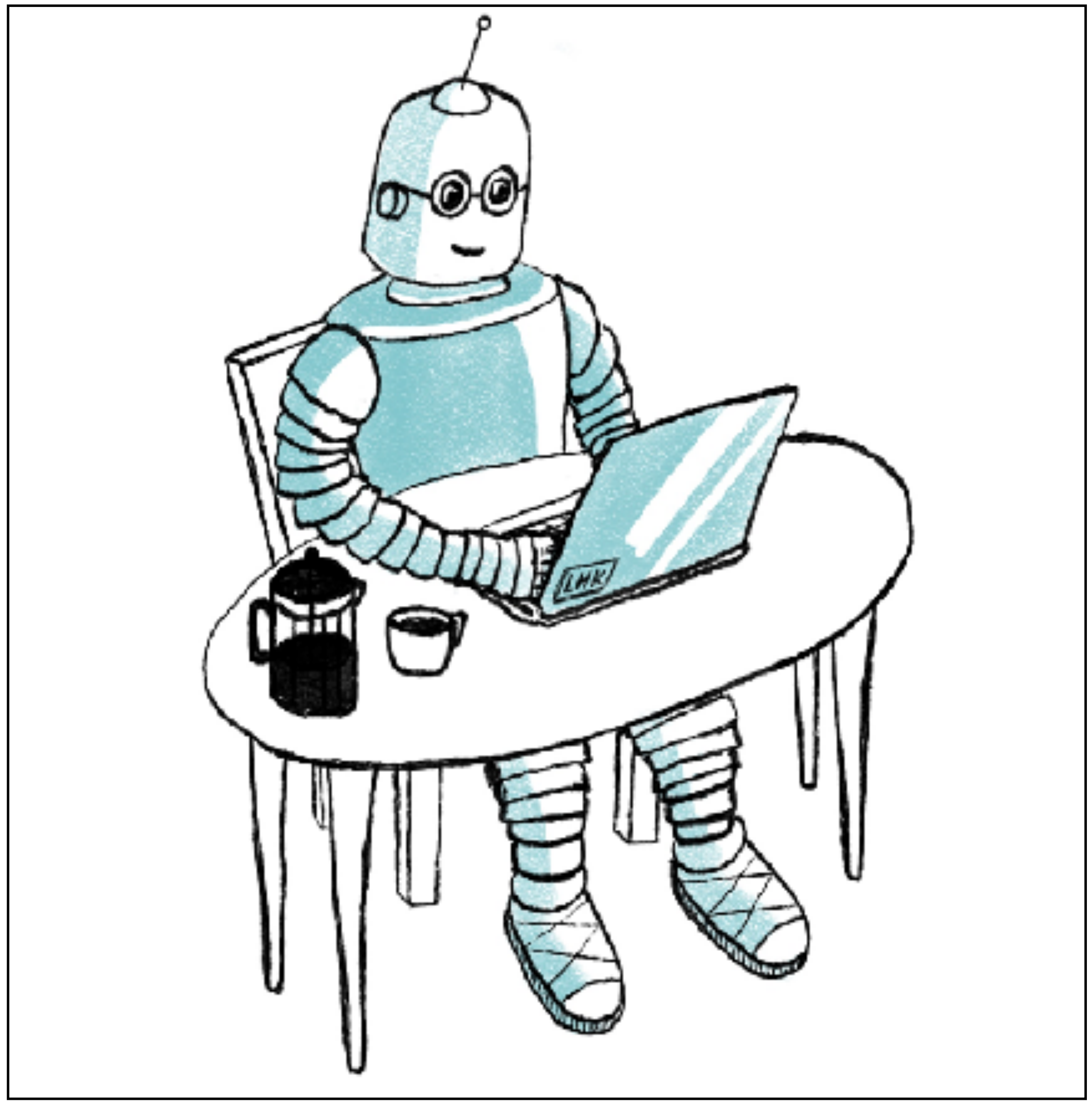
Logical scientific discovery



Andrew Cropper

My long-term goal

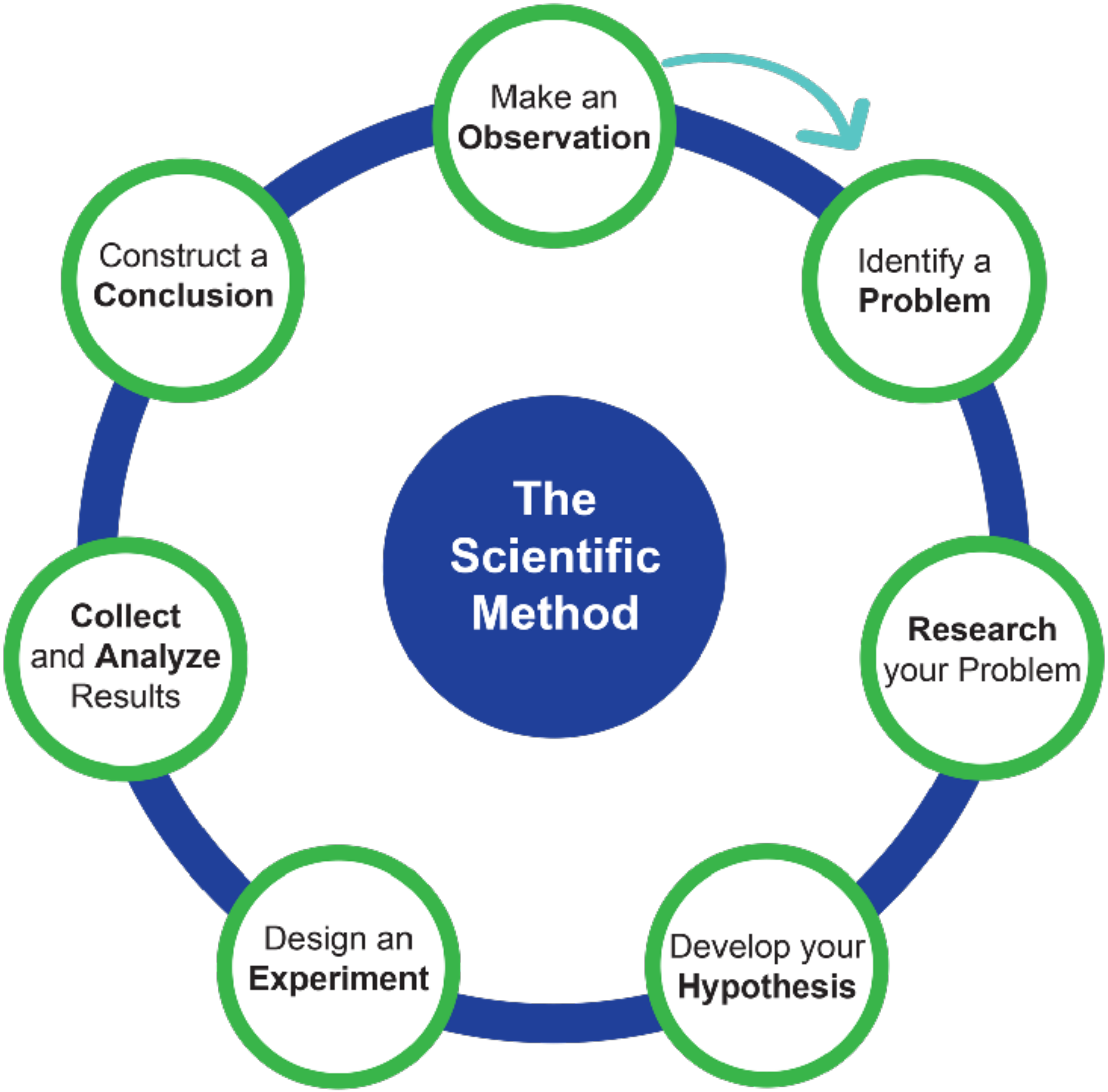
Accelerate scientific discovery

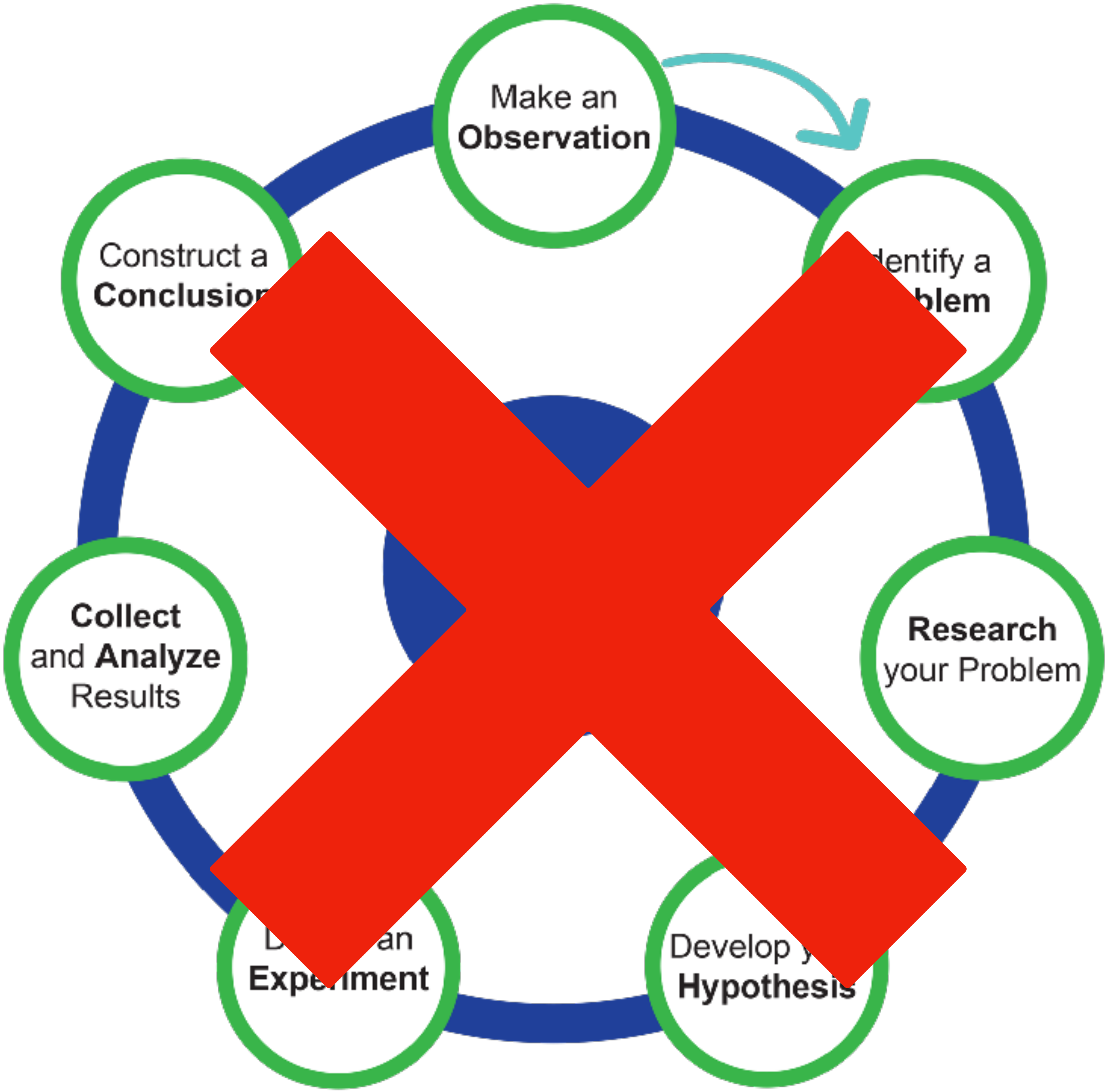
Why?

Science is important


SINGLE USE ONLY
Antibiotics

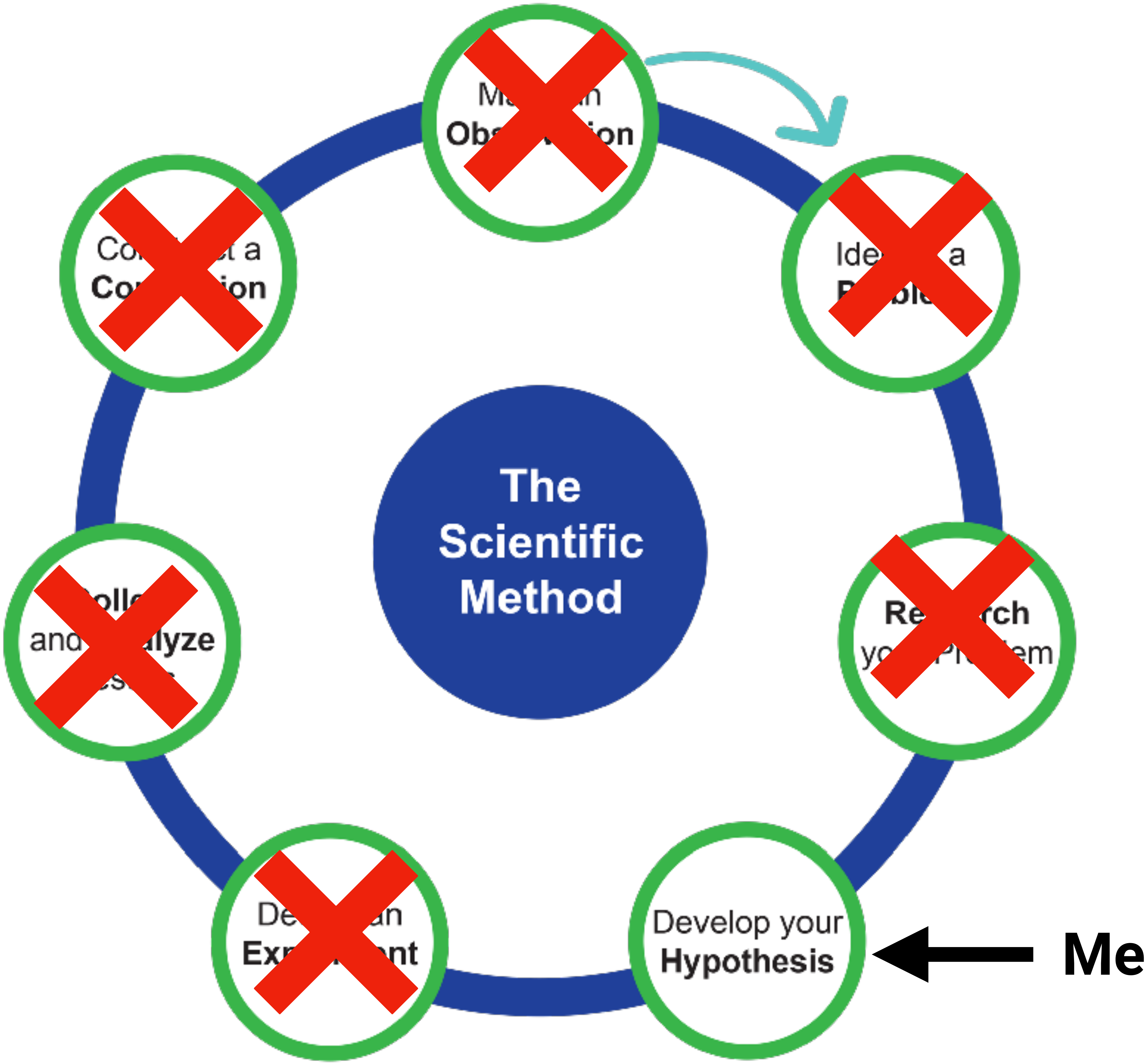
What exactly do I want to do?


