obs:** Definition of WPAXp is **non-monotonic** (from previous slide)

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[ABOS22]

What is known about PAXps?

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

Results for decision trees

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

Results for naive Bayes classifiers

Dataset ((#F	#I)	NBC	АХр			LmPAXp _≪ g	,			LmPAXp _{≤7}			$LmPAXp_{\leqslant 4}$				
	(11)	,	A%	Length	δ	Length	Precision	W%	Time	Length	Precision	W%	Time	Length	Precision	W%	Time	
adult (1					98	6.8± 1.1	100 ± 0.0	100	0.003	6.3± 0.9	99.61± 0.6	96	0.023	4.8± 1.3	98.73± 0.5	48	0.059	
	(12	200)	01 27	60110	95	6.8 ± 1.1	99.99± 0.2	100	0.074	5.9 ± 1.0	98.87 ± 1.8	99	0.058	3.9 ± 1.0	96.93 ± 1.1	80	0.071	
	(12	200)	01.37	0.6± 1.2	93	6.8 ± 1.1	99.97 ± 0.4	100	0.104	5.7 ± 1.3	98.34 ± 2.6	100	0.086	3.4 ± 0.9	95.21 ± 1.6	90	0.093	
					90	6.8 ± 1.1	99.95 ± 0.6	100	0.164	5.5 ± 1.4	97.86± 3.4	100	0.100	3.0 ± 0.8	93.46 ± 1.5	94	0.103	
					98	7.7±2.7	99.12± 0.8	92	0.593	6.4± 3.0	98.75± 0.6	87	0.763	6.0± 3.1	98.67± 0.5	29	0.870	
agarique	(22	200)	OF / 1	102125	95	6.9 ± 3.1	97.62 ± 2.1	95	0.954	5.3 ± 3.2	96.59 ± 1.6	92	1.273	4.8 ± 3.3	96.24 ± 1.2	55	1.217	
agancus	(23	200)	95.41	10.3 ± 2.3	93	6.5 ± 3.1	96.65 ± 2.8	95	1.112	4.8 ± 3.1	95.38 ± 1.9	93	1.309	4.3 ± 3.1	94.92 ± 1.3	64	1.390	
					90	5.9 ± 3.3	94.95 ± 4.1	96	1.332	4.0 ± 3.0	92.60 ± 2.8	95	1.598	$3.6{\pm}~2.8$	92.08 ± 1.7	76	1.830	
chess (37					98	8.1 ± 4.1	99.27± 0.6	64	0.383	5.9 ± 4.9	98.70± 0.4	64	0.454	5.7 ± 5.0	98.65± 0.4	46	0.457	
	(27	200)	00 21.	121 27	95	7.7 ± 3.8	98.51± 1.4	68	0.404	5.5 ± 4.4	97.90 ± 0.9	64	0.483	5.3 ± 4.5	97.85 ± 0.8	46	0.478	
	(37	200)	00.34	12.1± 3.7	93	7.3 ± 3.5	97.56 ± 2.4	68	0.419	5.0 ± 4.1	96.26 ± 2.2	64	0.485	4.8 ± 4.1	96.21 ± 2.1	64	0.493	
				90	7.3 ± 3.5	97.29± 2.9	70	0.413	4.9 ± 4.0	95.99 ± 2.6	64	0.483	4.8 ± 4.0	95.93 ± 2.5	64	0.543		
		81)			98	5.3± 1.4	100 ± 0.0	100	0.000	5.3± 1.3	99.95± 0.2	100	0.007	4.6± 1.1	99.60± 0.4	64	0.014	
viete	(17		0066	E 2 1 /	95	5.3 ± 1.4	100 ± 0.0	100	0.000	5.3 ± 1.3	99.93 ± 0.3	100	0.008	$4.1{\pm}~1.0$	98.25 ± 1.7	64	0.018	
vole	(1)		09.00	5.3± 1.4	93	5.3 ± 1.4	100 ± 0.0	100	0.000	5.2 ± 1.3	99.78 ± 1.1	100	0.012	$4.1{\pm}~0.9$	98.10 ± 1.9	64	0.018	
					90	5.3 ± 1.4	100 ± 0.0	100	0.000	5.2 ± 1.3	99.78± 1.1	100	0.012	4.0 ± 1.2	97.24± 3.1	64	0.022	
					98	7.8± 4.2	99.19± 0.5	64	0.387	6.5 ± 4.7	98.99± 0.4	64	0.427	6.1± 4.9	98.88 ± 0.3	43	0.457	
kr.vc.kp	(27	200)	0007	122120	95	7.3 ± 3.9	98.29 ± 1.4	64	0.416	6.0 ± 4.3	97.89 ± 1.1	64	0.453	5.5 ± 4.5	97.79 ± 0.9	43	0.462	
кі-vэ-кр	(37	200)	00.07	12.2± 3.9	93	6.9 ± 3.5	97.21± 2.5	69	0.422	5.6 ± 3.8	96.82 ± 2.2	64	0.448	5.2 ± 4.0	96.71 ± 2.1	43	0.468	
					90	6.8± 3.5	96.65± 3.1	69	0.418	5.4± 3.8	95.69± 3.0	64	0.468	5.0 ± 4.0	95.59± 2.8	61	0.487	
					98	7.5± 2.4	98.99± 0.7	90	0.641	6.5 ± 2.6	98.74± 0.5	83	0.751	6.3± 2.7	98.70± 0.4	18	0.828	
mushroom	(23	200)	95 51	107103	95	6.5 ± 2.6	97.35 ± 1.8	96	1.011	5.1 ± 2.5	96.52 ± 1.0	90	1.130	5.0 ± 2.5	96.39 ± 0.8	54	1.113	
Margues-Silva	(23	200)	JJ.JI	10.7 1 2.3	93	5.8 ± 2.8	95.77 ± 2.7	96	1.257	4.4 ± 2.5	94.67 ± 1.6	94	1.297	4.2 ± 2.4	94.48 ± 1.3	65	1.324	

