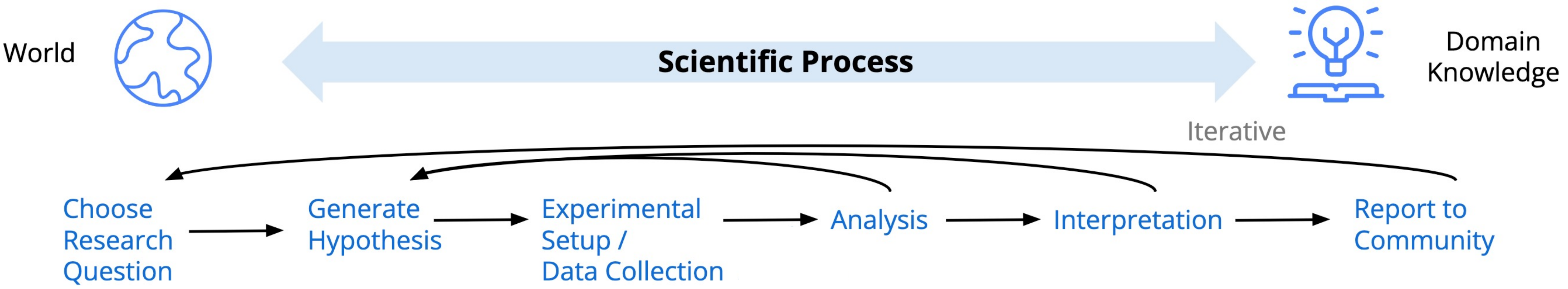


Goal: We want AI to achieve human level performance at *research in the natural sciences.*

World

Scientific Process

Domain Knowledge

Iterative

Choose Research Question → Generate Hypothesis → Experimental Setup / Data Collection → Analysis → Interpretation → Report to Community

Observation: Apparent Retrograde Planetary Motion

c.The Astronomical Revolution: Copernicus- Kepler-Borelli

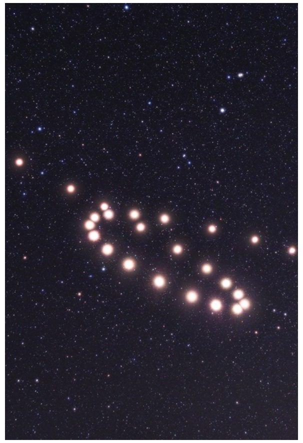
World

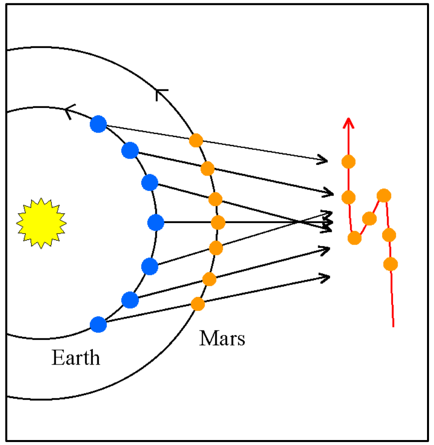
Scientific Process

Domain Knowledge

Iterative

Choose Research Question → Generate Hypothesis → Experimental Setup / Data Collection → Analysis → Interpretation → Report to Community





