

Akademia Górniczo-Hutnicza im. Stanisława Staszica w Krakowie

AGH University of Science and Technology

> In Search for Model-Driven eXplainable Artificial Intelligence

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AGH University of Science and Technology + KRaKEn Research Group https://kraken.edu.pl/

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#### Kilka uwag na wstępie





- To jest work in progress;
- Bliżej koncepcji niż finalnych rozwiązań,
- Prezentacja bardzo skrótowa i uproszczona,
- Także tendencyjna; zorientowana na przyjęte tezy,
- Proszę o wyrozumiałość.

#### Presentation Outline



- On AI. Towards XAI
- On XAI. Towards Model-Driven XAI
- 3 The SiCA Concept. 10 Examples
- AI & XAI Failures
- In Search for Model-Driven XAI. Towards Model-Discovery
- 6 Summary and What Next?

On AI. Towards XAI



#### On AI. Towards XAI



### What is Artificial Intelligence?



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#### Artificial Intelligence (AI)

The ability of a digital computer or computer-controlled robot to perform tasks commonly associated with intelligent beings. The term is frequently applied to the project of developing systems endowed with the intellectual processes characteristic of humans, such as the ability to reason, discover meaning, generalize, or learn from past experience (B.J. Copeland).

# Definitions of Artificial Intelligence

**Intelligence** = ability to solve new problems

- Artificial Intelligence (AI) is intelligence demonstrated by machines, as opposed to the natural intelligence displayed by humans or animals. <sup>1</sup>
- Artificial Intelligence, or AI, is the field that studies the synthesis and analysis of computational agents that act intelligently. <sup>2</sup>
- Artificial Intelligence: http://aima.cs.berkeley.edu/:
  - Systems that think like humans;
  - Systems that act like humans;
  - Systems that think rationally;
  - Systems that act rationally;
- Artificial Intelligence = Technology of Machine Thinking
- Artificial Intelligence  $\neq$  Computational Intelligence (CI)
- Artificial Intelligence  $\simeq$  Algorithmic Intelligence
- Can pass the Turing Test for Artificial Intelligence

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# Artificial Intelligence for Problem Solving. What is the Essence of it?



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The key issue: Black-Box Models (hidden knowledge) versus White-Box Models (explicit knowledge): Knowledge Representation and Reasoning – open, declarative/procedural, undergo analysis, design, verification; reliable and trustable solutions. On Al. Towards XAI

#### Taxonomy of AI methods: Diversified and Specilized





Figure: Source: Small Data Group

# AI-KRR: Basic Ideas behind this Course

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Key observation: There is no single, complete, consistent and uniform AI.

- to teach various, but selected methods of Al Knowledge Representation (KR),
- to teach various, but selected methods of AI Automated Reasoning (AR),
- with the focus on Symbolic Knowledge (Logical, Algebraic, Graph-Based)
- with the ultimate goal: Automated Problem Solving (APS);

# $\mathsf{KR} + \mathsf{AR} + \mathsf{Control} \longrightarrow \mathsf{APS}$

• to keep the course practical rather than *just theory*:

- some background knowledge but in an informal way,
- modern tools if available (Prolog, MiniZinc, Problog, PDDL, Picat, Logica,...Python, Julia),

# Human Intelligence vs. Artificial Intelligence

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- Curiosity human tend to observe, explore and explain the environment;
- Flexibility single brain explores a wide spectrum of problems;
- Model Discovery human tend to understand the problem nature and build a model;
- Combining Knowledge commonsense and domain knowledge is combined;
- eXplanation ability to discuss, explain, reconsider and modify the analysis.

- Must be initiated started by man, event, clock, another program, ...
- Specialization AI is task oriented, tools are efficient but of narrow domains;
- Pre-programmed Knowledge Processing - applied to solve a particular problem,
- Machine Learning purely syntax-based, mechanical decision engines;
- Shallow eXplanation if present, it is based on the same data as used for learning.

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#### Black Box



In science, computing, and engineering, a **black box** is a device, system, or object which can be viewed in terms of its inputs and outputs, without any knowledge of its internal workings. Its implementation is opaque or "black".