Results for decision diagrams

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

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[IHI+23]

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

[IMM24]

Changing Assumptions

Inflated Explanations

Probabilistic Explanations

Constrained Explanations

Distance-Restricted Explanations

Additional Topics

[GR22, YIS+23]

- The (implicit) assumption that all inputs are possible is often unrealistic
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- Constrained AXps/CXps find other applications!

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 - Q: can we relate AXps with adversarial examples?
 - Obs: we already proved some basic (duality) properties for global explanations
- Change definition of WAXp/WCXp to account for l_p distance to **v**:

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

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

- Norm l_p is arbitrary, e.g. Hamming, Manhattan, Euclidean, etc.
- Distance-restricted explanations: dAXp/dCXp



• Plain AXps/CXps:



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 \cdot Given ϵ , larger adversarial examples are excluded





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Relating explanations with adversarial examples

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$$\begin{aligned} \forall (\mathbf{x} \in \mathbb{F}). \left[\bigwedge_{j \in \mathcal{X}} (X_j = V_j) \land \left(\| \mathbf{x} - \mathbf{v} \|_{l_p} \leq \epsilon \right) \right] \to (\sigma(\mathbf{x})) \\ \exists (\mathbf{x} \in \mathbb{F}). \left[\bigwedge_{j \in \mathcal{X}} (X_j = V_j) \land \left(\| \mathbf{x} - \mathbf{v} \|_{l_p} \leq \epsilon \right) \right] \land (\neg \sigma(\mathbf{x})) \end{aligned}$$

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[BMB⁺23]

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- Clear scalability improvements for explaining NNs (see next)
 [HM23b, WWB23, IHM+24a, IHM+24b]

[BMB⁺23]
Basic algorithm

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

- 1: **function** FindAXpDel($\epsilon; \mathcal{E}, p$)
- 2: $\mathcal{S} \leftarrow \mathcal{F}$
- 3: for $i \in \mathcal{F}$ do
- 4: $\mathcal{S} \leftarrow \mathcal{S} \setminus \{i\}$
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- 6: if outc then

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8: return S

▷ Initially, no feature is allowed to change▷ Invariant: ∂WAXp(S)

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- Limitation: Running time grows with number of features

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

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

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Scales to a few hundred neurons

