

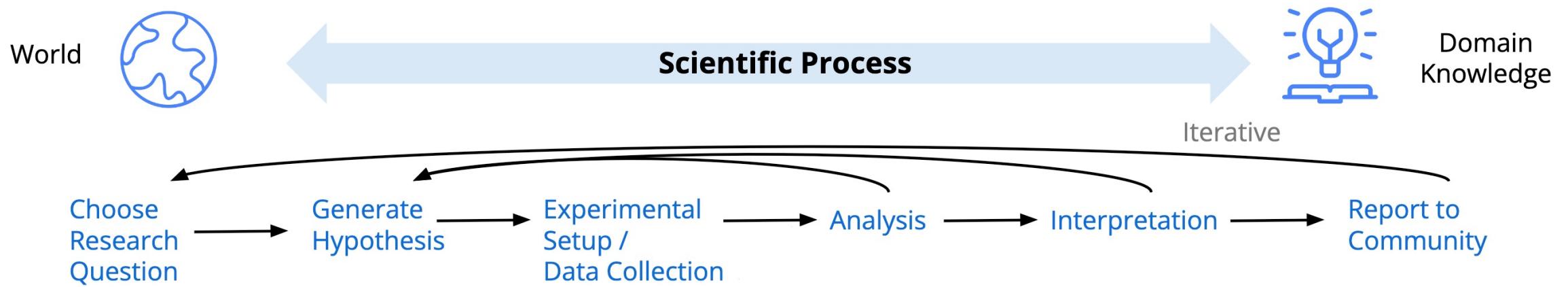
Neurosymbolic Programming for Scientific Discovery

Atharva Sehgal

atharvas@utexas.edu

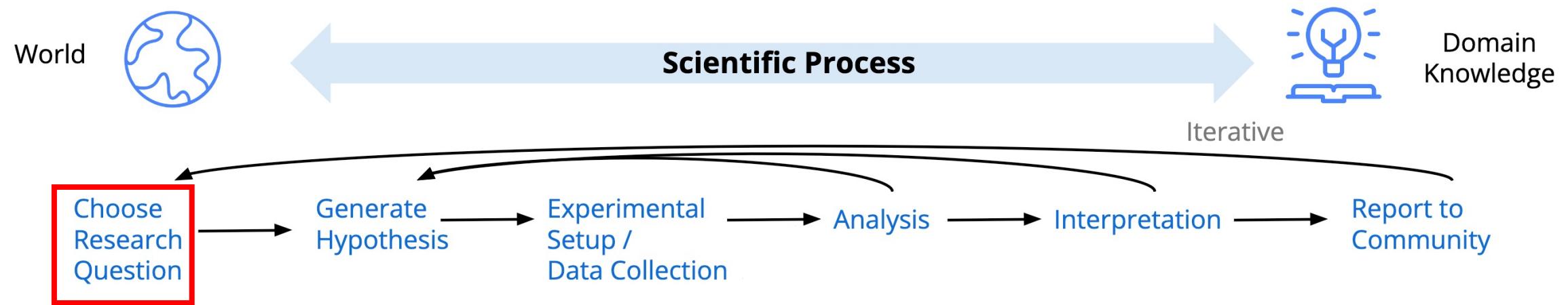


Scientific Discovery



Goal: We want AI to achieve human level performance at *research in the natural sciences*.

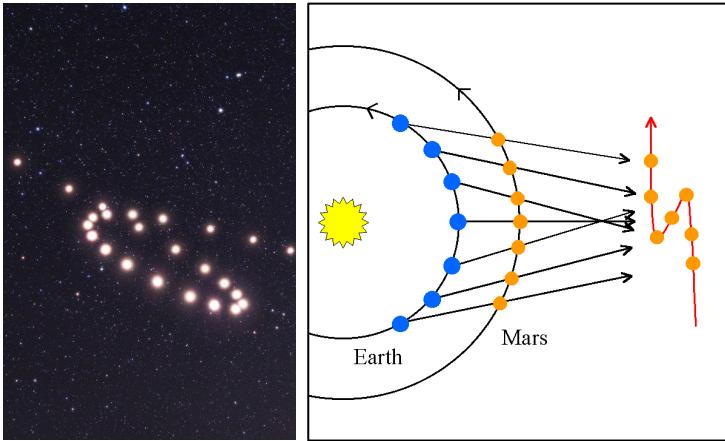
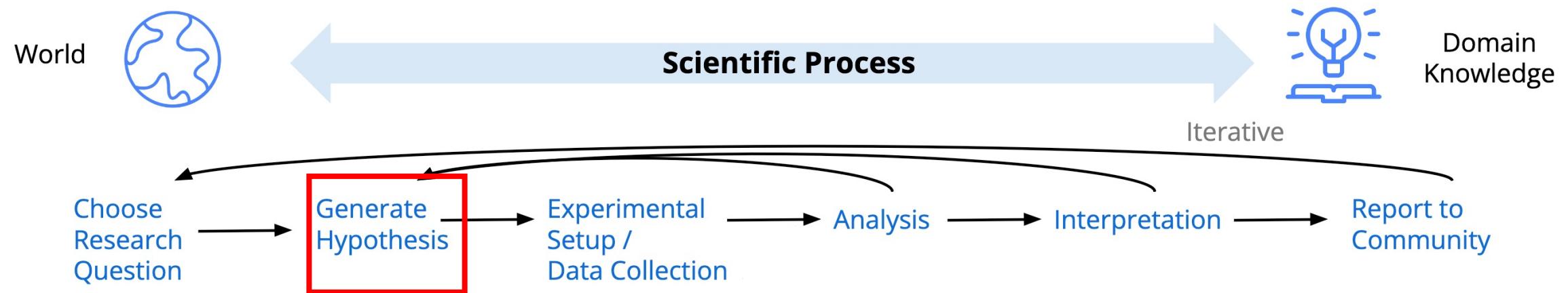
Lifecycle of a Scientific Process



Observation: Apparent
Retrograde Planetary Motion

c.The Astronomical Revolution: Copernicus- Kepler-Borelli

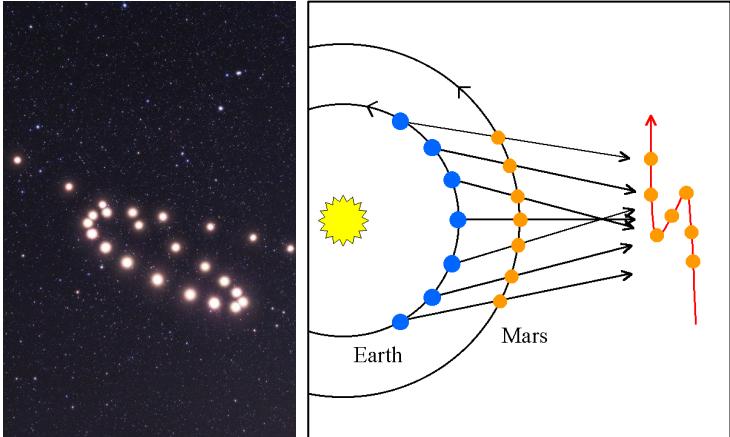
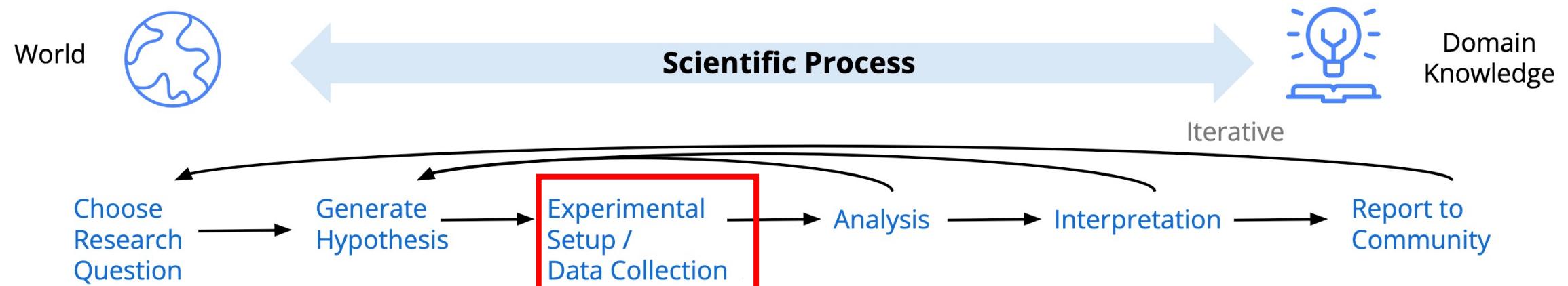
Lifecycle of a Scientific Process



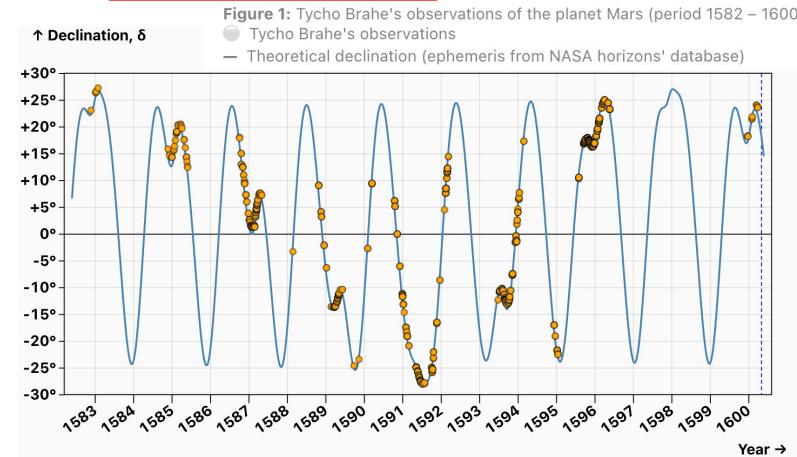
Observation: Apparent
Retrograde Planetary Motion
Theory: Heliocentric Model

c. The Astronomical Revolution: Copernicus- Kepler-Borelli

Lifecycle of a Scientific Process



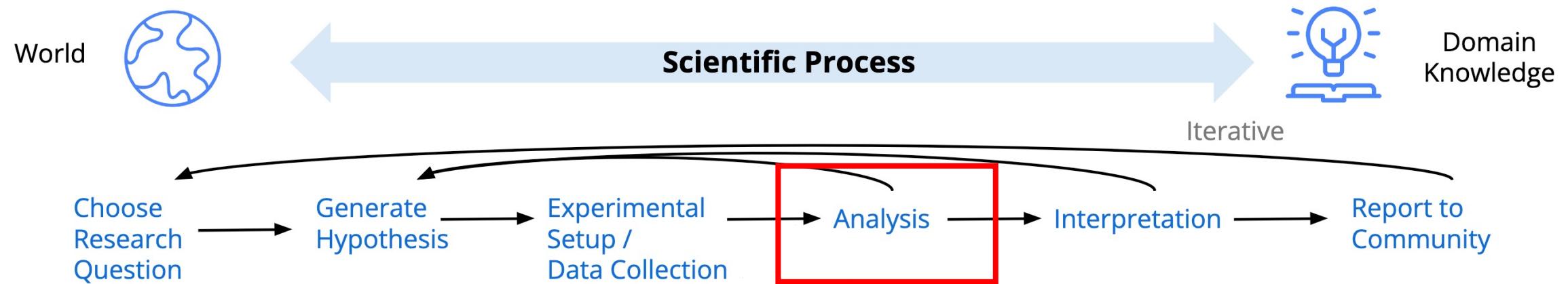
Observation: Apparent
Retrograde Planetary Motion
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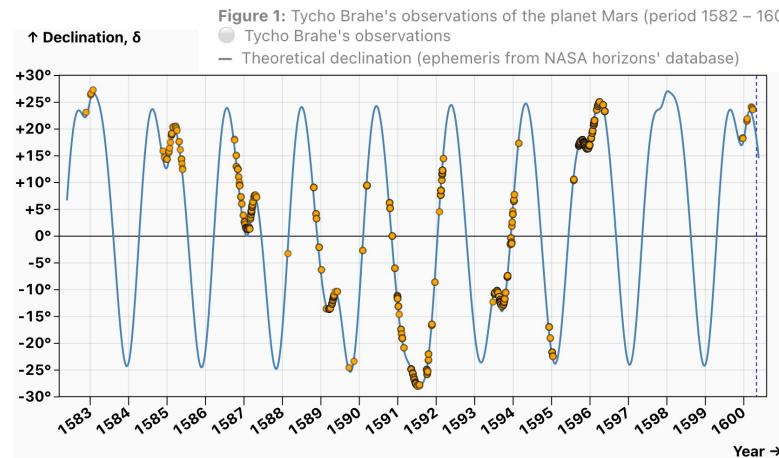
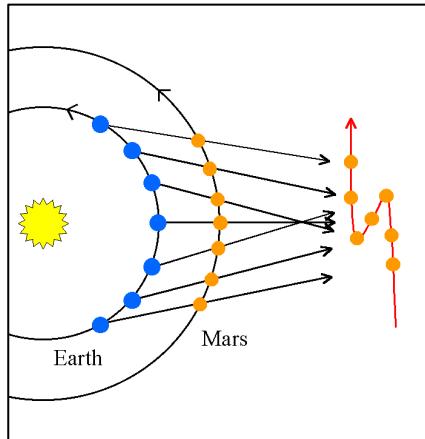
Data Collection: Sample data in regime
of interest.