Figure: Source: Black Box Model in Investopedia

On AI. Towards XAI

#### Model-Based Reasoning: Logical Model



#### Declarative Modeling Components & Causal Structure

 $\begin{array}{l} \mathsf{ADD}(x) \land \neg \mathsf{AB}(x) \Rightarrow \mathsf{Output}(x) = \mathsf{Input1}(x) + \mathsf{Input2}(x), \\ \mathsf{MULT}(x) \land \neg \mathsf{AB}(x) \Rightarrow \mathsf{Output}(x) = \mathsf{Input1}(x) * \mathsf{Input2}(x), \\ \mathsf{ADD}(a1), \ \mathsf{ADD}(a2), \ \mathsf{MULT}(m1), \ \mathsf{MULT}(m2), \\ \mathsf{MULT}(m3), \\ \mathsf{Output}(m1) = \mathsf{Input1}(a1), \ \mathsf{Output}(m2) = \mathsf{Input2}(a1), \\ \mathsf{Output}(m2) = \mathsf{Input1}(a2), \ \mathsf{Output}(m3) = \mathsf{Input2}(a2), \\ \mathsf{Input2}(m1) = \mathsf{Input1}(m3), \\ \mathsf{Input1}(m1) = \mathsf{A} \dots \mathsf{Output}(a2) = \mathsf{G} \end{array}$ 

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# Taxonomy of AI methods in ML

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#### • White-box models:

- Logical Models; declarative KRR,
- Rule Based Models/Learners, Rule Induction
- Model-Based Reasoning, Causal Modelling, Structure Discovery, Qualitative Physics, ...

#### • Semi-White-box models:

- Linear/Logistic Regression
- Decision Trees
- Decision Graphs (including BPMN)

#### Black-box models:

- Tree Ensembles
- Computational Intelligence and Bio-Inspired Models
- Multi-layer Neural Network
- Convolutional Neural Network
- Deep Learning

# IS AI just ML: Induction of Trees or Rules





Problem: shallow knowledge  $\implies$  Does work — but why?

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#### Better Model: Bayes Nets Causal Model ?



#### A further step on...



#### of an epidemiologic system analysis of cardiovascular risk

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<sup>1</sup> Comparison parties of Department of Mathematics and Computer Interior, Universital Eles Robert, Palena de Mallaren, Educare 16/07120, pages 194 - 04 AUTURES. Ensait address plan Interiorbuits on (P. Faster Paras).

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On AI. Towards XAI

#### Bayes Nets: Even More Precise Model



#### Towards Model-Driven Explainability



#### Model Discovery. Motivation:

- majority of ML models cover shallow knowledge only,
- most of them are of decision/classification type; no functional output,
- no investigation of the guts what is inside?
- Eternal question: How does it work? No answer...
- variables, values,
- Components,
- Causal links,
- Connections struCture,
- input internal state output,
- functionality.



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# The Role of Abduction and Creativity



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- abduction: what, why and where — what for?
- abduction: investigation of causality,
- abduction: a method of logical inference (but invalid),
- abduction vs. deduction,
- abduction: primary method used by Sherlock Holmes!
- abduction: inevitable ambiguity (potential/admissible solutions; many of them),
- abduction: more constraints better abduction,





# On XAI. Towards Model-Driven XAI



# XAI: Explainable Artificial Intelligence – WHY?

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Why do we care about **Explainability in Artificial** Intelligence?

- readable and interpretable models,
- reduction of models (knowledge is more concise than data),
- well-defind domain of application,
- predictable behavior,
- Reliable Artificial Intelligence,
- safe AI solutions,
- easy adaptation and modification,
- Trustable Artificial Intelligence,

...

# XAI: Explainable Artificial Intelligence – HOW?

Direct approaches to **Explainable in Artificial Intelligence** (in contrast to a posteriori explanation mechanisms).

- declarative programming; Prolog,
- rule-based systems (Why, How, What-is questions),
- automated deduction; the Resolution Method,
- automated planning systems; STRIPS, PDDL,
- Bayes Networks, causal graphs,
- Model-Based Reasoning (MBR),
- Model Checking,
- Abductive vs. Inductive reasoning,
- Explainability by Design,
- Constraint Programming, Functional Constraint Programming,

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### What is XAI NOW?



#### Explainable Artificial Intelligence

XAI will create a suite of machine learning techniques that enables human users to understand, appropriately trust, and effectively manage the emerging generation of artificially intelligent partners.