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

- 1: function FindAXpDel($\epsilon; \mathcal{E}, p$)
- 2: $\mathcal{S} \leftarrow \mathcal{F}$
- 3: for $i \in \mathcal{F}$ do
- 4: $\mathcal{S} \leftarrow \mathcal{S} \setminus \{i\}$
- 5: outc \leftarrow FindAdvEx $(\epsilon, S; \mathcal{E}, p)$
- 6: if outc then
- 7: $\mathcal{S} \leftarrow \mathcal{S} \cup \{i\}$
- 8: return S

ightarrow Initially, no feature is allowed to change ightarrow Invariant: ∂ WAXp(S)

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- \cdot To drop features from $\mathcal{S}\subseteq\mathcal{F}$, it is open whether paralellization might be applicable
 - Algorithm FindAXpDel is mostly sequential (see above)
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[IHM+24b]

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

[IHM+24b]

[IHM+24b]

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

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

Inflated Explanations

Probabilistic Explanations

Constrained Explanations

Distance-Restricted Explanations

Additional Topics

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- $\cdot\,$ Report computed explanation as explanation for the complex ML model

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

- Lecture 01 units:
 - #01: Foundations
- Lecture 02 units:
 - #02: Principles of symbolic XAI feature selection
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 - #08: Conclusions & research directions

Questions?

Lecture 05

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

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

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

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- + Each minimal winning coalition $\mathcal C$ corresponds to an AXp of $\mathcal E=(\mathcal M,(\mathbb 1,1))$
- \therefore WVGs can be analyzed by studying the AXps/CXps of monotonically increasing boolean classifiers

• WVG: [25; 10, 9, 7, 1, 1, 1, 1, 1]

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• Q: How should features be ranked in terms of importance?

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Unit #07

Principles of Symbolic XAI – Feature Attribution

Exact Shapley Values for XAI

Myth #03: Shapley Values for XAI

Corrected SHAP Scores

Voting Power & Power Indices

Feature Importance Scores
Detour: Standard SHAP Intro (from another course...)

What are Shapley values?

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[Sha53]

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

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In m	achine learning [edit]			
The Sha model t	The Shapley value provides a principled way to explain the predictions of nonlinear models common in the field of machine learning. By interpreting a model trained on a set of features as a value function on a coalition of players. Shapley values provide a natural way to compute which features contribute			
to a pre	a prediction. ^[17] This unifies several other methods including Locally Interpretable Model-Agnostic Explanations (LIME), ^[18] DeepLIFT, ^[19] and Layer-Wise			
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 ^{*} Lundberg, Scott M.; Lee, Su-In (2017). ^{*}A Unified Approach to Interpreting Model Predictions[®] *Advances in Neural Information Processing* Systems. 30: 4765–4774. arXiv:1705.07874 (2). Retrieved 2021-01-30.

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

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

......

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

[1117]

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

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

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Marginal contribution (in SHAP lingo)!



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How are Shapley values computed in practice?

• Exact evaluation is computationally (very) hard

[VLSS21, ABBM21, VLSS22, ABBM23, HMS24]

- SHAP proposes a sample-based approach; with **no** guarantees of rigor
 - Recent experiments revealed little to no correlation between Shapley values and SHAP's results

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• Polynomial-time algorithm for deterministic decomposable boolean circuits [ABBM21]

• Polynomial-time algorithm for boolean functions represented with a truth-table

• [SK10] reads:

"According to the 2nd axiom, if two features values have an identical influence on the prediction they are assigned contributions of equal size. The 3rd axiom says that if a **feature has no influence** on the prediction **it is assigned a contribution of 0**." (Obs: the axioms refer to the axiomatic characterization of Shapley values.)

What do Shapley values tell in terms of feature importance?

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

Exact Shapley Values for XAI

Myth #03: Shapley Values for XAI

Corrected SHAP Scores

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Feature Importance Scores

Shapley values vs. feature (ir)relevancy – identified issues [HM23G,]

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

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

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 $\operatorname{Relevant}(i) \wedge (\operatorname{Sv}(i) = 0)$

• Issue I4 occurs if,

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

Shapley values vs. feature (ir)relevancy – identified issues [HM23c,

- Boolean classifier, instance (\mathbf{v}, c) , and some $i, i_1, i_2 \in \mathcal{F}$:
 - Issue I1 occurs if,

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• Issue I5 occurs if,

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

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

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

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











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



DT1

Tabular representations

Computing XPs – make sense...