Observation: Apparent Retrograde Planetary Motion

Theory: Heliocentric Model

c.The Astronomical Revolution: Copernicus- Kepler-Borelli

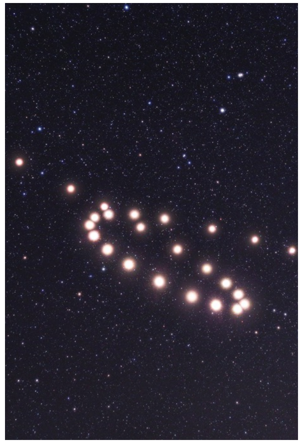
World

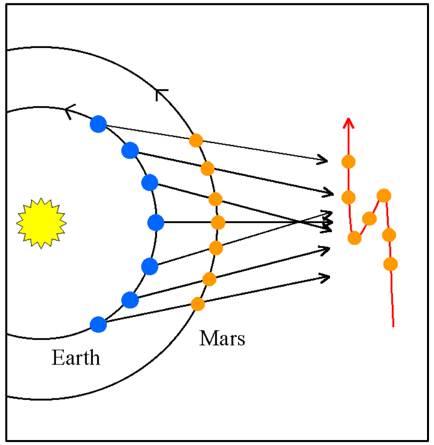
Scientific Process

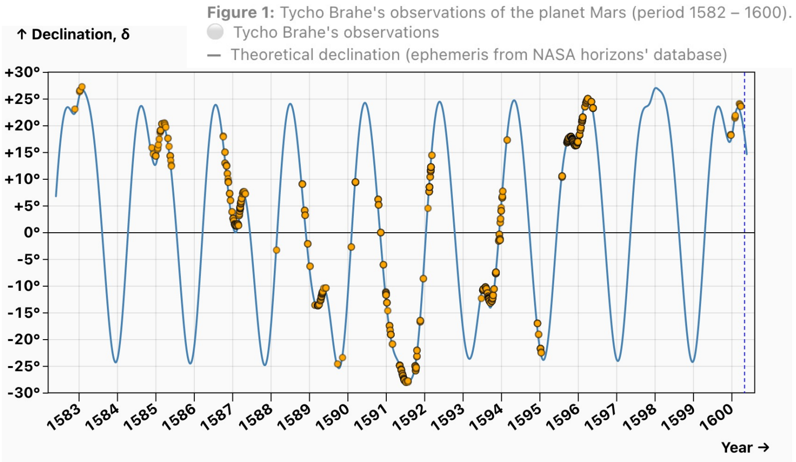
Domain Knowledge

Iterative

Choose Research Question → Generate Hypothesis → Experimental Setup / Data Collection → Analysis → Interpretation → Report to Community







Observation: Apparent Retrograde Planetary Motion
Theory: Heliocentric Model

Data Collection: Sample data in regime of interest.

c.The Astronomical Revolution: Copernicus- Kepler-Borelli

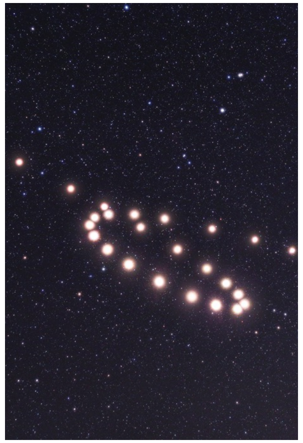
World

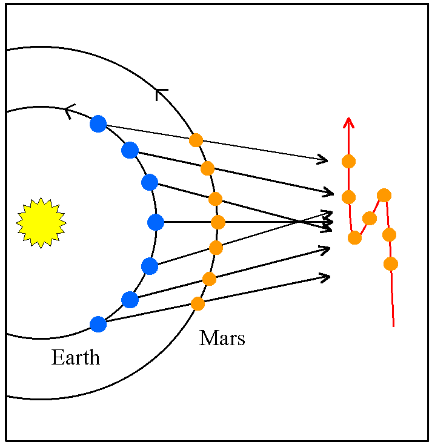
Scientific Process

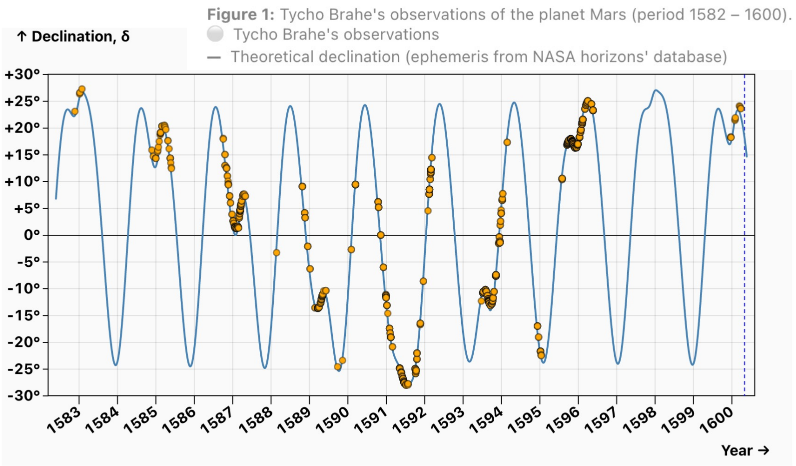
Domain Knowledge

Iterative

Choose Research Question → Generate Hypothesis → Experimental Setup / Data Collection → Analysis → Interpretation → Report to Community







Observation: Apparent Retrograde Planetary Motion
Theory: Heliocentric Model

Data Collection: Sample data in regime of interest.

