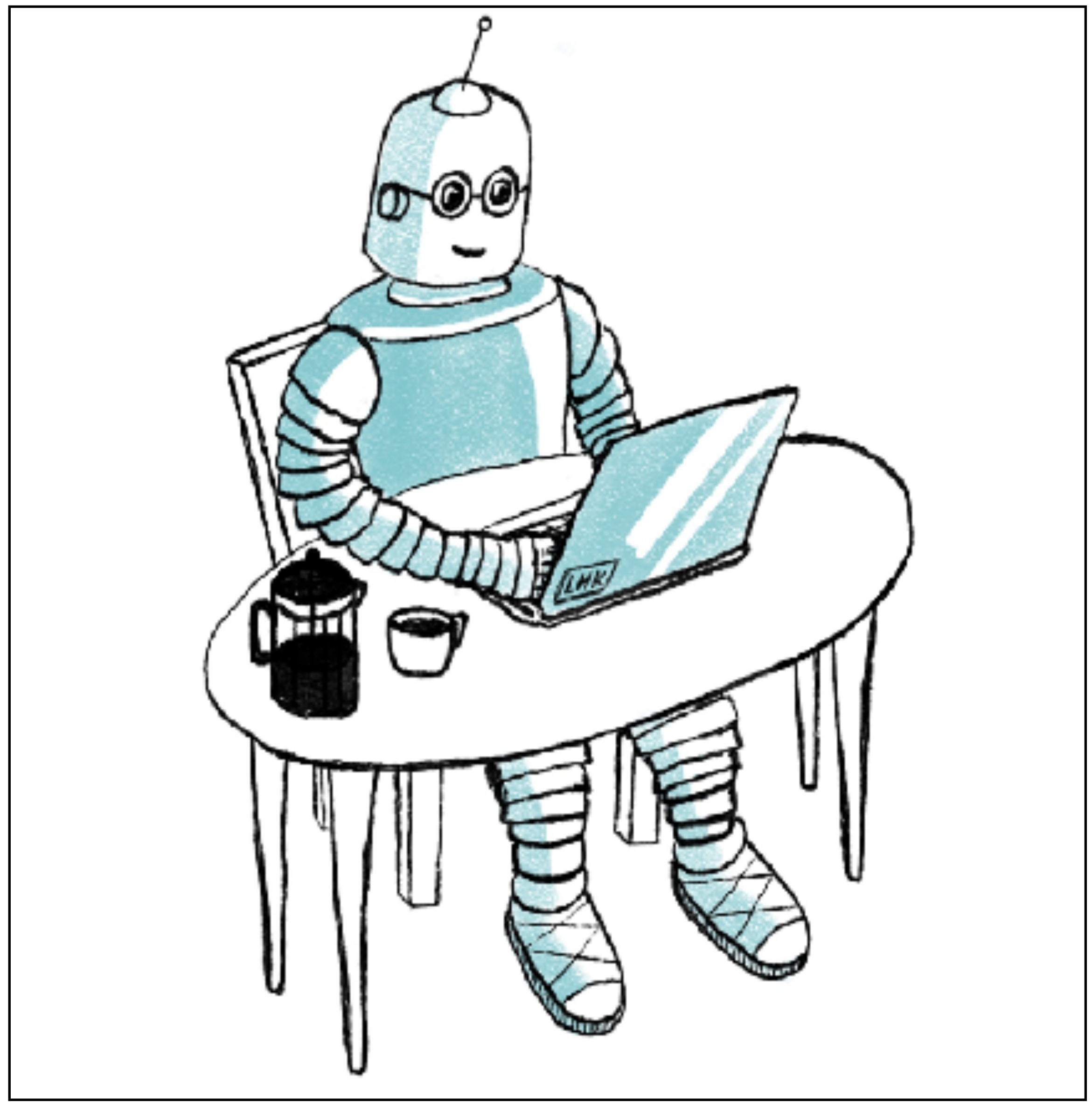
# Logical scientific discovery



Andrew Cropper

# My long-term goal

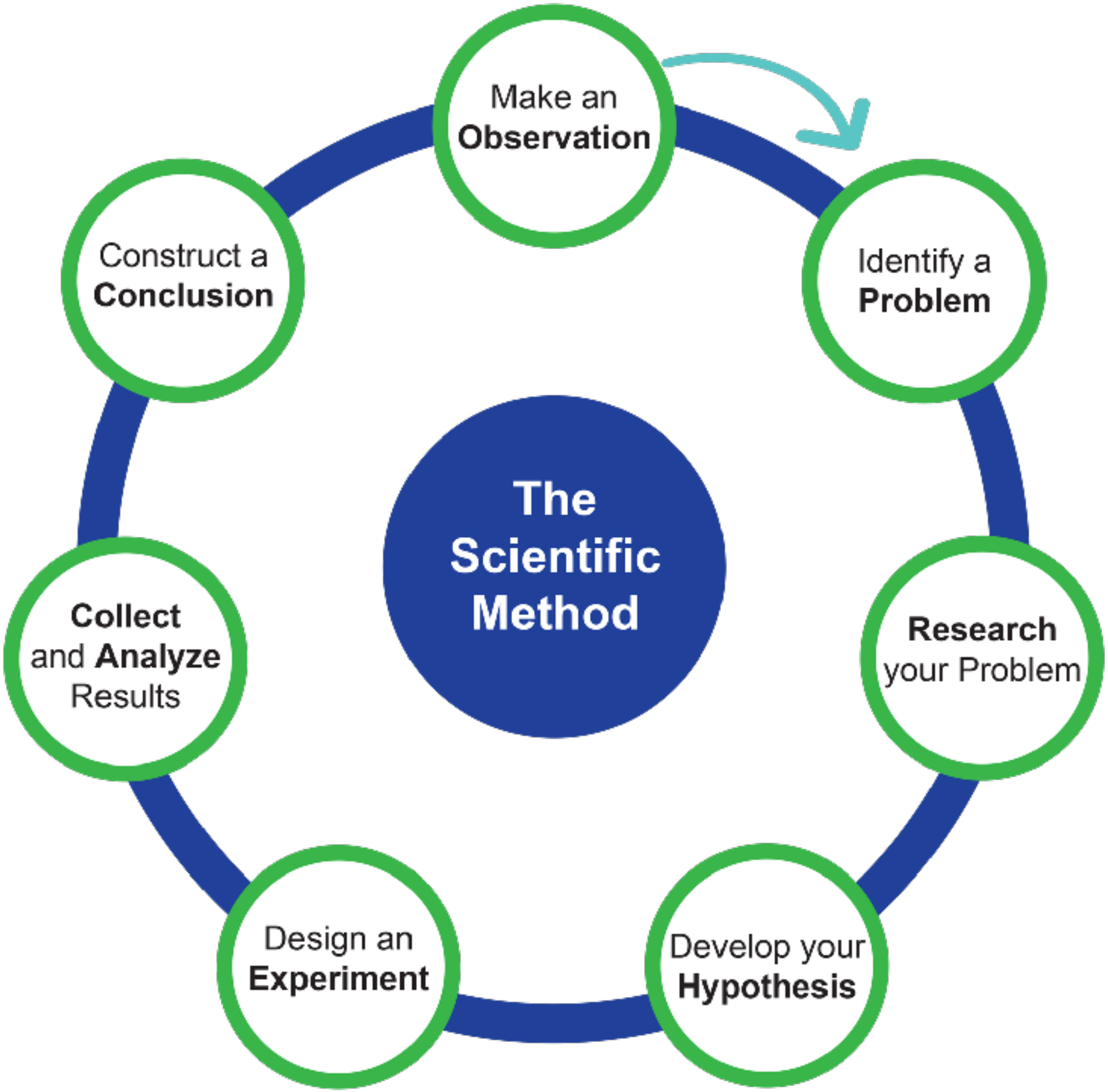
Accelerate scientific discovery

# Why?

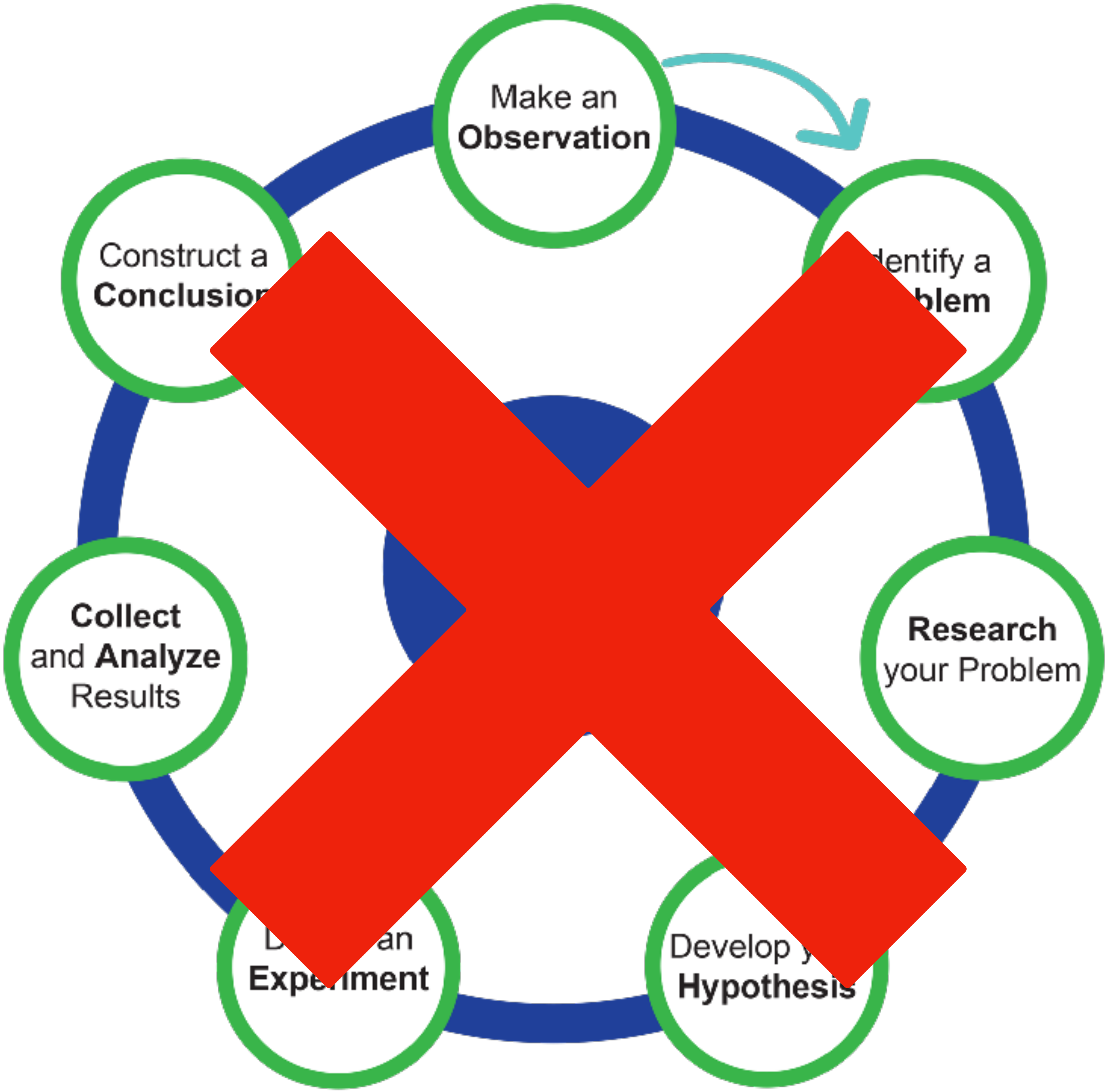
Science is important


SINGLE USE ONLY
Antibiotics

What exactly do I want to do?