c. The Astronomical Revolution: Copernicus- Kepler-Borelli

Lifecycle of a Scientific Process



Observation: Apparent Retrograde Planetary Motion
Theory: Heliocentric Model



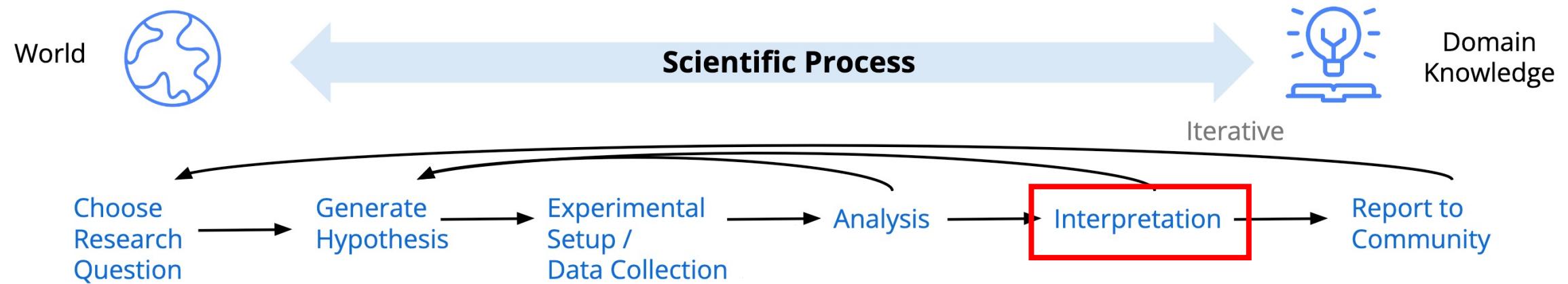
Data Collection: Sample data in regime of interest.

$$T^2 \propto r^3$$

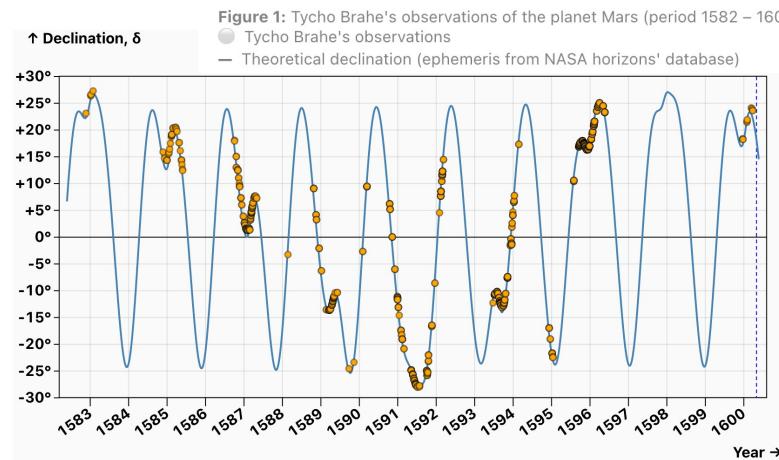
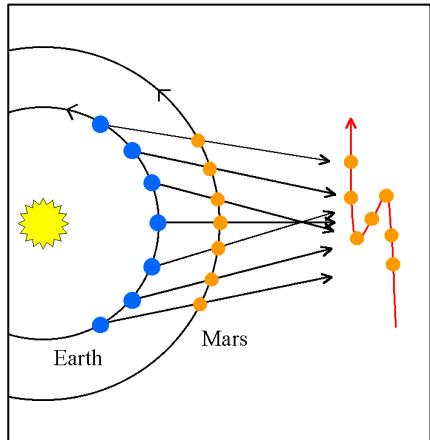
Analysis: Kepler's Third Law

c. The Astronomical Revolution: Copernicus- Kepler-Borelli

Lifecycle of a Scientific Process



Observation: Apparent Retrograde Planetary Motion
Theory: Heliocentric Model



Data Collection: Sample data in regime of interest.

$$T^2 \propto r^3$$

Analysis: Kepler's Third Law

$$mr \left(\frac{2\pi}{T} \right)^2 = G \frac{mM}{r^2}$$

Interpretation: Newton's Law of Gravitation

c. The Astronomical Revolution: Copernicus- Kepler-Borelli

Symbolic Regression

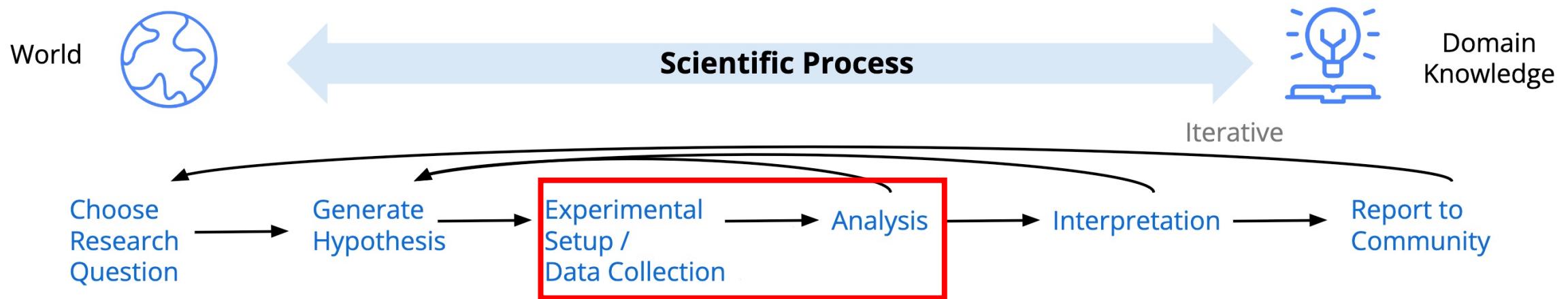
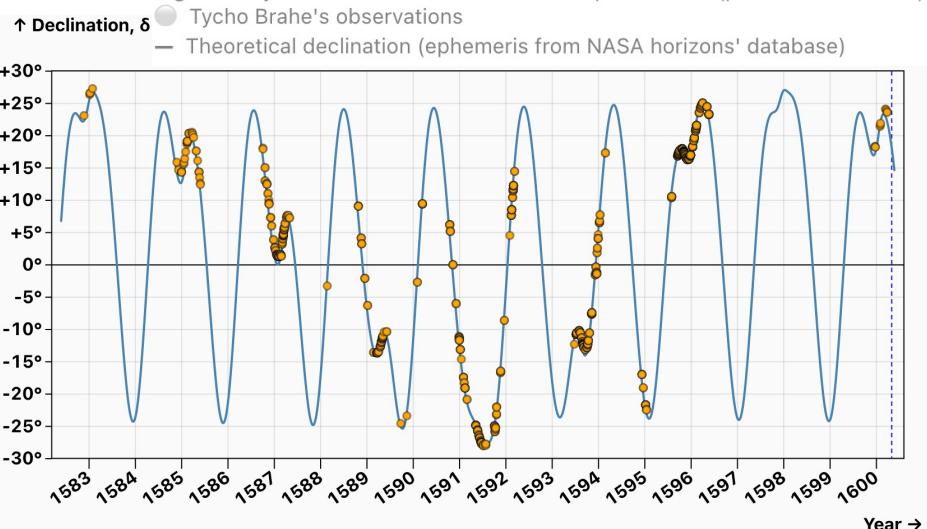


Figure 1: Tycho Brahe's observations of the planet Mars (period 1582 – 1600).



Kepler's Third Law

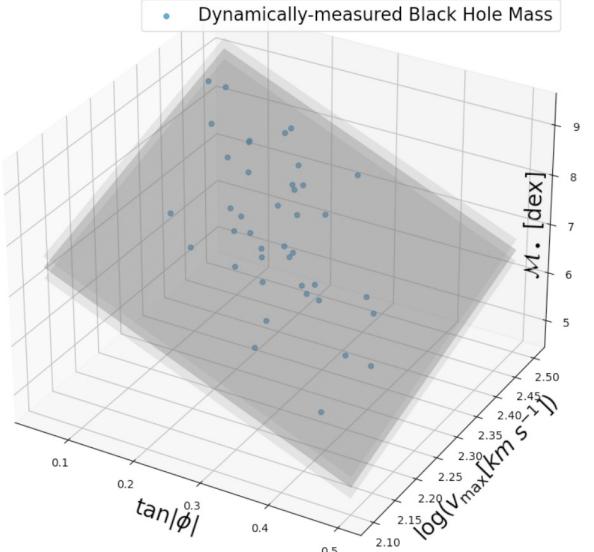
$$T^2 \propto r^3$$

c. The Astronomical Revolution: Copernicus- Kepler-Borelli

Symbolic Regression Algorithms

Symbolic Regression Algorithms

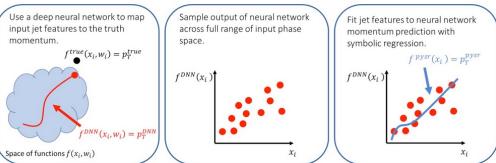
PySR's impact



Discovery of a Planar Black Hole Mass Scaling Relation for Spiral Galaxies

Benjamin L. Davis ¹, Zehao Jin ¹

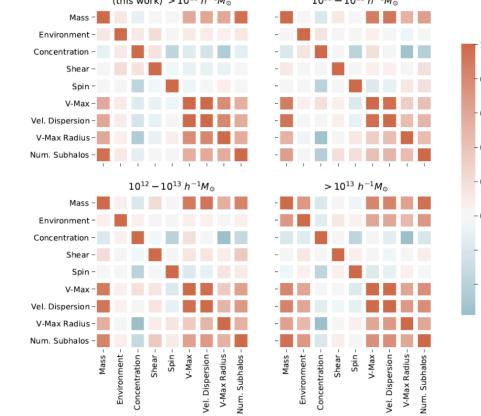
¹Center for Astrophysics and Space Science, New York University Abu Dhabi



Interpretable machine learning methods applied to jet background subtraction in heavy-ion collisions

Tanner Mengel ¹, Patrick Steffanic ¹, Charles Hughes ^{1,2}, Antonio Carlos Oliveira da Silva ^{1,2}, Christine Natrass ¹

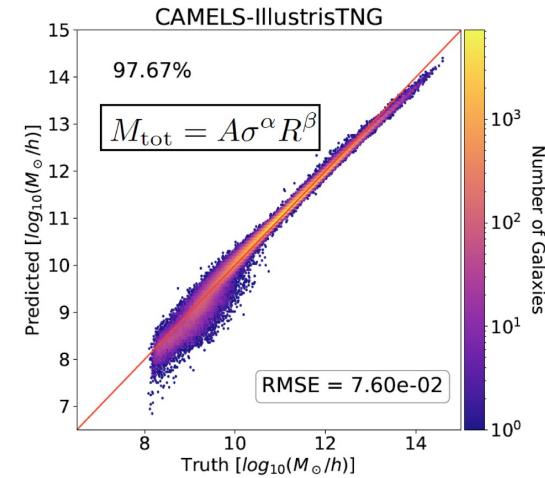
¹University of Tennessee, Knoxville, ²Iowa State University of Science and Technology



Modeling the galaxy-halo connection with machine learning

Ana Maria Delgado ¹, Digvijay Wadekar ^{2,3}, Boryana Hadzhiyska ¹, Sownak Bose ^{1,7}, Lars Hernquist ¹, Shirley Ho ^{2,4,5,6}

¹Center for Astrophysics | Harvard & Smithsonian, ²New York University, ³Institute for Advanced Study, ⁴Flatiron Institute, ⁵Center for Astrophysics | Harvard & Smithsonian, ⁶Carnegie Mellon University, ⁷Durham University

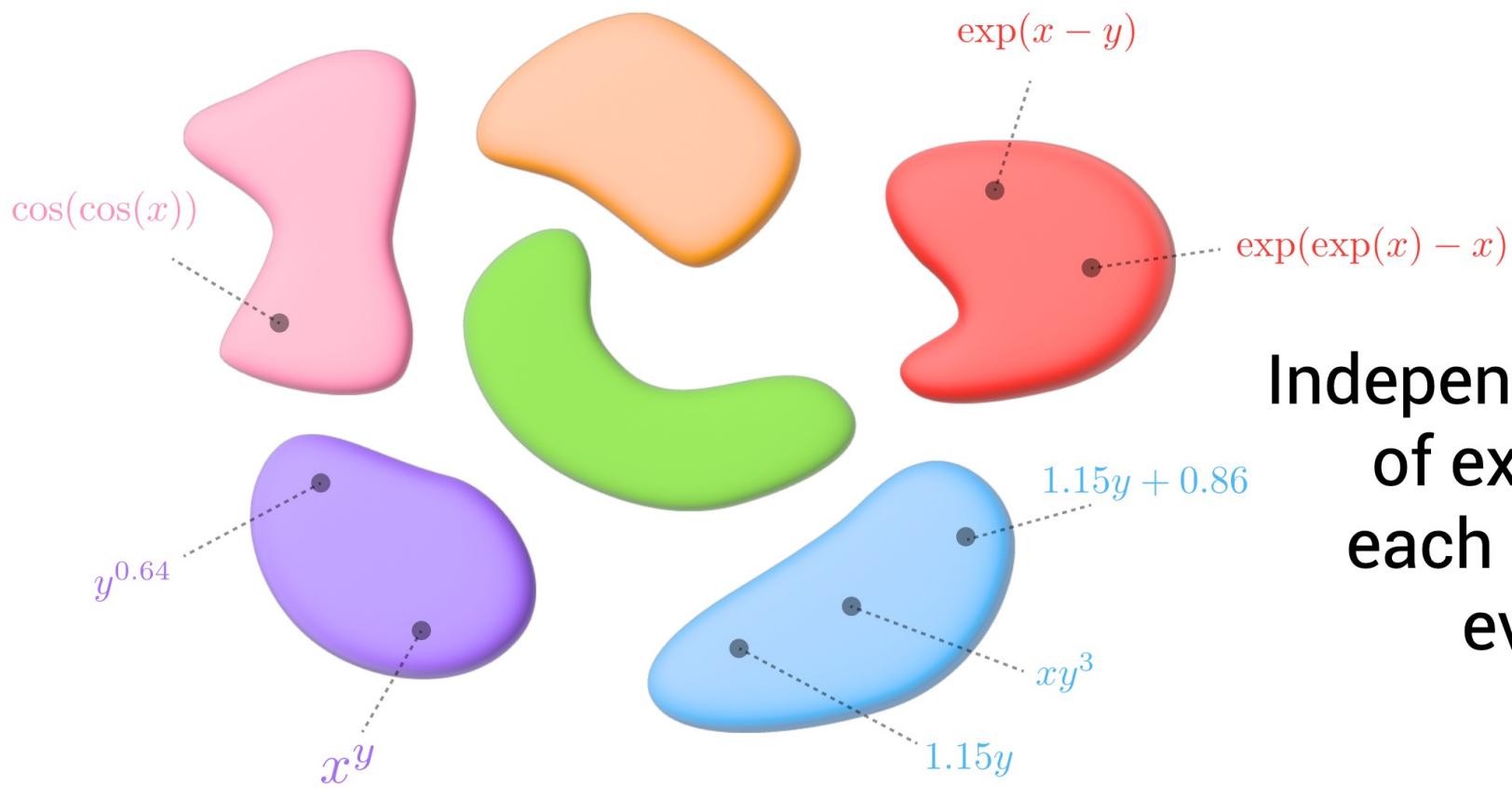


Finding universal relations in subhalo properties with artificial intelligence

Helen Shao ¹, Francisco Villaescusa-Navarro ^{1,2}, Shy Genel ^{2,3}, David N. Spergel ^{2,1}, Daniel Angles-Alcazar ^{4,2}, Lars Hernquist ⁵, Romeel Dave ^{6,7,8}, Desika Narayanan ^{9,10}, Gabriella Contardo ², Mark Vogelsberger ¹¹