DT1

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



Tabular representations



Computing XPs, AEs – also make sense...



DT1

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

row #	X_1	X_2	X_3	$\kappa_1(\mathbf{x})$	$\kappa_2(\mathbf{x})$
1	0	0	0	0	0
2	0	0	1	4	2
3	0	0	2	0	0
4	0	1	0	0	0
5	0	1	1	7	3
6	0	1	2	0	0
7	1	0	0	1	1
8	1	0	1	1	1
9	1	0	2	1	1
10	1	1	0	1	1
11	1	1	1	1	1
12	1	1	2	1	1

Tabular representations

Adversarial Examples				
DT	<i>l</i> ₀ -minimal AEs			
DT1	{1}			
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Computing XPs, AEs & Svs



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Tabular representations

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Shapley values				
DT	Sc(1)	Sc(2)	Sc(3)	
DT1	0.000	0.083	-0.500	
DT2	0.278	0.028	-0.222	

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row #

 X_1

 $X_2 \quad X_3$



DT1

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 $\{1\}$

DT2

 $\kappa_1(\mathbf{x})$

 $\kappa_2(\mathbf{x})$





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Another example – arbitrary mistakes!

[LHAMS24]



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[LHAMS24]



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Example devised by O. Letoffe, PhD student at IRIT

More detail



<i>i</i> = 1						
S	$v_e(\mathcal{S})$	$v_e(\mathcal{S} \cup \{1\})$	$\Delta_1(\mathcal{S})$	$\varsigma(\mathcal{S})$	$\varsigma(\mathcal{S}) \times \Delta_1(\mathcal{S})$	
Ø	$1 - \alpha$	1	α	$^{1/2}$	$\alpha/2$	
$\{2\}$	$1 + \alpha$	1	$-\alpha$	$^{1/2}$	$-\alpha/2$	
		$Sc_E(1) = 0$				
i = 2						
S	(\mathbf{O})					
	$v_e(\mathcal{S})$	$v_e(\mathcal{S} \cup \{2\})$	$\Delta_2(\mathcal{S})$	$\varsigma(\mathcal{S})$	$\varsigma(\mathcal{S}) \times \Delta_2(\mathcal{S})$	
Ø	$v_e(\mathcal{S})$ $1 - \alpha$	$\frac{v_e(\mathcal{S} \cup \{2\})}{1 + \alpha}$	$\frac{\Delta_2(\mathcal{S})}{2\alpha}$	$\frac{\zeta(S)}{1/2}$	$\frac{\varsigma(\mathcal{S}) \times \Delta_2(\mathcal{S})}{\alpha}$	
Ø {1}	$\frac{v_e(\mathcal{S})}{1-\alpha}$ 1	$\frac{v_e(\mathcal{S} \cup \{2\})}{1+\alpha}$ 1	$\begin{array}{c} \Delta_2(\mathcal{S}) \\ \hline 2\alpha \\ 0 \end{array}$	$\frac{\varsigma(\mathcal{S})}{\frac{1/2}{1/2}}$	$\frac{\varsigma(\mathcal{S}) \times \Delta_2(\mathcal{S})}{\begin{array}{c} \alpha \\ 0 \end{array}}$	

Exact Shapley Values for XAI

Myth #03: Shapley Values for XAI

Corrected SHAP Scores

Voting Power & Power Indices

Feature Importance Scores

[LHMS24, LHAMS24]

• Is the theory of Shapley values incorrect?

[LHMS24, LHAMS24]

• Is the theory of Shapley values incorrect? No!

[LHMS24, LHAMS24]

[SK10, SK14, LL17]

- Is the theory of Shapley values incorrect? No!
- What is inadequate is the characteristic function used in XAI
 - $\cdot\,$ In XAI: characteristic function uses the expected value
 - This defines the marginal contribution in SHAP lingo...