Analysis: Kepler's Third Law

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

c.The Astronomical Revolution: Copernicus- Kepler-Borelli

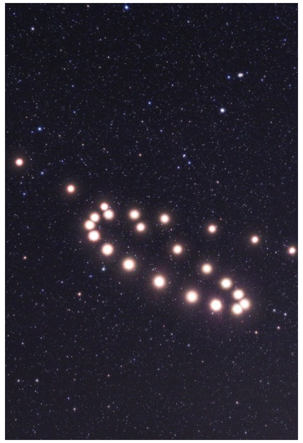
World

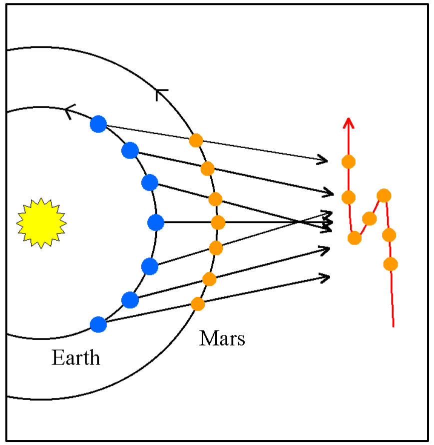
Scientific Process

Domain Knowledge

Iterative

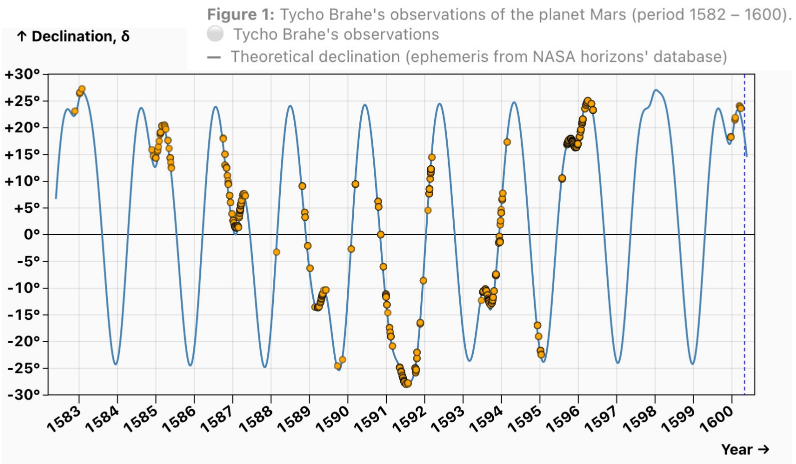
Choose Research Question → Generate Hypothesis → Experimental Setup / Data Collection → Analysis → $\boxed{\text{Interpretation}}$ → Report to Community





Observation: Apparent Retrograde Planetary Motion

Theory: Heliocentric Model



Data Collection: Sample data in regime of interest.