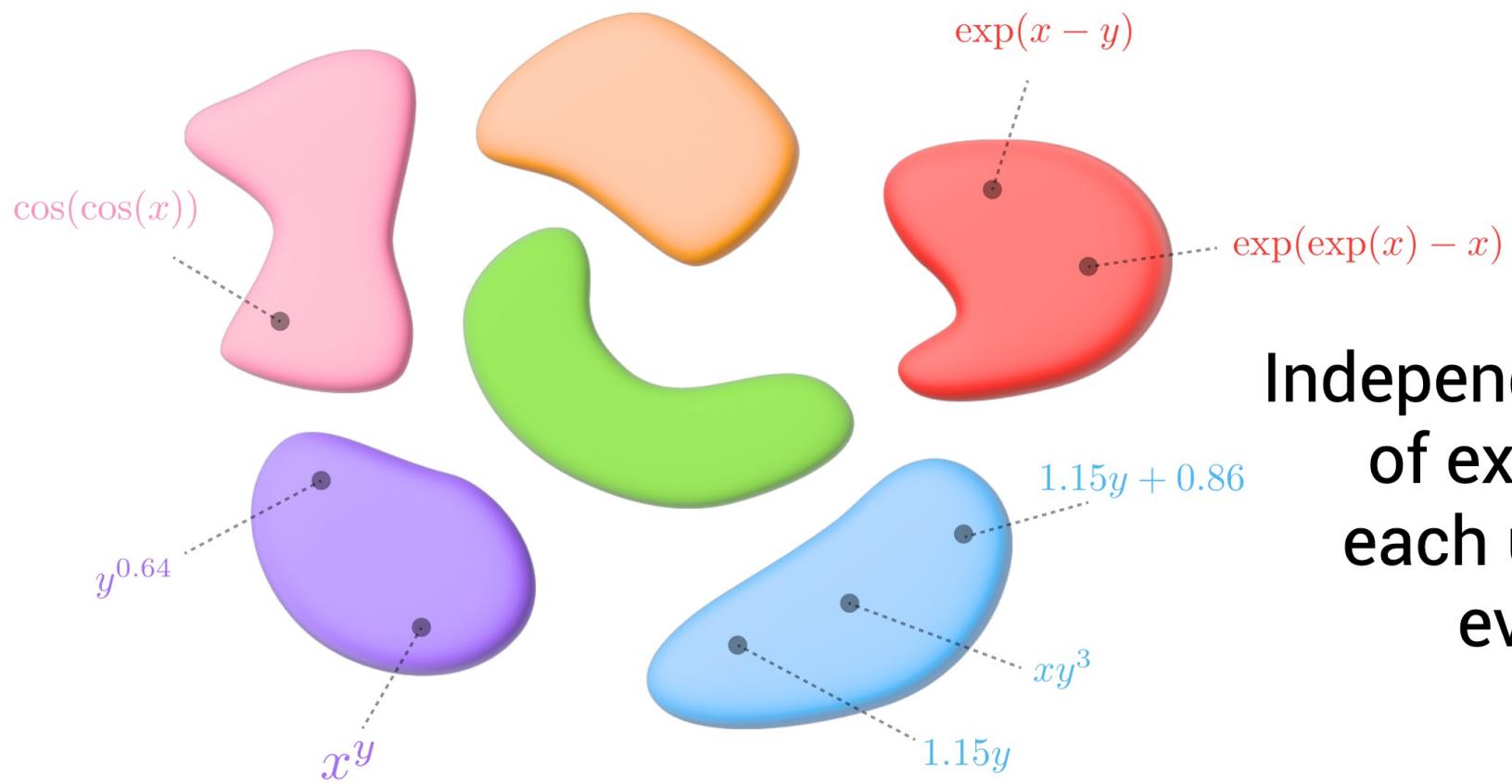
¹Princeton University, ²Flatiron Institute, ³Columbia University, ⁴University of Connecticut, ⁵Center for Astrophysics | Harvard & Smithsonian, ⁶University of Edinburgh, ⁷University of the Western Cape, ⁸South African Astronomical Observatories, ⁹University of Florida, ¹⁰University of Florida Informatics Institute, ¹¹MIT

Sketch of PySR's Exploration Space



Independent “islands”
of expressions,
each undergoing
evolution

Sketch of PySR's Exploration Space



Independent “islands”
of expressions,
each undergoing
evolution

Goal: How can we increase exploration in
relevant parts of the search space?



TEXAS
The University of Texas at Austin



UNIVERSITY OF
CAMBRIDGE



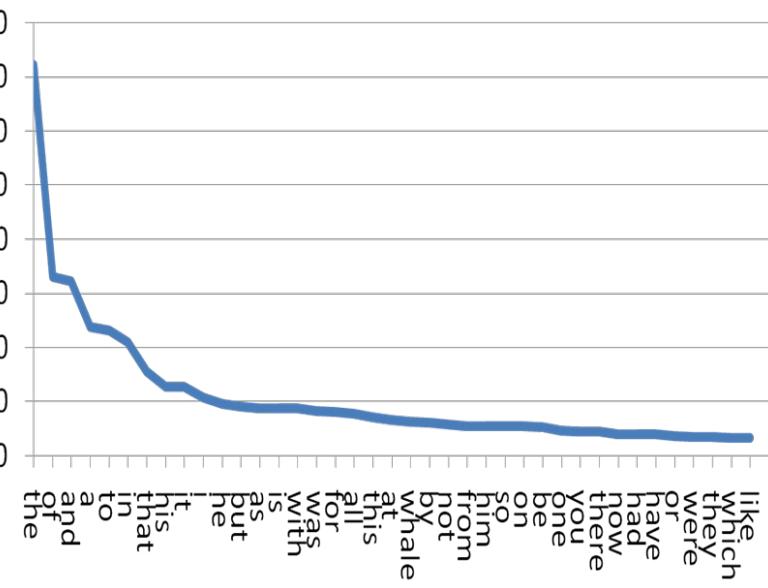
LaSR: Symbolic Regression with a Learned Concept Library

Arya Grayeli*, Atharva Sehgal*, Omar Costilla-Reyes, Miles Cranmer, Swarat Chaudhuri

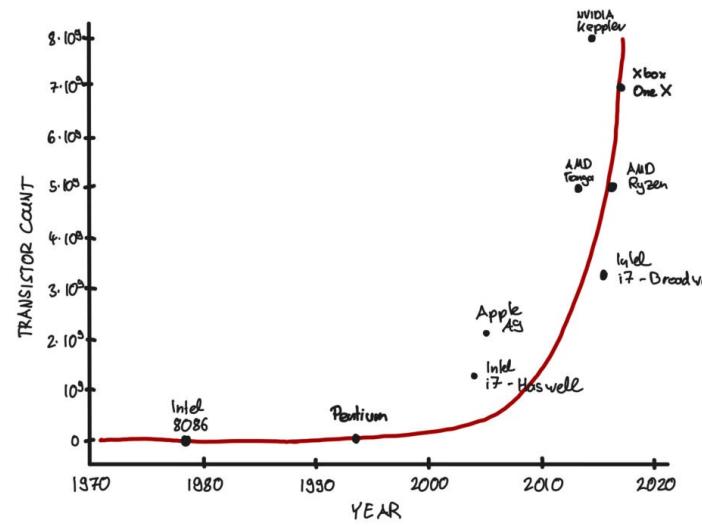
What is a Concept?

Desiderata I: Symbolic Abstraction

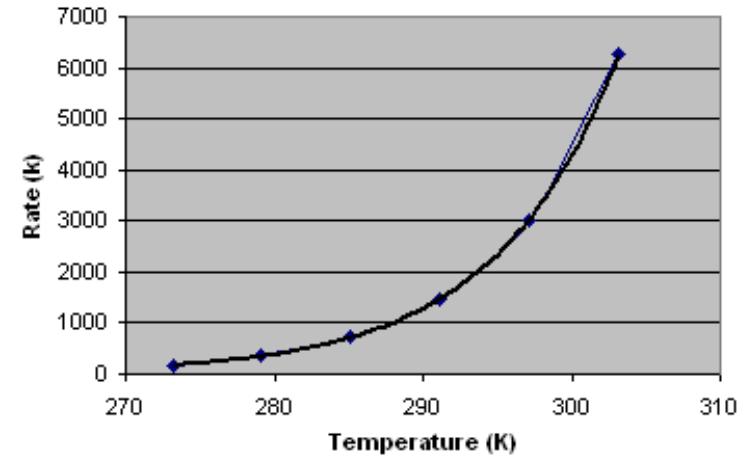
Zipf's Law



Moore's Law



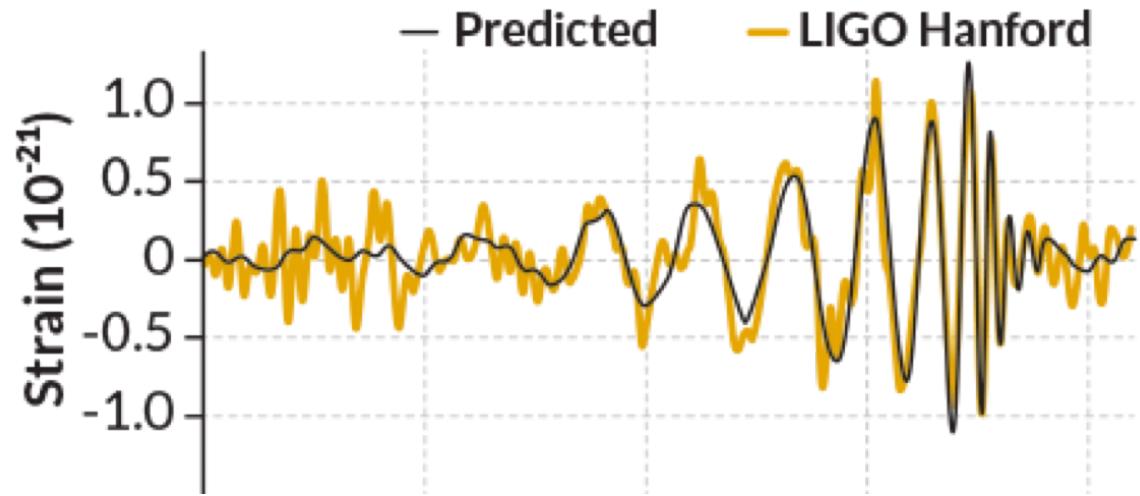
Arrhenius' Equation



$$y = ax^k + \epsilon \Leftrightarrow \text{"Power Law Trend"}$$

What is a Concept?

Desiderata II : Symbolic Guidance



Concepts (by Physicist or LLM)

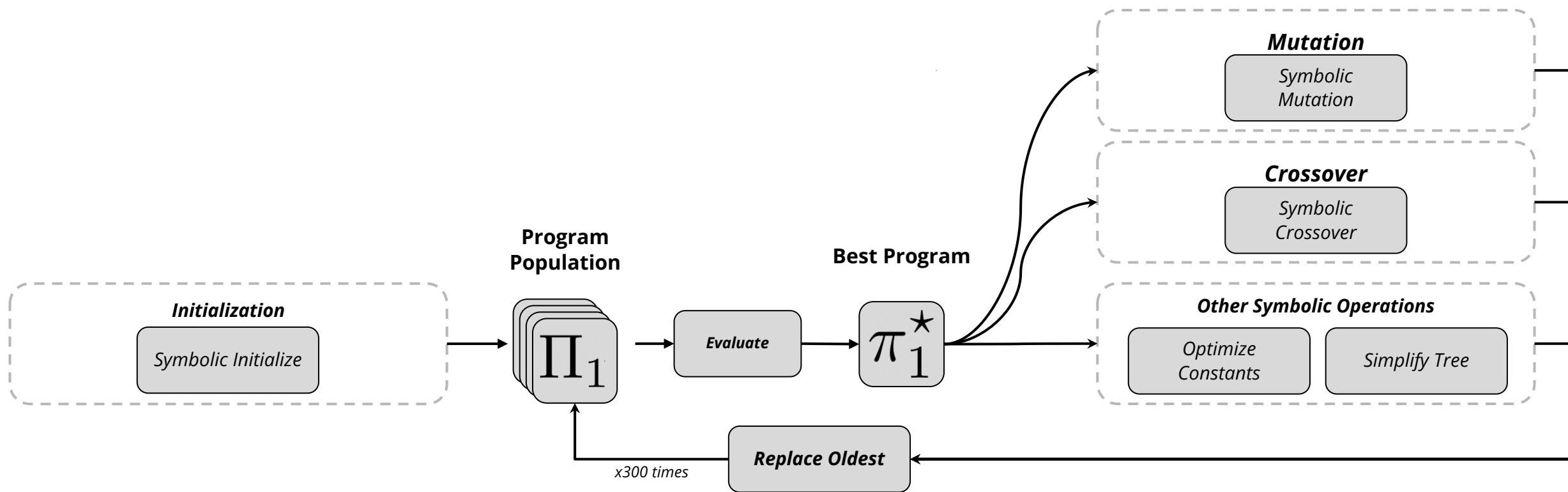
“Wave strain diminishes as distance increases”