[LHMS24, LHAMS24]

[SK10, SK14, LL17]

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- Replace characteristic function based on expected values by new characteristic function based on AXps/WAXps
 - Resulting scores are (still) Shapley values & identified issues no longer observed

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Feature importance scores:	[LHAMS24]
Generalize recent axiomatic aggregations	[BIL+24]
 Adapt best known power indices 	

Devise new scores for XAI

• Replace the characteristic function used for SHAP scores:

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

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

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- · Issues with non-boolean classifiers disappear; issues with boolean classifiers remain
- Developed SSHAP prototype using SHAP's code base

[LHMS24]

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

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

Exact Shapley Values for XAI

Myth #03: Shapley Values for XAI

Corrected SHAP Scores

Voting Power & Power Indices

Feature Importance Scores

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

• Power indices assign a measure of importance to each voter

What are power indices?

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

• Penrose	[Pen46]
• Shapley-Shubik	[SS54]
• Banzhaf	[BI65]
• Coleman	[Col71]
• Johnston	[Joh78]
• Deegan-Packel	[DP78]
• Holler-Packel	[HP83]
• Andjiga	[ACL03]
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- ...
- What characterizes power indices?
 - Account for the cases when voter is *critical* for a winning coalition
 - E.g. in previous example, Luxembourg is never critical for a winning coalition
 - · Account for whether coalition is subset-minimal or cardinality-minimal

• Understanding criticality (used at least since 1954):

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 - Since the work of Shapley-Shubik [SS54], the criticality of a voter has been accounted for: "Our definition of the power of an individual member depends on the chance he has of being critical to the success of a winning coalition."

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 "Our definition of the power of an individual member depends on the chance he has of being critical to the success of a winning coalition."
 - This means that a voter *i* is **critical** when:
 - If the voter votes Yes, then we have a winning coalition; and
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[SS54]

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 - A winning coalition is cardinality-minimal if it has the smallest cardinality among subset-minimal winning coalitions

[SS54]

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

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

$$\begin{split} \mathbb{W} \mathbb{A}_{i}(\mathcal{E}) &= \{ \mathcal{S} \subseteq \mathcal{F} \mid \mathbb{W} \mathsf{AXp}(\mathcal{S}; \mathcal{E}) \land i \in \mathcal{S} \} \\ \mathbb{W} \mathbb{C}_{i}(\mathcal{E}) &= \{ \mathcal{S} \subseteq \mathcal{F} \mid \mathbb{W} \mathsf{CXp}(\mathcal{S}; \mathcal{E}) \land i \in \mathcal{S} \} \\ \mathbb{A}_{i}(\mathcal{E}) &= \{ \mathcal{S} \subseteq \mathcal{F} \mid \mathsf{AXp}(\mathcal{S}; \mathcal{E}) \land i \in \mathcal{S} \} \\ \mathbb{C}_{i}(\mathcal{E}) &= \{ \mathcal{S} \subseteq \mathcal{F} \mid \mathsf{CXp}(\mathcal{S}; \mathcal{E}) \land i \in \mathcal{S} \} \end{split}$$

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- $\cdot\,$ Definitions of WA, WC, A, and C mimic the ones above, but without specifying a voter
- Power indices of Holler-Packel and Deegan-Packel:

[HP83, DP78]

$$\begin{aligned} \mathsf{Sc}_{H}(i;\mathcal{E}) &= \sum_{\mathcal{S} \in \mathbb{A}_{i}(\mathcal{E})} \left(\frac{1}{|\mathbb{A}(\mathcal{E})|} \right) \\ \mathsf{Sc}_{D}(i;\mathcal{E}) &= \sum_{\mathcal{S} \in \mathbb{A}_{i}(\mathcal{E})} \left(\frac{1}{|\mathcal{S}| \times |\mathbb{A}(\mathcal{E})|} \right) \end{aligned}$$

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

$$\begin{split} \mathbb{W}\mathbb{A}_{i}(\mathcal{E}) &= \{ \mathcal{S} \subseteq \mathcal{F} \mid \mathbb{W}\mathsf{AXp}(\mathcal{S}; \mathcal{E}) \land i \in \mathcal{S} \} \\ \mathbb{W}\mathbb{C}_{i}(\mathcal{E}) &= \{ \mathcal{S} \subseteq \mathcal{F} \mid \mathbb{W}\mathsf{CXp}(\mathcal{S}; \mathcal{E}) \land i \in \mathcal{S} \} \\ \mathbb{A}_{i}(\mathcal{E}) &= \{ \mathcal{S} \subseteq \mathcal{F} \mid \mathsf{AXp}(\mathcal{S}; \mathcal{E}) \land i \in \mathcal{S} \} \\ \mathbb{C}_{i}(\mathcal{E}) &= \{ \mathcal{S} \subseteq \mathcal{F} \mid \mathsf{CXp}(\mathcal{S}; \mathcal{E}) \land i \in \mathcal{S} \} \end{split}$$