#### **Crucial problems:**

- ML is not Al! Al is not ML!
- no background/commonsense/domain knowledge allowed!
- explanations a created (i) a posteriori (ii) on the base of the same data!

#### Hot topic



### Who needs explanations?



Figure: Source: XAI: Concepts, Taxonomies...

#### Explainability workflow



Figure: Source: A brief explanation of XAI, DARPA

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#### Accuracy vs Explainability



#### How to explain black-boxes?



### XAI Approaches



#### Goal of XAI?



Figure: Source: XAI: Concepts, Taxonomies...





#### XAI: Model-Driven Approach – WHY?

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#### Explainability in Artificial Intelligence – observations:

- often only limited, and incomplete data is available,
- on the other hand, some domain knowledge is present:
  - on Components,
  - on Connections,
  - on Causal Dependencies;
- partial inspection of the system is possible,
- abductive reasoning is used instead of induction,
- creative reasoning seems to be the key,
- domain knowledge is available,
- commonsense knowledge plays a role.

In such a case, ML is out of play. Such a case will be referred to as SiCA: Singular Case Analysis. Some 10 examples follow...

The eternal question: How does it work? is answered with Model-Based Reasoning.

#### An Eternal Question: How Does it Work?



Figure: The Antikythera mechanism; recovered on May 17, 1901. The instrument has been variously dated to about 87 BC, or between 150 and 100 BC, or in 205 BC https://en.wikipedia.org/wiki/Antikythera\_mechanism

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#### How Does it Work? Model-Based Reasoning





Components + Connections + Causality = Operation

#### An Eternal Question: How Does it Work?





Figure: XAI: Model-Driven eXplainable AI System

#### An Eternal Question: How Does it Work?



#### An Eternal Question: How Does it Work?





Components + Connections + Causality = Operation System: mechanical, hydraulic, pneumatic, electric, electromechanical.

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## An Eternal Question: How Does it Work?







Components + Connections + Causality = Operation System: mechanical, hydraulic, pneumatic, electric, electromechanical.

## An Eternal Question: How Does it Work?



Components + Connections + Causality = Operation

Boeing 737 Max 8: Introduced into exploitation 2017
1. Crash: October 2018, Lion Air (Malaysia)
2. Crash: March 2019, Ethiopian Airlines
Explanation: MCAS System (Maneuvering Characteristics Augmentation System).

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## An Eternal Question: How Does it Work?



## An Eternal Question: How Does it Work?



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Components + Connections + Causality = Operation The viaduct was built between 1963 and 1967 costing 3.8 billion Italian lire and opened on 4 September 1967. It had a length of 1,182 meters (3,878 ft), a height above the valley of 45 meters (148 ft) at road level, and three reinforced concrete pylons reaching 90 meters (300 ft) in height; the maximum span was 210 meters (690 ft). On 14 August 2018, a 210-metre (690 ft) section of the viaduct collapsed during a rainstorm, killing forty-three

## An Eternal Question: How Does it Work?



Input	Output
1	5
2	10
3	15
10	???

- Find the missing value;
- Find the rule.

## An Eternal Question: How Does it Work?



Input	Output
1	5
2	10
3	55
10	???

- Find the missing value;
- Find the rule.

From: MindYourDecisions by Presh Talwalkar
(https://www.youtube.com/watch?v=Pb7N6wqhjhg)

## An Eternal Question: How Does it Work?



Input	Output
1	5
2	10
3	55
10	1490

- The missing value is given;
- Find the rule.

From: MindYourDecisions by Presh Talwalkar
(https://www.youtube.com/watch?v=Pb7N6wqhjhg)

## An Eternal Question: How Does it Work?

Input	Output
1	5
2	10
3	55
10	1490

The output is given by:

$$f(x) = ax^2 + bx + c$$

where: a = 20, b = -55, c = 40.

This explanation is rational, correct, complete, minimal. From: MindYourDecisions by Presh Talwalkar (https://www.youtube.com/watch?v=Pb7N6wqhjhg)

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## An Eternal Question: How Does it Work?

Find all integer functions f such that:

$$f(2a) + 2f(b) = f(f(a+b))$$

- This is a Functional Equation;
- In fact, one looks for Components, Connections and Causality (well, functional dependencies) = the 3C principle;

• From AI point of view this is a Model Discovery task. From: MindYourDecisions by Presh Talwalkar (https://www.youtube.com/watch?v=uJqbHaFqjmI)

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## Chihuahua or Muffin?