The Scientific Method
Make an Observation
Identify a Problem
Research your Problem
Develop your Hypothesis
Design an Experiment
Collect and Analyze Results
Construct a Conclusion


Make an Observation
Construct a
Collect and Analyze Results
Research your Problem
Hypothesis

Robot scientist

Robot scientist



The Scientific Method
Develop your Hypothesis
Me

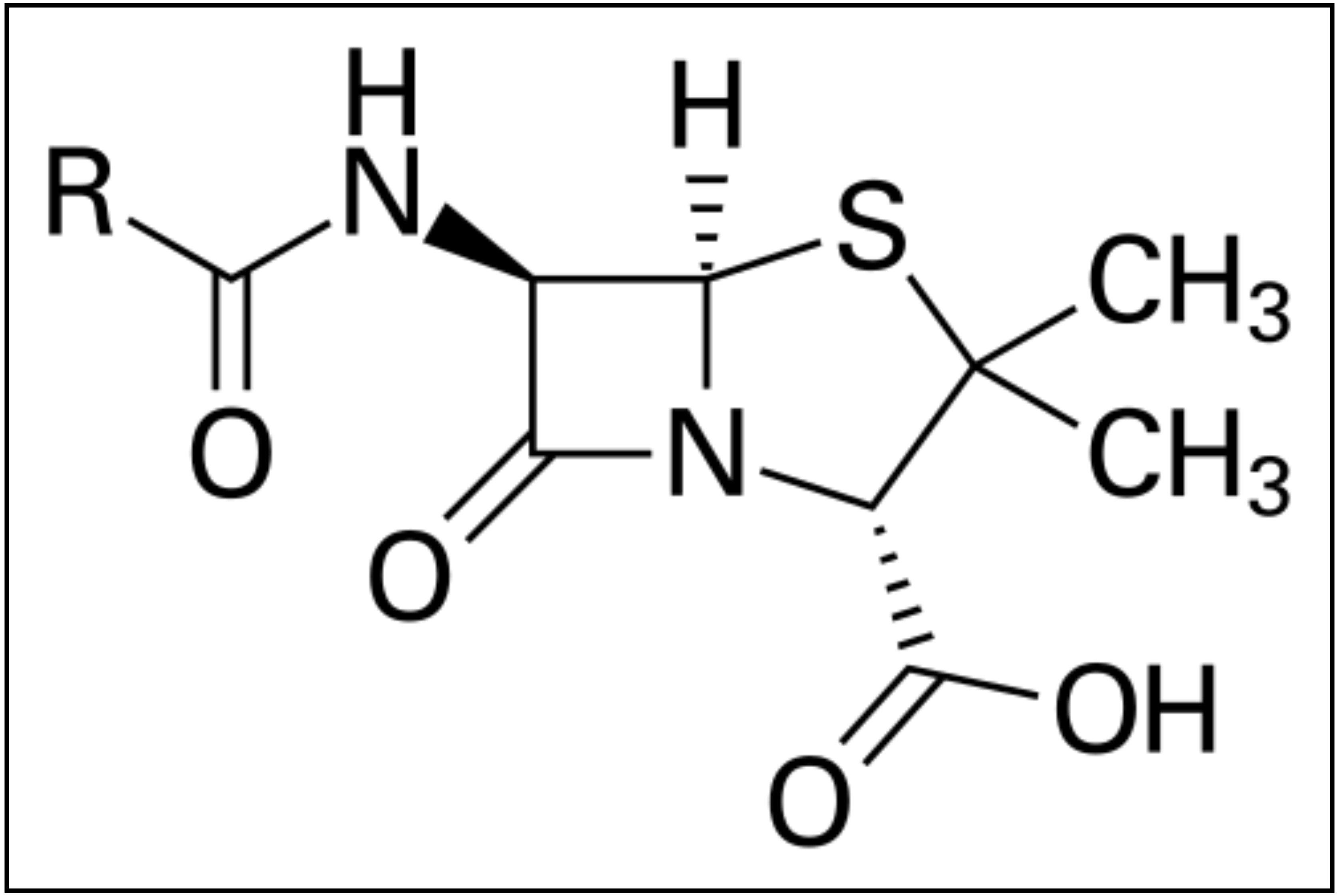
My research

My research

Prior knowledge

My research

Prior knowledge



My research

Observations

My research

Observations

My research

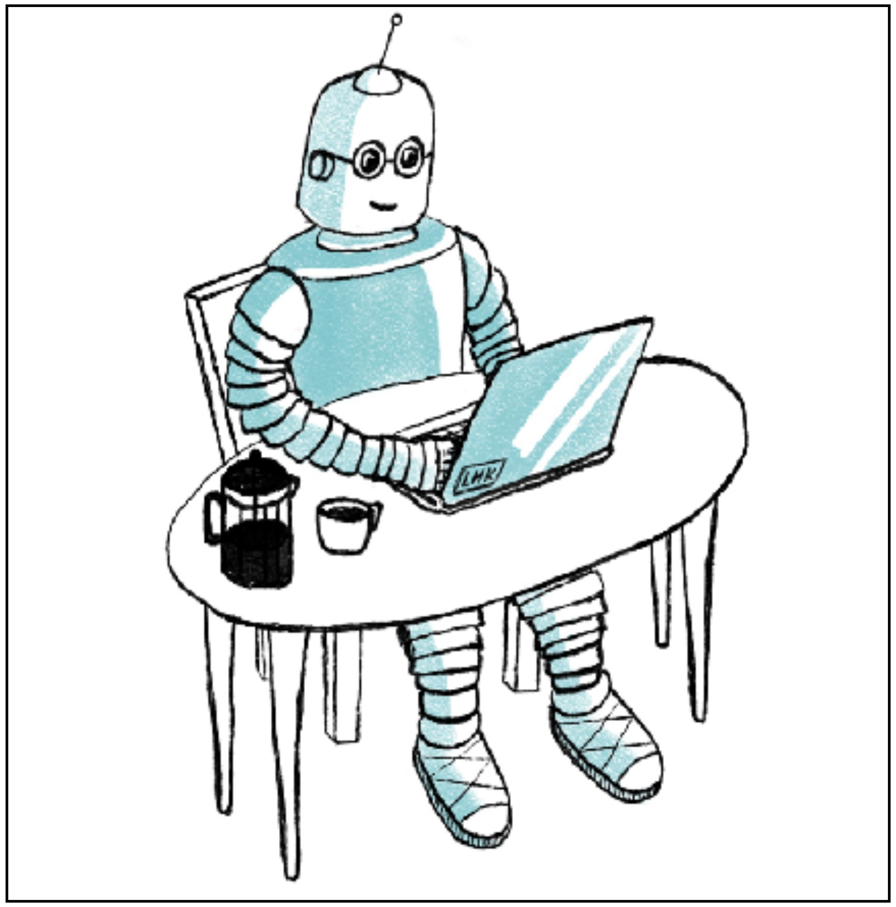
Prior knowledge

Observations

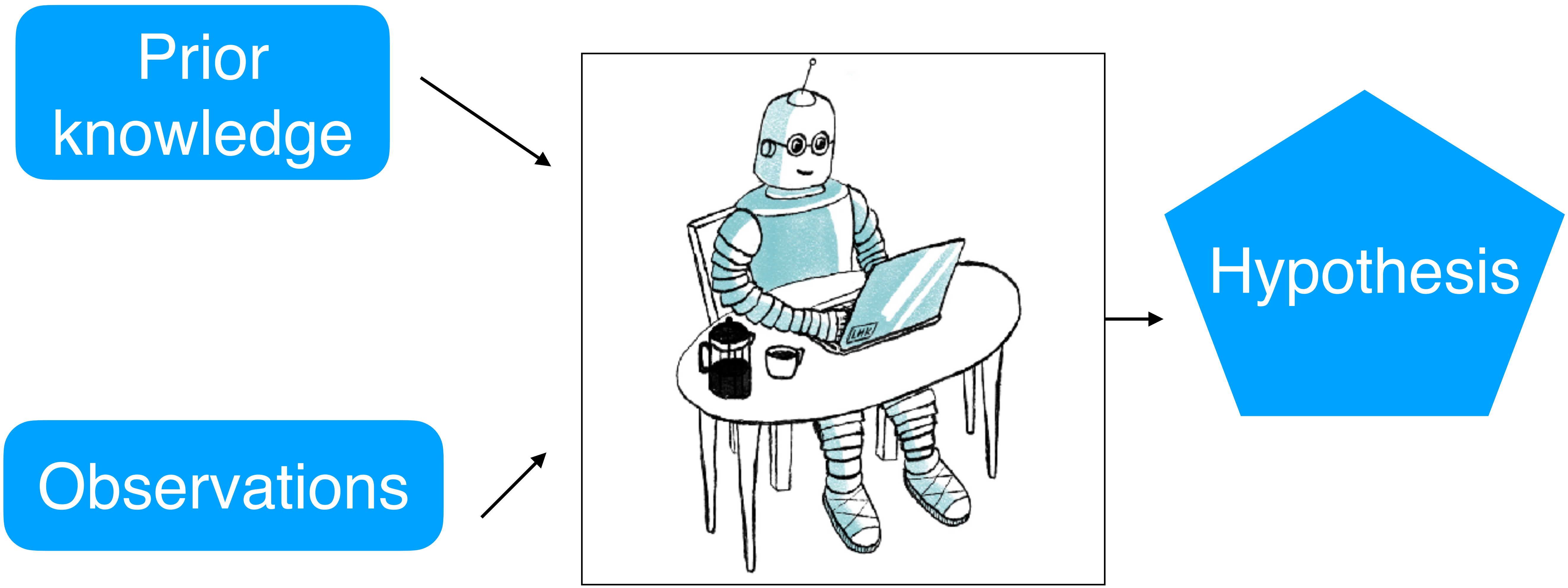
My research

Prior knowledge

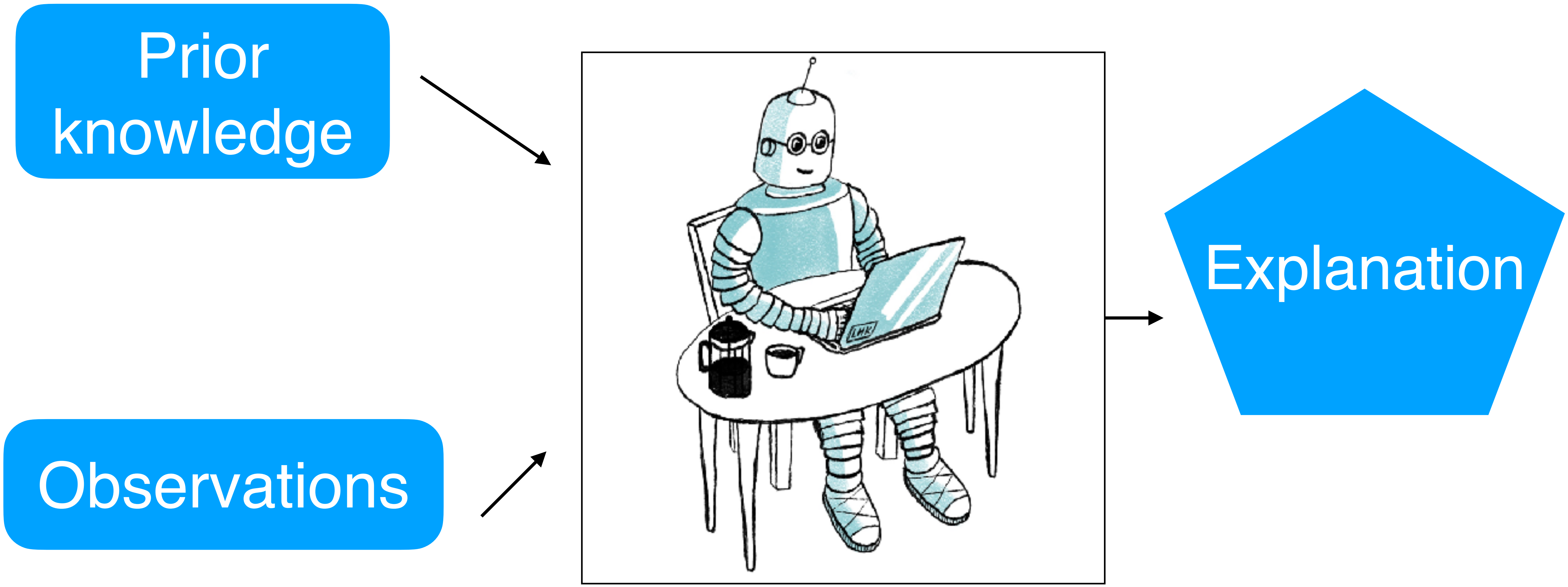
Observations



My research



My research



My research

A drug works if it has both a hydroxyl group and an amine group and the oxygen atom of the hydroxyl group is connected to the nitrogen atom of the amine group

Explanation

What do we need?