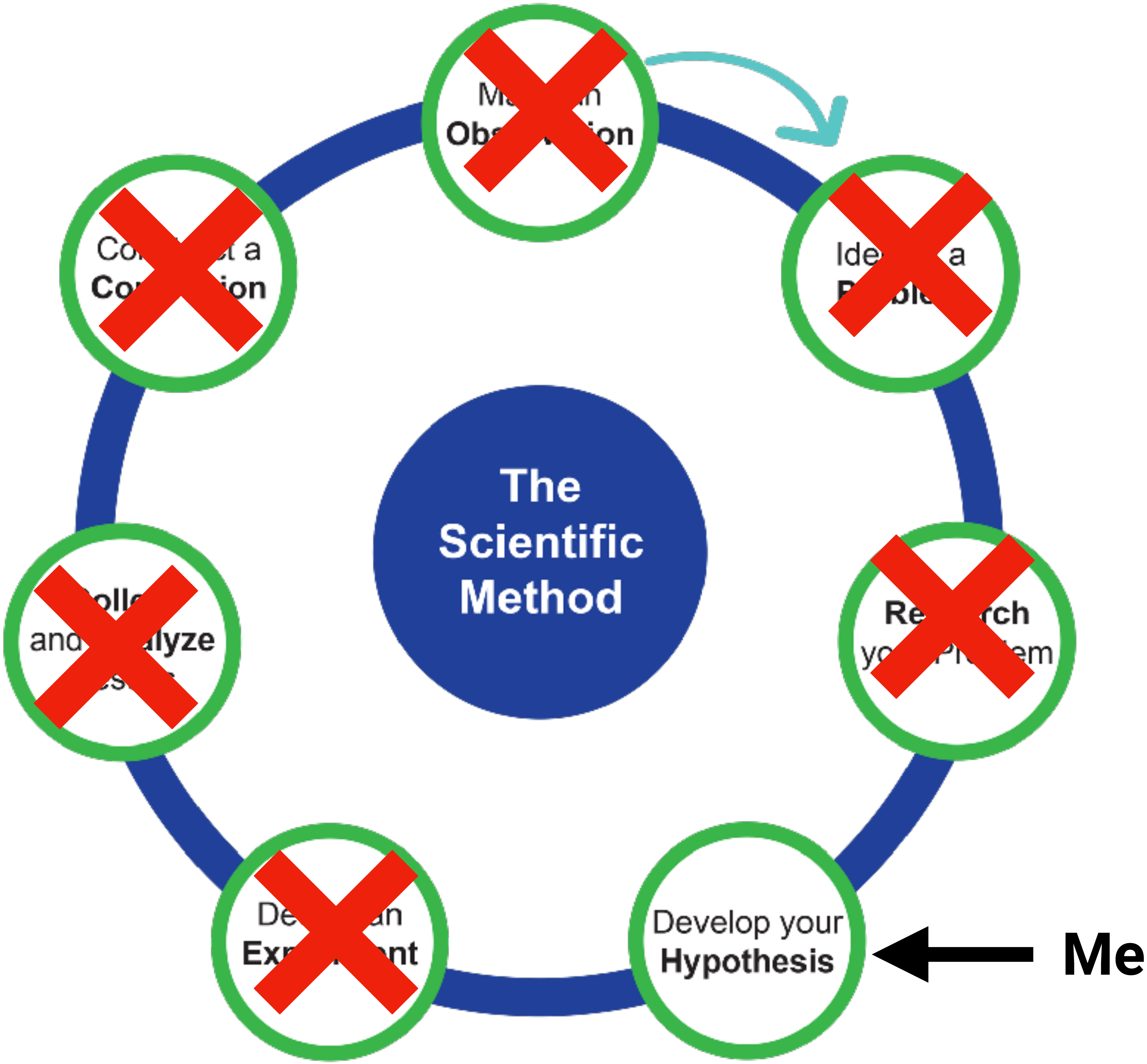


The Scientific Method
Make an Observation
Identify a Problem
Research your Problem
Develop your Hypothesis
Design an Experiment
Collect and Analyze Results
Construct a Conclusion