“Wave strain has extraordinarily small magnitude”

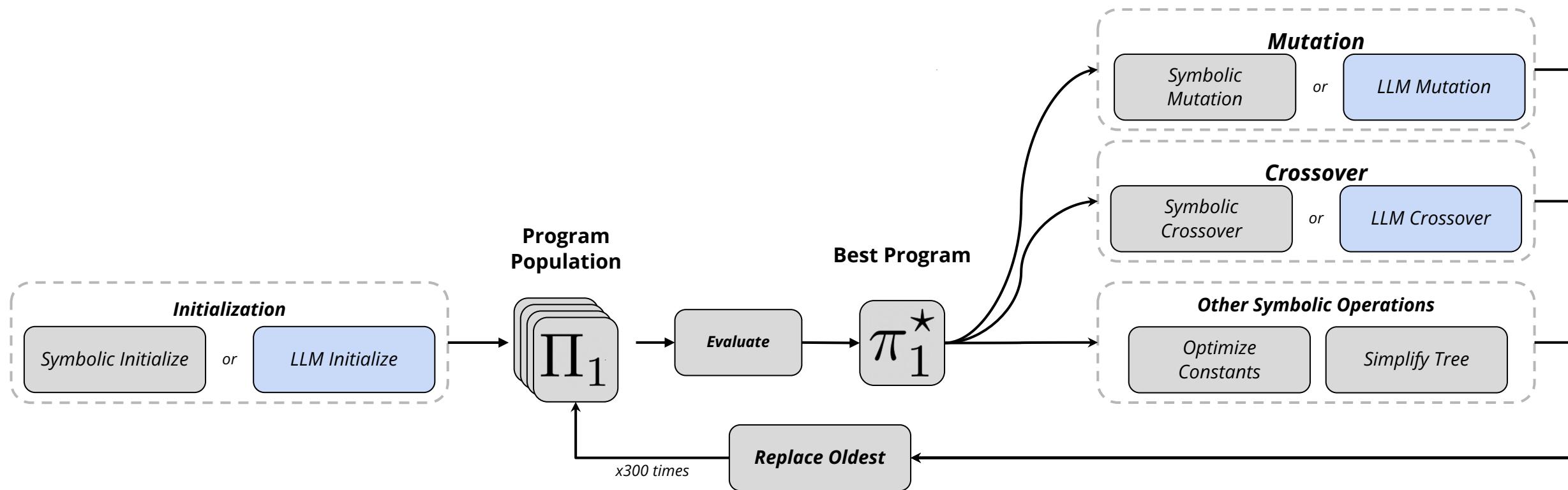
Guide the search for

$$h = \frac{2G}{c^4} \frac{1}{r} \frac{\partial^2 Q}{\partial t^2}$$

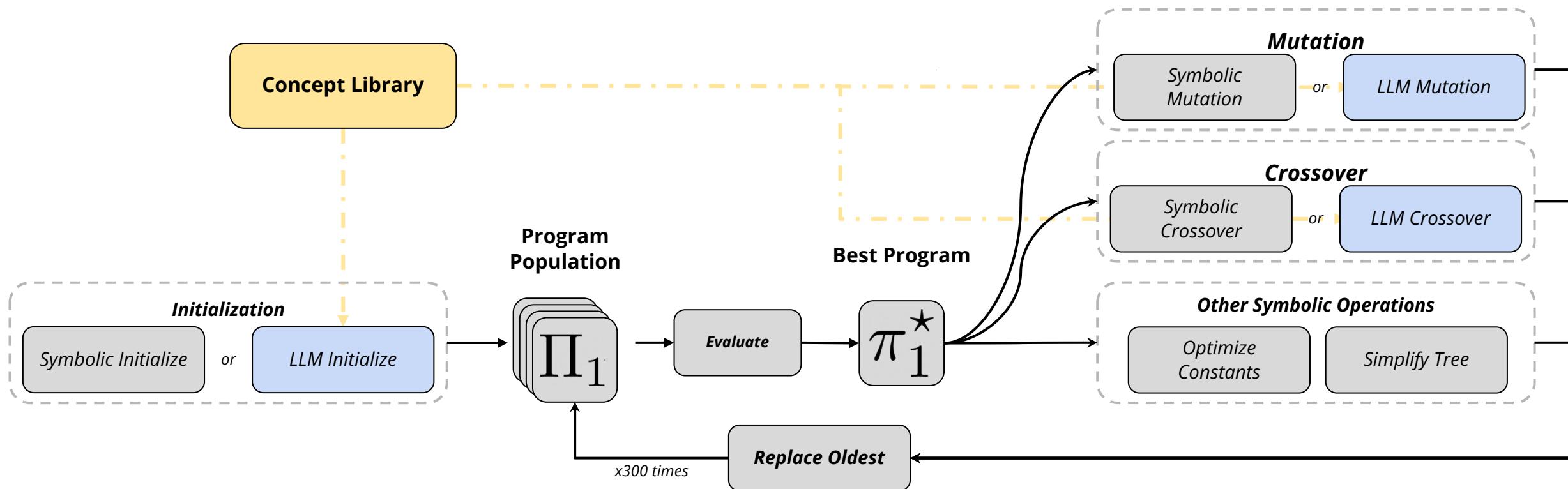
Hypothesis Evolution



Hypothesis Evolution + Concept guidance



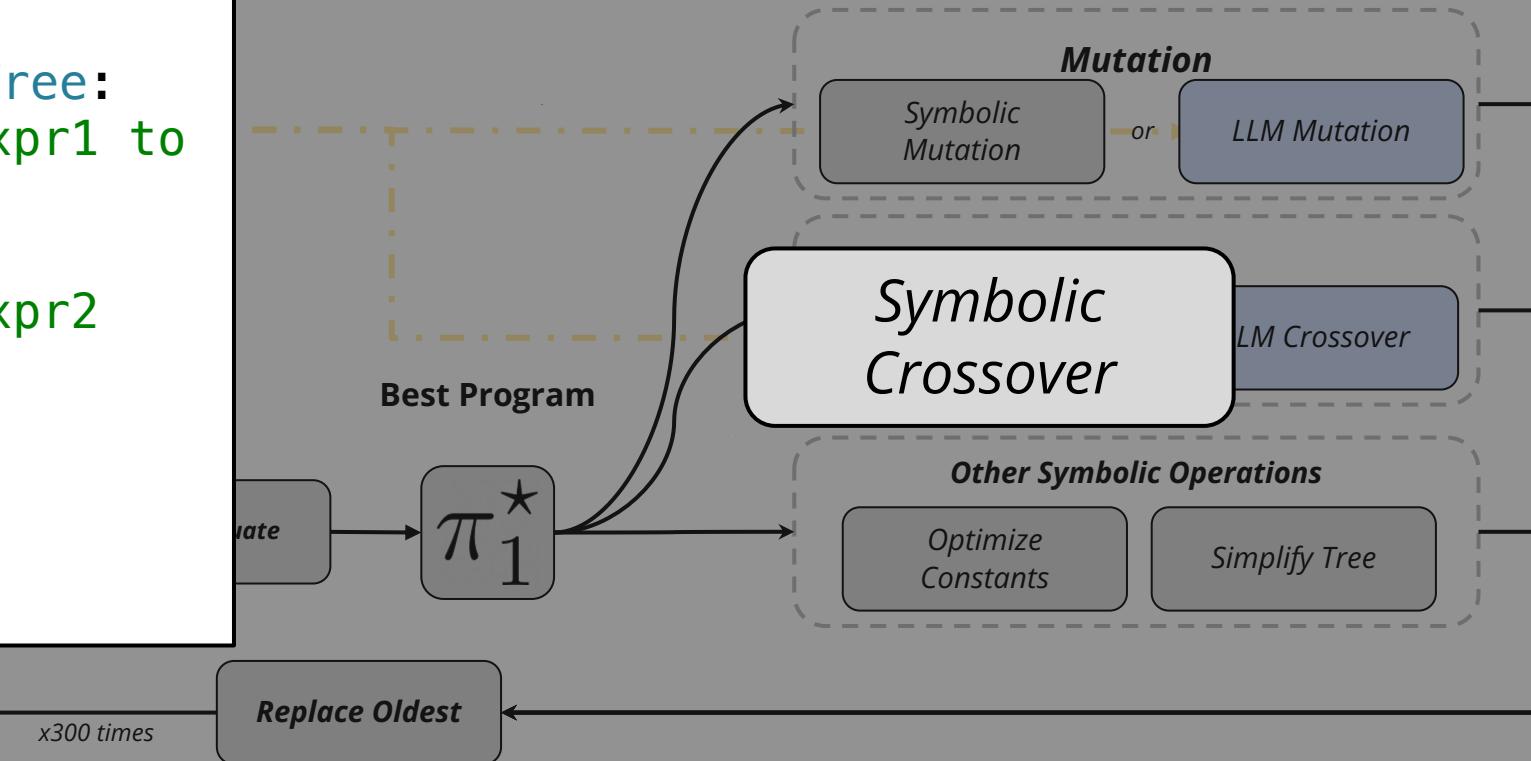
Hypothesis Evolution + Concept guidance



Hypothesis Evolution + Concept guidance

```
import random

def crossover(
    expr1: SymTree,
    expr2: SymTree) -> SymTree:
# Randomly choose a node in expr1 to
remove
...
# Randomly choose a node in expr2
which will be added to eq1
...
# Return new tree
new_expr = ...
return new_expr
```



Hypothesis Evolution + Concept guidance

(System)
Header

You are a helpful assistant that recombines two mathematical expressions by following a few provided suggestions. You will be given three suggestions and two expressions to recombine.

An expression must consist of the following variables: {{variables}}. All constants will be represented with the symbol C. Each expression will only use these operators: {{operators}}.

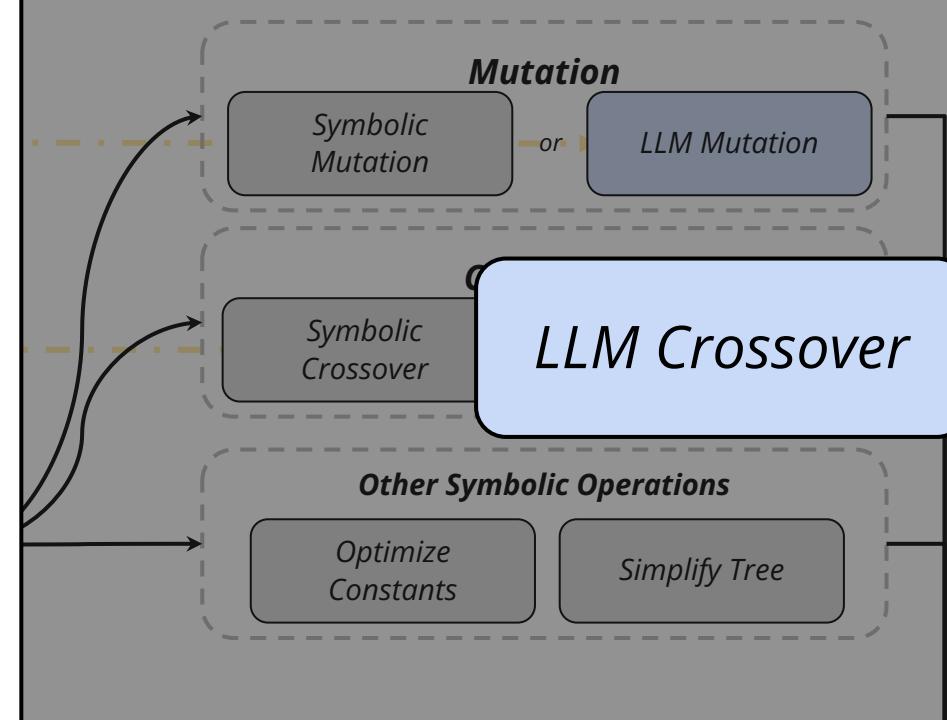
(User)
Crossover
Prompt

Suggestion 1: {{assump1}}
Suggestion 2: {{assump2}}
Suggestion 3: {{assump3}}
Expression 1: {{expr1}}
Expression 2: {{expr2}}