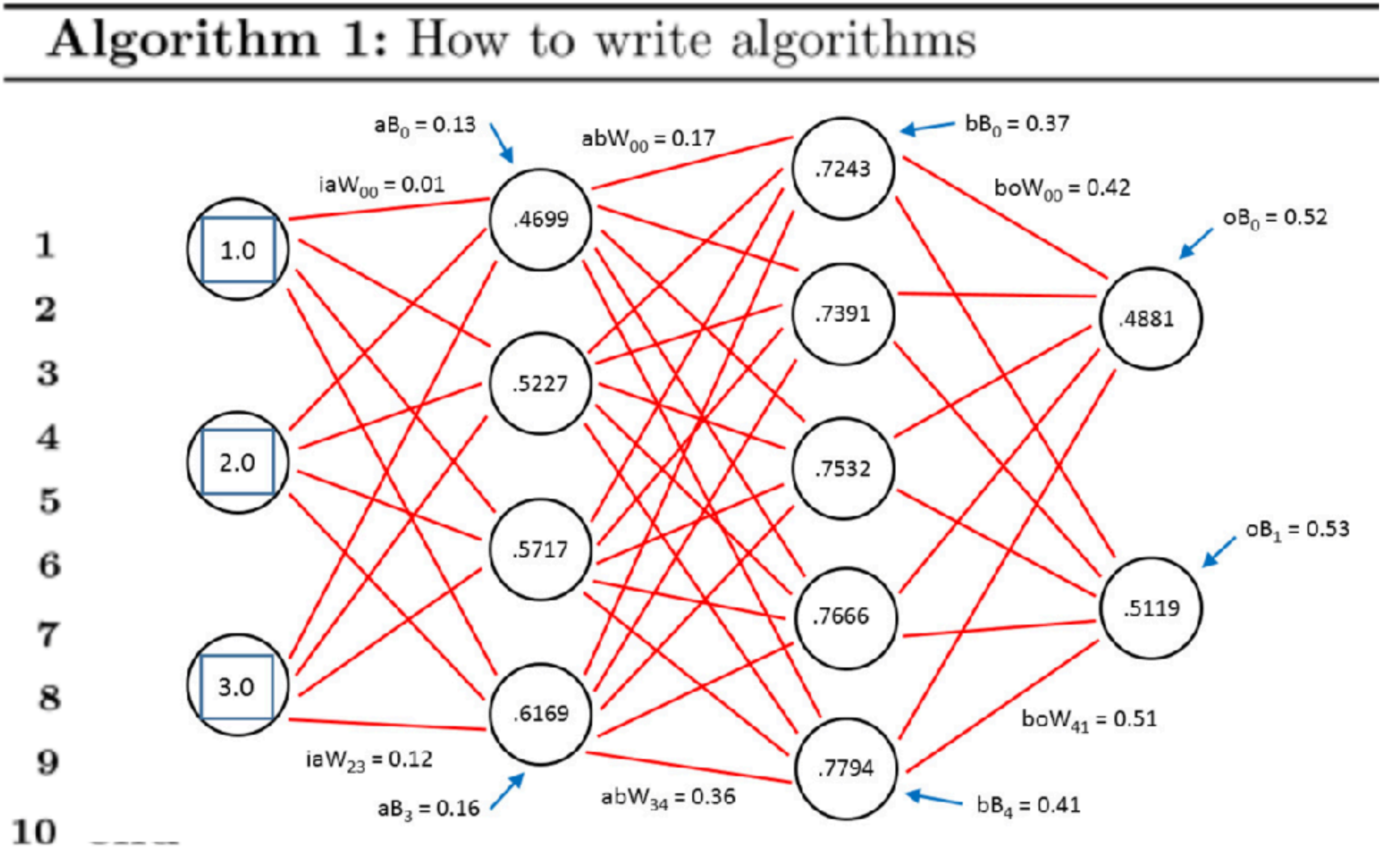
Efficiency


MasterControl

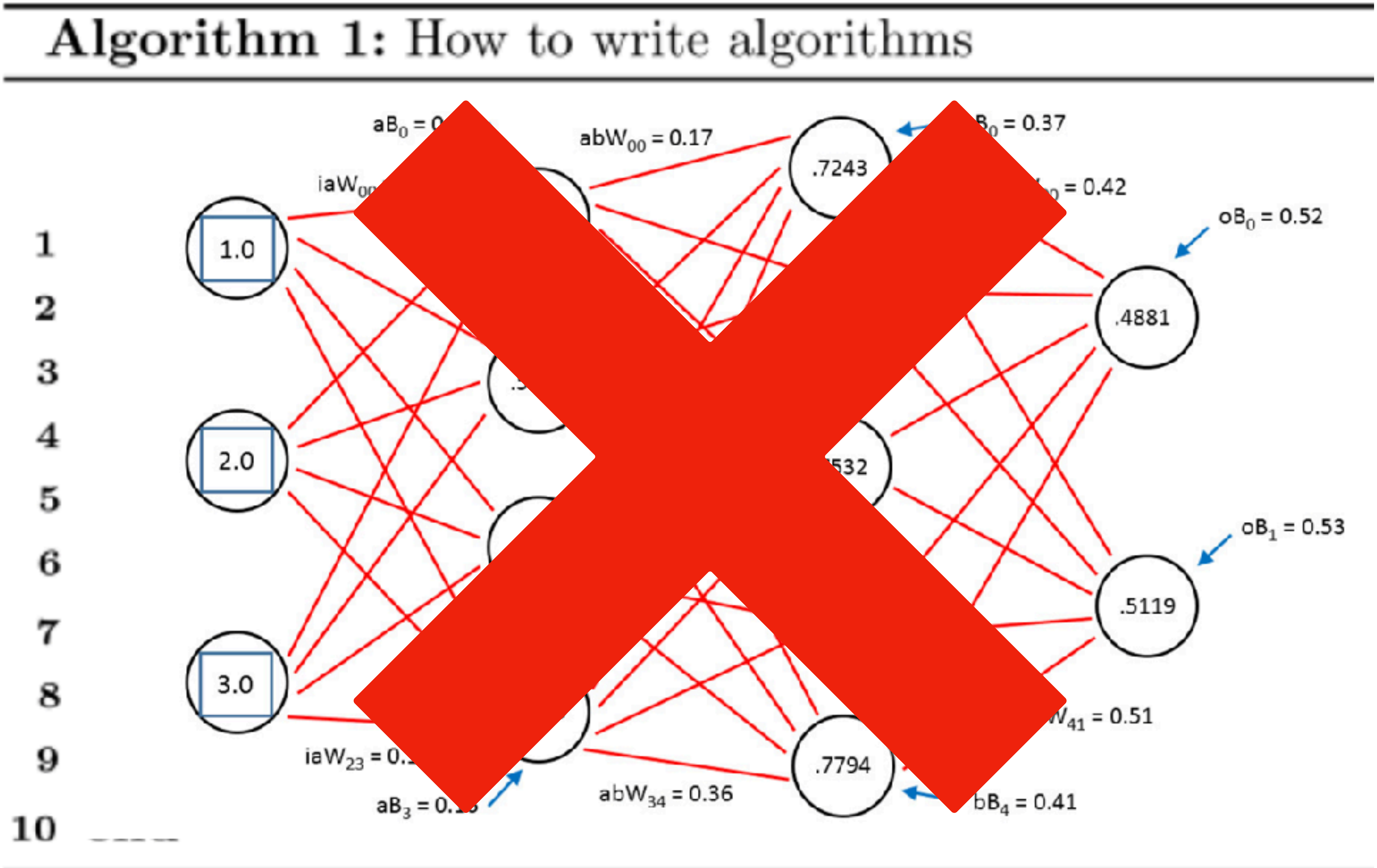
Explainability

To publish a discovery, we must **explain** it

Explainability

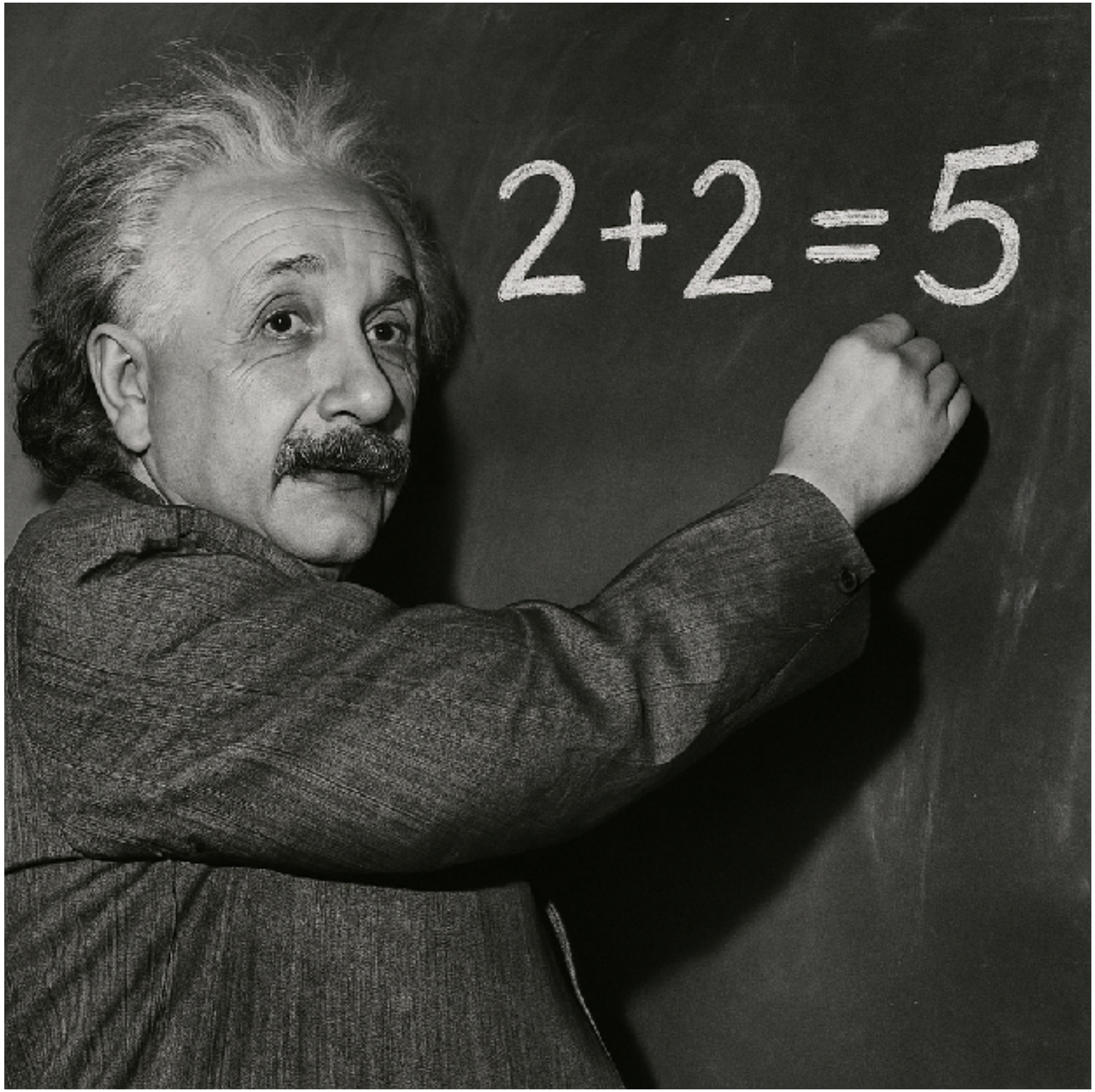


Explainability

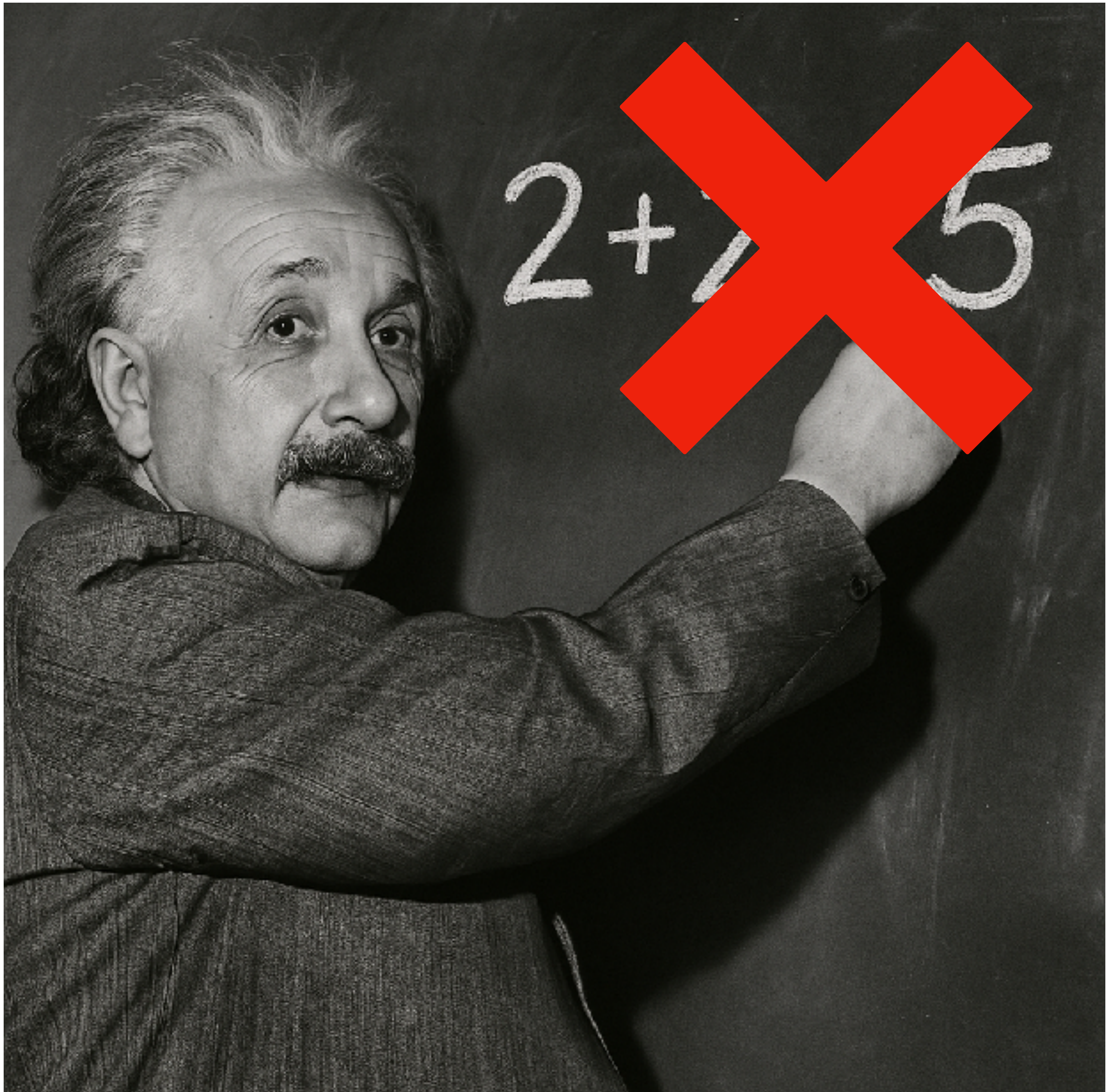


Trustworthy

Trustworthy



Trustworthy



A problem

FCAI

Key objectives: data efficiency, trust & ethics, understandability

To create Real AI, we have set up three grand scientific objectives: data efficiency, trust & ethics, and understandability.