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

# Robot scientist

# Robot scientist


The Scientific Method
Develop your Hypothesis
Me

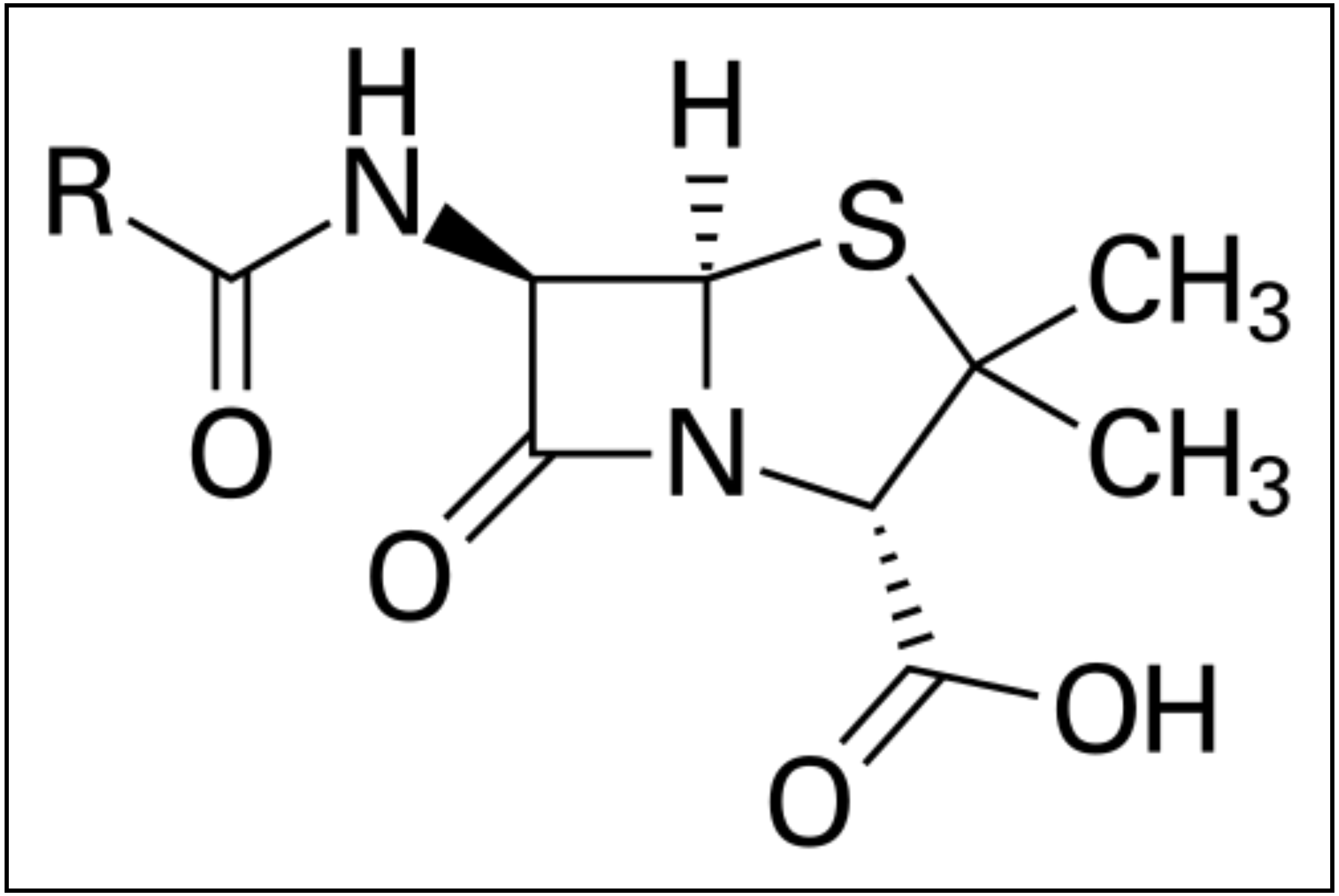
# My research

# My research

Prior knowledge

# My research

Prior knowledge



# My research

Observations

# My research


Observations

# My research

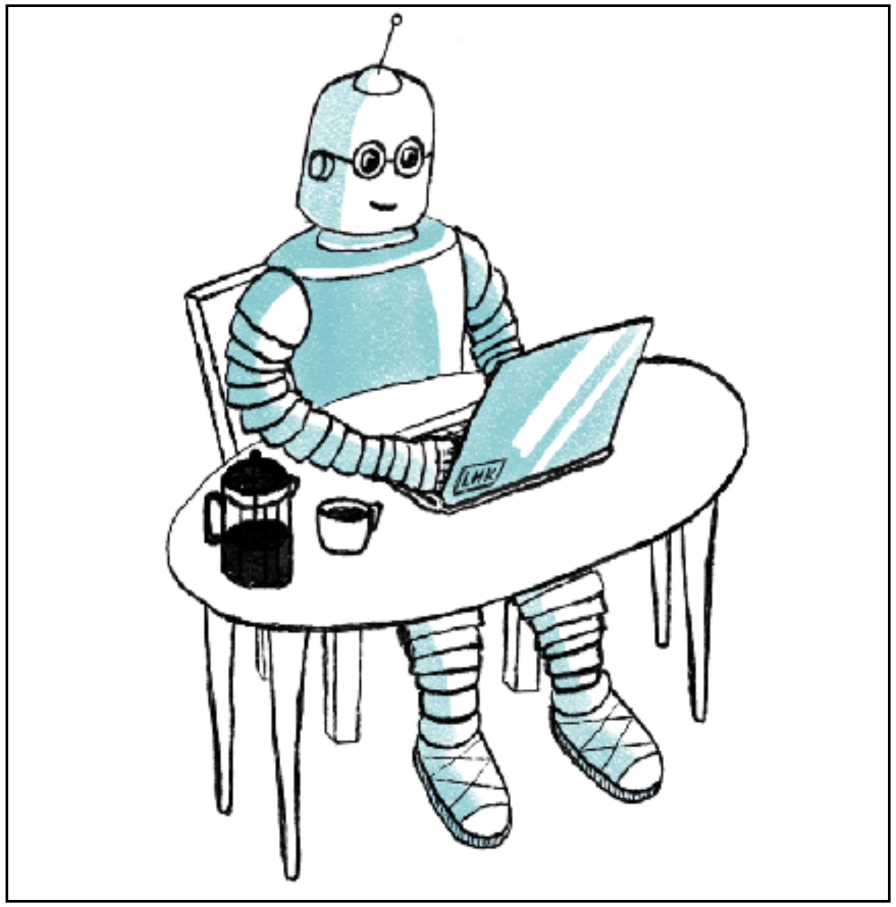
Prior knowledge

Observations

# My research

Prior knowledge

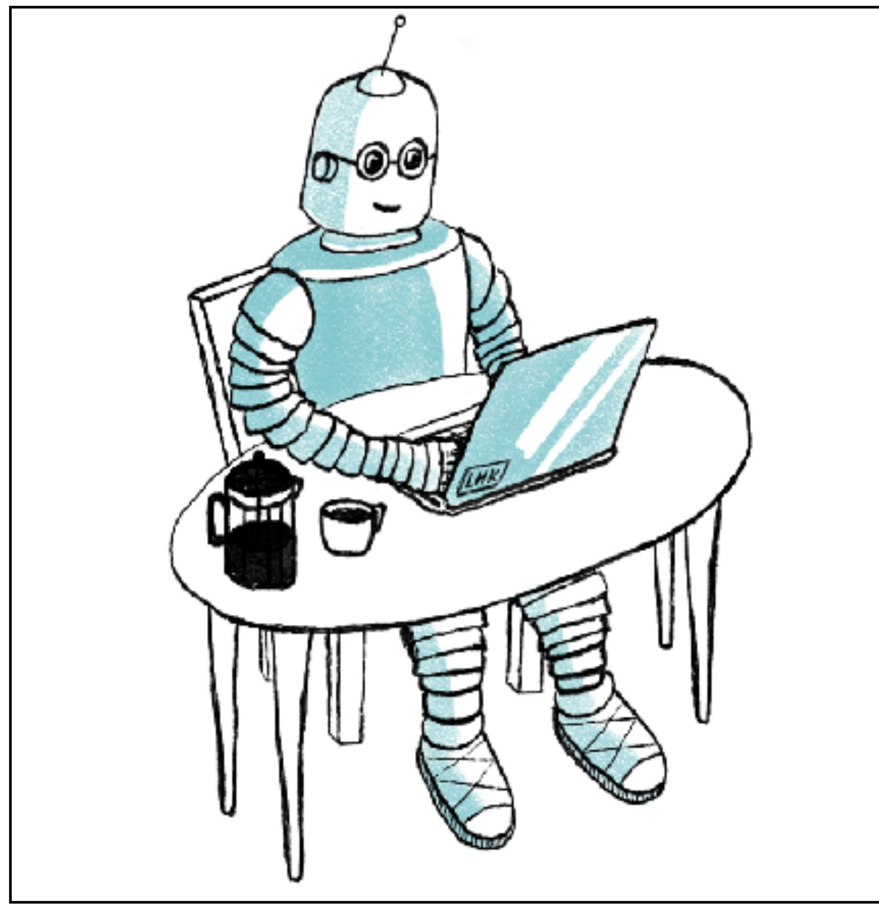
Observations



# My research

Prior knowledge

Observations

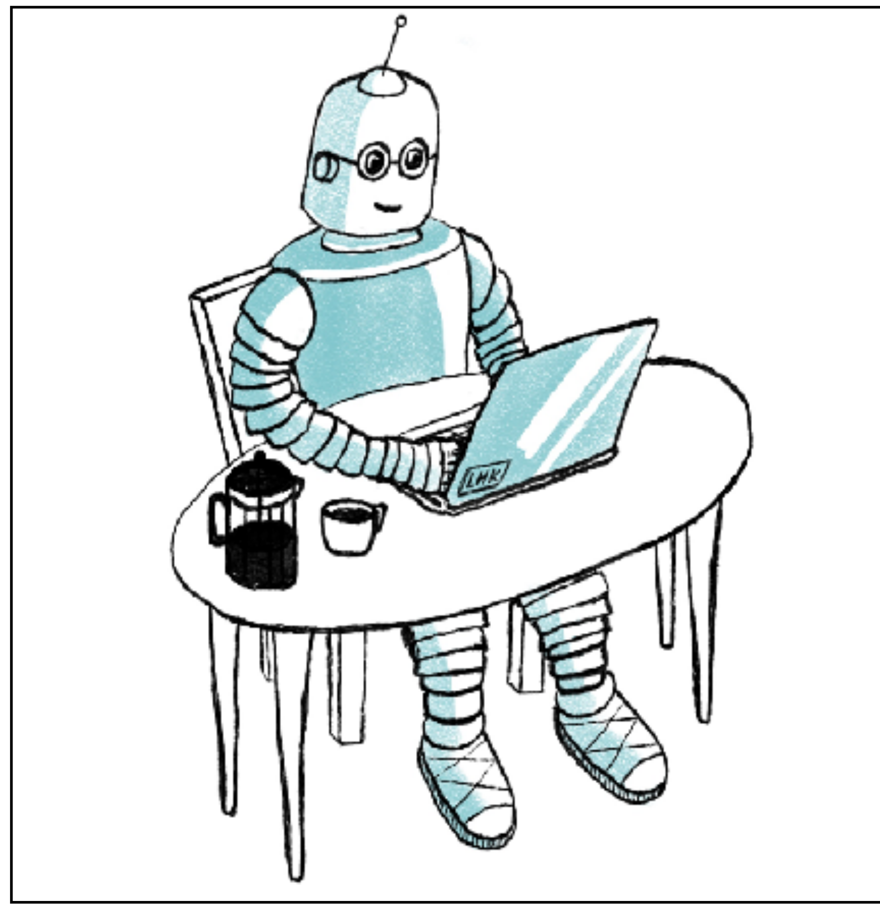


Hypothesis

# My research

Prior knowledge

Observations



Explanation

# 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

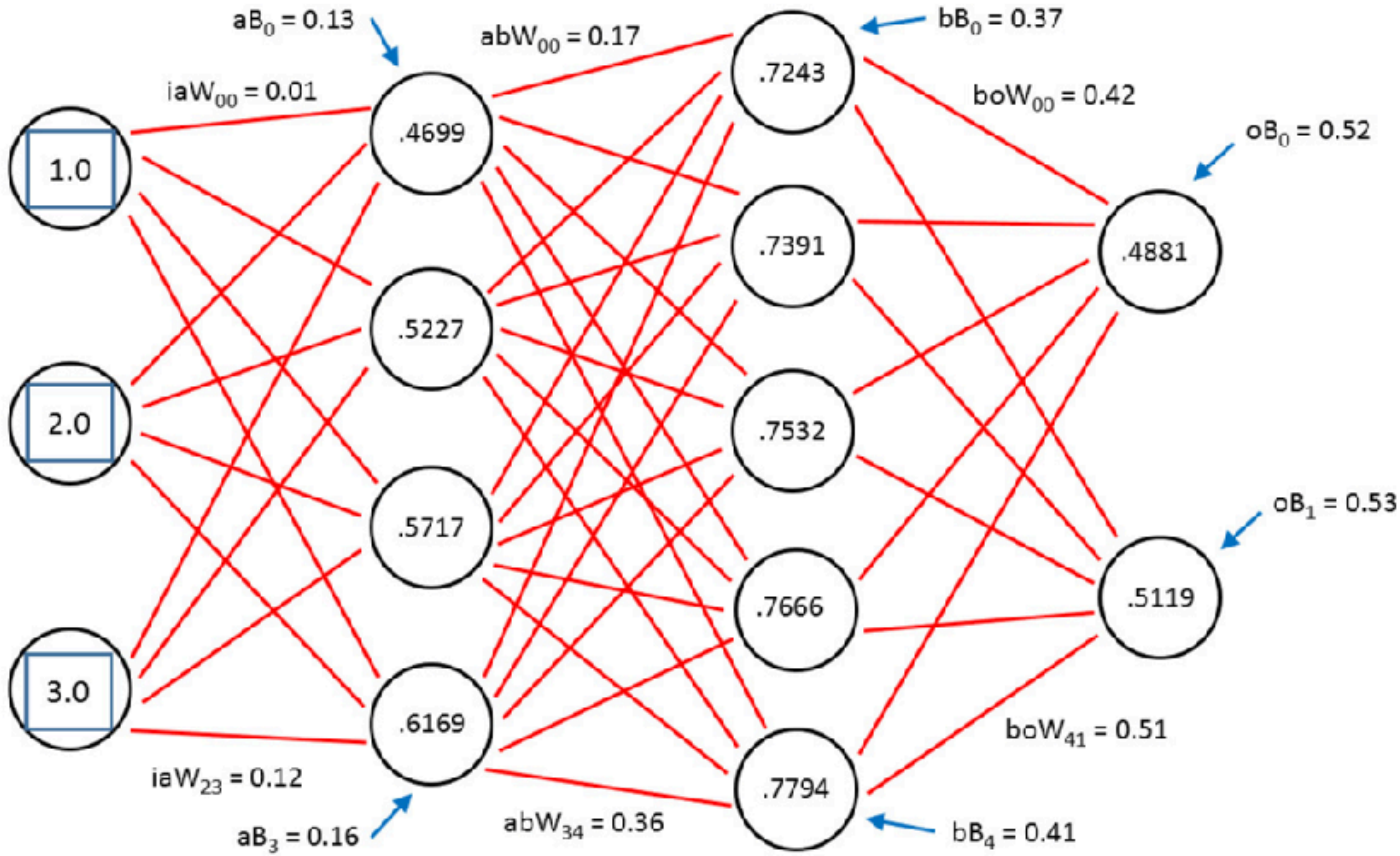

MasterControl

# Explainability

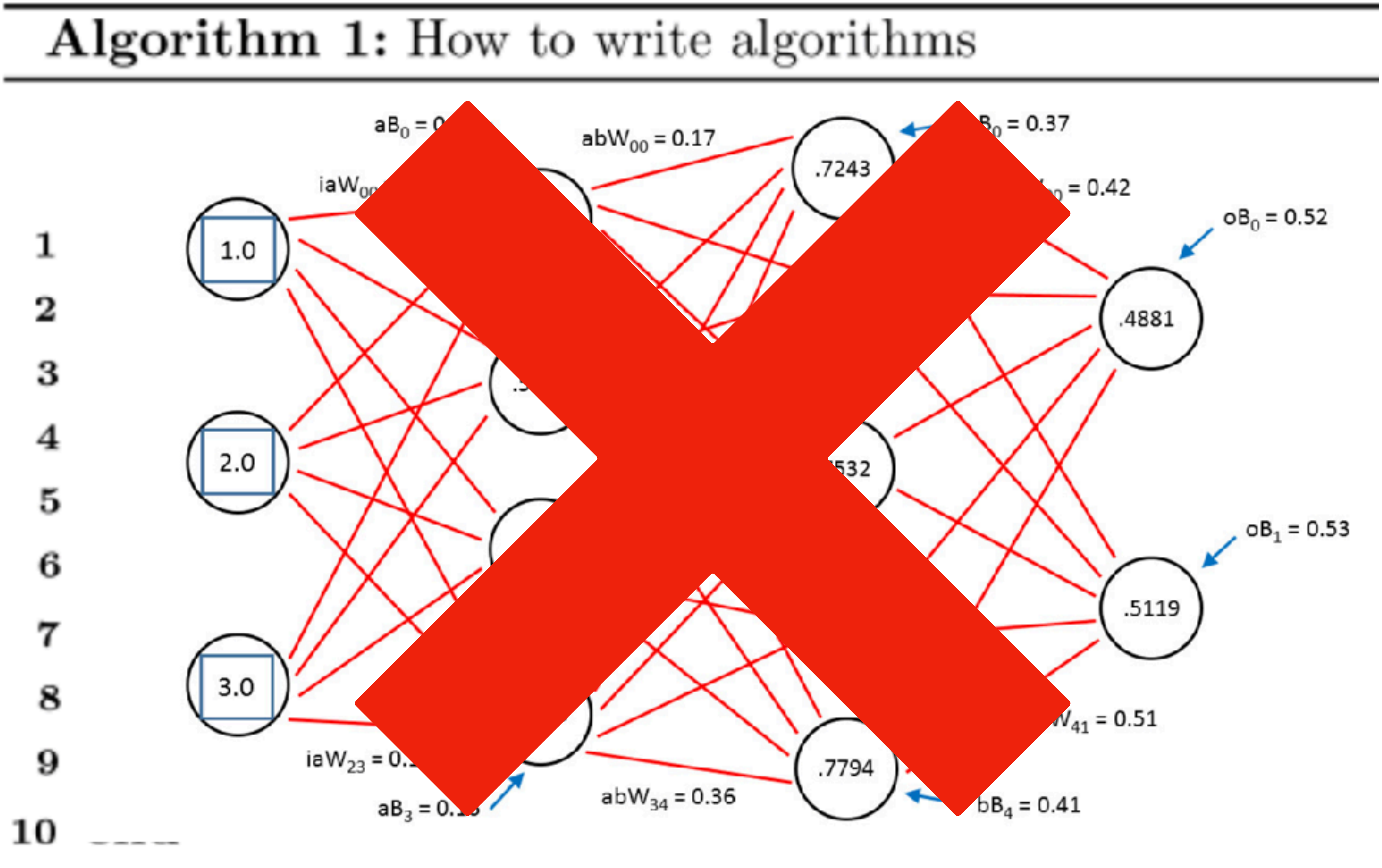
To publish a discovery, we must **explain** it