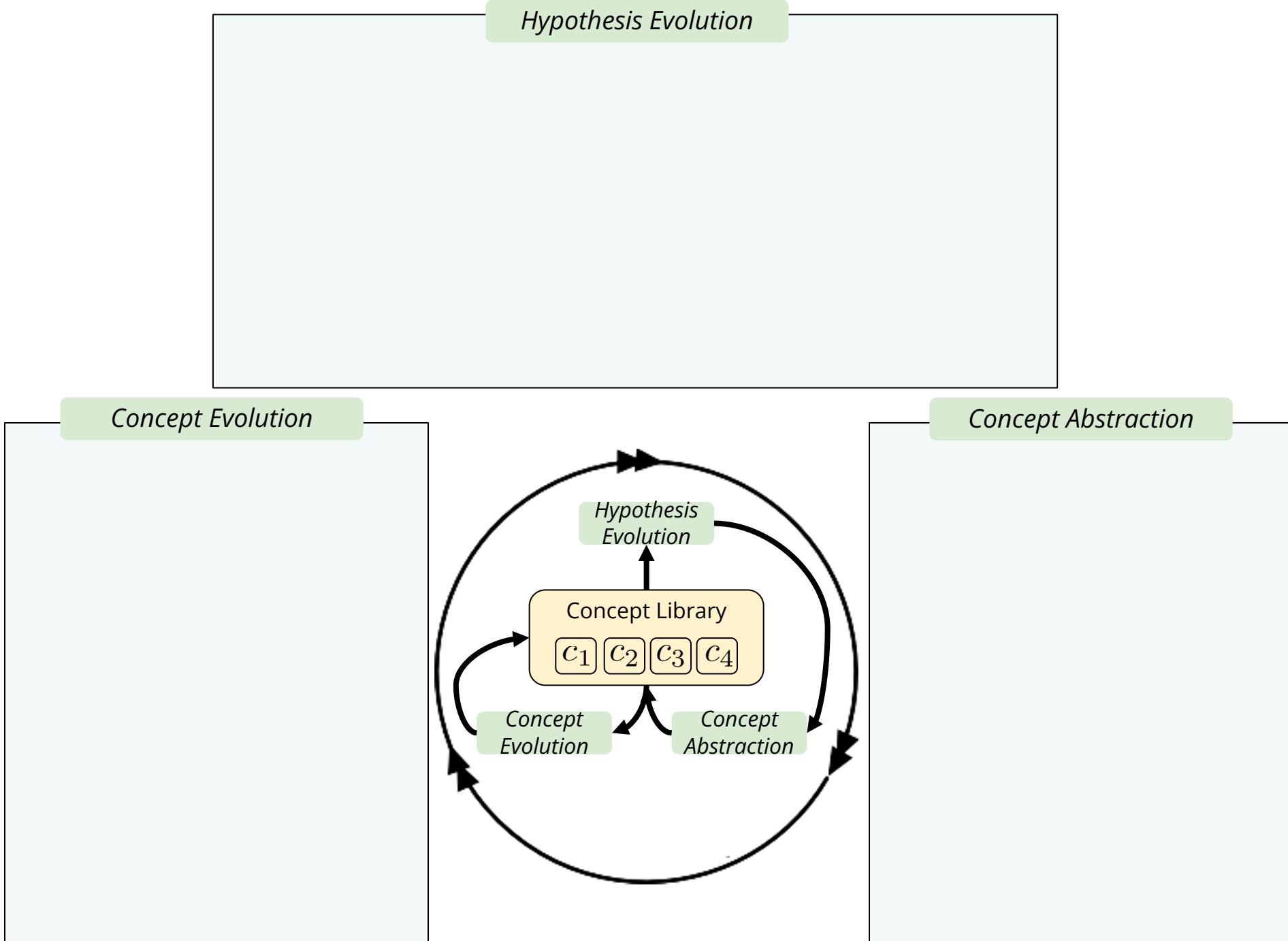
Propose {{N}} expressions that would be appropriate given the suggestions and expressions. Provide short commentary for each of your decisions. End with a JSON list that enumerates the proposed expressions following this format:

(User)
JSON
Formatting
Instructions

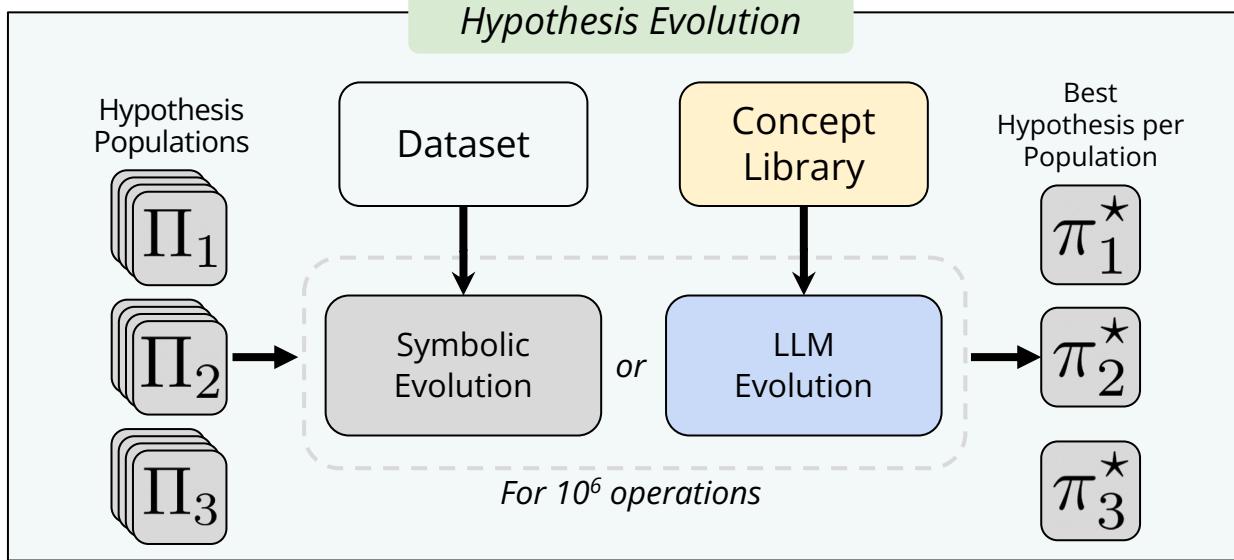
```
```json
["expr1",
 "expr2",
 ...
 "expr{{N}}"]
```
```



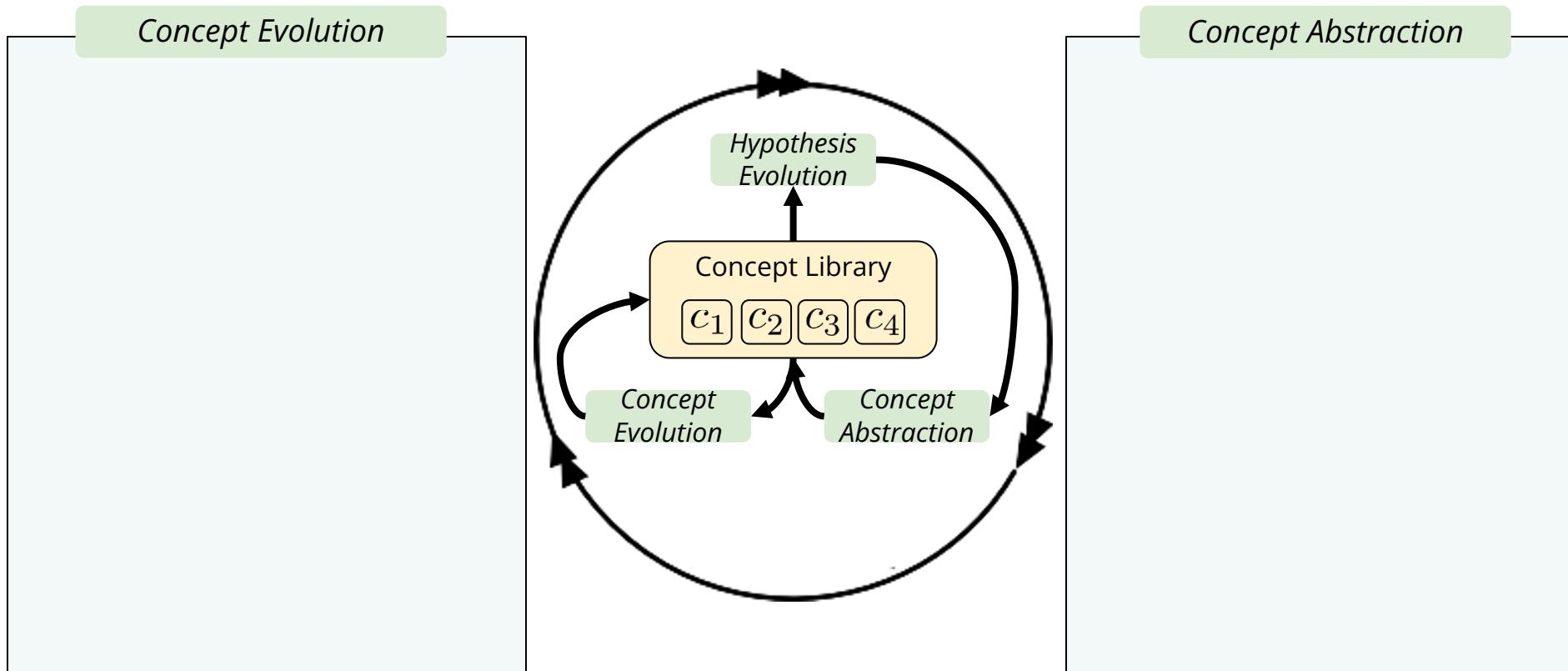
LaSR



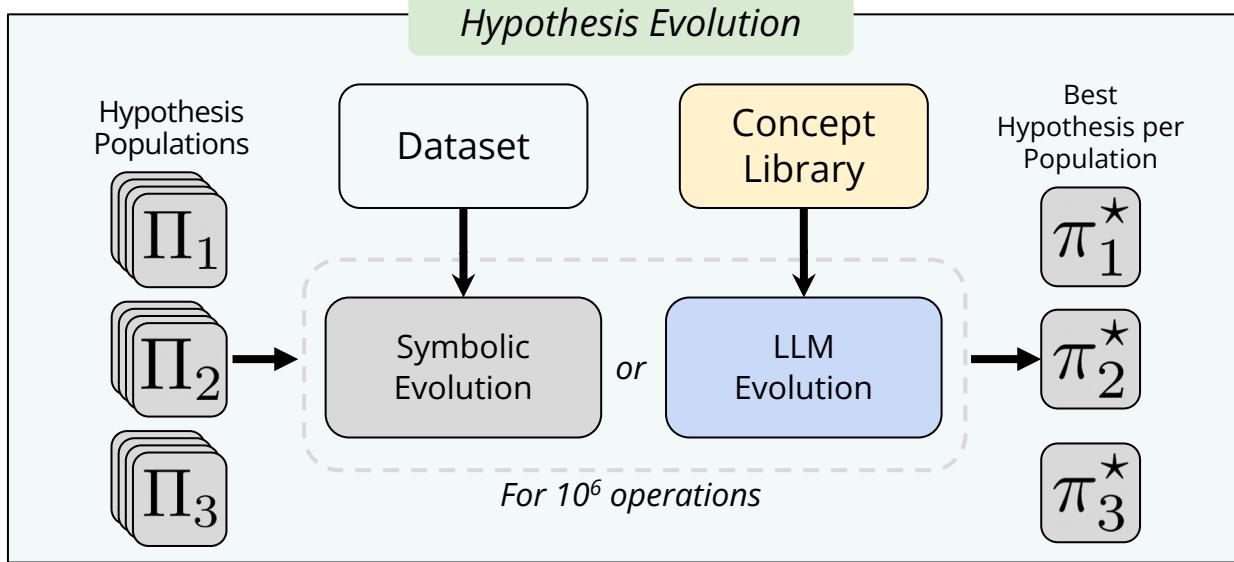
LaSR



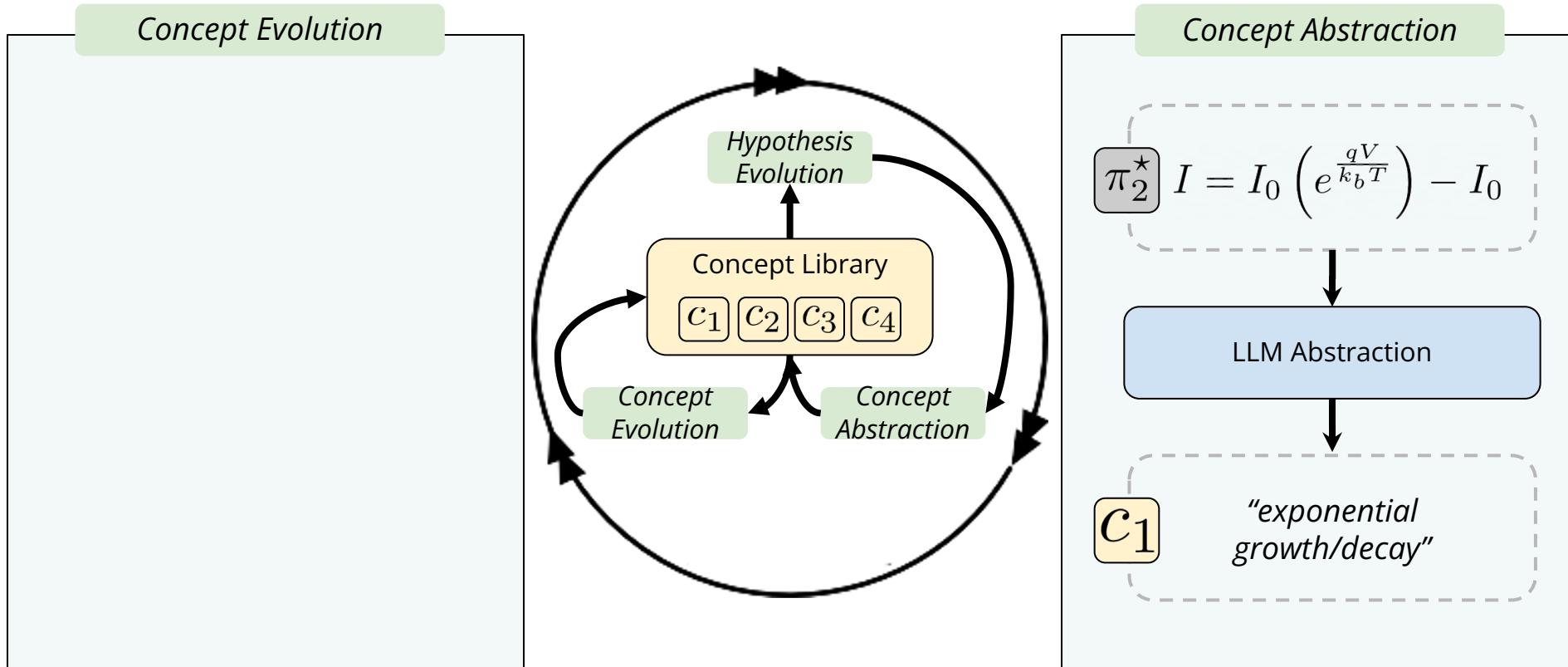
LLM Evolution provides neural guidance (over a language prior)