Present-day AI solutions work well only in a very small subset of simple domains. In order to expand the deployment of AI further, we need new AI tools that overcome the key shortcomings of current AI systems.

DATA EFFICIENCY

Current AI solutions can be very successful in domains where tasks are relatively simple and well-defined and an abundance of high-quality, properly annotated data are available. Existing AI methods do not, however, easily extend to domains where such data are not available or are difficult or expensive to acquire. Real AIs will be able to work with real-world scarce data – ill-defined, hard to acquire or unavailable.

TRUST & ETHICS

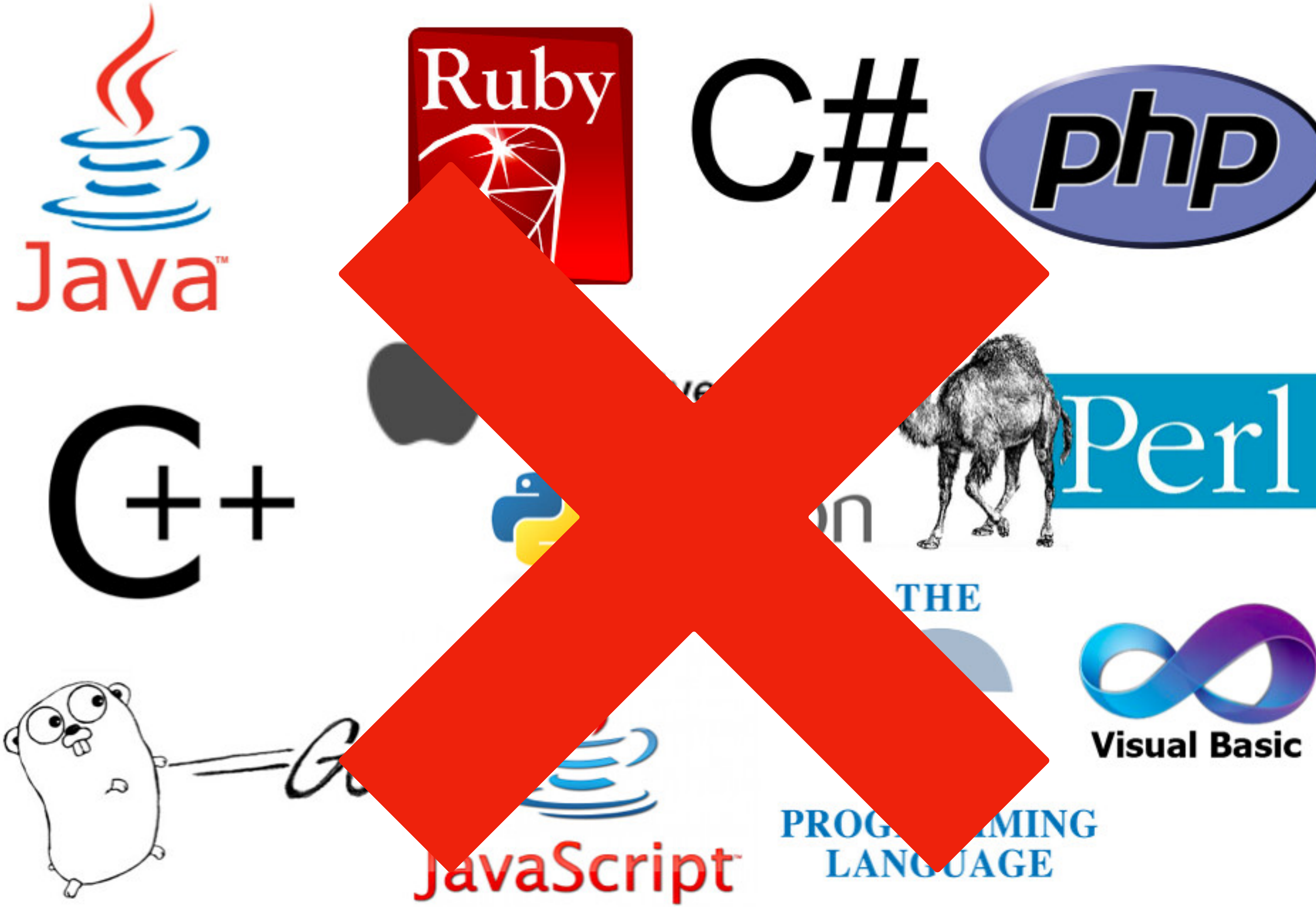
We will create AIs that are secure, give trustworthy results, preserve privacy, are fair, and whose use is ethically sustainable. We will develop the required privacy-preserving and secure methods to address challenges related to susceptibility to manipulation, information stealing and unethical approaches. We will provide new resilient deep learning approaches for the currently popular and successful deep neural networks.

UNDERSTANDABILITY

AI does not yet understand users. We need to open the "black box" of many AI methods: to understand how methods such as neural networks operate and what are the uncertainties inherent to their outputs. Modeling the user and the interaction will help the AI understand the user and vice versa. The outcome is AIs that are able to augment human capabilities in a multitude of tasks.

How?