# Explainability

**Algorithm 1:** How to write algorithms

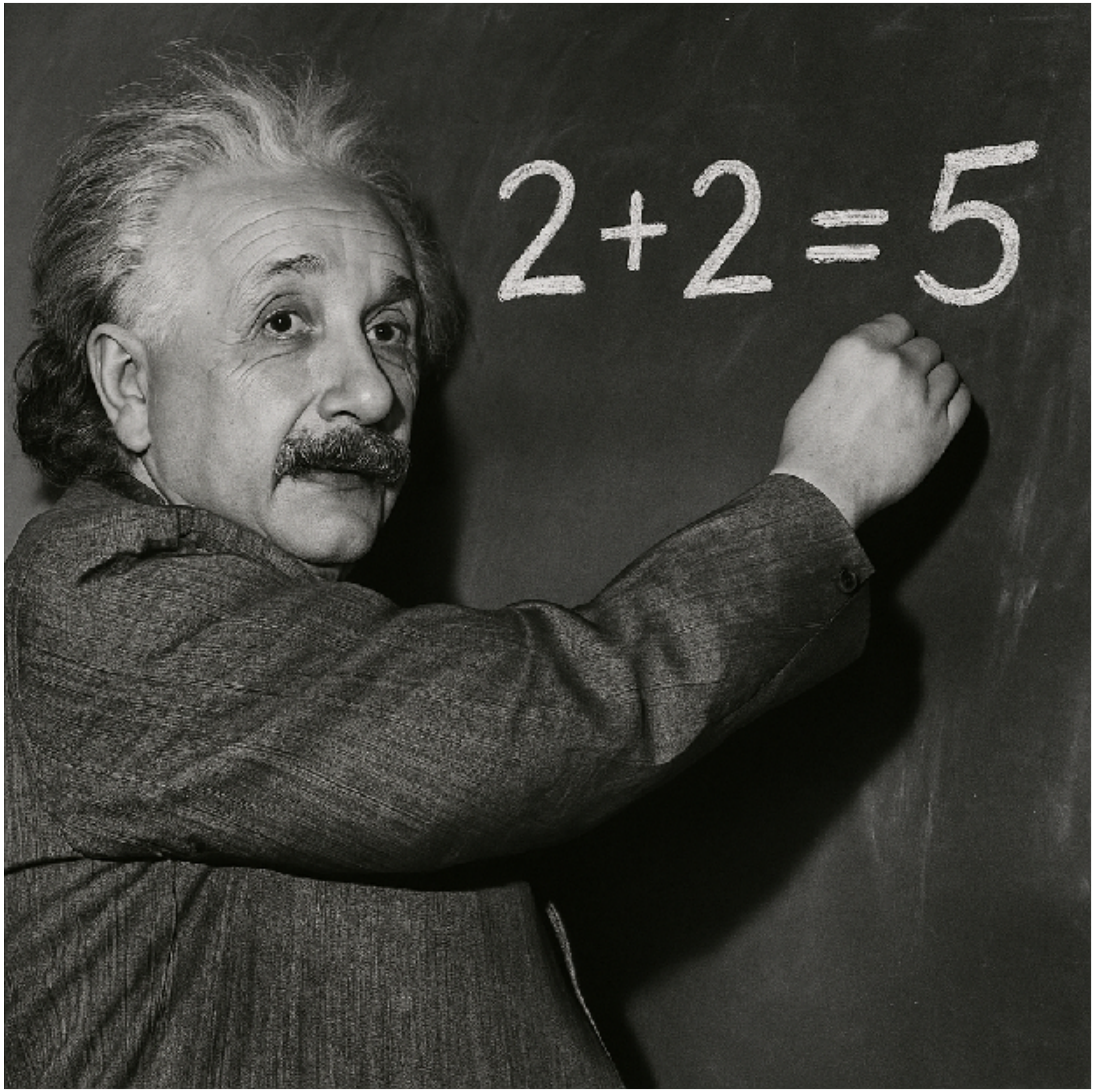


# Explainability

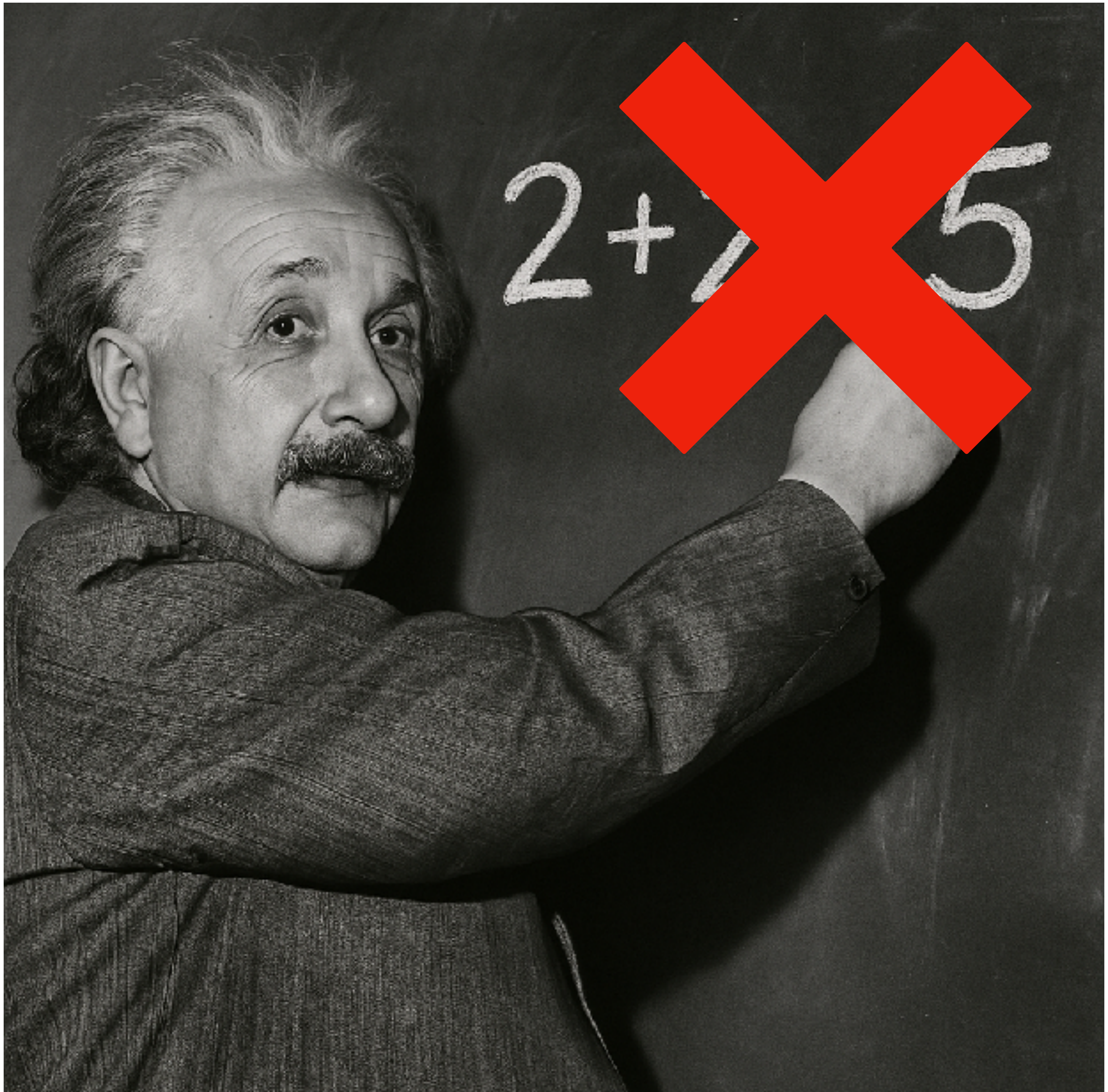


# Trustworthy

# 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

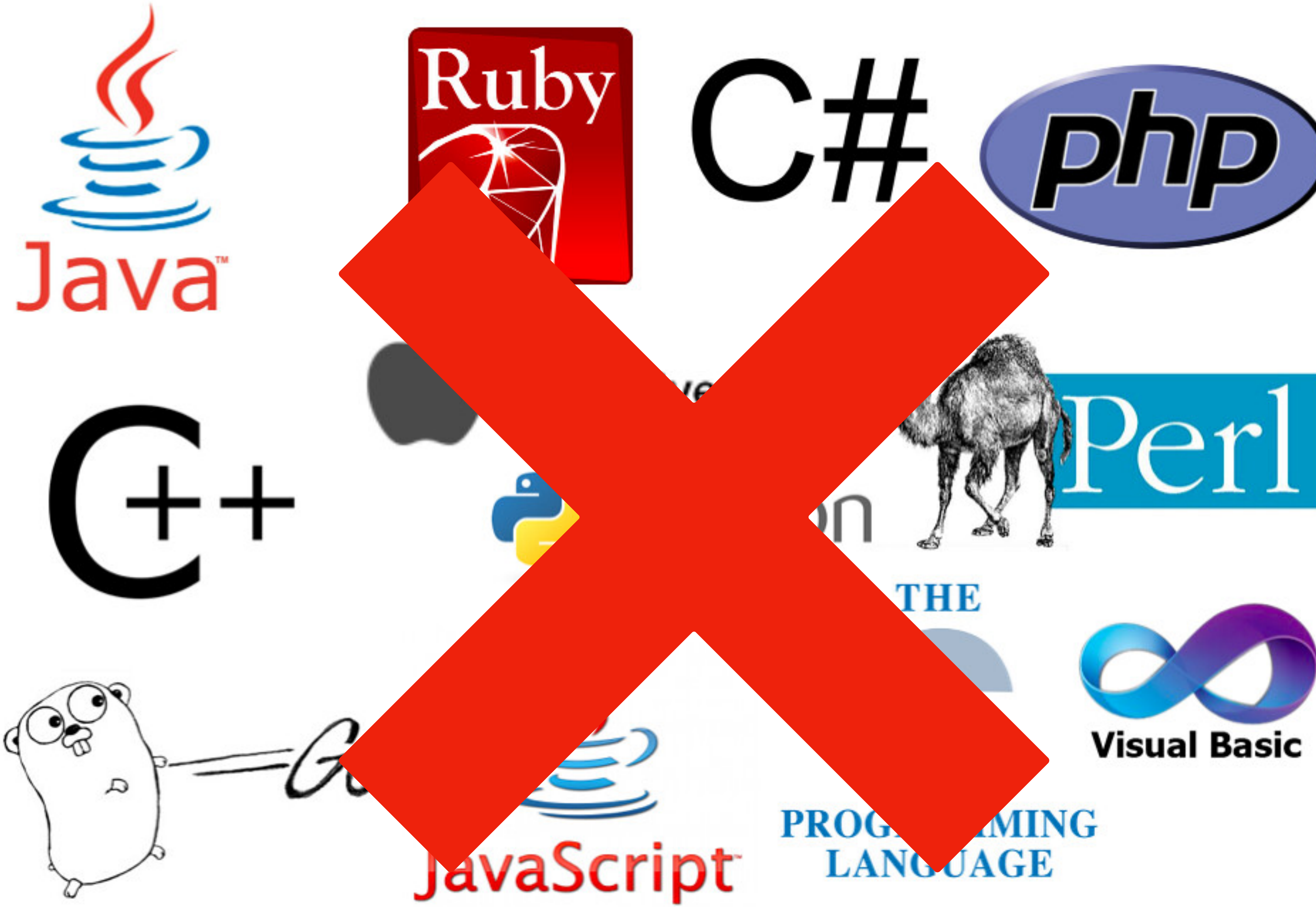
We will create AIs that are secure, give trustworthy results, preserve privacy, are fair, and whose use is ethically sustainable. We will develop the required privacy-preserving and secure methods to address challenges related to susceptibility to manipulation, information stealing and unethical approaches. 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