Figure: Source: https://skywell.software/blog/top-artificial-intelligence-fails/

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## Husky or wolf?



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A husky (on the left) is confused with a wolf, because the pixels (on the right) characterizing wolves are those of the snowy background. This artifact is due to a learning base that was insufficiently representative



Figure: Source: Can Everyday AI be Ethical? Machine Learning Algorithm Fairness

AI & XAI Failures

## Shallow Rule Induction – A Naive Example



#### But why ???

Problem: no semantics; no background knowledge.

## Shallow Rule Induction – A Naive Example

шĬ		Car colo	or Car turns	]
	IJ	red	left	
AC	6 H	red	left	
		:		$Car\_color = red \longrightarrow Car\_turns = left$
		black	right	$Car\_color = black \longrightarrow Car\_turns = right$
		black	right	
	I	:	:	
		- C	car_turns(X,le car_turns(X,ri	ft) :- drives(X,university). ght) :- drives(X,court).
		d	lrives(X,unive	rsity) :- young(X).
drives(X,court) :- old(X).				) :- old(X).
.edu.	young(X) :- write(X),			
ı.agh			wr	ite(' is young and preferes red cars.').
www		C	old(X) :- writ	e(X),
			writ	e(' is old and preferes black cars.').



# In Search for Model-Driven XAI. Towards Model-Discovery

## Model-Driven XAI - The Concept



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#### Model-Driven eXplainable Artificial Intelligence - to be:

- transparent, readable and interpretable models,
- visible knowledge component,
- maybe simplified and therefore inaccurate,
- but still useful,
- well-defined domain of application,
- predictable behavior,
- Reliable Artificial Intelligence,
- safe Al solutions,
- flexible an so easy adaptation and modification,
- The 3C Principle:
  - Components,
  - Connections,
  - Causality
- Functional Characteristics if available.

## XAI: Explainable Artificial Intelligence – HOW?

Direct approaches to **Model-Driven XAI**; (in contrast to a posteriori explanation mechanisms).

- declarative programming; Prolog,
- rule-based systems (Why, How, What-is questions),
- automated deduction; the Resolution Method,
- automated planning systems; STRIPS, PDDL,
- Bayes Networks, Causal Graphs,
- Model-Based Reasoning (MBR),
- Model Checking,
- Abductive vs. Inductive reasoning,
- Explainability by Design,
- Declarative Programming, Constraint Programming, Logic Programming,

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## Model-Based Reasoning: Logical Model



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# Model Discovery: If Not Hand-Coded - Then Guided Search



- Ancient Math:
  - Differential Equations,
  - Variational Calculus,
  - Functional Equations,
- Inductive Logic Programming,
- Symbolic Regression,
- Grammatical Evolution,
- Functional Constraint Programming,
- Bayes Nets Discovery,

• ...

## Selected Tools



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#### Symbolic Regression<sup>3</sup> – 11 tools, e.g.:

- uDSR (Deep Symbolic Optimization)
- QLattice (a quantum-inspired simulation and machine learning technology)
- geneticengine (Genetic Engine)
- PySR Python Symbolic Regression,
- ...

Grammatical Evolution<sup>4</sup> – 12 tools, e.g:

- GELab (Matlab),
- PonyGE2 (Python),
- gramEvol (R),

• ...

<sup>3</sup>https://en.wikipedia.org/wiki/Symbolic\_regression
<sup>4</sup>https://en.wikipedia.org/wiki/Grammatical\_evolution

# XAI by Now: LIME





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## XAI by Now: SHAP



## Motivation



#### • Limitations of current XAI task formulation:

- No holistic, general framework; only local peep-hole view,
- No Causal Models; lack of structural approach,
- The explanation is based on the same data as learning!,
- No deep, background knowledge is taken into account.
- Towards Model-Driven XAI: Introduction of Knowledge-Based Component
- Trustworthy Decision-Making
- Building Model-Based (Model-Driven) XAI techniques

## Grammatical Evolution



## Simple Experiment

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- A series of experiments in order to create models that calculate the BMI function
- Decision Tree, Random Forest, Grammatical Evolution
- 10, 50, and 100 observations