LaSR

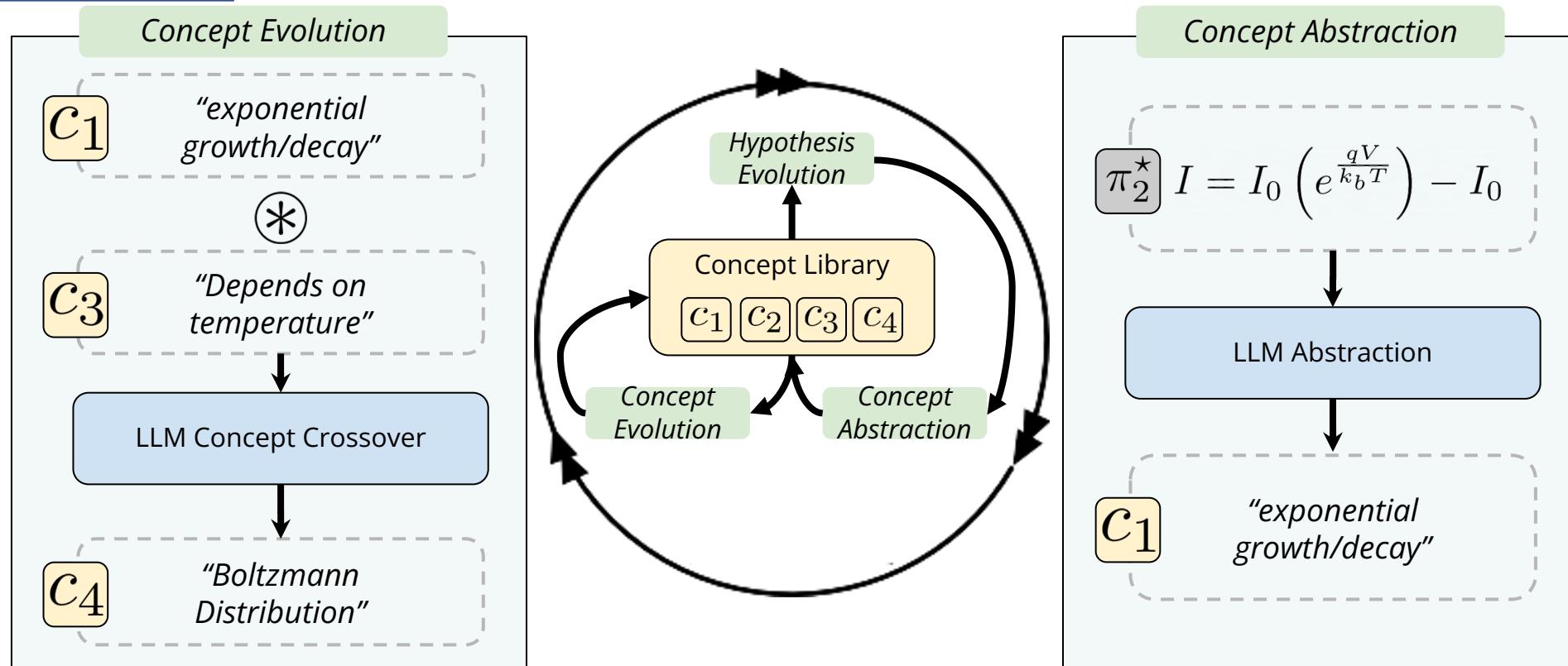
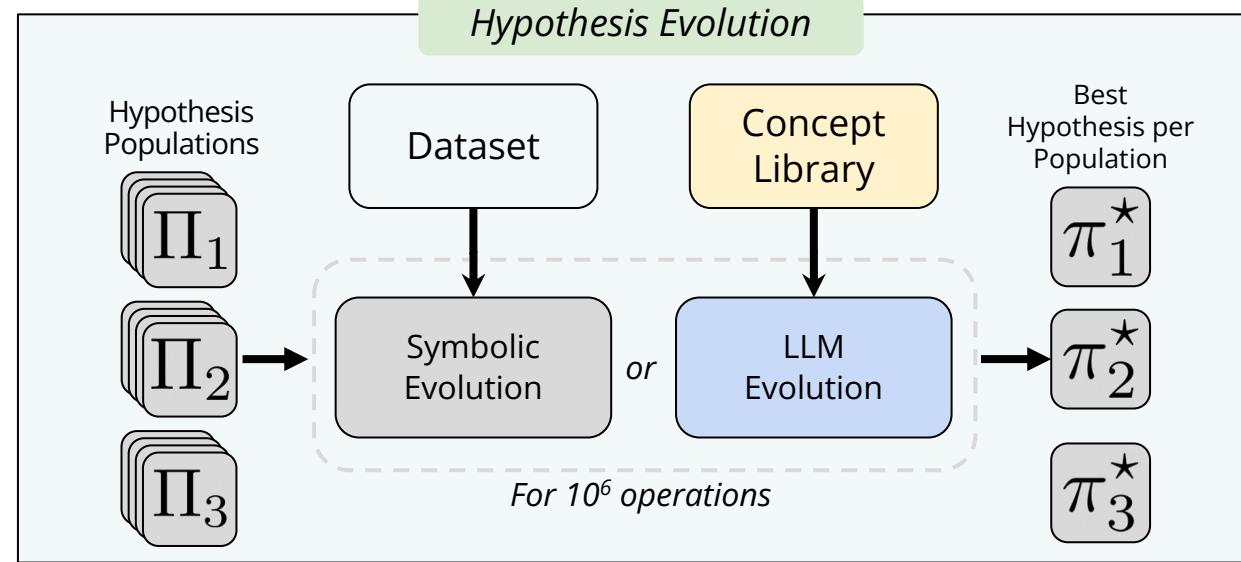


LLM Abstraction
induces *useful** abstractions.

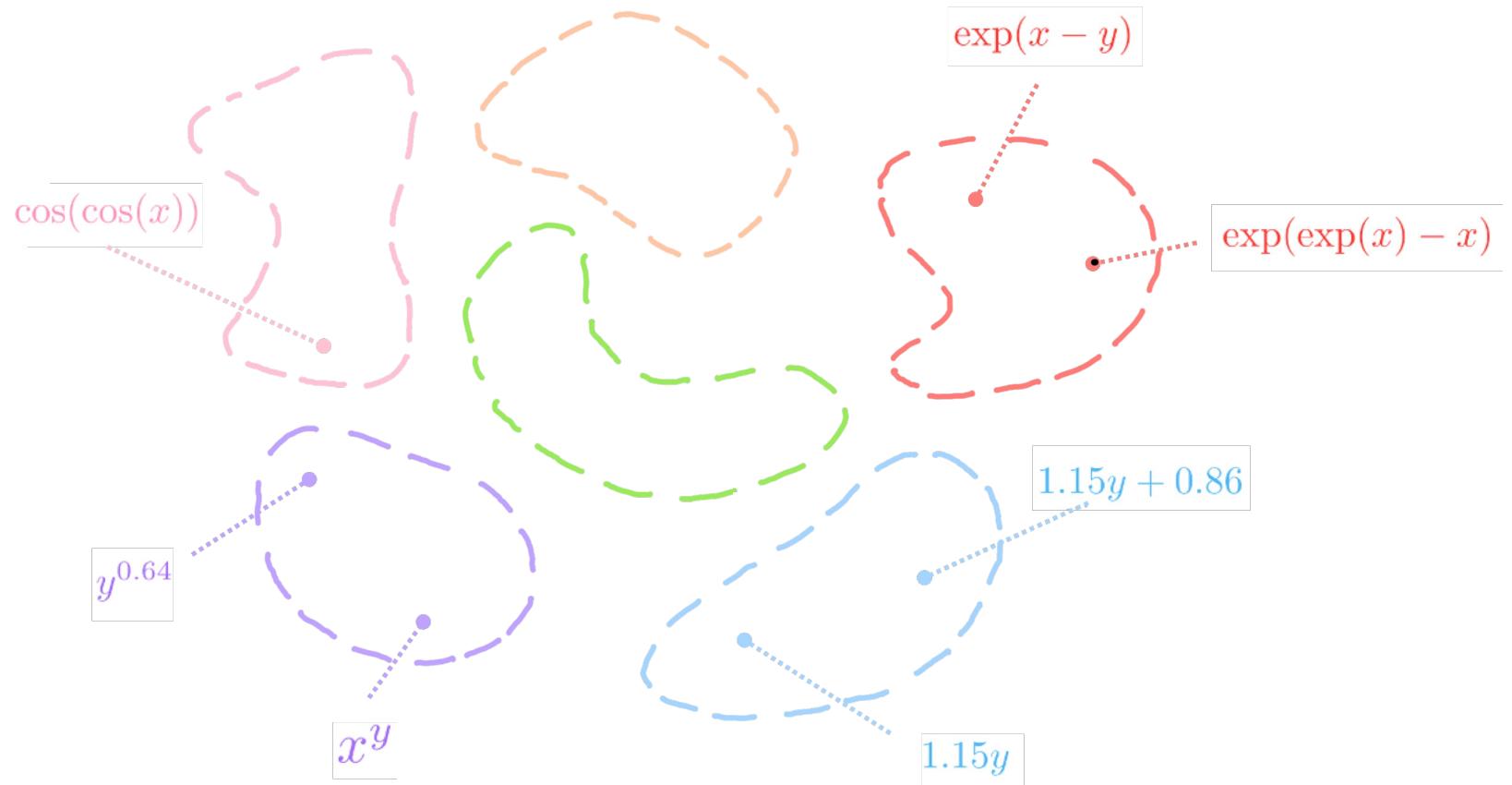


LaSR

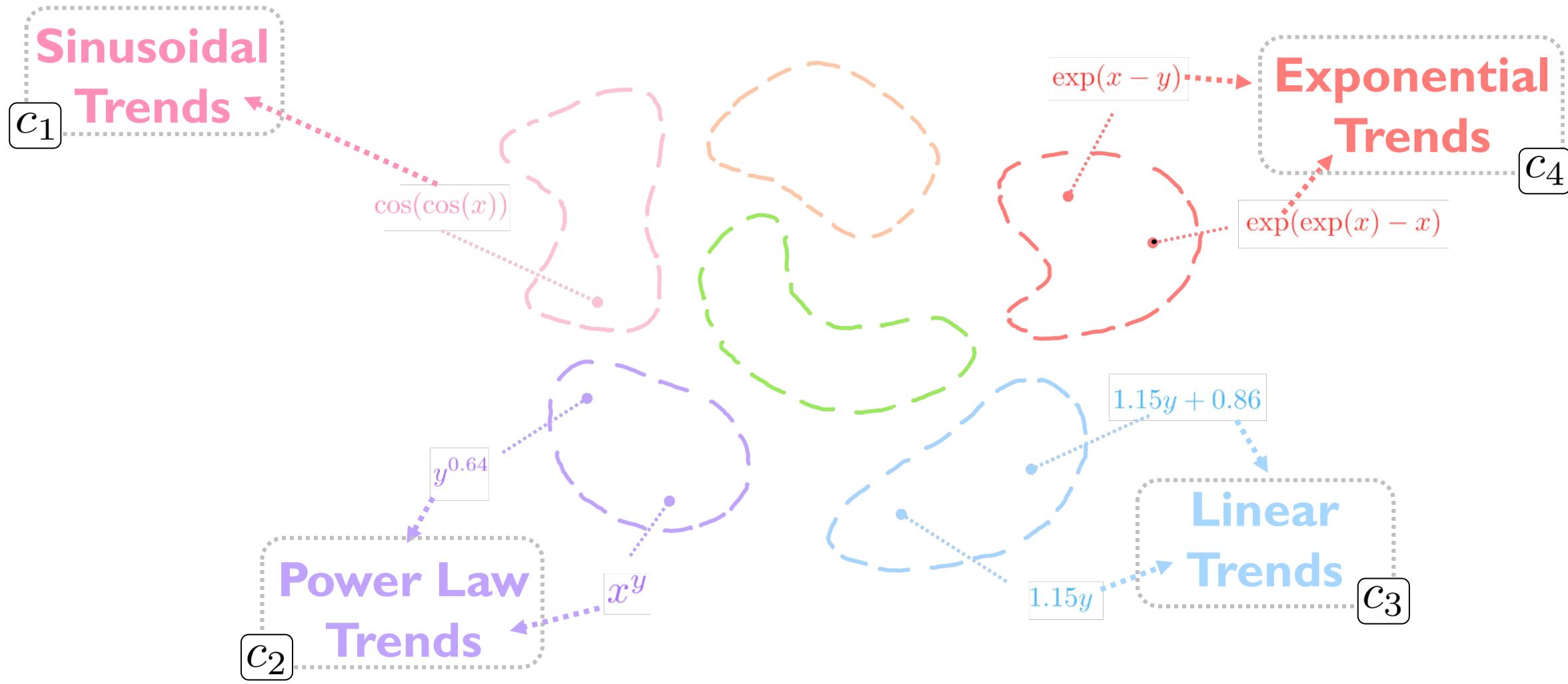
LLM Concept
Crossover evolves
all concepts.