# Logical machine learning

# Inductive logic programming

# Inductive logic programming

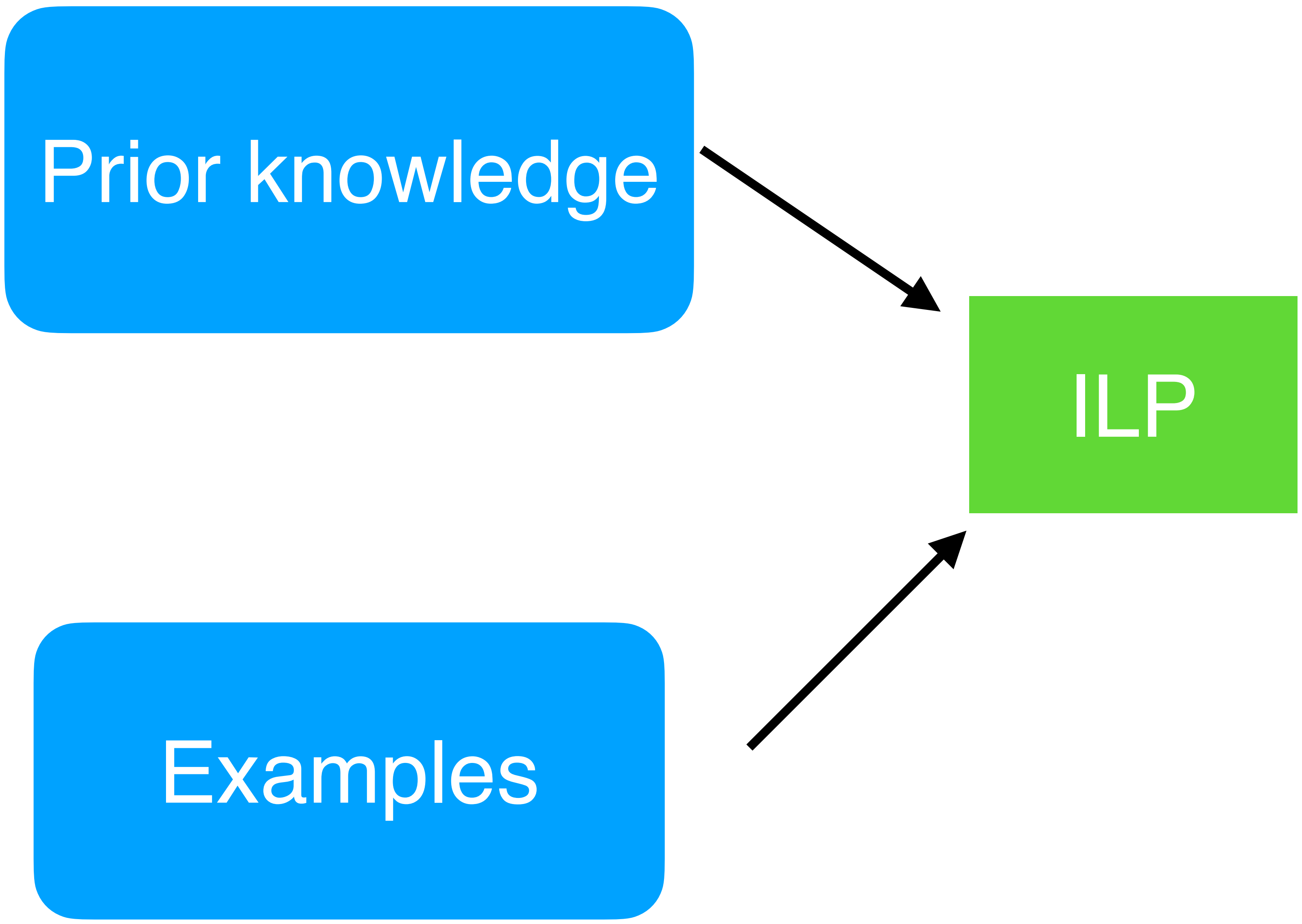
Prior knowledge

# Inductive logic programming

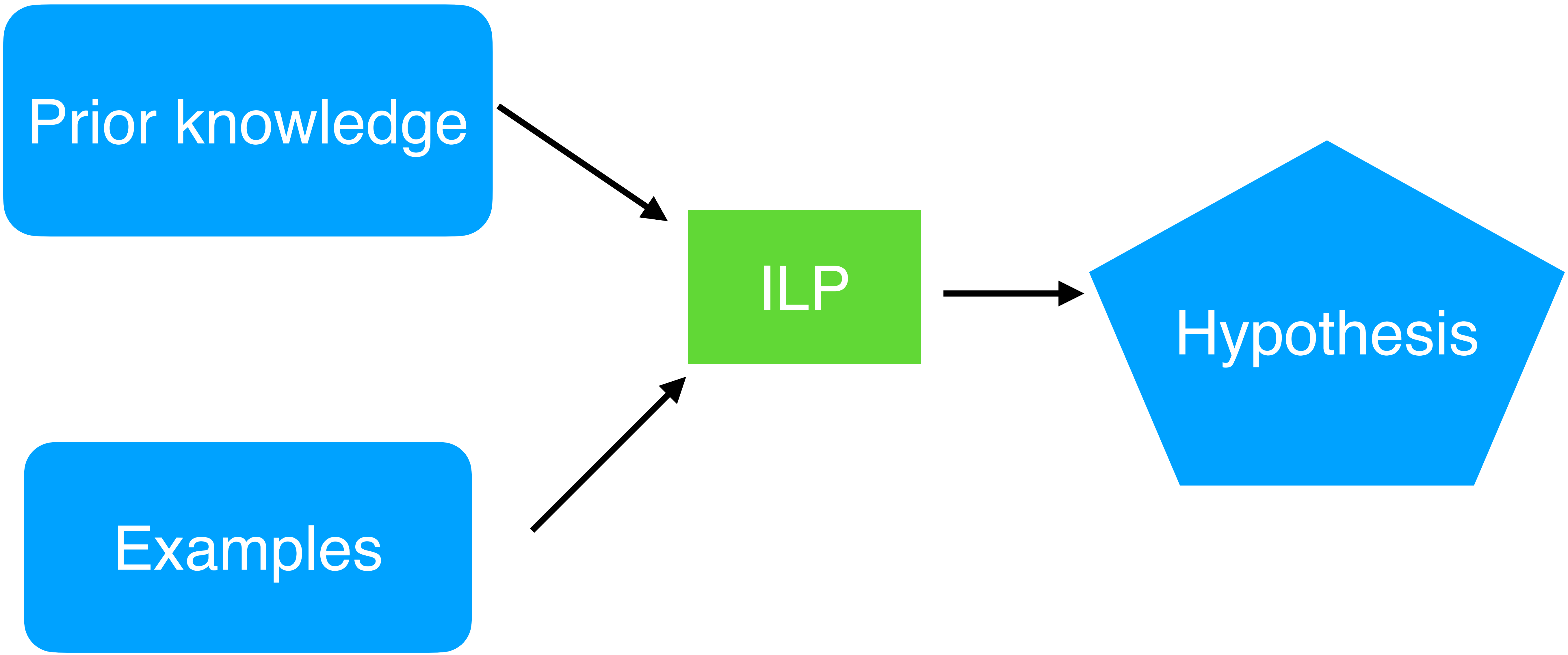
Prior knowledge

Examples

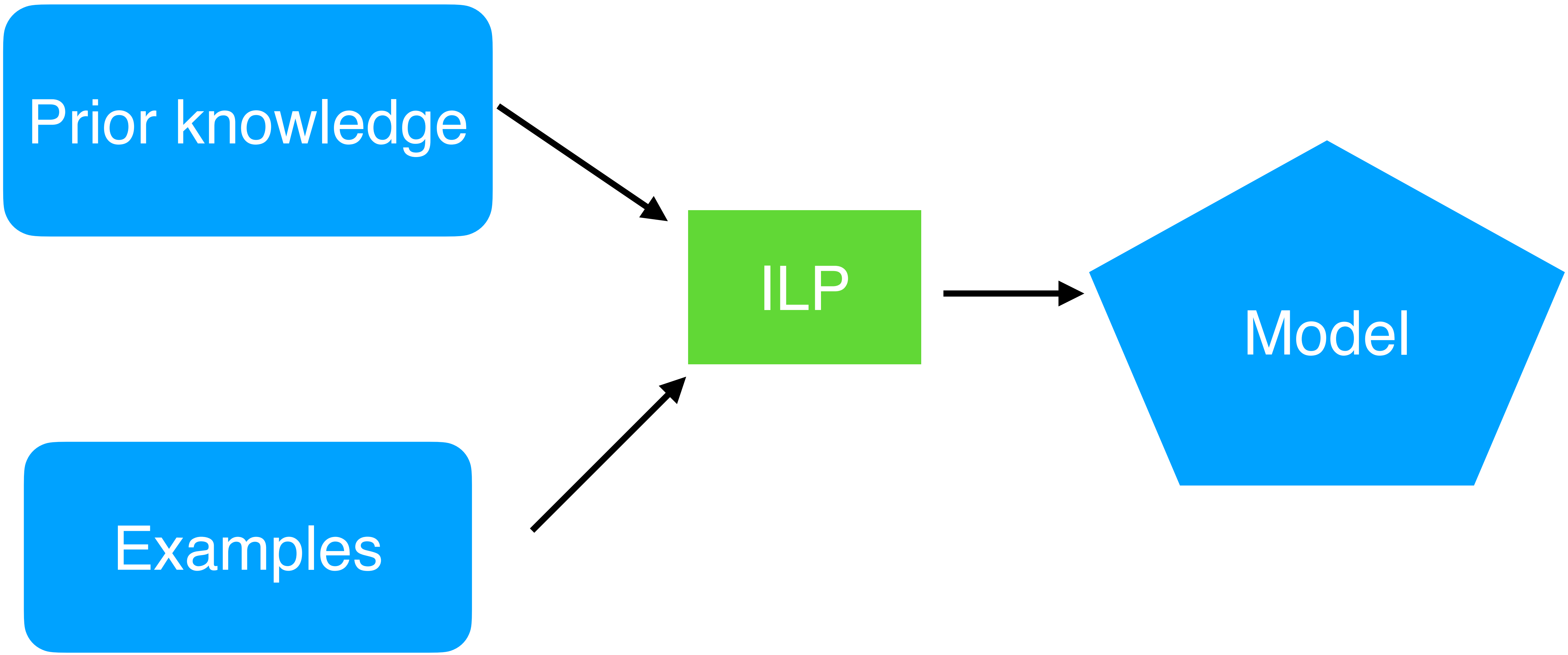
# Inductive logic programming



# Inductive logic programming

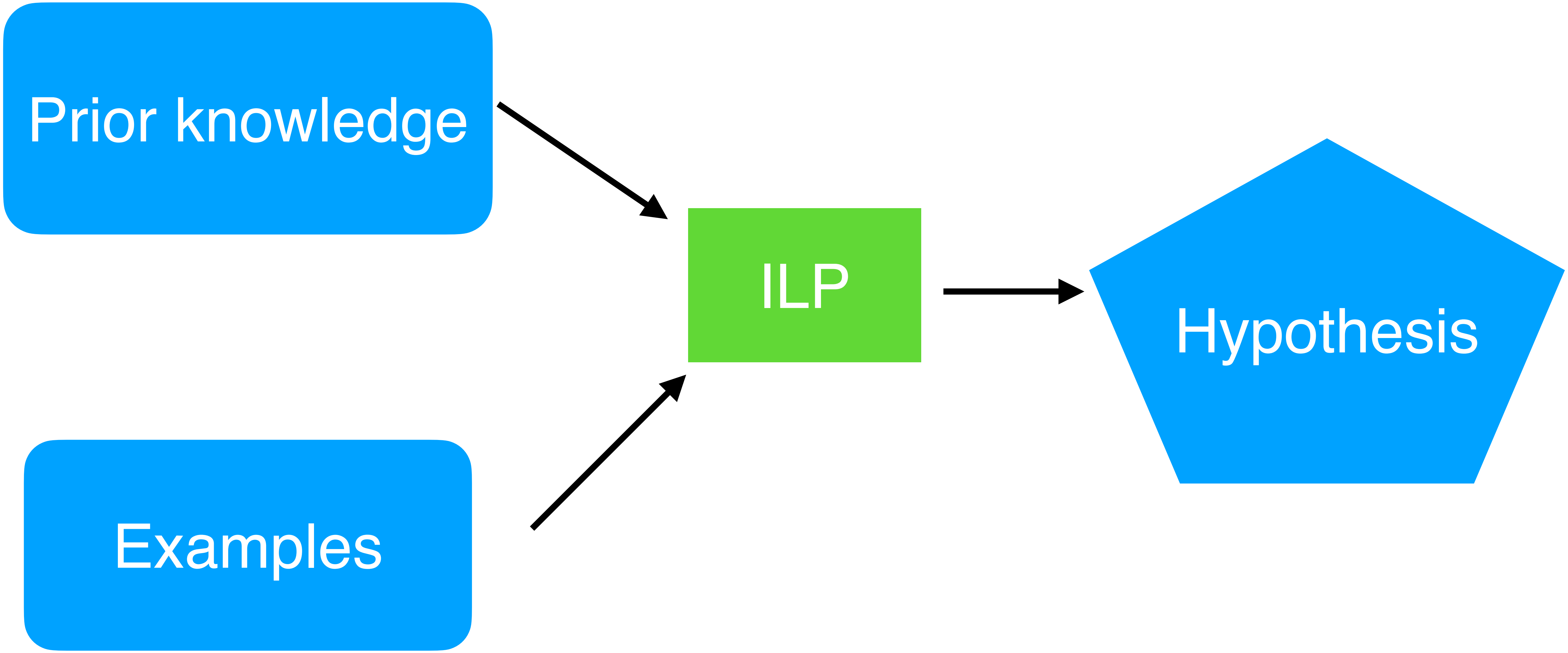


# Inductive logic programming



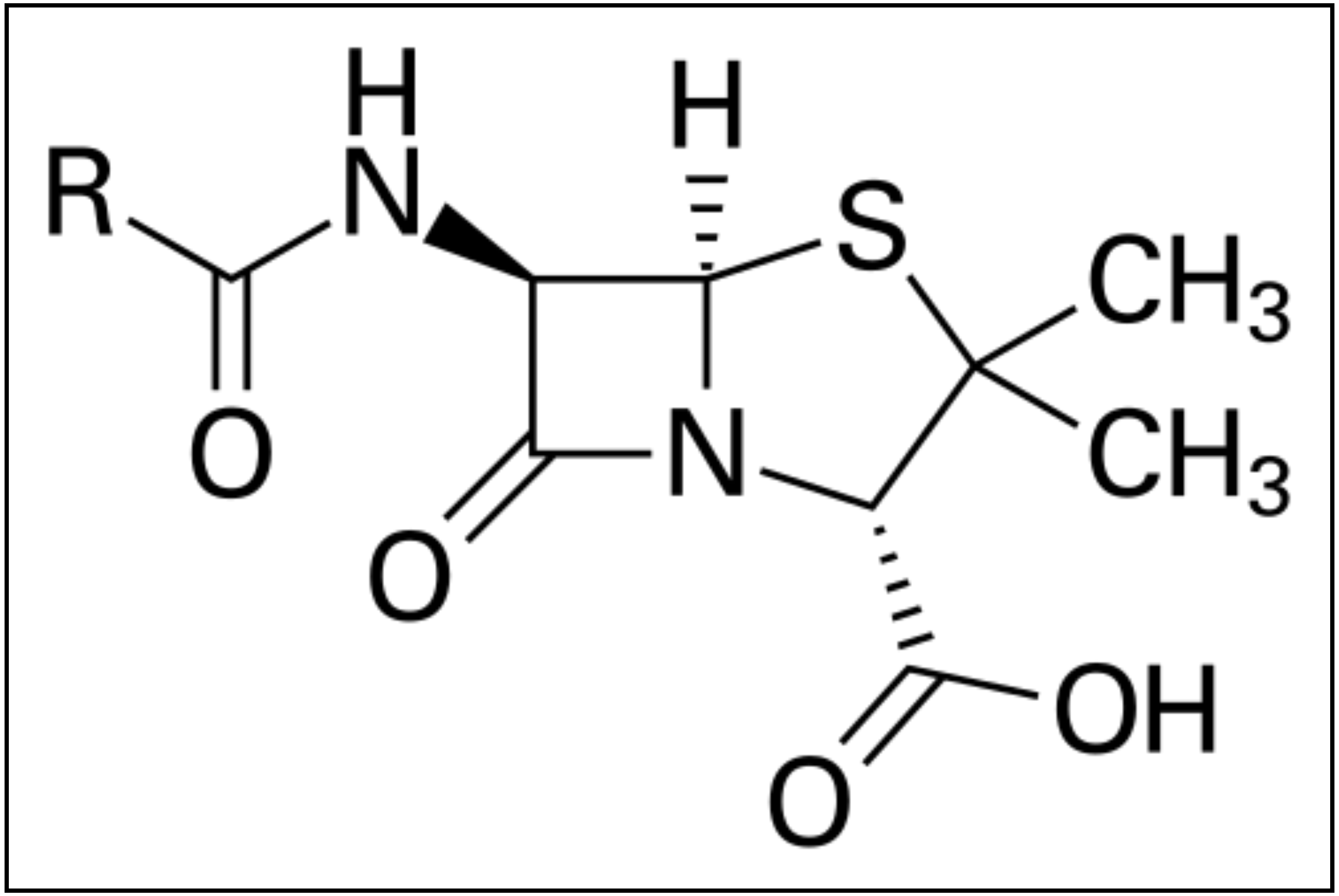

**Supervised machine learning**

# 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

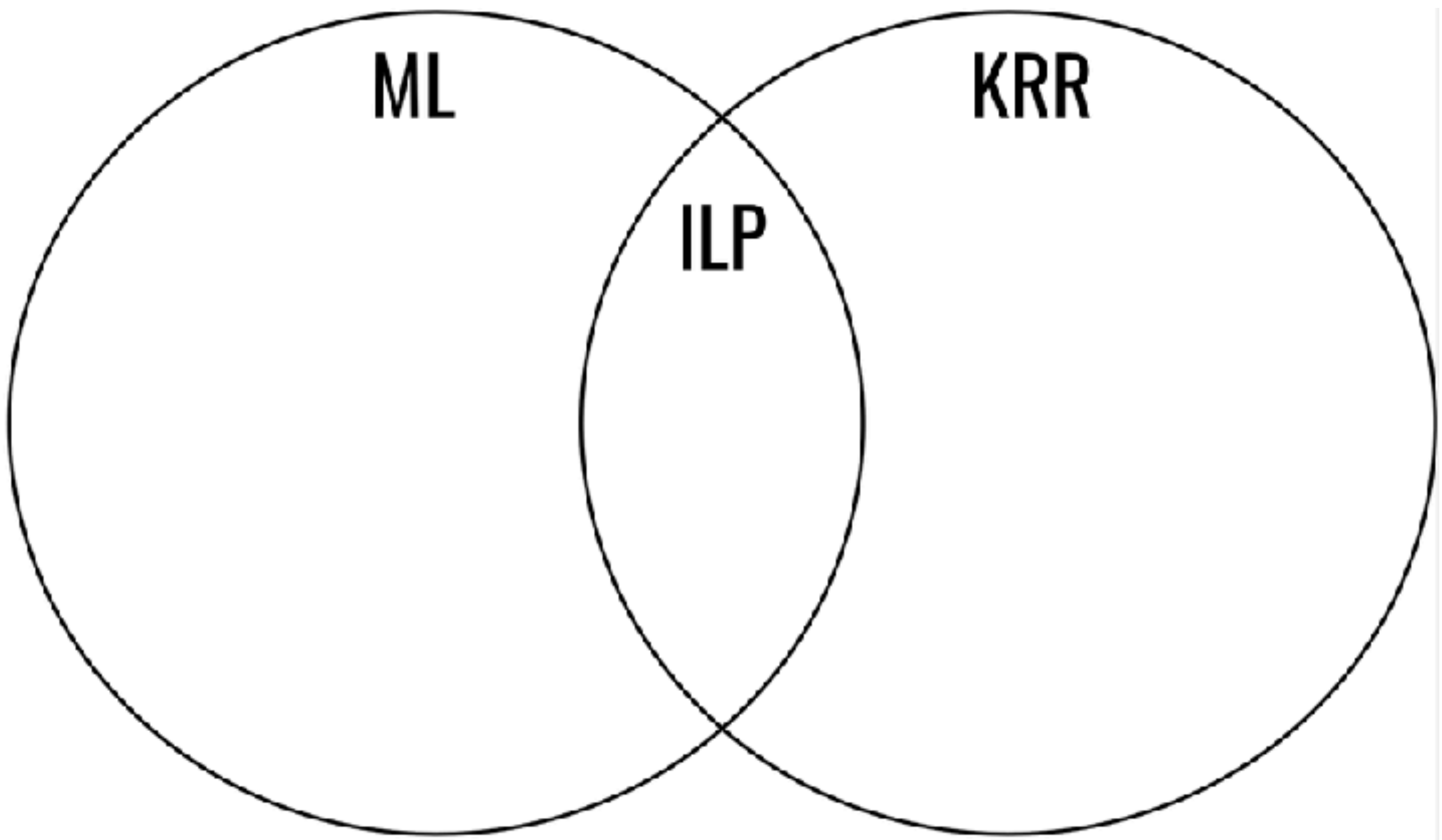
$$\forall Mol((has\_hydroxyl(Mol) \\ \land\ has\_amine(Mol) \\ \land\ \exists A1,A2(bond(A1,A2,Mol) \\ \land\ atom(Mol,A1,oxygen) \\ \land\ atom(Mol,A2,nitrogen))) \\ \rightarrow\ active(Mol))$$