Inductive logic programming



Java
Ruby
C#
php
C++
Perl
THE
Visual Basic
JavaScript
PROG
MING
LANG
UAGE

Logical machine learning

Inductive logic programming

Inductive logic programming

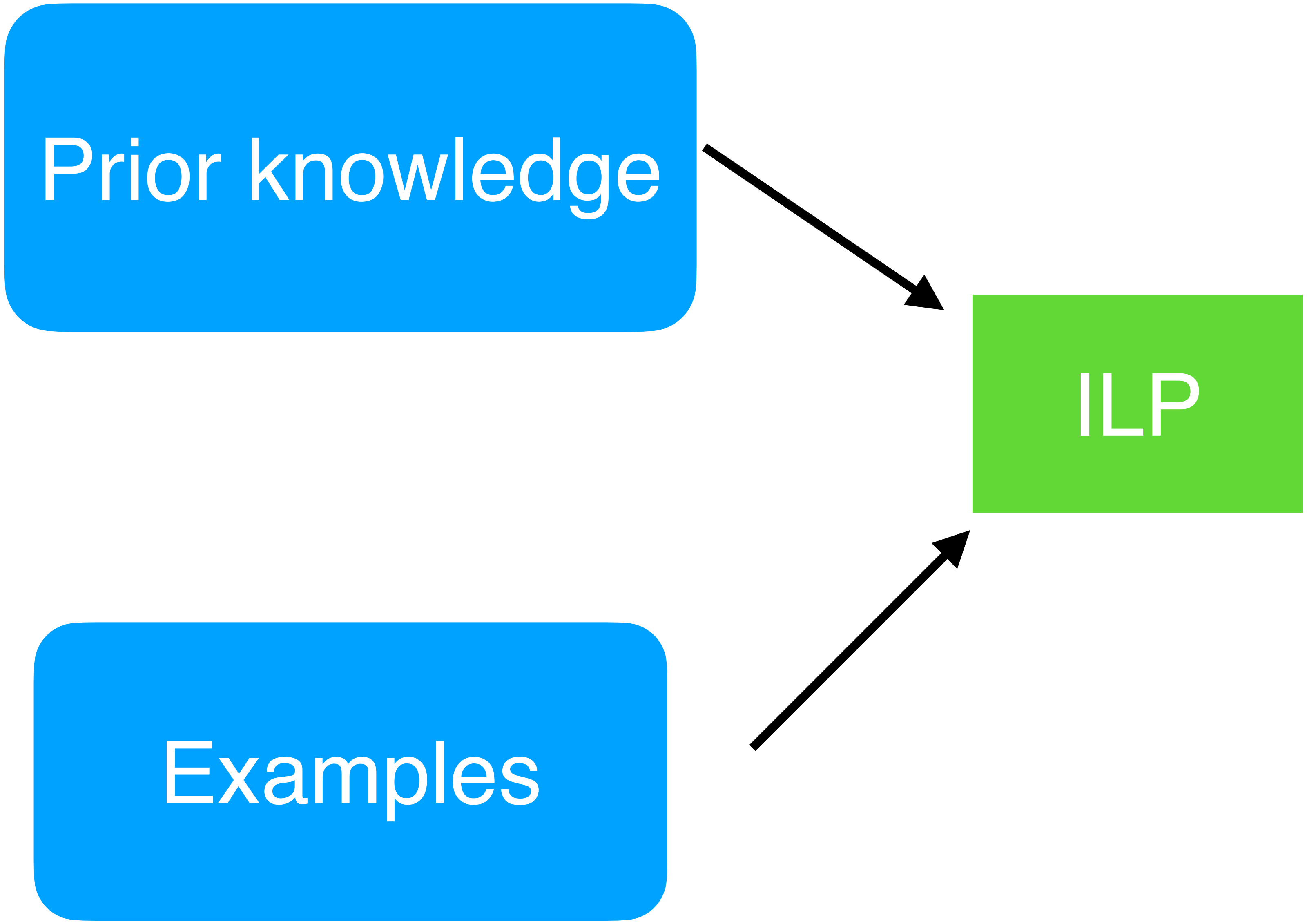
Prior knowledge

Inductive logic programming

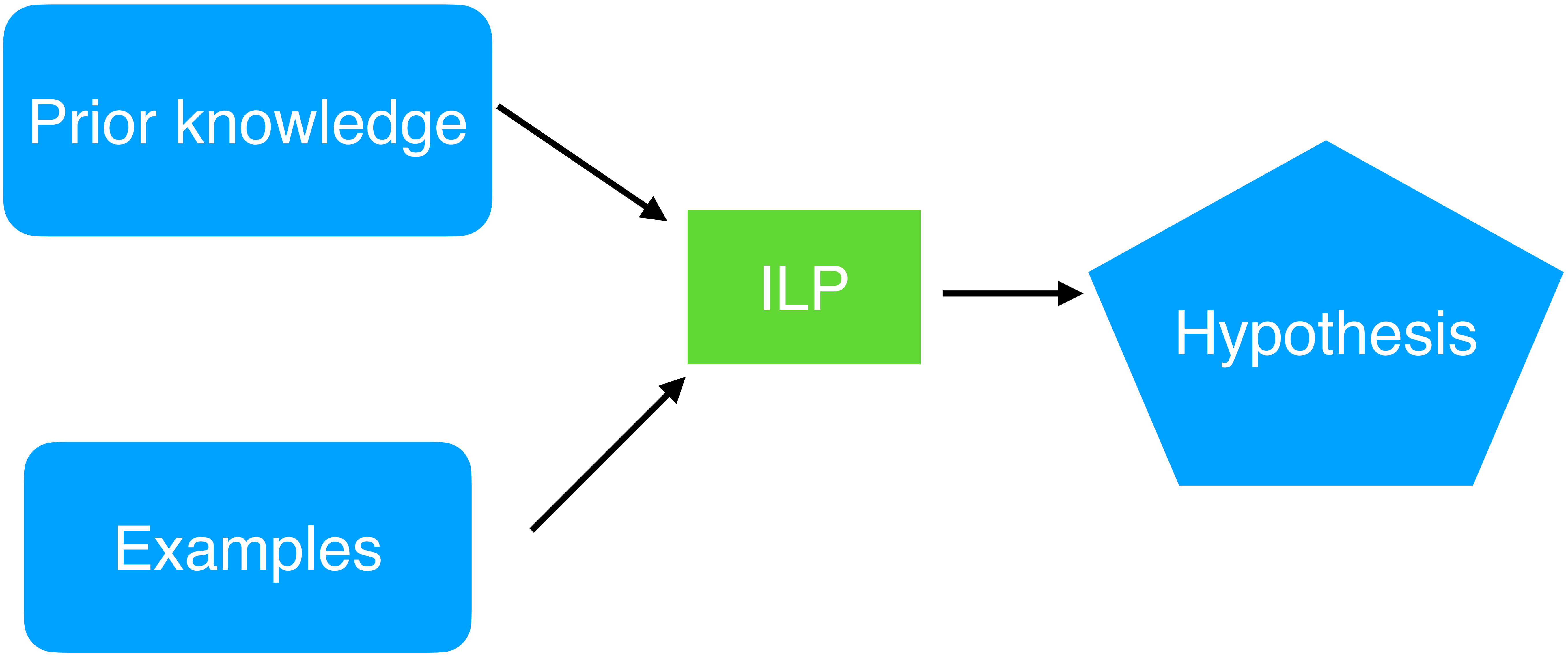
Prior knowledge

Examples

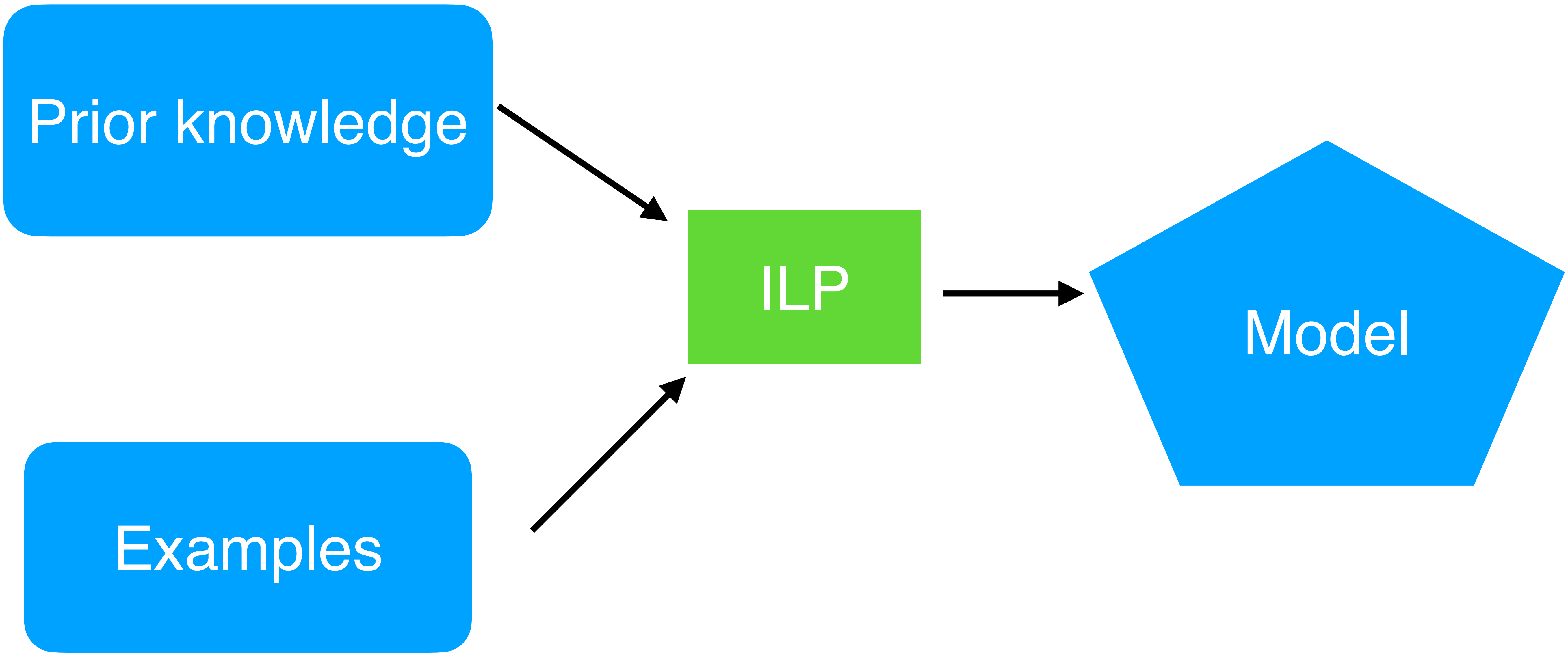
Inductive logic programming



Inductive logic programming

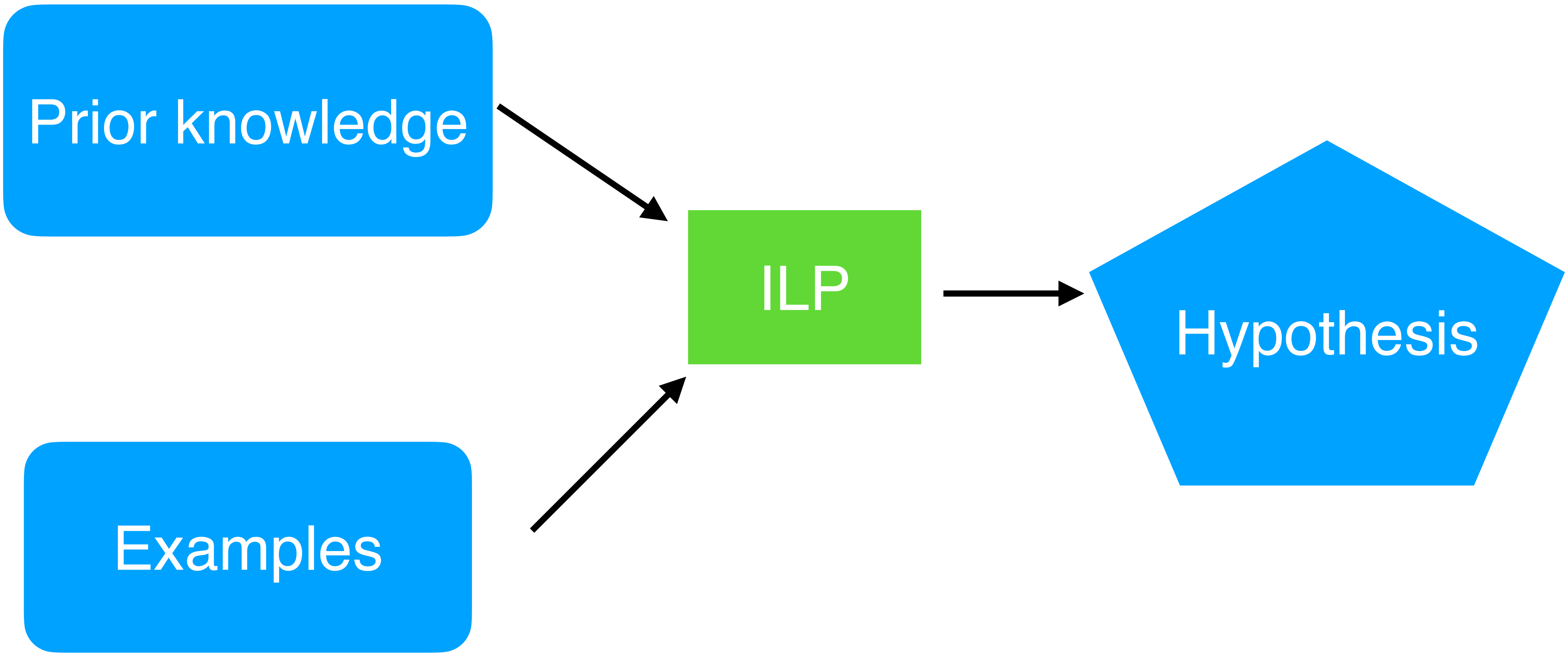


Inductive logic programming



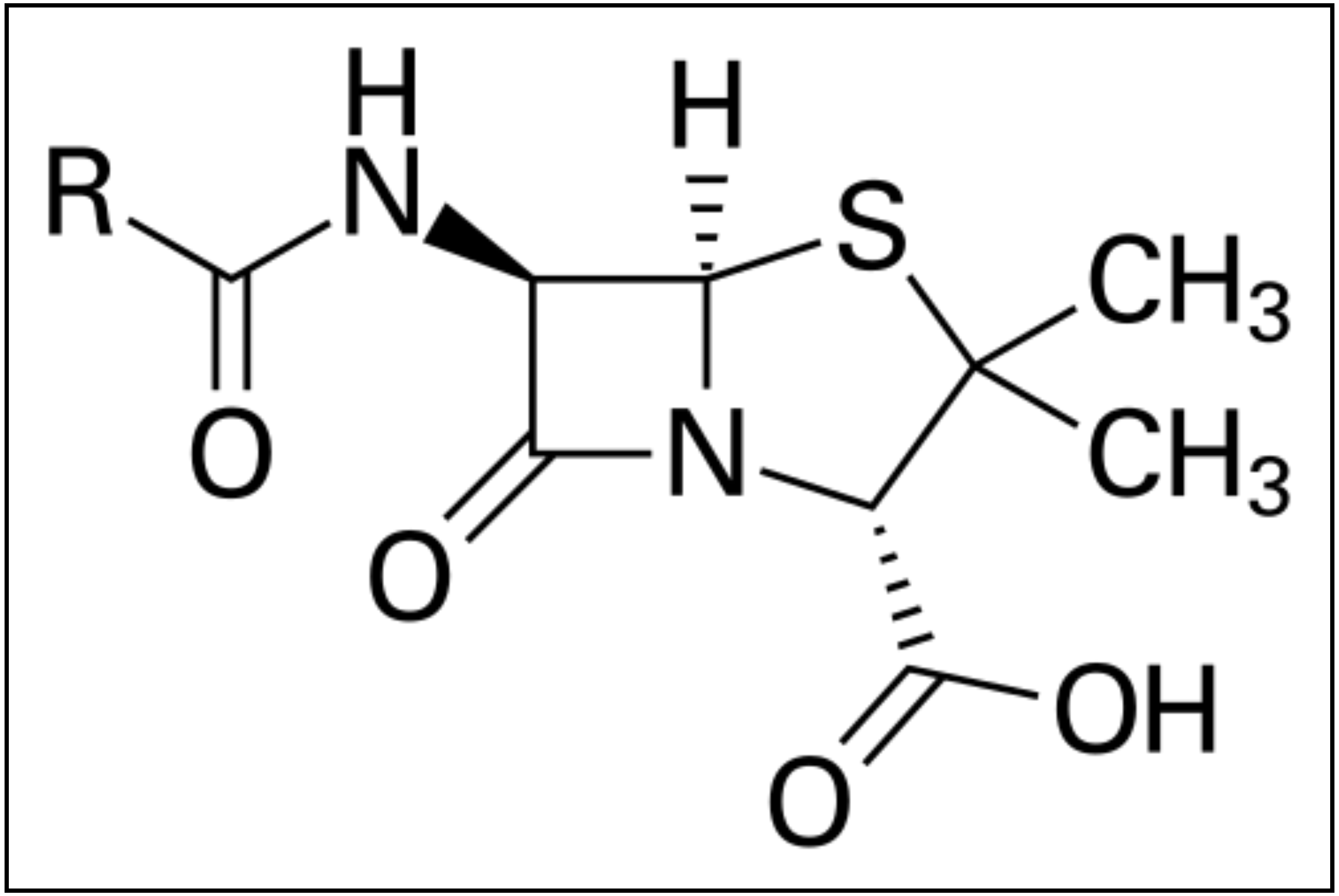
Supervised machine learning

Inductive logic programming



Uses logic to represent data

Prior knowledge



Prior knowledge

```
atom(7, o).
atom(8, o).
atom(9, h).
atom(10, h).
atom(11, h).
atom(12, h).
...
bond(1, 2, single).
bond(2, 3, single).
bond(3, 4, single).
bond(4, 5, single).
...
```

Observations

Hypothesis

```
∀Mol((has_hydroxyl(Mol)
∧ has_amine(Mol)
∧ ∃A1,A2(bond(A1,A2,Mol)
∧ atom(Mol,A1,oxygen)
∧ atom(Mol,A2,nitrogen)))
→ active(Mol))
```

Hypothesis

A drug works if it has both a hydroxyl group and an amine group and the oxygen atom of there is a bond between the hydroxyl group and the nitrogen atom of the amine group

Why ILP?

- Interpretable ✓
- **Efficient** ✓
- **Trustworthy** ✓

What have I done?

Design ILP algorithms and package them into open-source tools

Contributions

scalability

data efficiency

handling noisy numerical data

How does old ILP work?

Old ILP

Pick a hypothesis and tweak it to fit the data

My contribution

Automate Karl Popper’s
logic of scientific discovery

Science progresses by eliminating false theories

My contribution

Popper ILP system

What is the impact?