- $\cdot\,$ Definitions of WA, WC, A, and C mimic the ones above, but without specifying a voter
- Power indices of Holler-Packel and Deegan-Packel:

[HP83, DP78]

$$Sc_{H}(i; \mathcal{E}) = \sum_{\mathcal{S} \in \mathbb{A}_{i}(\mathcal{E})} (1/|\mathbb{A}(\mathcal{E})|)$$
$$Sc_{D}(i; \mathcal{E}) = \sum_{\mathcal{S} \in \mathbb{A}_{i}(\mathcal{E})} (1/(|\mathcal{S}| \times |\mathbb{A}(\mathcal{E})|))$$

• Obs: One only needs the AXps
• Additional definitions:

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

• Additional definitions:

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

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

[SS54, BI65, Joh78]

$$\begin{aligned} \mathsf{SC}_{\mathsf{S}}(i;\mathcal{E}) &= \sum_{\mathcal{S} \subseteq \mathcal{F} \land \mathsf{Crit}(i,\mathcal{S};\mathcal{E})} \left(\frac{1}{|\mathcal{F}| \times \binom{|\mathcal{F}| - 1}{|\mathcal{S}| - 1}} \right) \end{aligned}$$
$$\begin{aligned} \mathsf{SC}_{\mathsf{B}}(i;\mathcal{E}) &= \sum_{\mathcal{S} \subseteq \mathcal{F} \land \mathsf{Crit}(i,\mathcal{S};\mathcal{E})} \frac{1}{2^{|\mathcal{F}| - 1}} \end{aligned}$$
$$\begin{aligned} \mathsf{SC}_{\mathsf{J}}(i;\mathcal{E}) &= \sum_{\mathcal{S} \subseteq \mathcal{F} \land \mathsf{Crit}(i,\mathcal{S};\mathcal{E})} \frac{1}{\Delta(\mathcal{S})} \end{aligned}$$

• Additional definitions:

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

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

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$$\begin{aligned} \mathsf{SC}_{\mathsf{S}}(i;\mathcal{E}) &= \sum_{\mathcal{S} \subseteq \mathcal{F} \land \mathsf{Crit}(i,\mathcal{S};\mathcal{E})} \left(\frac{1}{|\mathcal{F}| \times \binom{|\mathcal{F}| - 1}{|\mathcal{S}| - 1}} \right) \end{aligned}$$
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$$\begin{aligned} \mathsf{SC}_{\mathsf{J}}(i;\mathcal{E}) &= \sum_{\mathcal{S} \subseteq \mathcal{F} \land \mathsf{Crit}(i,\mathcal{S};\mathcal{E})} \binom{1}{\Delta(\mathcal{S})} \end{aligned}$$

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

• WVG: [9; 9, 2, 2, 2, 2, 1, 1]

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

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

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

• WVG: [16; 10, 6, 4, 2, 2]

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

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

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

• WVG: [6; 4, 2, 1, 1, 1, 1]

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

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

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

• WVG: [21; 12, 9, 4, 4, 1, 1, 1]

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

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

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

Exact Shapley Values for XAI

Myth #03: Shapley Values for XAI

Corrected SHAP Scores

Voting Power & Power Indices

Feature Importance Scores

- A Feature Importance Score (FIS) is a measure of feature importance in XAI, parameterizable on an explanation problem and a chosen characteristic function
 - + Explanation problem: $(\mathcal{M}, (\mathbf{v}, q))$
 - Define characteristic function using explanation problem (more next slide)

- Obs: Can adapt (generalized) power indices as templates for feature importance scores
- Obs: Can devise new templates and/or new FISs

• More notation:

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

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

Some examples (1 of 2)

• More notation:

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

- Can use **any** characteristic function, including those presented earlier in this lecture
- Some templates:
 - Shapley-Shubik:

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

• Banzhaf:

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

Some examples (1 of 2)

• More notation:

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

- Can use **any** characteristic function, including those presented earlier in this lecture
- Some templates:
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$$\mathsf{TSC}_{\mathsf{S}}(i;\mathcal{E},v) := \sum_{\mathcal{S} \in \{\mathcal{T} \subseteq \mathcal{F} \mid i \in \mathcal{T}\}} \left(\frac{\Delta_i(\mathcal{S};\mathcal{E},v)}{|\mathcal{F}| \times \binom{|\mathcal{F}|-1}{|\mathcal{S}|-1}} \right)$$

• Banzhaf:

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

• Can use other templates

Some examples (1 of 2)

 \cdot More notation:

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

- Can use **any** characteristic function, including those presented earlier in this lecture
- Some templates:
 - Shapley-Shubik:

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

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- Can use other templates
- Can devise FISs without exploiting existing templates

Some examples (2 of 2)

• Recall WAXp based characteristic function:

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

Some examples (2 of 2)

• Recall WAXp based characteristic function:

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

- Some FISs:
 - Shapley-Shubik:

$$Sc_{S}(i;\mathcal{E}) := TSc_{S}(i;\mathcal{E},v_{a}) := \sum_{\mathcal{S} \in \{\mathcal{T} \subseteq \mathcal{F} \mid i \in \mathcal{T}\}} \left(\frac{\Delta_{i}(\mathcal{S};\mathcal{E},v_{a})}{|\mathcal{F}| \times \binom{|\mathcal{F}|-1}{|\mathcal{S}|-1}} \right)$$

• Banzhaf:

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

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



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



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



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



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



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



Questions?

Unit #08

Conclusions & Research Directions

Some Words of Concern

Conclusions & Research Directions

LIME on 2023/05/31:

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Any time Since 2023 Since 2022 Since 2019 Custom range Sort by relevance Sort by date Any type Review articles ☐ include patents ☑ include citations	" Why should i trust you?" Explaining the predictions of any classifier <u>MT Ribeiro</u> , <u>S Singh</u> , <u>C Guestrin</u> - Proceedings of the 22nd ACM, 2016 - dLacm.org Despite widespread adoption, machine learning models remain mostly black boxes. Understanding the reasons behind predictions is, however, quite important in assessing trust, which is fundamental if one plans to take action based on a prediction, or when choosing whether to deploy a new model. Such understanding also provides insights into the model, which can be used to transform an untrustworthy model or prediction into a trustworthy one. In this work, we propose LIME, a novel explanation technique that explains ☆ Save IST Cite Cited by 12683 Related articles All 36 versions Showing the best result for this search. See all results	[PDF] arxiv.org

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Since 2020 Custom range	Despite widespread adoption, machine learning models remain mostly black boxes. Understanding the reasons behind predictions is, however, quite important in assessing				
Sort by relevance Sort by date	trust, which is fundamental if one plans to take action based on a prediction, or when choosing whether to deploy a new model. Such understanding also provides insights into the model, which can be used to transform an untrustworthy model or prediction into a trustworthy cana.				
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SHAP on 2023/05/31:

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≡ Google Scholar	A unified approach to interpreting model predictions	Q SIGN IN
Articles		🌎 My profile 🔺 My library
Any time Since 2023 Since 2022 Since 2019 Custom range Sort by relevance Sort by date Any type Review articles ☐ include patents ☑ include citations	A unified approach to interpreting model predictions SM Lundberg, SI Lee - Advances in neural information, 2017 - proceedings.neurips.cc Understanding why a model makes a certain prediction can be as crucial as the prediction's accuracy in many applications. However, the highest accuracy for large modern datasets is often achieved by complex models that even experts struggle to interpret, such as ensemble or deep learning models, creating a tension between accuracy and interpretability. In response, various methods have recently been proposed to help users interpret the predictions of complex models, but it is often unclear how these methods are related and ☆ Save 59 Cite Cited by 13080 Related articles All 17 versions ≫ Showing the best result for this search. See all results	[PDF] neurips.cc

SHAP on 2024/07/02:

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Since 2020 Custom range	Abstract Understar	ding why a model makes a certain prediction can be as crucial as the			
Sort by relevance Sort by date	prediction's accuracy in many applications. However, the highest accuracy for large modern datasets is often achieved by complex models that even experts struggle to interpret, such as ensemble or deep learning models, creating a tension between				
Any type Review articles	to help us	and interpretability. In response, various methods have recently been proposed ars interpret the predictions of complex models, but it is often unclear how these RE ~			
include patents	☆ Save ₪	Cite Cited by 23321 Related articles All 22 versions ⊗ st result for this search. See all results			

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• (Heuristic) XAI research experiences a persistent "Don't Look Up" moment...



• (Heuristic) XAI research experiences a persistent "Don't Look Up" moment...



BTW, there are a multitude of proposed uses of LIME/SHAP in medicine... A

• For DTs:

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

[IIM20, HIIM21, IIM22]

[HIIM21, IIM22]

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

Declarative Reasoning on Explanations Using Constraint Logic Programming

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

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

[IIM20, HIIM21, IIM22]

[HIIM21, IIM22]

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

[IIM20, HIIM21, IIM22]

[HIIM21, IIM22]

HHAI 2024: Hybrid Human AI Systems for the Social Good F. Lorig et al. (Eds.) © 2024 The Authors. This article is published online with Open Access by IOS Press and distributed under the terms of the Creative Commons Attribution Non-Commercial License 4.0 (CC BY-NC 4.0). doi:10.3233/FAIA240183

Exploring Large Language Models Capabilities to Explain Decision Trees

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

[IIM20, HIIM21, IIM22]

[HIIM21, IIM22]

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

FAccT '24, June 03-06, 2024, Rio de Janeiro, Brazil © 2024 Copyright held by the owner/author(s). ACM ISBN 979-8-4007-0450-5/24/06 https://doi.org/10.1145/3630106.3658953

- For DTs:
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[HIIM21, IIM22]



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 - One AXp in polynomial-time
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[IIM20, HIIM21, IIM22]

[HIIM21, IIM22]



Some Words of Concern

Conclusions & Research Directions

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

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

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- Demonstrated tight connection between (rigorous) feature selection and (rigorous) feature attribution in XAI

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 - Explainability using intrinsic interpretability is a **myth**
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 - The rigor of SHAP scores as a measure of relative feature importance is a **myth**
- Demonstrated tight connection between (rigorous) feature selection and (rigorous) feature attribution in XAI
- Symbolic XAI exhibits links with many fields of research: machine learning, artificial intelligence, formal methods, automated reasoning, optimization, computational social choice (& game theory), etc.

• Scalabilitty, scalability, and scalability

- Scalabilitty, scalability, and scalability
- Probabilitistic explanations

- Scalabilitty, scalability, and scalability
- Probabilitistic explanations
- Distance-restricted explanations

- \cdot Scalabilitty, scalability, and scalability
- Probabilitistic explanations
- Distance-restricted explanations
- Rigorous feature attribution

- Scalabilitty, scalability, and scalability
- Probabilitistic explanations
- Distance-restricted explanations
- Rigorous feature attribution
- Preferred explanations

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- Distance-restricted explanations
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- Preferred explanations
- Certified XAI tools

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- New topics from discussions with participants of ESSAI'24 Thank you!

- Scalabilitty, scalability, and scalability
- Probabilitistic explanations
- Distance-restricted explanations
- Rigorous feature attribution
- Preferred explanations
- Certified XAI tools
- New topics from discussions with participants of ESSAI'24 Thank you!
- ... And trying to curb the massive momentum of (heuristic) XAI myths!

- Lecture 01 units:
 - #01: Foundations
- Lecture 02 units:
 - #02: Principles of symbolic XAI feature selection
 - #03: Tractability in symbolic XAI (& myth of interpretability)
- Lecture 03 units:
 - #04: Intractability in symbolic XAI (& myth of model-agnostic XAI)
 - #05: Explainability queries
- Lecture 04 units:
 - #06: Advanced topics
- Lecture 05 units:
 - #07: Principles of symbolic XAI feature attribution (& myth of Shapley values in XAI)
 - #08: Conclusions & research directions

Q & A

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

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