# 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

# Inductive logic programming

Combines logical reasoning with data-driven learning



# Why ILP?

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

What have I done?

Design ILP algorithms and package them into open-source tools

# Scalability

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

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

# Data efficiency

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

MLJ 2021

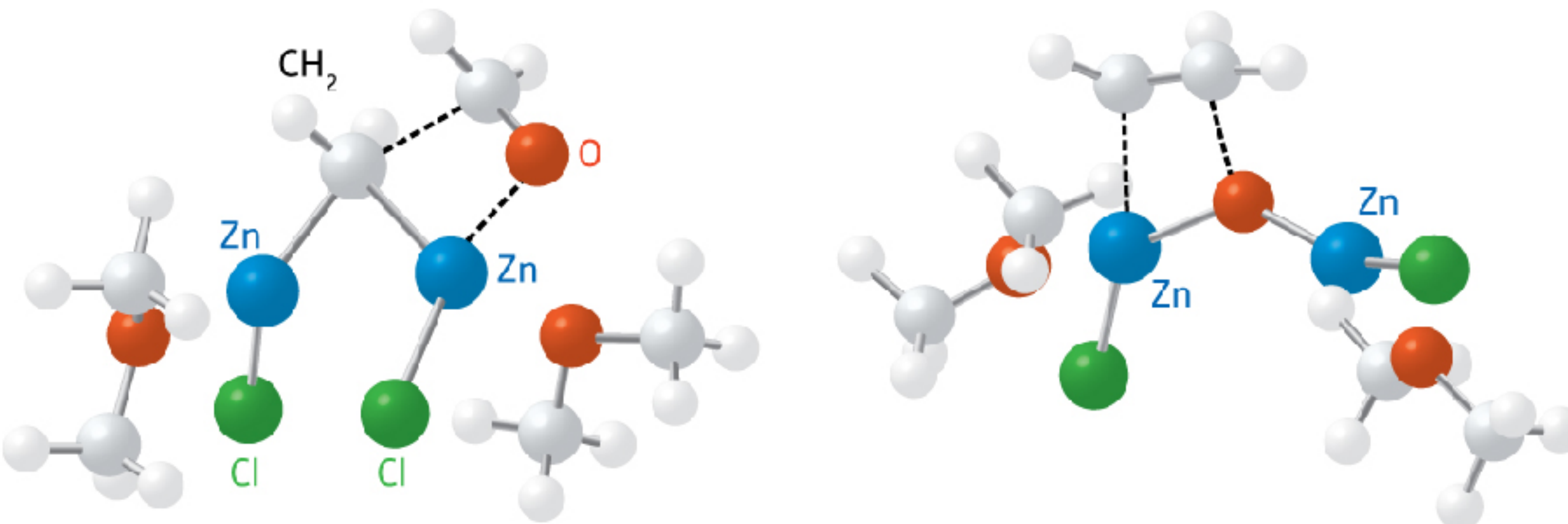
# Noisy data

Handle noisy data by learning **MDL** hypotheses

What is the actual impact?