Learn hypotheses **100x bigger** than traditional approaches

MLJ21, AAAI22, ECAI23, MLJ23, AA23, ECAI24, IJCAI24

Learn from less data by learning **recursive** hypotheses

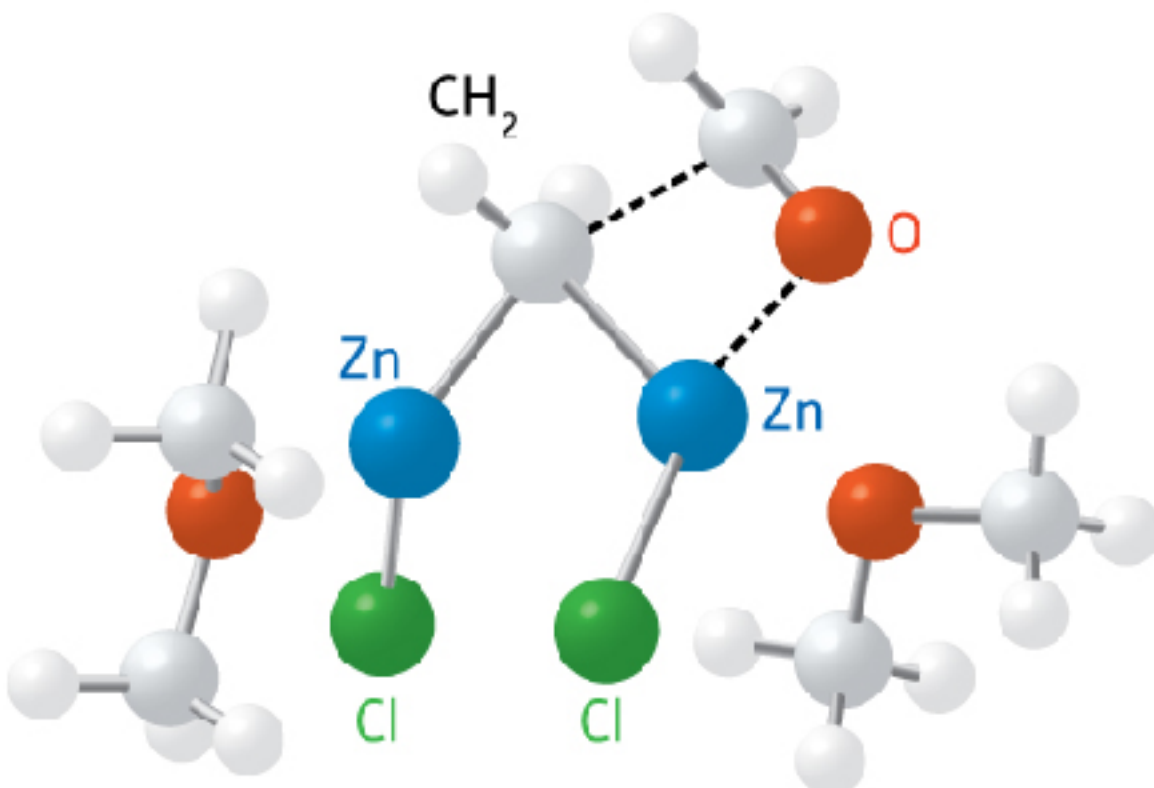
MLJ 2021

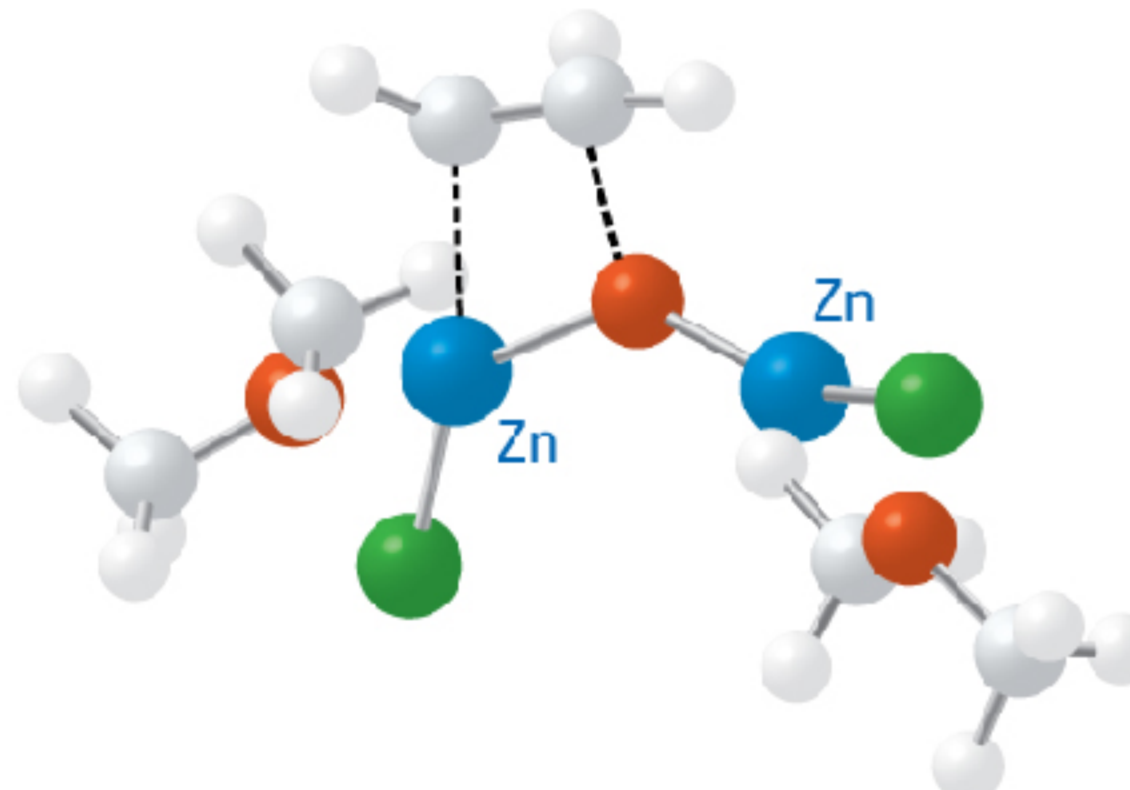
Handle noisy data by learning **MDL** hypotheses

But what is the actual impact?

People use it

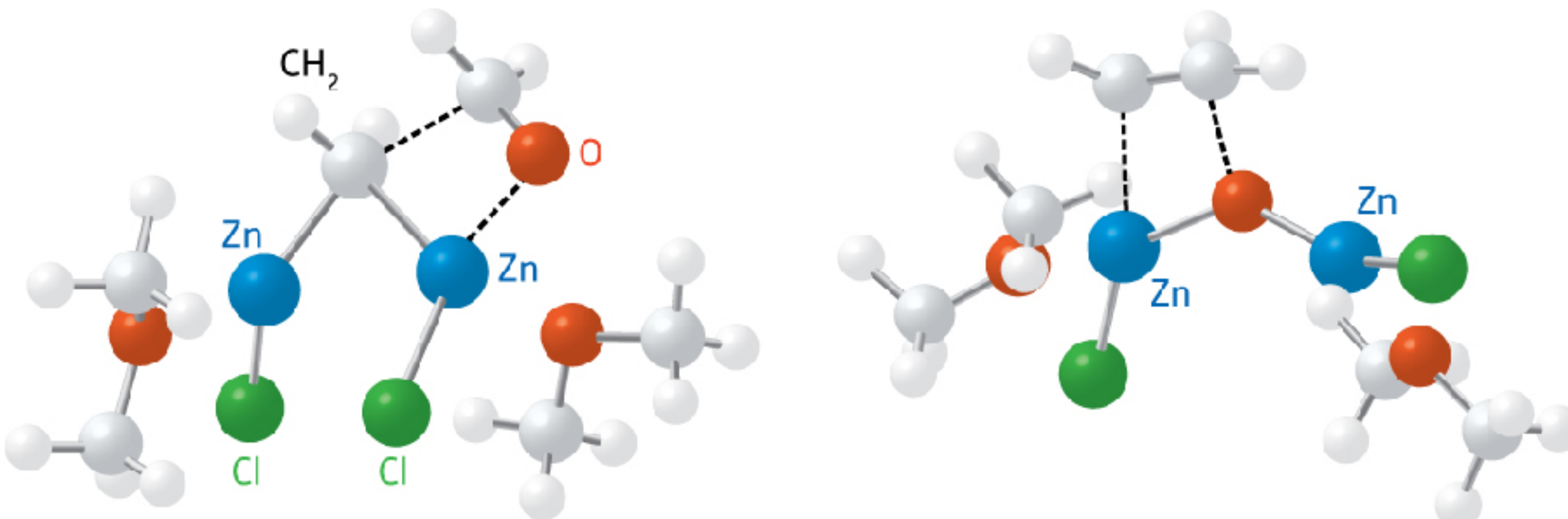
Explainable drug design





AAAI23

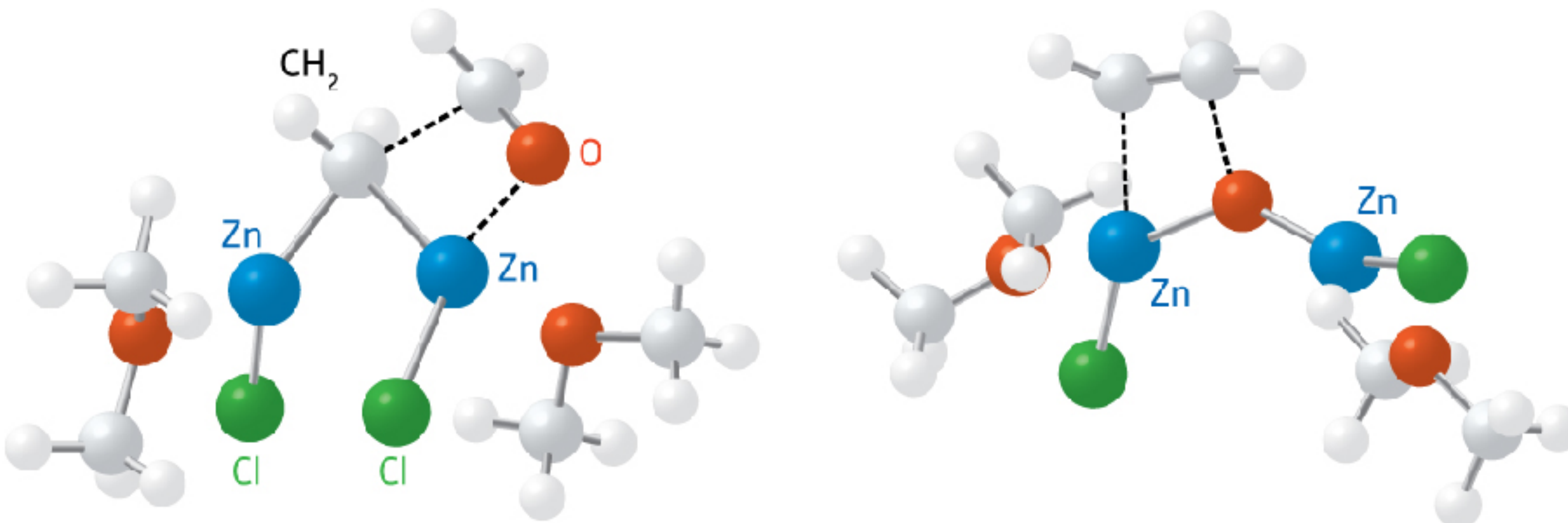
Explainable drug design



active(A) ← zinc(A,C), zinc(A,B), bond(B,C,du), dist(A,B,C,D), leq(D,1.23).