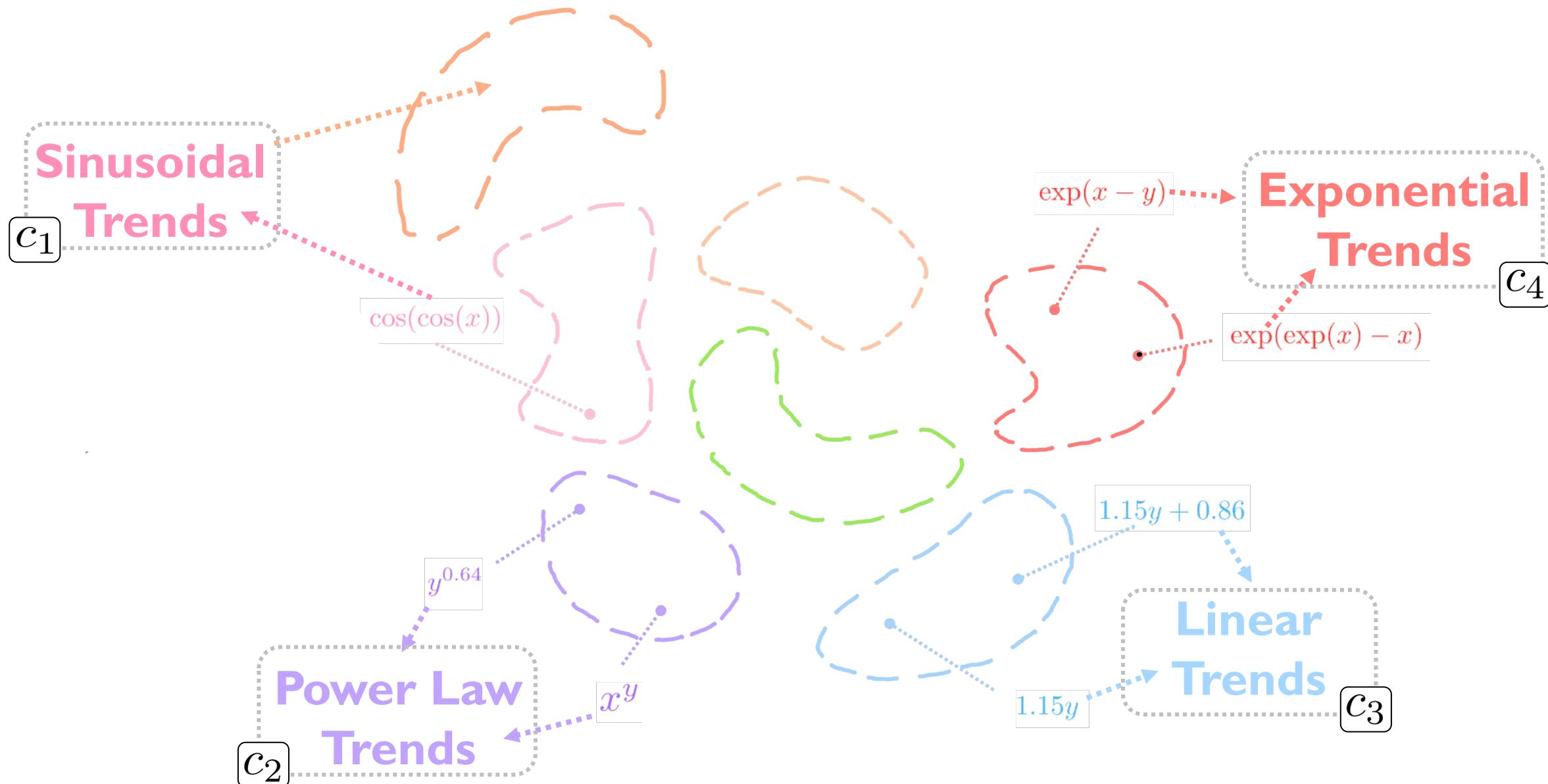
LaSR - Sketch of Search Space



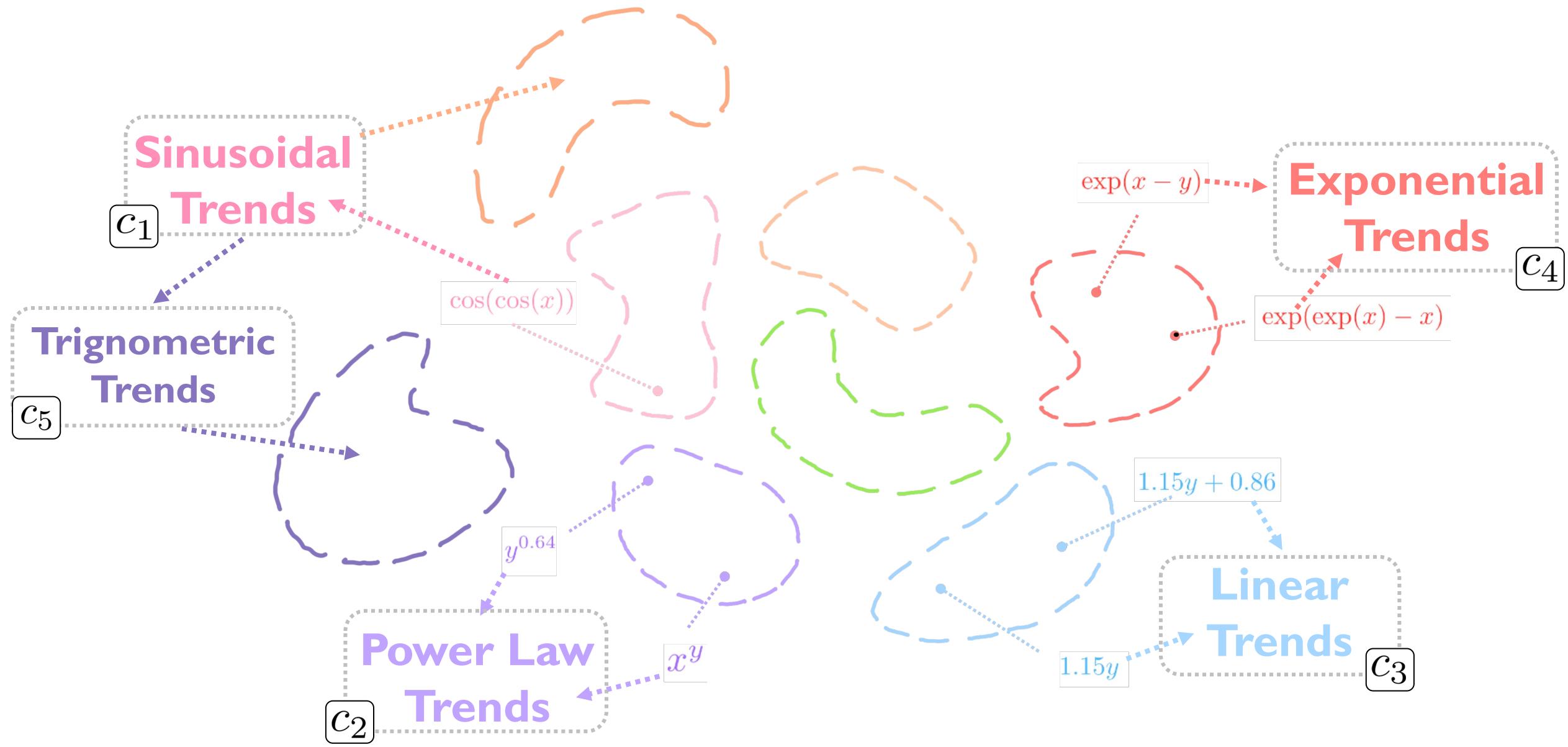
LaSR - Sketch of Search Space



LaSR - Sketch of Search Space



LaSR - Sketch of Search Space



LaSR Results I - Performance

- Concept Guidance accelerates scientific discovery.
- LaSR outperforms PySR even with local language models (llama-3-7b, 1%)

| GPlearn | AFP | AFP-FE | DSR | uDSR | AIFeynman | PySR | LaSR |
|---------|--------|--------|--------|--------|-----------|--------|-------------------|
| 20/100 | 24/100 | 26/100 | 23/100 | 40/100 | 38/100 | 59/100 | 59 + 7/100 |

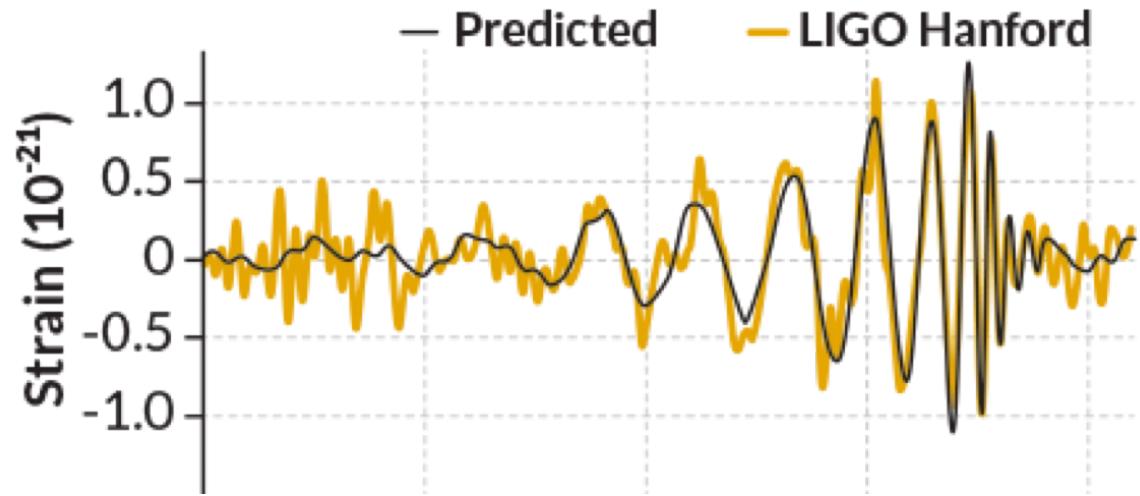
Table 1: Results on 100 Feynman equations from [41]. We report exact match solve rate for all models. LASR achieves the best exact match solve rate using the same hyperparameters as PySR [8].

| Type of Solve | PySR | LASR (Llama3-8B) | | | LASR (GPT-3.5) |
|---------------|--------|------------------|-----------|------------|----------------|
| | | $p = 1\%$ | $p = 5\%$ | $p = 10\%$ | $p = 1\%$ |
| Exact Solve | 59/100 | 63/100 | 65/100 | 65/100 | 66/100 |
| Almost Solve | 7/100 | 6/100 | 9/100 | 12/100 | 13/100 |
| Close | 16/100 | 13/100 | 14/100 | 11/100 | 9/100 |
| Not Close | 18/100 | 18/100 | 12/100 | 13/100 | 13/100 |

Table 2: Evaluation results on Feynman dataset by cascading LASR’s LLM backbone (llama3-8b, gpt-3.5-turbo) and changing the probability of calling the model ($p = [0.01, 0.05, 0.10]$) in the order of increasing concept guidance. LASR outperforms PySR even with minimal concept guidance using an open-source LLM.

What is a Concept?

Desiderata II : Symbolic Guidance



Concepts (by Physicist or LLM)

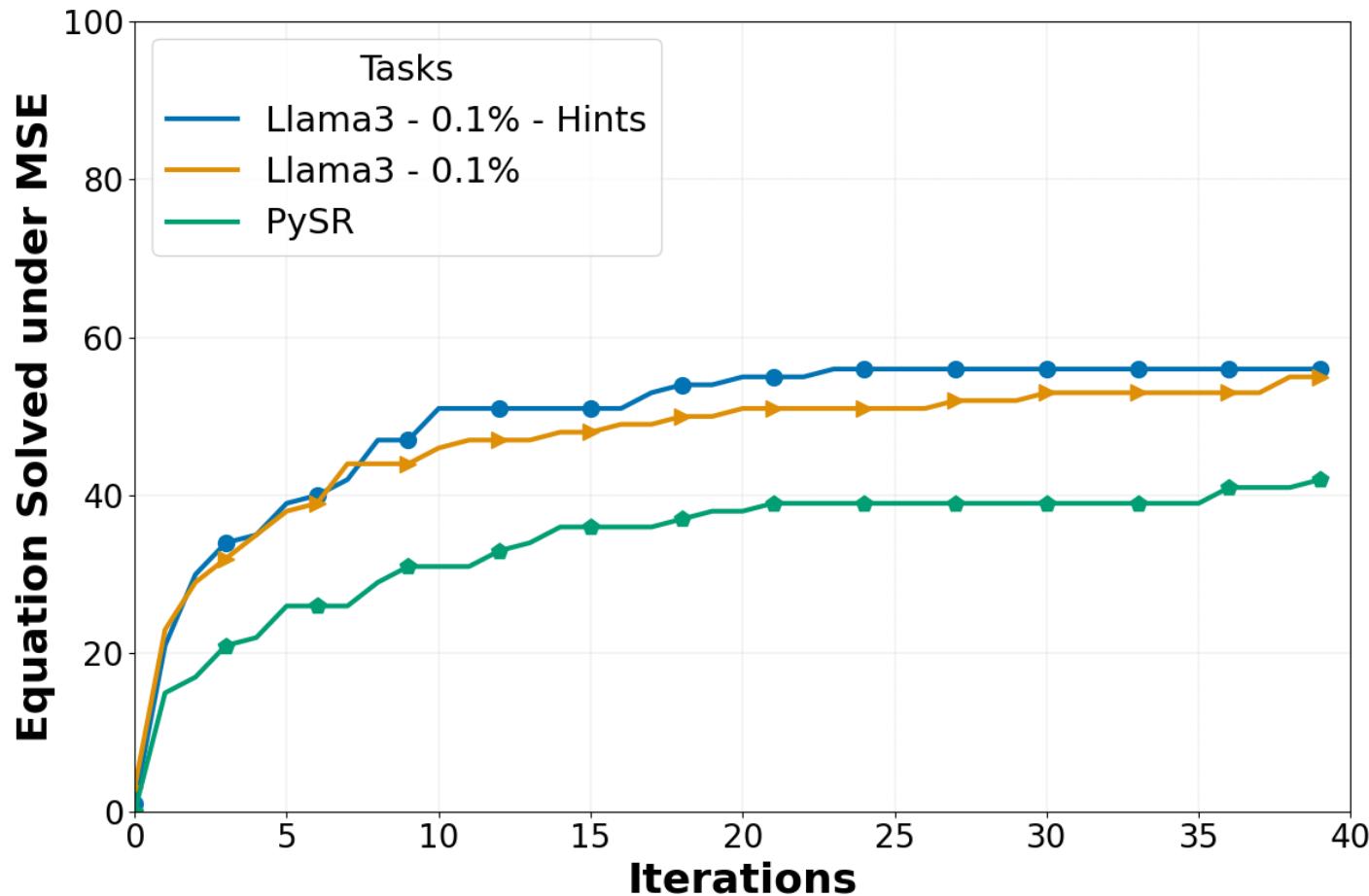
“Wave strain diminishes as distance increases”

“Wave strain has extraordinarily small magnitude”

Guide the search for

$$h = \frac{2G}{c^4} \frac{1}{r} \frac{\partial^2 Q}{\partial t^2}$$

LaSR Results II - Hints



User provided hints accelerate hypothesis search

Results III - Case Study

$$F = \frac{1}{4\pi\epsilon} \frac{q_1 q_2}{r^2}$$

$$F = \frac{\left(\left(\frac{q_2 \cdot 3.382}{r} \right) - \left(\frac{\sin\left(\frac{0.017}{\exp(B)}\right)}{\exp(C)} \right) \right) / 0.712 \right) \cdot q_1 \right) \cdot 0.087 \right) / \epsilon \right) \cdot 0.191 \right)$$

Eq 10: Coulomb's Law

- Inverse Square Law
- Directly proportional to charges
- Force symmetric w.r.t charges

PySR's Solution

- Reduces to ground truth after 10 steps of simplification.
- Unwieldy
- Fitting more constants => more optimization errors

Results III - Case Study

$$F = \frac{1}{4\pi\epsilon} \frac{q_1 q_2}{r^2}$$

Eq 10: Coulomb's Law

- Inverse Square Law
- Directly proportional to charges
- Force symmetric w.r.t charges

$$\begin{aligned} F &= \frac{q_1}{\left(\frac{r}{q_2}\right) \left(r + \frac{1.9181636 \times 10^{-5}}{q_2}\right) \epsilon} \cdot 0.07957782 \\ &= \frac{q_1}{\left(\frac{r}{q_2}\right) \left(r + \frac{1.9181636 \times 10^{-5}}{q_2}\right) \epsilon} \cdot \frac{1}{4\pi} && \text{(Substitute constant)} \\ &= \frac{q_1 q_2}{r \left(r + \frac{1.9181636 \times 10^{-5}}{q_2}\right) \epsilon} \cdot \frac{1}{4\pi} && \text{(Simplify denominator)} \\ &\approx \frac{q_1 q_2}{r(r)\epsilon} \cdot \frac{1}{4\pi} && \text{(Negligible. } \frac{1.9181636 \times 10^{-5}}{q_2} \approx 0) \end{aligned}$$

LaSR's Solution

- Reduces to ground truth after 4 steps of simplification
- Smaller models synthesize simpler equations!