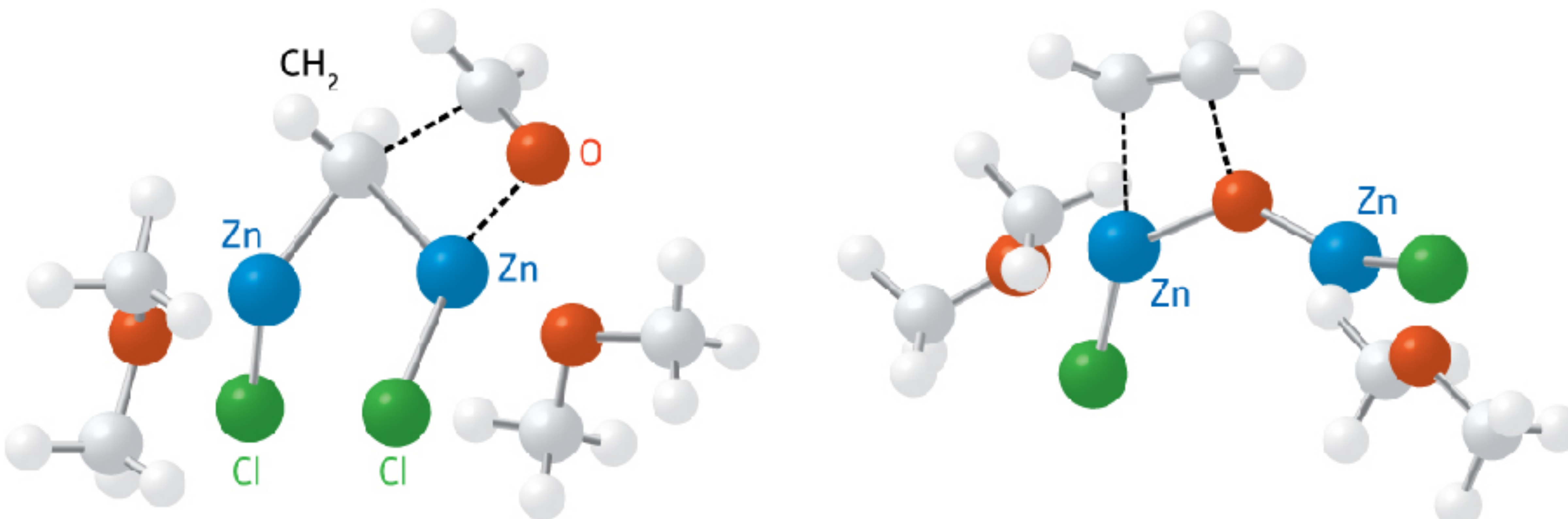
People use it

# Explainable drug design




AAAI23

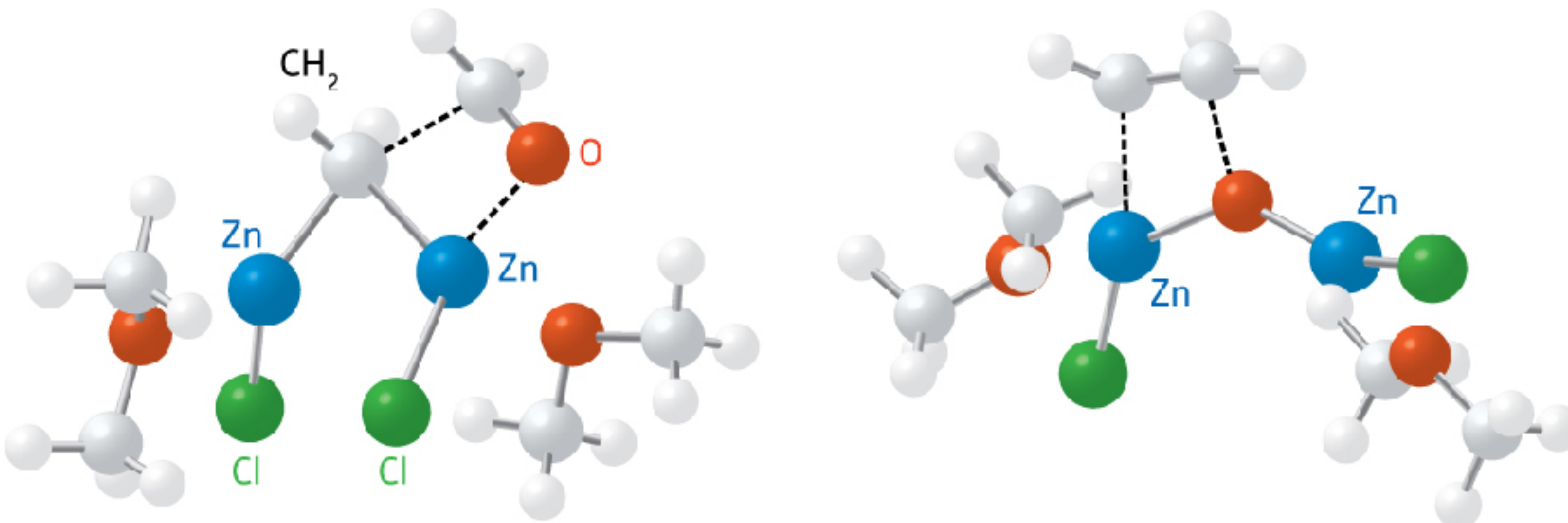
# Explainable drug design




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

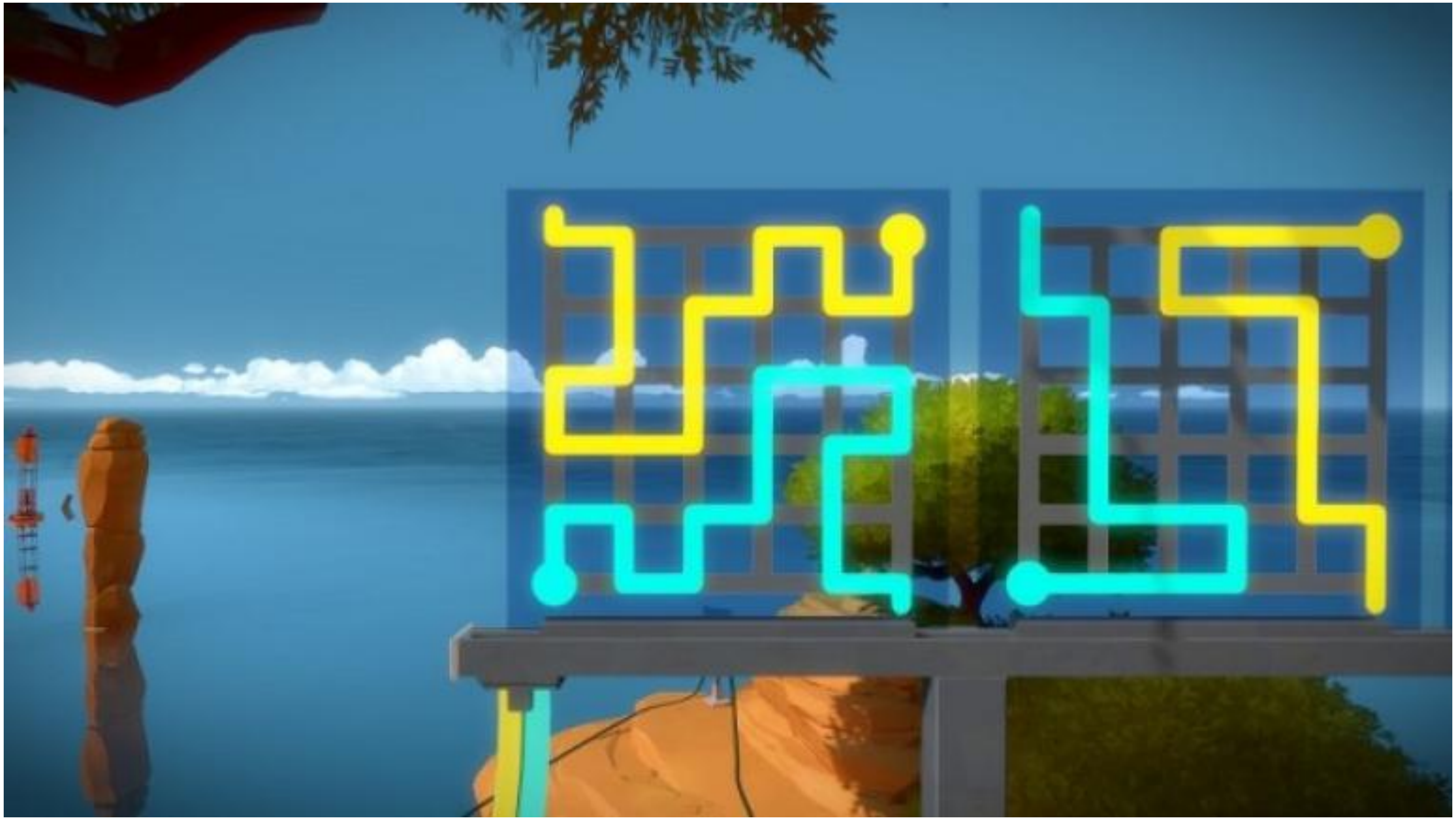



active if there are two zinc atoms

and there is a 'du' bond type between them

and the distance between them is <= 1.23

# Games



Learned explanations for bad game states

Stevens et al, 2023

# Puzzles

Lakkaraju et al, 2022

# Program synthesis

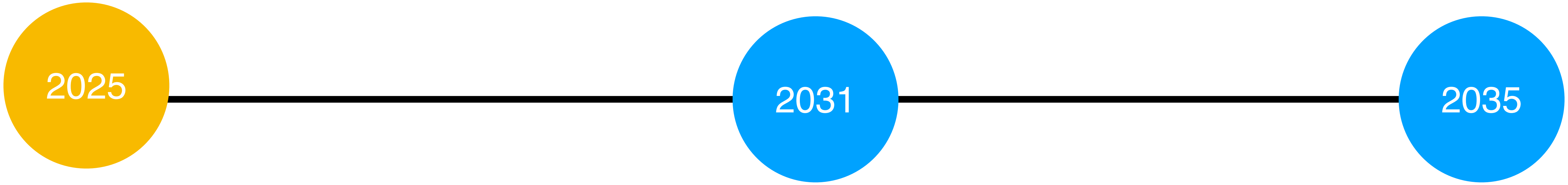
$$
\begin{aligned}
&[3,1,9,0,7] &&\rightarrow [1,9,0]\\
&[2,1,3,4,6,9] &&\rightarrow [1,3]\\
&[4,1,2,3,5,0,7,6,9,8] &&\rightarrow [1,2,3,5]\\
&[1,5,4,2,8,3,0,6] &&\rightarrow [5]\\
&[5,2,1,0,4,3,7,6] &&\rightarrow [2,1,0,4,3]
\end{aligned}
$$

Nature Communications 2024, IJCAI25?

What is missing?

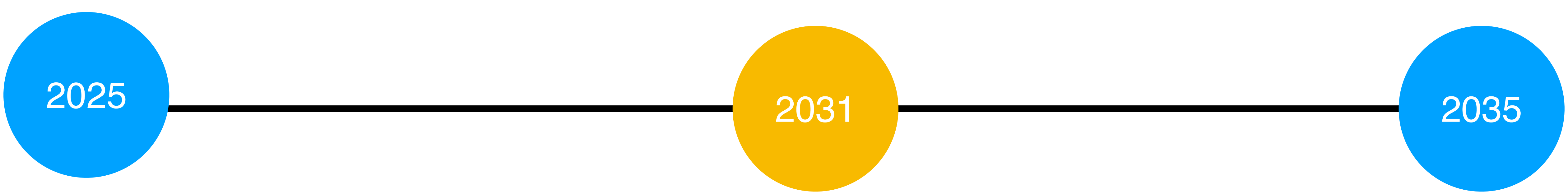
# Now: undergraduate

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



# Five-years: professor

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



# How?

**Better search**

Complex prior knowledge

Scientist-aligned methods

# Neural-symbolic

Can we learn which hypothesis to try next?

# How?

Better search

**Complex prior knowledge**

Scientist-aligned methods

# Uncertainty

Elbow Ruler


Scale

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**

# My job

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

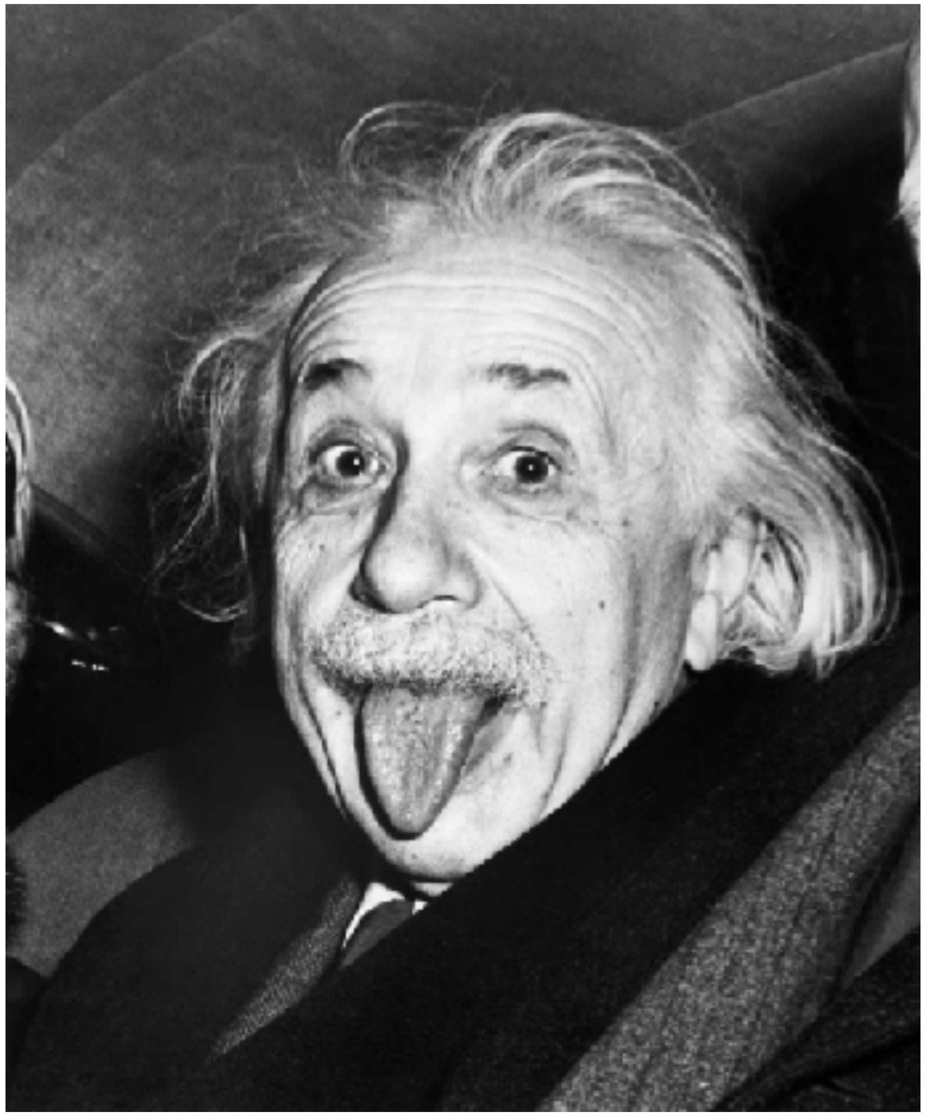
The ability to **understand a hypothesis** is equally, if not more, important than how well it performs

# Explainability

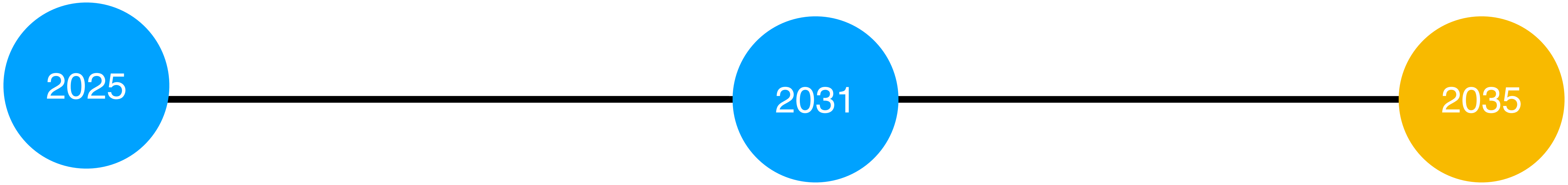
How do we trade-off accuracy vs explainability?

# Multidisciplinary collaborations

# 10-year goal: genius



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



# Questions?

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

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

# Me

- Algorithmics and Computational Intelligence group

# Teaching

1. TKO_7092 Evaluation of Machine Learning Methods, 5 ECTS
2. TKO_3120 Machine Learning and Pattern Recognition, 5 ECTS

# 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

# 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

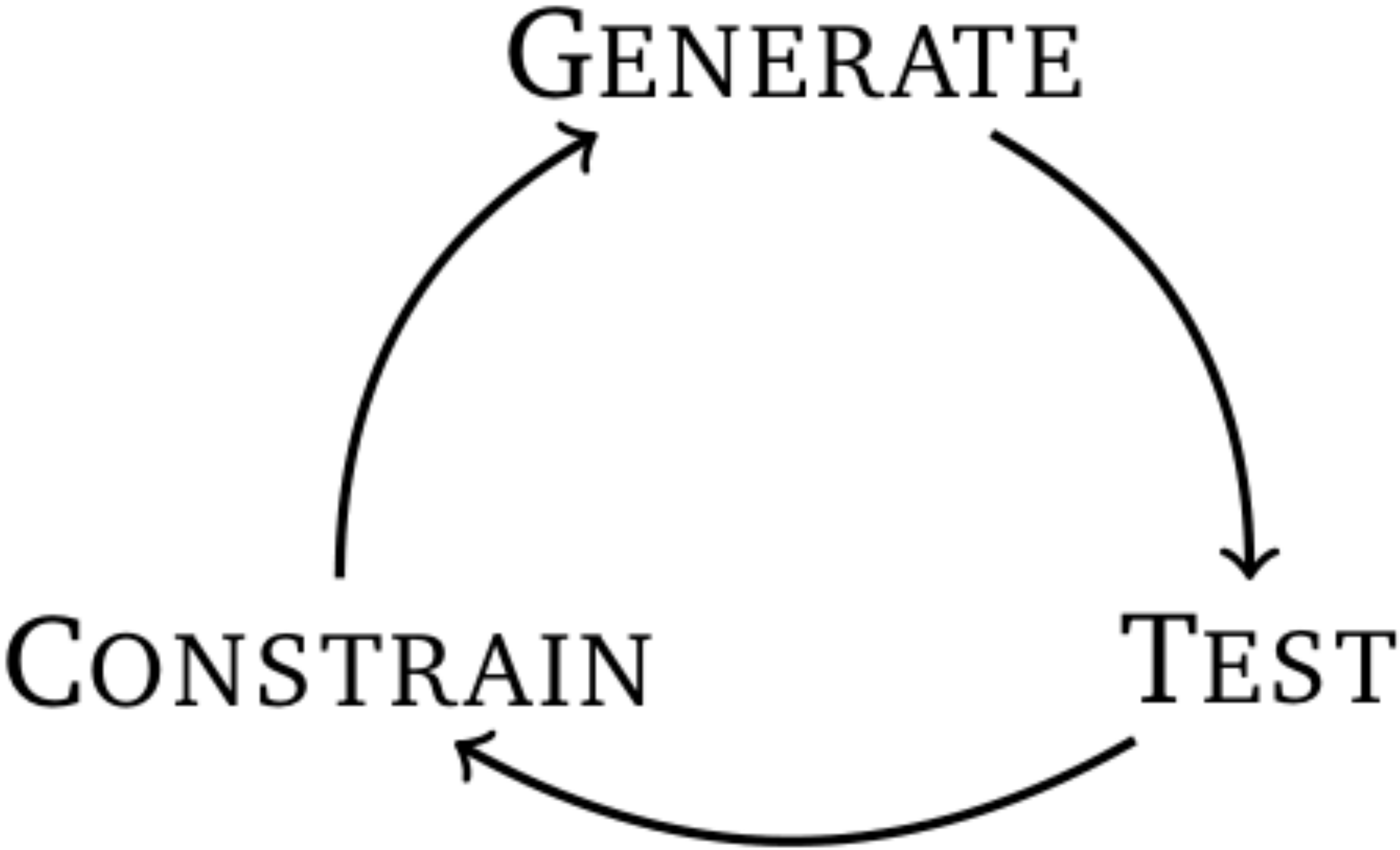
0. Start with a hypothesis space
1. Select a hypothesis
2. Empirically try to refute it
3. If the hypothesis is falsified, determine **why**