AAAI23

Explainable drug design

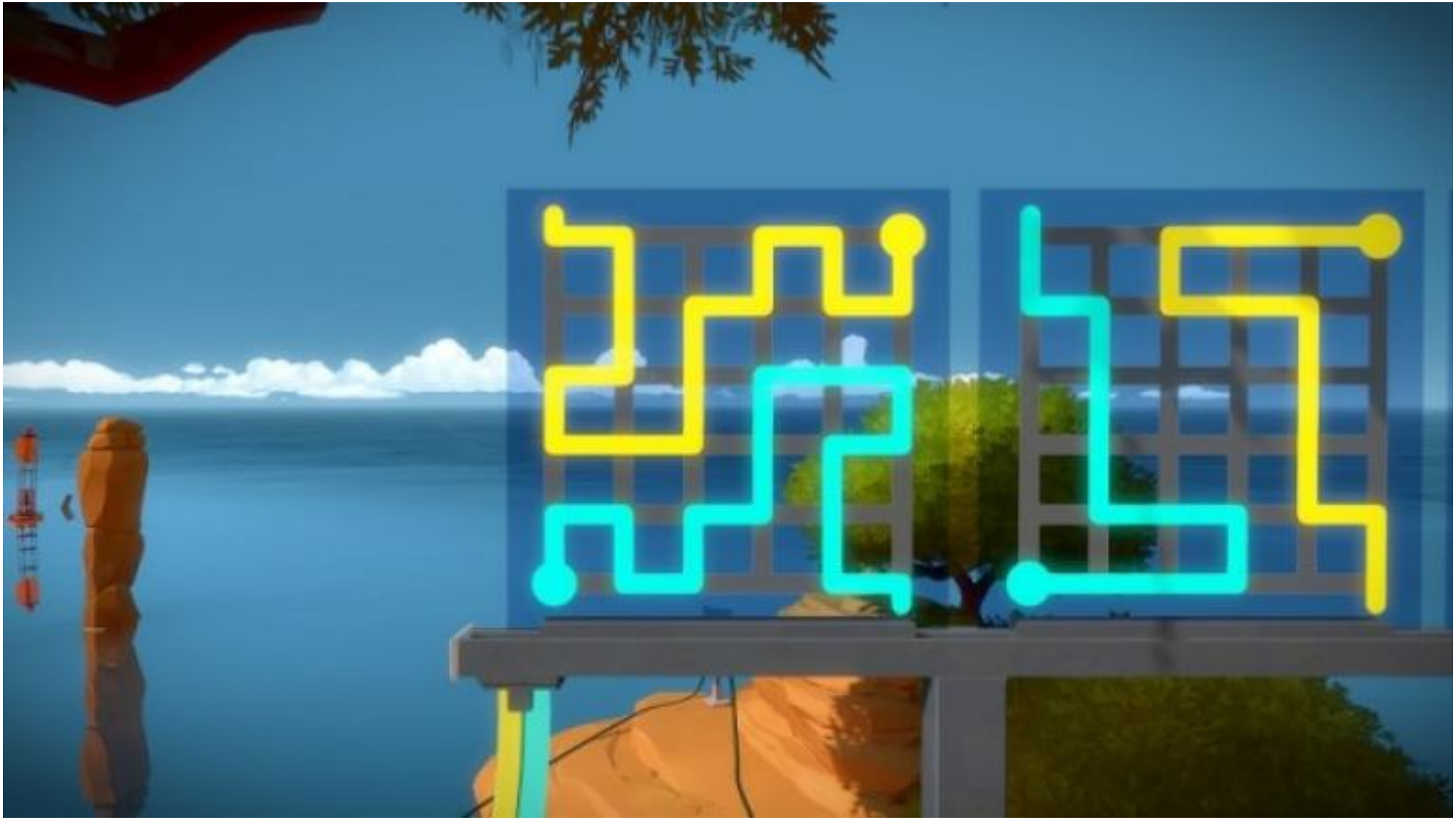


active if there are two zinc atoms

and there is a 'du' bond type between them

and the distance between them is <= 1.23

Games

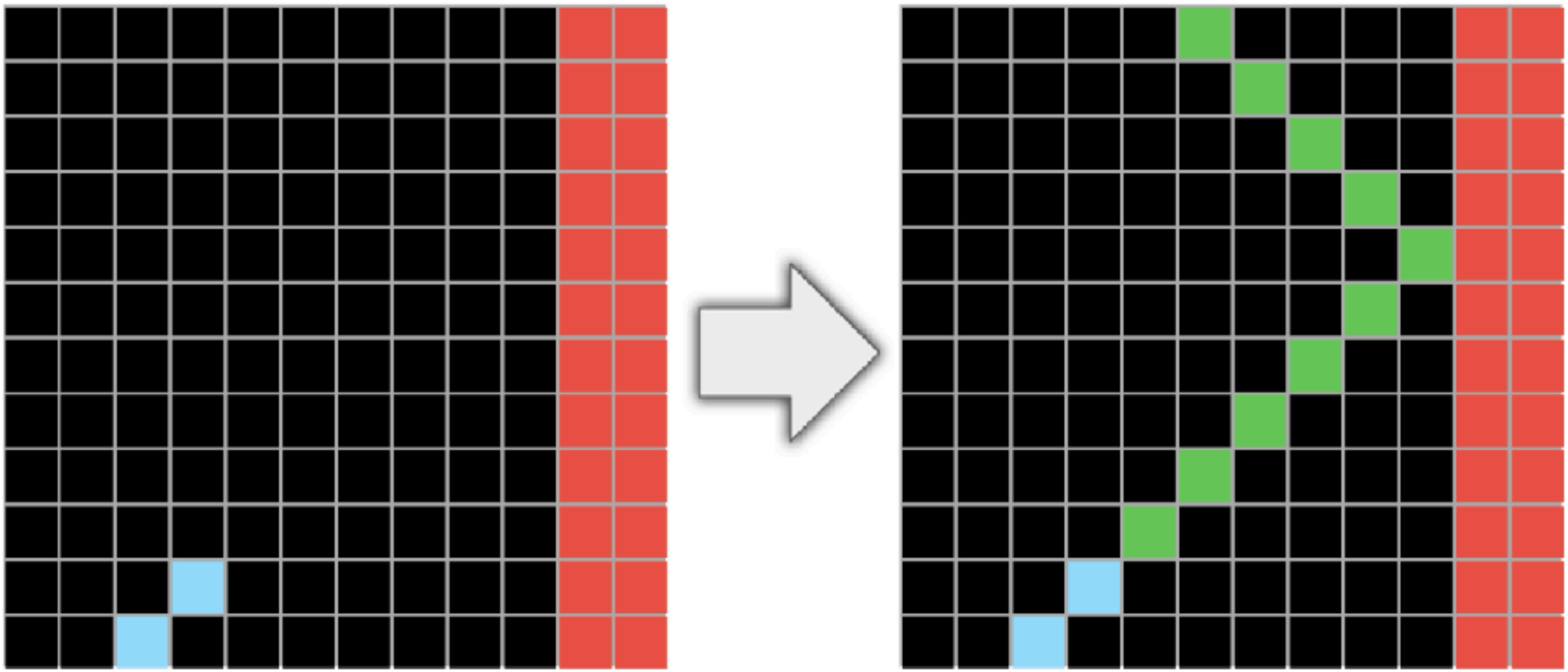


Stevens et al, 2023

Puzzles

Lakkaraju et al, 2022

Visual reasoning



IJCAI 2025?

Human learning / program synthesis

$[3,1,9,0,7] \rightarrow [1,9,0]$

$[2,1,3,4,6,9] \rightarrow [1,3]$

$[4,1,2,3,5,0,7,6,9,8] \rightarrow [1,2,3,5]$

$[1,5,4,2,8,3,0,6] \rightarrow [5]$

$[5,2,1,0,4,3,7,6] \rightarrow [2,1,0,4,3]$

Nature Communications 2024

What is missing?

Now: **undergraduate**

Given **much** guidance learn **complex** hypotheses

2025 — 2031 — 2035

Five-years: professor

Given **little** guidance learn **publishable** hypotheses

2025

2031

2035

How?

Better search

Complex prior knowledge

Scientist-aligned methods

Neural-symbolic

Can we learn which hypothesis to try next?

SMiLE research group?

How?

Better search

Complex prior knowledge

Scientist-aligned methods

Uncertainty

Scale

Elbow Ruler

Calipers

Stopwatch

Thermometer

Ruler

Roll Meter

Micrometer

Beaker Glass

Angle Ruler

Uncertainty

Can we combine Bayes and Popper?

***ProbFOIL**

How?

Better search

Complex prior knowledge

Scientist-aligned methods

There are significant discrepancies between
what AI researchers do and what scientists need

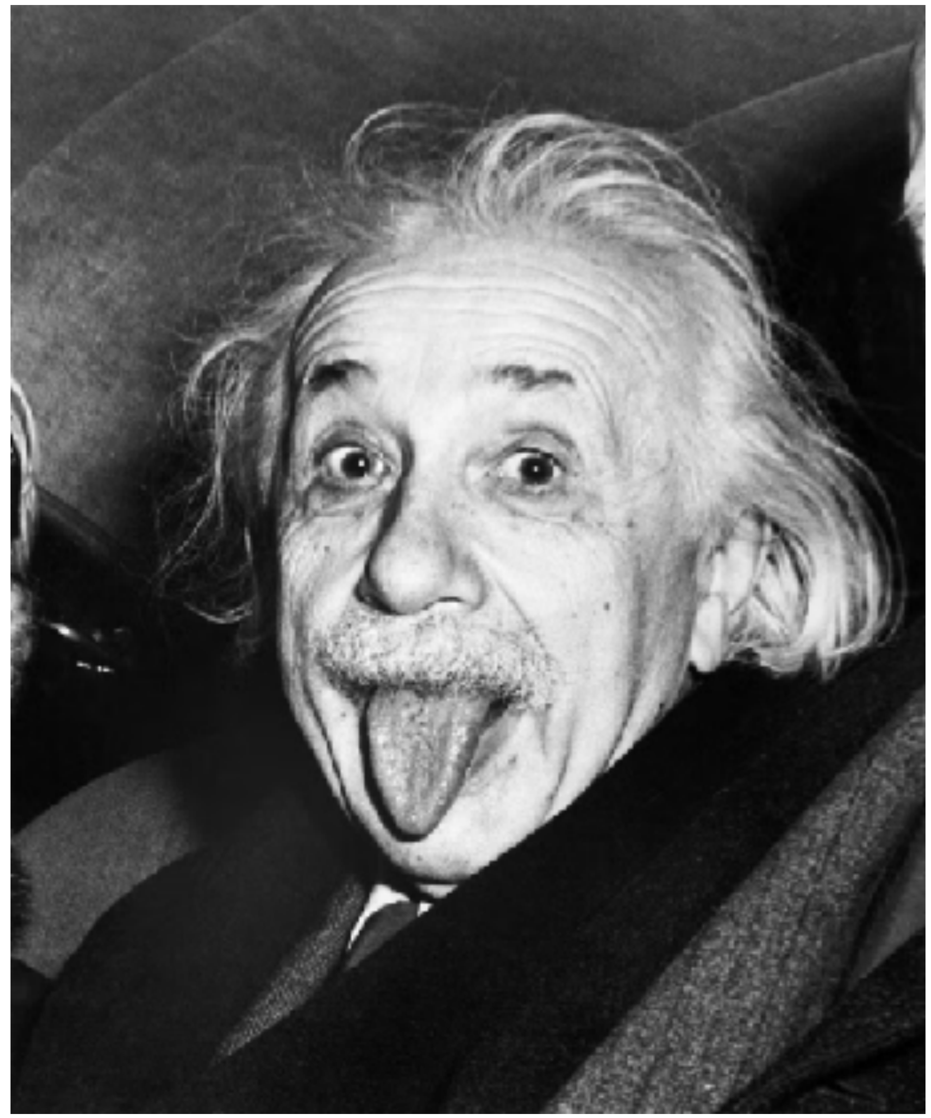
The ability to **understand a hypothesis** is equally, if not more, important than how well it performs

Explainability

How do we trade-off accuracy vs explainability?

Multidisciplinary collaborations

10-year goal: genius



Give **little** guidance make **Nobel-prize** worthy discoveries

2025 — 2031 — 2035

Questions?

Inductive logic programming at 30: a new introduction. Cropper and Dumančić. JAIR 2022

https://github.com/logic-and-learning-lab/Popper

Me

- Computer Engineering
- **Data Science**
- **Human-Technology Interaction**
- **Mathematics**
- Network and Information Security
- **Signal Processing**
- **Software Engineering**

Teaching

1. DATA.ML.310 Artificial Intelligence
2. DATA.ML.100 Introduction to Machine Learning
3. FIL.FIA.002. Logic

Popper

Popper

0. Start with a hypothesis space

Popper

0. Start with a hypothesis space
1. Select a hypothesis

Popper

0. Start with a hypothesis space
1. Select a hypothesis
2. Empirically try to refute it

Popper

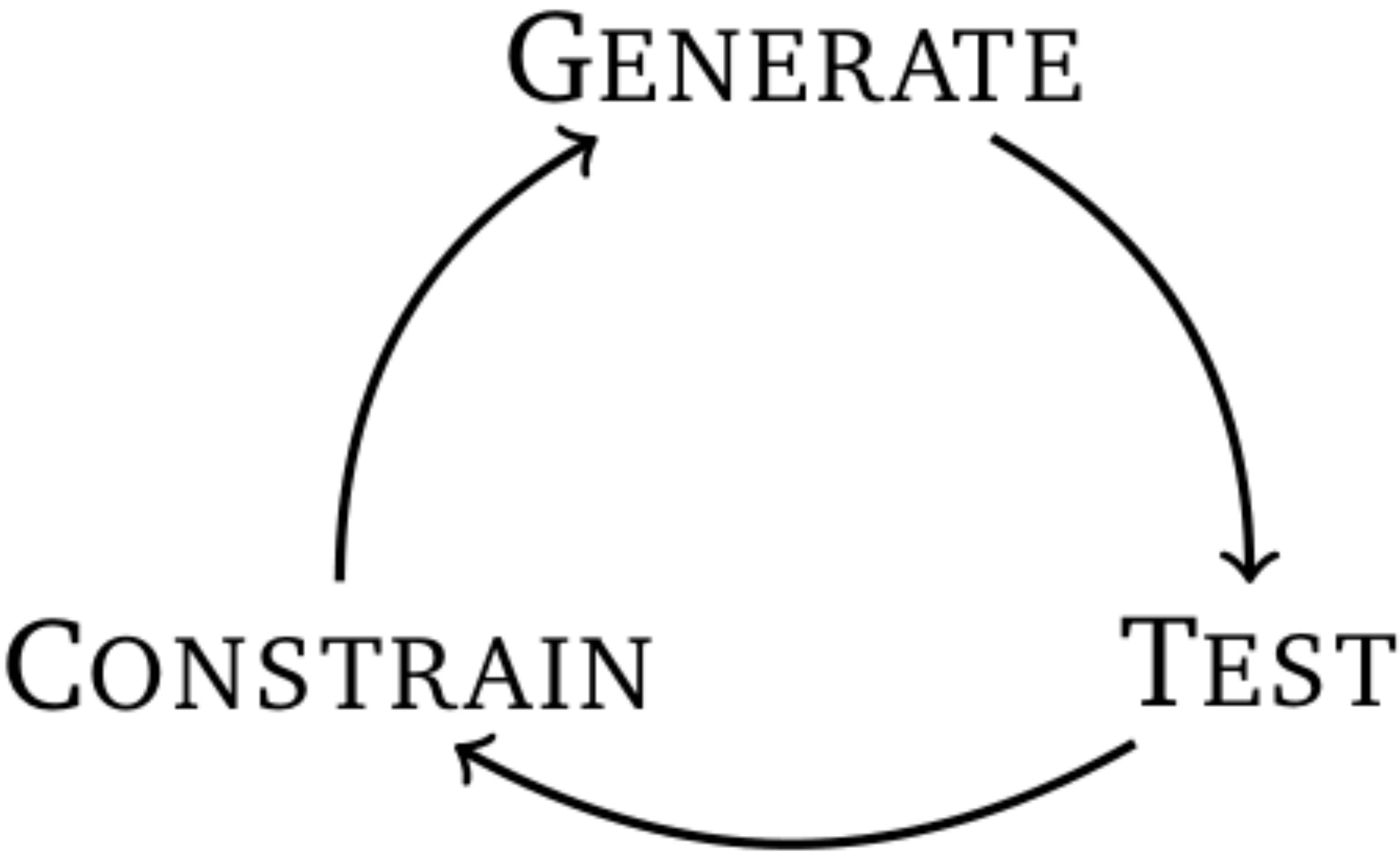
0. Start with a hypothesis space
1. Select a hypothesis
2. Empirically try to refute it
3. If the hypothesis is falsified, determine **why**