Figure: BMI chart

## **Decision** Tree



## Random Forest



## Grammatical Evolution



The Proposed Grammar:

```
<expr> ::= <op>(<expr>, <expr>) | <func>(<expr>) | <var>
<func> ::= 'log ' | 'sqrt '
<op> ::= "+" | "-" | "*" | "/" | "^"
<var> ::= Weight | Height | <n>
\langle n \rangle ::= -3 | -2 | -1 | 0 | 1 | 2 | 3
```

The Best Expression: Weight \* Height<sup>-2</sup>

## A Second Test Example



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Table: A schematic presentation of the input data. The table contains a sample of the data used for experiments.

а	b	С	decision
3	9	7	0
1	4	4	1
5	9	4	2
:	÷	÷	:

Table: RMSE for selected ML techniques.

	RMSE train	RMSE test
Linear Regression	0.8267	0.8239
Decision Tree	0.5431	0.8142
Random Forest	0.2284	0.5883

## Frame Title



## A Knowledge Component Supplied



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Table: A Meaningful Intermediate Variable (MIV) added.

а	b	С	d	decision
3	9	7	-3	0
1	4	4	0	1
5	9	4	16	2
:	÷	÷	÷	÷

Table: RMSE for selected ML models with KC.

	RMSE train	RMSE test	
Linear Regression	0.4778	0.5779	
Decision Tree	0.0000	0.0000	
Random Forest	0.0386	0.0266	

## A GE Model



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<op>(<expr>, <expr>)</expr></expr></op>
<op> ::= "-"   "*"   "^"</op>
<var> ::= a   'c'   b</var>
<n> ::= 1   2   3   4</n>
Best Expression for d: $b^2 - c * 4 * a$
The rules:
ifelse(d > 0, "two", "other no. of roots")
<pre>ifelse(d == 0, "one", "other no. of roots")</pre>
ifelse(d < 0, "zero", "other no. of roots")

<expr> ::= <var> | <op>(<n>, <var>) | <op>(<var>,

## Final Model-Driven eXplanation



Best Expression for d: b<sup>2</sup> - c \* 4 \* a

ifelse(d > 0, "two", "other no. of roots")
ifelse(d == 0, "one", "other no. of roots")
ifelse(d < 0, "zero", "other no. of roots")</pre>

ifelse(d > 0, "two", ifelse ( d == 0 , "one", "zero"))





# Summary and What Next?



## Observations

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#### • Limitations of current XAI task formulation:

- No holistic, general framework; only local, peep-hole view,
- No Causal Models; lack of structural approach,
- The explanation is based on the same data as learning!; an intrinsic, born-in limitation,
- No deep, background knowledge is taken into account.
- Towards Model-Driven XAI: Introduction of Knowledge-Based Components, Connections, Causality,
- Reliable, Trustworthy Decision-Making,
- Incorporation of Model-Based (Model-Driven) XAI techniques.

## Summary

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- Using only shallow explainability techniques can lead to inconsistent and misleading explanations, having nothing to do with the real, Model-Driven understanding of the decision procedure,
- Simple decision models but deep explainability techniques should be preferred,
- Grammatical Evolution can be applied for identification of functional dependencies in data,
- Perhaps the 3C approach seems reasonable for trustworthy XAI:
  - Components identification (also functional ones),
  - Causality causal dependencies discovery,
  - Connections struCture identification.

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## Further Work



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- Larger data sets... The A case,
- $\bullet$  Structure Discovery: combined KB + automated,
- Incorporation of Automated Planning Techniques,
- Incorporation of Functional Constraint Programming,
- Combination of Logical, Causal, Functional and Probabilistic Models.
- Combination with LLM; perhaps some synergy effect?

## Challenges of XAI



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## Some current research trends

- New research field promising trustability,
- Explanation quality measures; accuracy vs. simplicity,
- Explanation discrepancies exceptions,
- Complexity of Model-Generation,
- Implications for Law.

## Alternative Approaches: Deep Models vs. Shallow Ones

- eXplainability by Design,
- eXplainability by Structure Discovery,
- using Model-Based Reasoning,
- Knowledge Graph Models, Functional Constraint Programming, Constructive Abduction,...



Thank you for your kind attention! Questions? Remarks? Constructive critics?