Results III - Case Study

$$F = \frac{1}{4\pi\epsilon} \frac{q_1 q_2}{r^2}$$

Eq 10: Coulomb's Law

- Inverse Square Law
- Directly proportional to charges
- Force symmetric w.r.t charges

| Iteration | Discovered Concept |
|-----------|--|
| 2 | The good mathematical expressions exhibit [...] with a focus on power functions and trigonometric functions [...] |
| 6 | The good mathematical expressions exhibit [...] symmetry or regularity [...] |
| 24 | The good mathematical expressions have [...] with a specific pattern of division and multiplication |

LaSR's Concepts (Limitations)

- Cannot guarantee factuality or correctness.
- Good concepts depend on LLM training.
Concepts can mislead scientists.

Outline of this Talk

- I. What is Scientific Discovery?
 - I. Symbolic Regression
2. Symbolic Regression with a Concept Library
3. **Additional Application: Visual Reasoning**
4. Discussion

Recap: Symbolic Regression

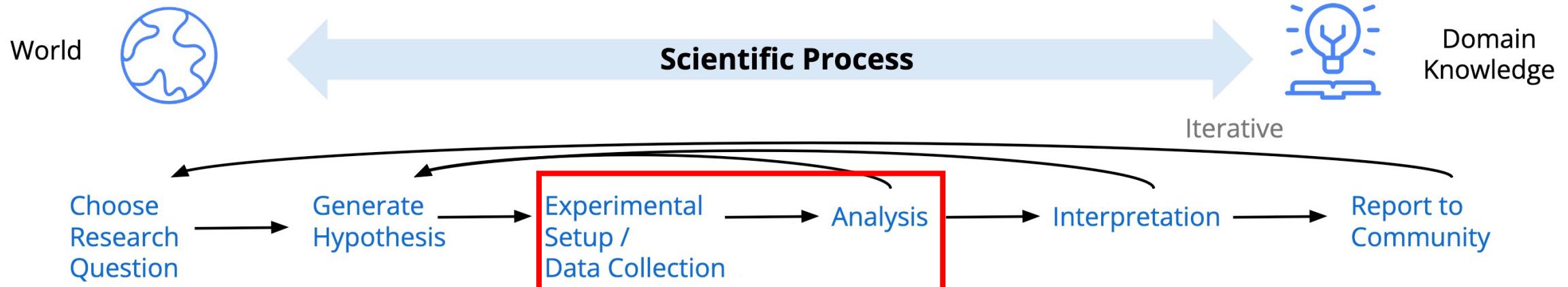
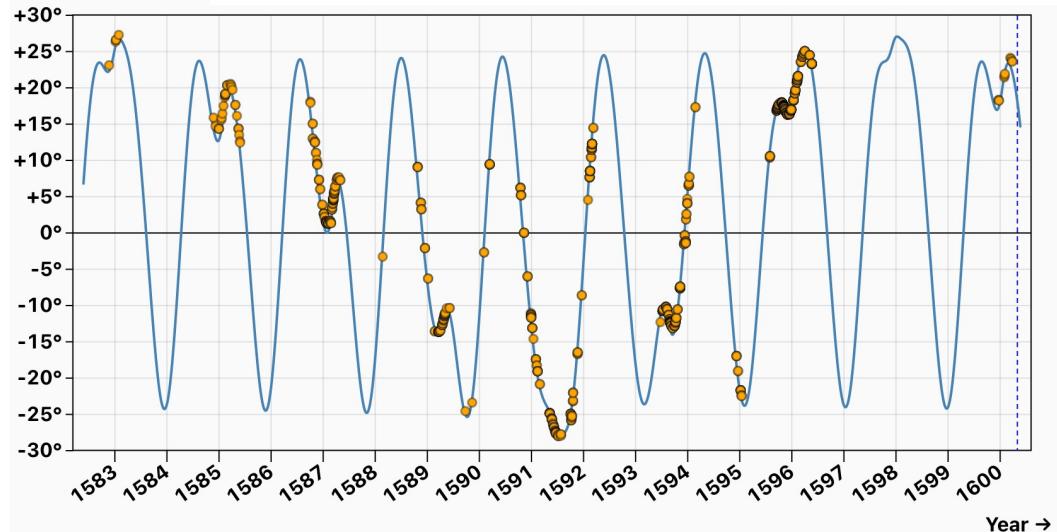


Figure 1: Tycho Brahe's observations of the planet Mars (period 1582 – 1600).

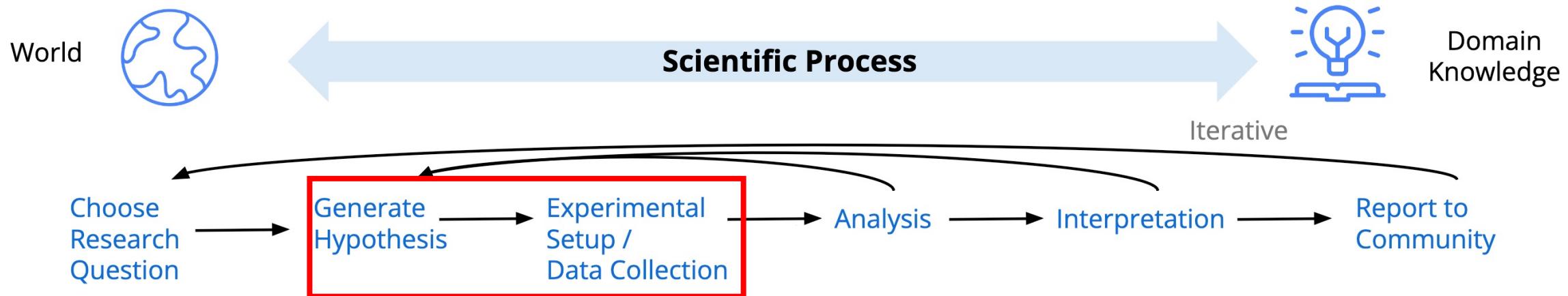
↑ Declination, δ
● Tycho Brahe's observations
— Theoretical declination (ephemeris from NASA horizons' database)



Kepler's Third Law

$$T^2 \propto r^3$$

Visual Reasoning



Observation: Geolocated Picture

finatic suggested an ID Ø ID Withdrawn 9y

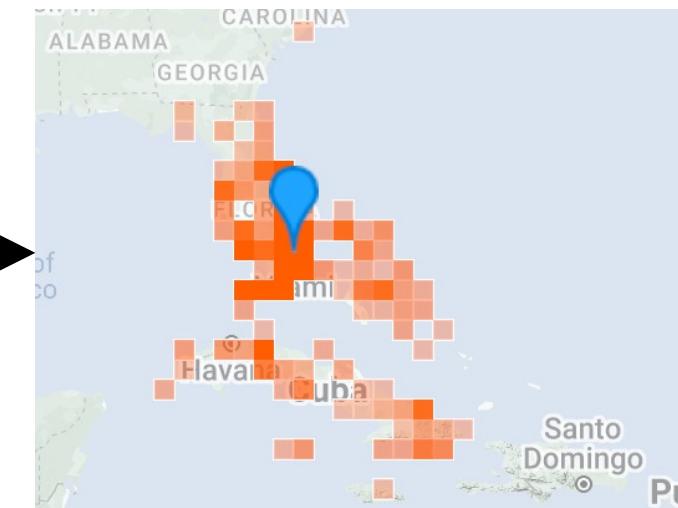
Florida Scrub Lizard
Sceloporus woodi

hydaticus suggested an ID 🏆 Improving 9y

Northern Curly-tailed Lizard
Leiocephalus carinatus

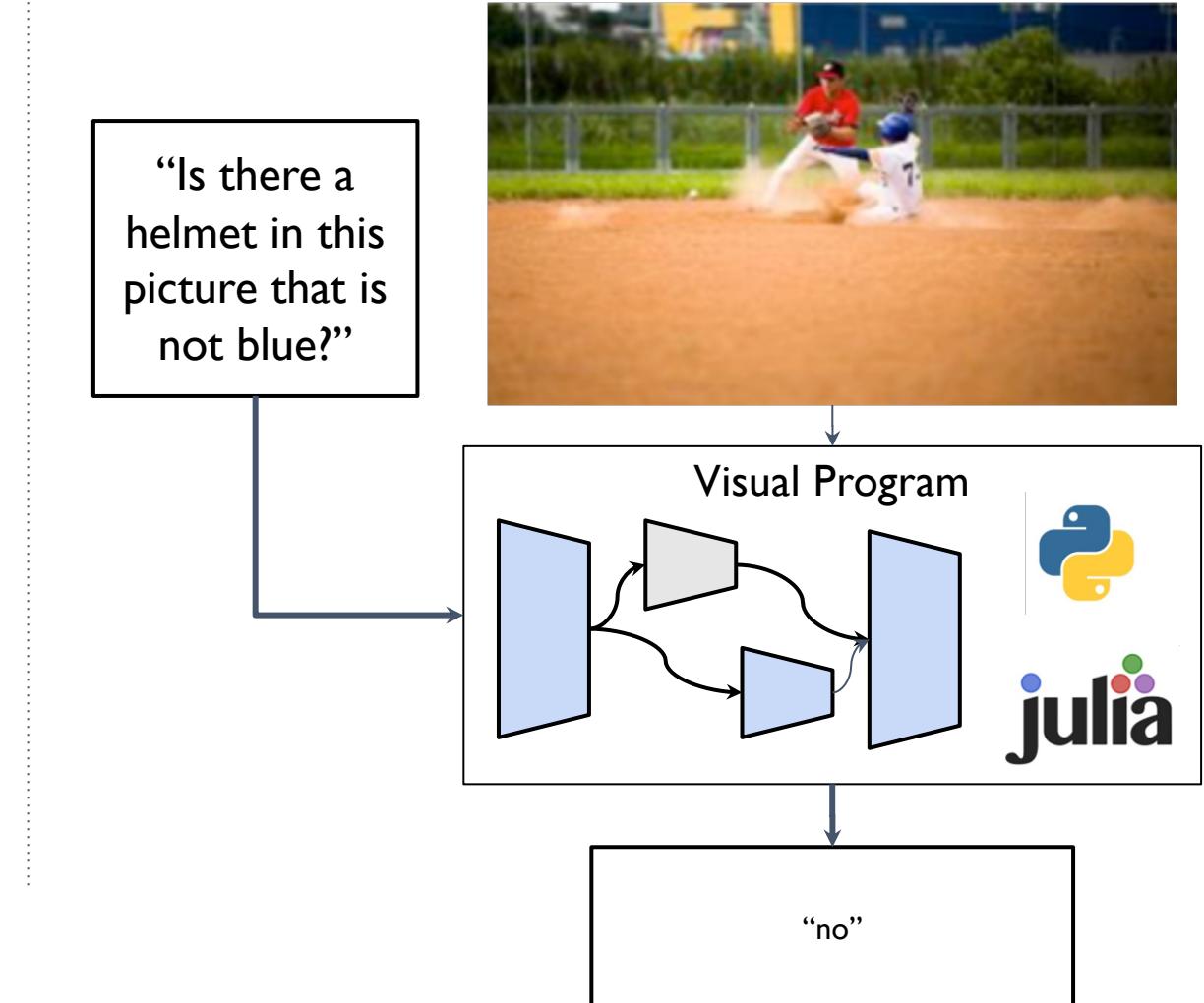
The tail looks too strongly keeled to be Sceloporus.

Theory: Crowdsourced identification



Data: Geotagged sightings

Visual Programming



Compositional Question Answering

Is there a helmet in the photo that is not blue?



Prediction: no

| | |
|------|--|
| |  IMAGE |
| | <code>BOX0=Loc(image=IMAGE, object='helmet')</code> |
| |  <code>IMAGE0=Crop(bbox=BOX0)</code> |
| blue | <code>ANSWER0=Vqa(image=IMAGE0, question='What color is the helmet?')</code> |
| no | <code>ANSWER1=Eval(expr="'yes' if {ANSWER0} != 'blue' else 'no'")</code>
<code>=Eval(expr="'yes' if 'blue' != 'blue' else 'no'")</code> |

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 - I. Symbolic Regression**
- 2. Symbolic Regression with a Concept Library**
- 3. Additional Application: Visual Reasoning**
- 4. Discussion**