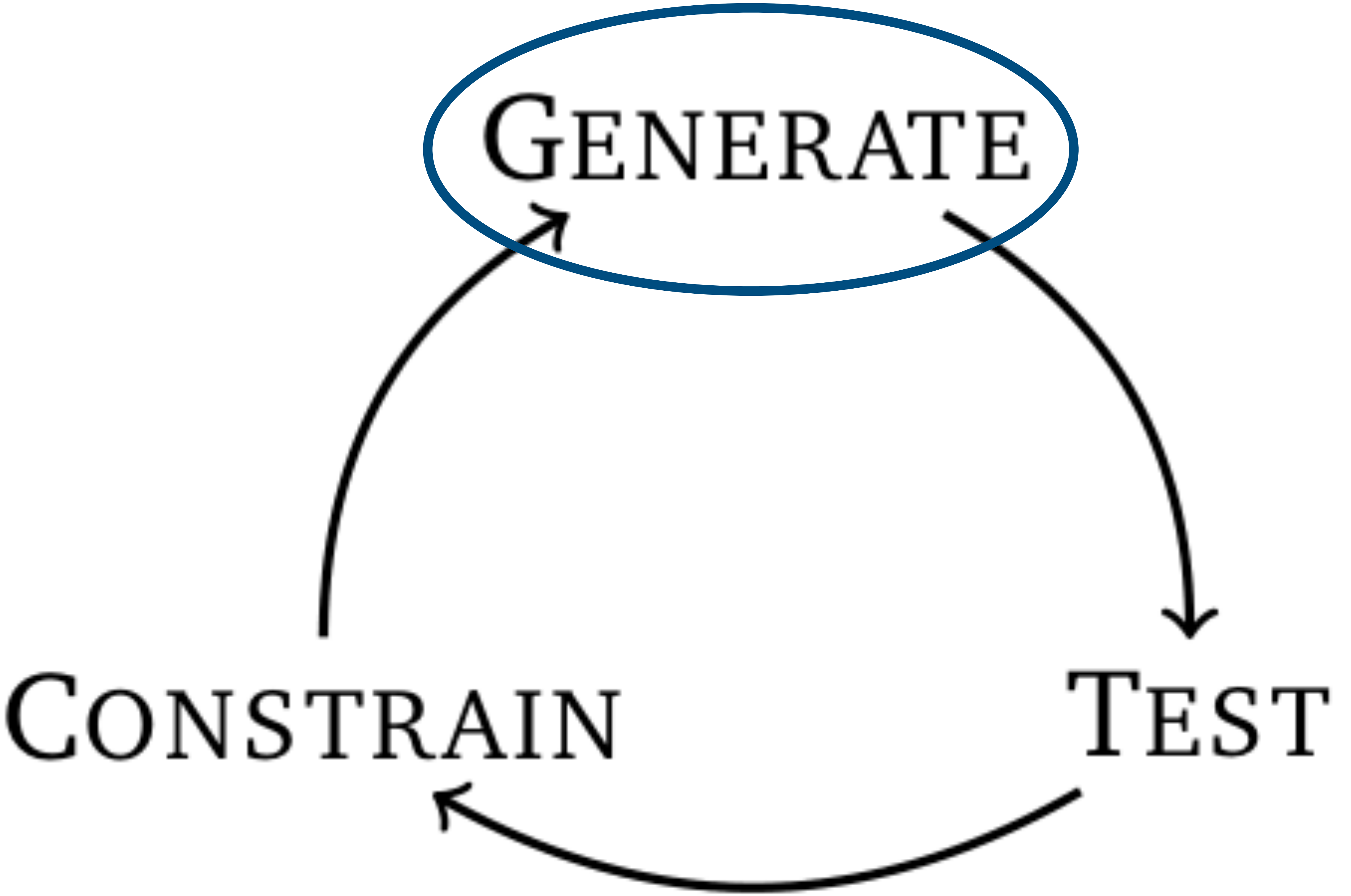
Popper

0. Start with a hypothesis space
1. Select a hypothesis
2. Empirically try to refute it
3. If the hypothesis is falsified, determine **why**
4. Use the **explanation** to prune the hypothesis space

Popper

0. Start with a hypothesis space
1. Select a hypothesis
2. Empirically try to refute it
3. If the hypothesis is falsified, determine **why**
4. Use the **explanation** to prune the hypothesis space
5. Go to 1


Generate
Test
Constrain



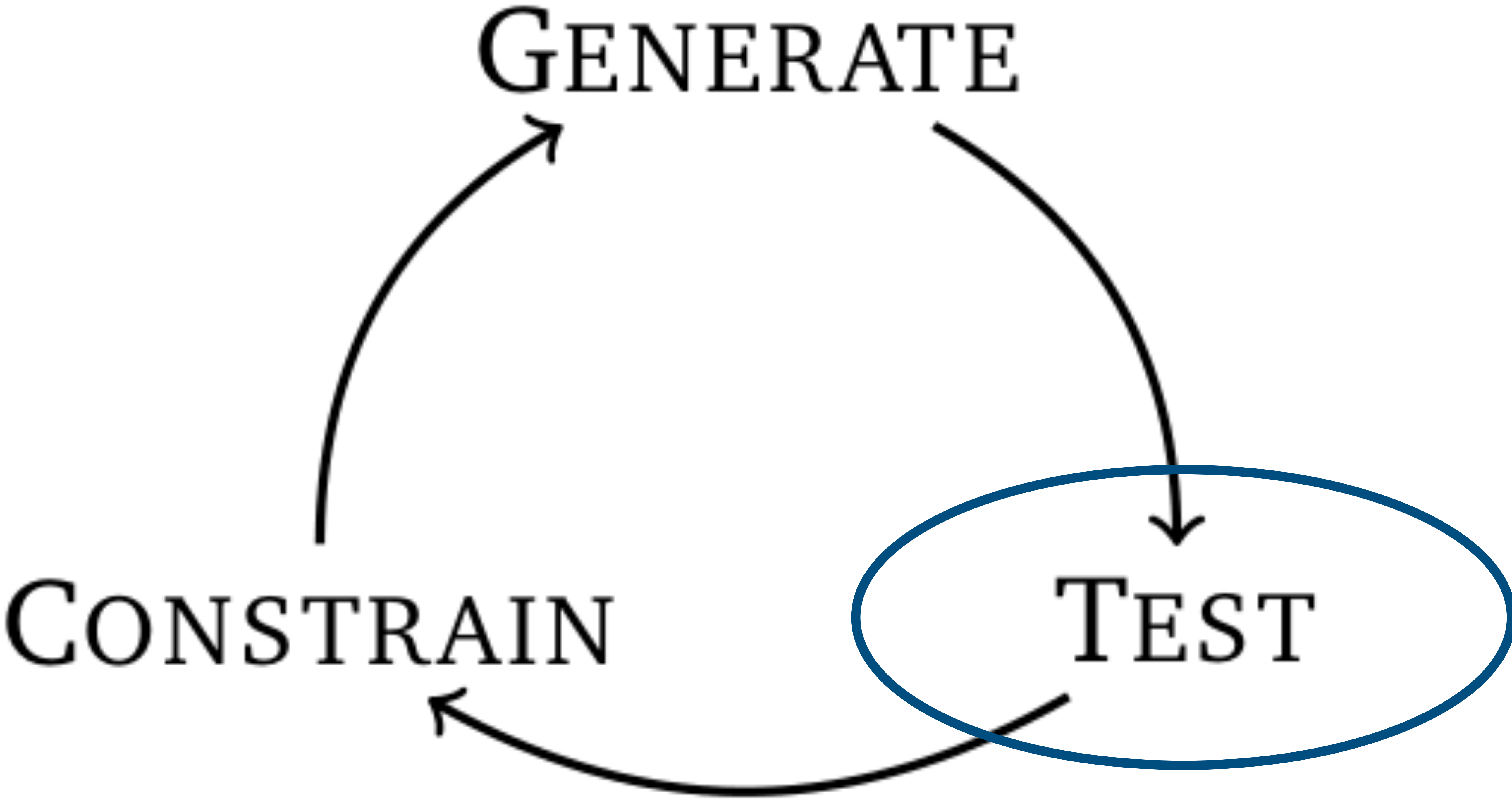
Generate
Test
Constrain

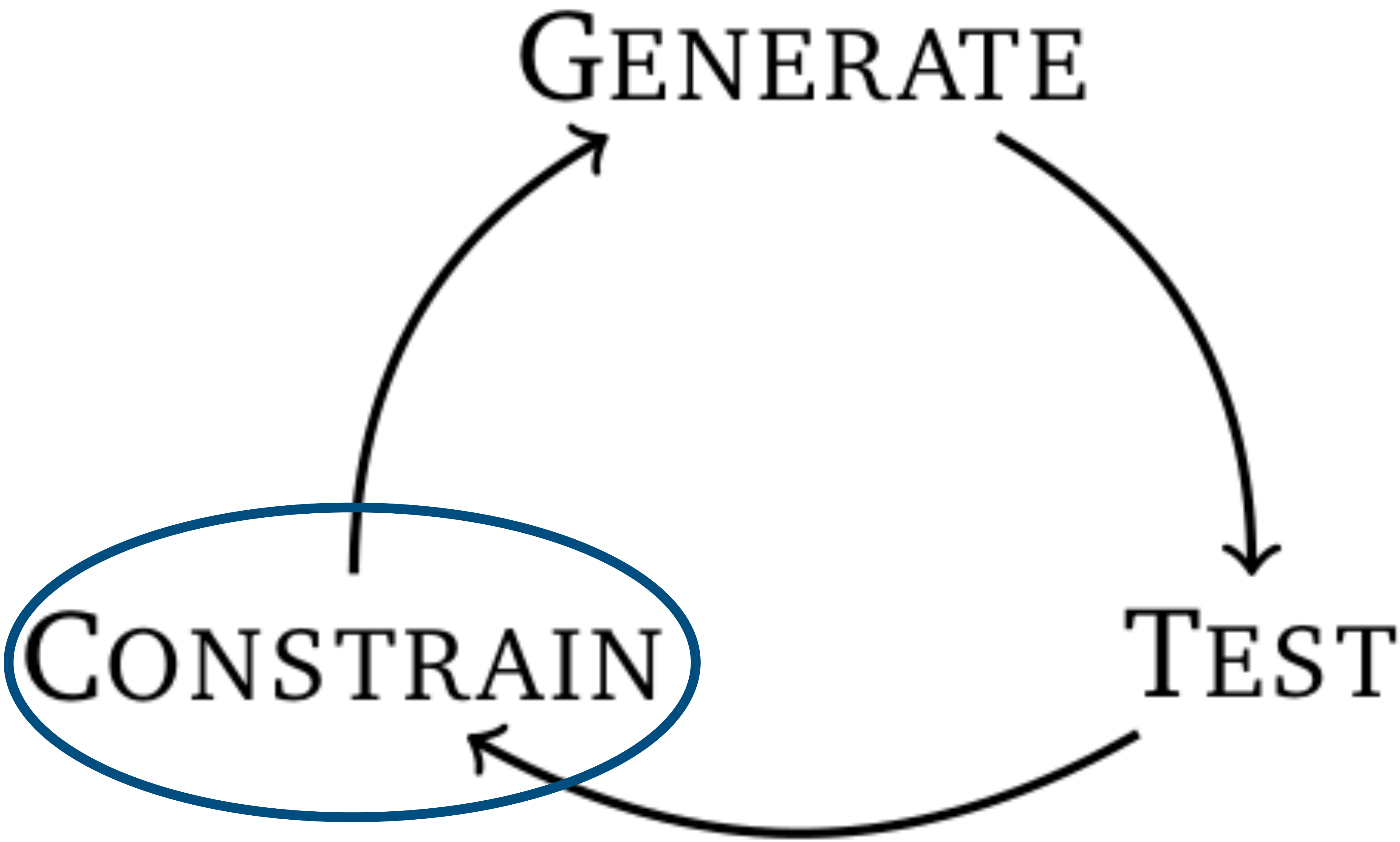
Generate

We construct a logical formula where every truth assignment is a hypothesis

Satisfiability problem

We ask a SAT solver to find a model/hypothesis


Generate
Constrain
Test


GENERATE
TEST
CONSTRAIN

Constrain

Adding constraints prunes models thus hypotheses

MLJ21, MLJ23, ECAI24

Popper can learn **recursive** hypotheses

MLJ 2021

Recursion

Grand challenge in ILP for 30 years


Edgware Road
Marylebone
St John's Wood
Euston
Edgware Road
Baker Street
Great Portland Street
Euston Square
Warren Street
Regent's Park
Goodge Street
Russell Square
Bayswater
Bond Street
Oxford Circus
Marble Arch
Notting Hill Gate
Tottenham Court Road
Holborn
Covent Garden
Lancaster Gate
Queensway
Green Park
Leicester Square
Hyde Park Corner
Piccadilly Circus
High Street Kensington
Knightsbridge
Charing Cross
Gloucester Road
Victoria
Westminster
Embankment
Earl's Court
South Kensington
Sloane Square
St James's Park
Temple

```
edge(oxford_circus, bond_street).
edge(oxford_circus, piccadilly_circus).
edge(south_kensington, gloucester_road).
```

Old ILP

```
connected(A,B):-?
```

Old ILP

```
connected(A,B):- edge(A,B).
```

A and B are connected if there is an edge between them

Old ILP

```
connected(A,B):- edge(A,C),edge(C,B).
```

A and B are connected via an intermediate edge C

Old ILP

```
connected(A,B):- edge(A,C),edge(C,D),edge(D,B).
```

A and B are connected via intermediate edges C and D

Old ILP

```
connected(A,B):- edge(A,B).
connected(A,B):- edge(A,C),edge(C,B).
connected(A,B):- edge(A,C),edge(C,D),edge(D,B).
connected(A,B):- edge(A,C),edge(C,D),edge(D,E),edge(E,B).
….. .
```

Old ILP

```
connected(A,B):- edge(A,B).
connected(A,B):- edge(A,C),edge(C,B).
connected(A,B):- edge(A,C),edge(C,D),edge(D,B).
connected(A,B):- edge(A,C),edge(C,D),edge(D,E),edge(E,B).
….. .
```

Cannot generalise to arbitrary depth

Old ILP

```
connected(A,B):- edge(A,B).
connected(A,B):- edge(A,C),edge(C,B).
connected(A,B):- edge(A,C),edge(C,D),edge(D,B).
connected(A,B):- edge(A,C),edge(C,D),edge(D,E),edge(E,B).
….. .
```

Difficult to learn because of its size

Old ILP

```
connected(A,B):- edge(A,B).
connected(A,B):- edge(A,C),edge(C,B).
connected(A,B):- edge(A,C),edge(C,D),edge(D,B).
connected(A,B):- edge(A,C),edge(C,D),edge(D,E),edge(E,B).
…. . .
```

Need to see an example of all path lengths

Popper

```
connected(A,B):- edge(A,B).
```

A and B are connected if there is an edge between them

Popper

```
connected(A,B):- edge(A,C),connected(C,B).
```

A and B are connected if there is an edge between A and C and C is **connected** to B

Popper

```
connected(A,B):- edge(A,B).
connected(A,B):- edge(A,C),connected(C,B).
```

Generalises to arbitrary depth

Popper

```
connected(A,B):- edge(A,B).
connected(A,B):- edge(A,C),connected(C,B).
```

Reduces sample complexity