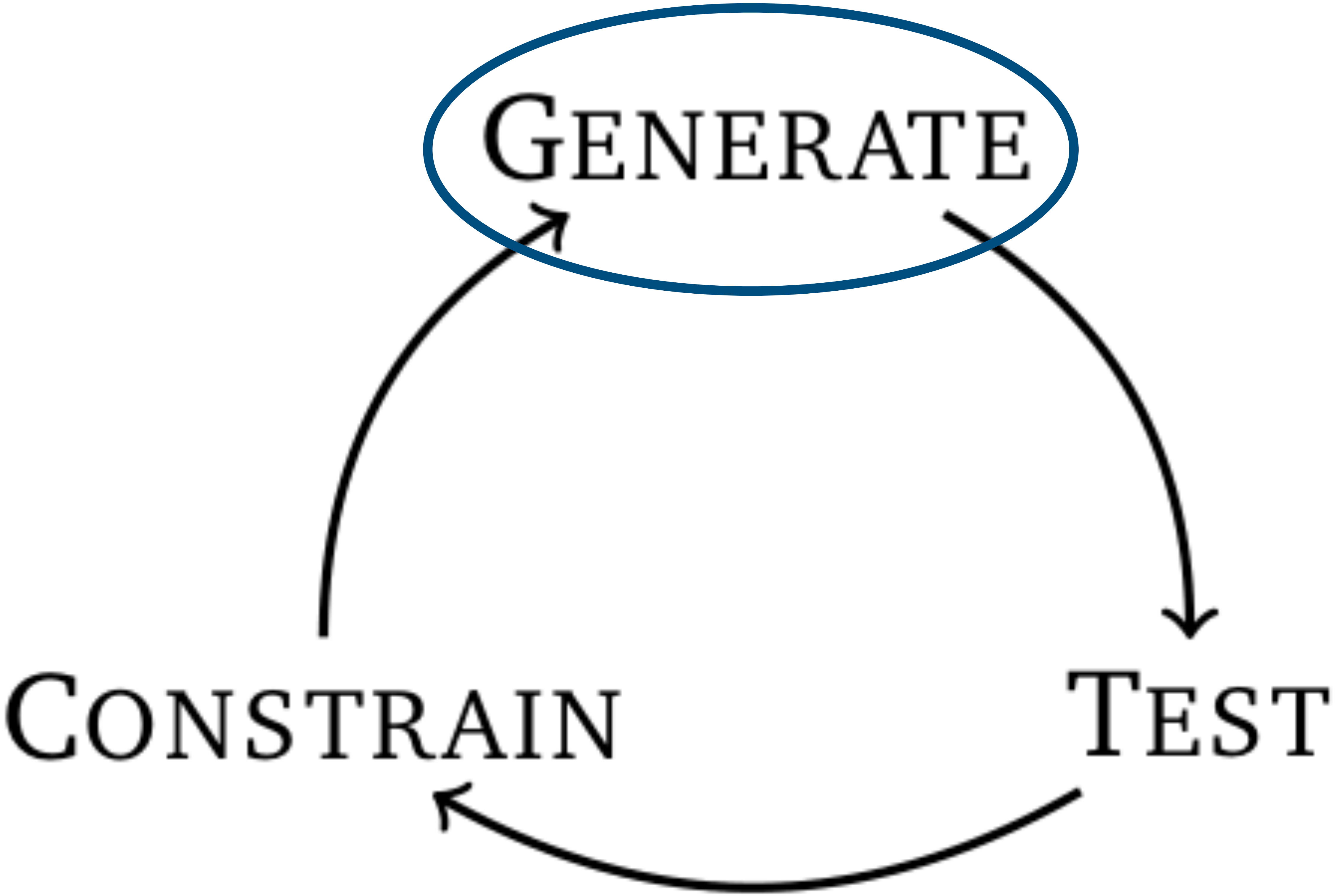
# Popper

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
CONSTRAIN
TEST



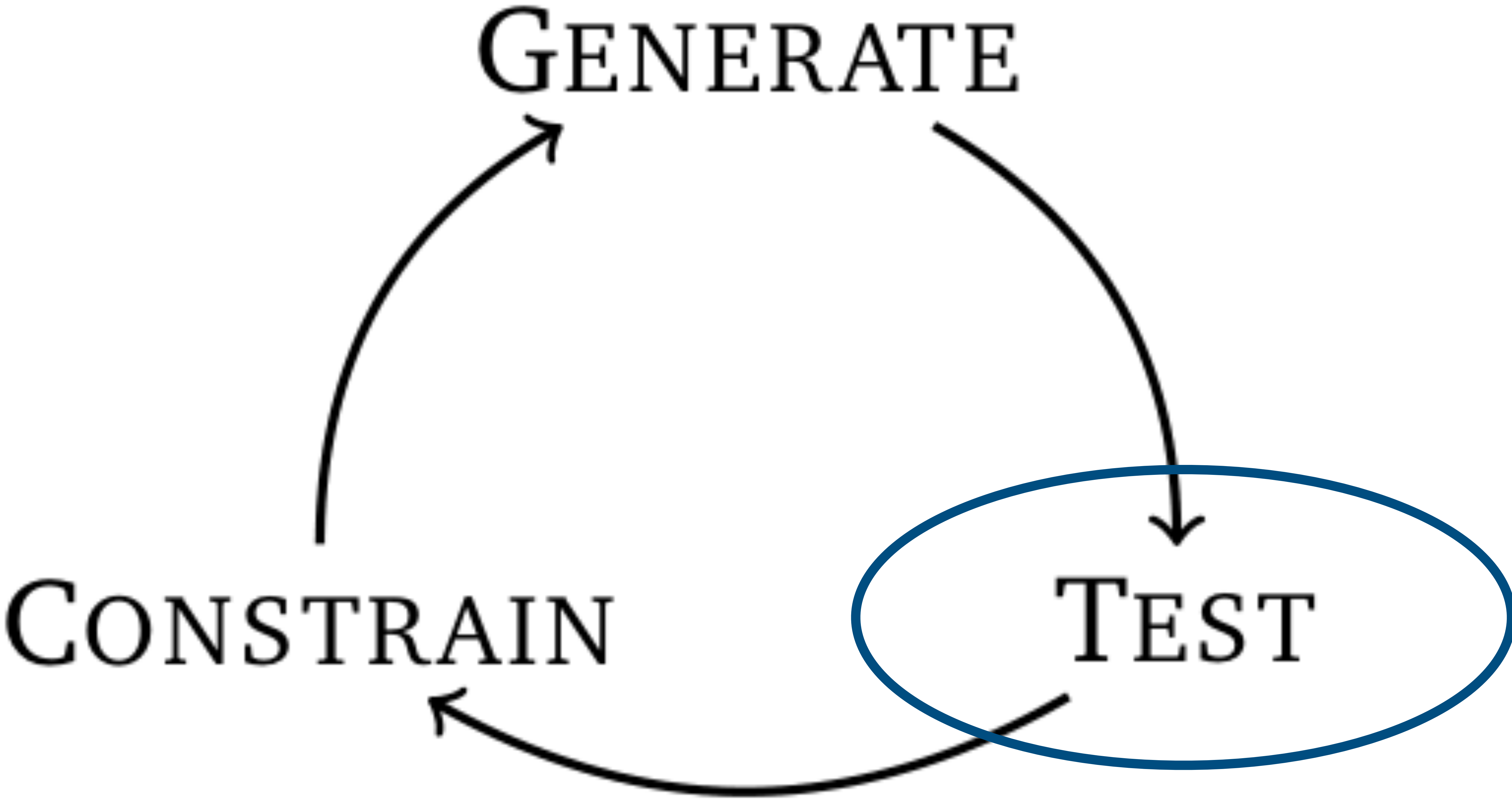
Generate
Test
Constrain

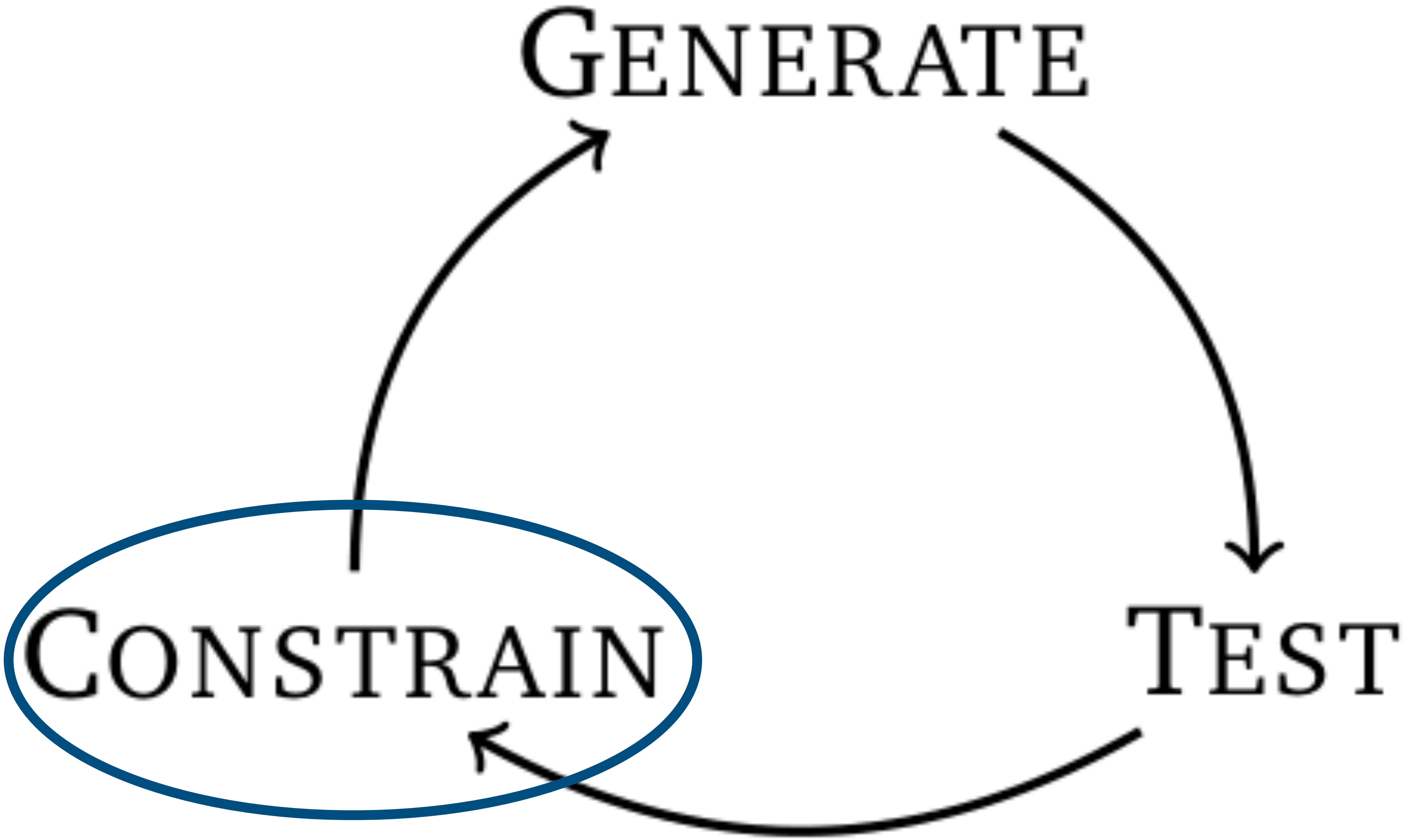
# Generate

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
Tottenham Court Road
Holborn
Notting Hill Gate
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**