Analysis: Kepler's Third Law

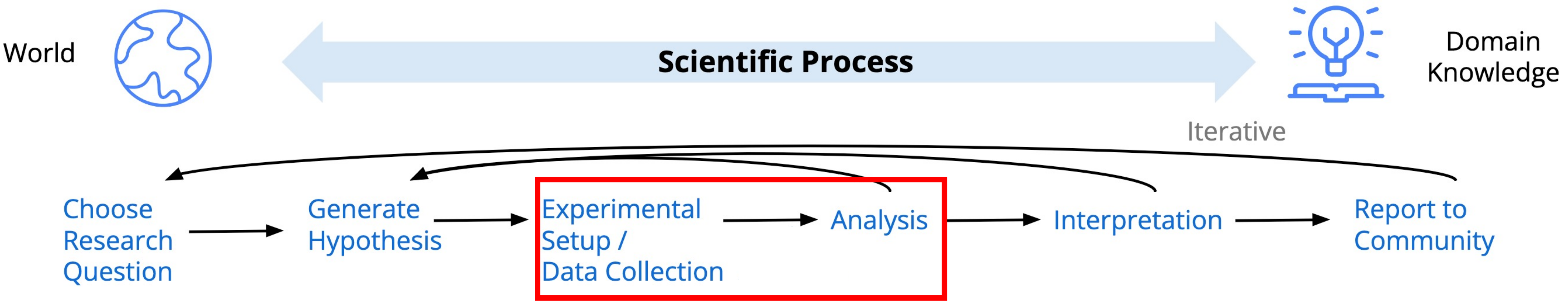
$$T^2 \propto r^3$$

$$\Downarrow$$

Interpretation: Newton's Law of Gravitation

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

c. The Astronomical Revolution: Copernicus- Kepler-Borelli



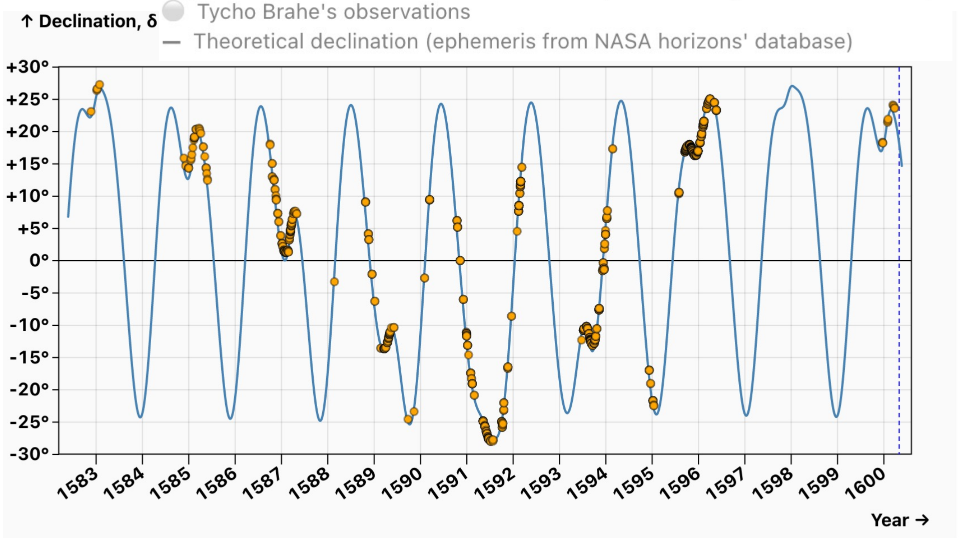


Figure 1: Tycho Brahe's observations of the planet Mars (period 1582 – 1600).

Kepler's Third Law

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

c.The Astronomical Revolution: Copernicus- Kepler-Borelli

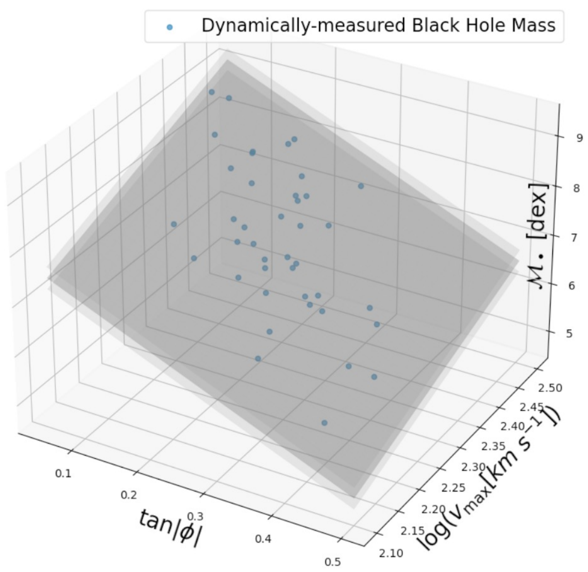
Symbolic Regression Algorithms

c. PySR. Miles Cranmer

Symbolic Regression Algorithms

c. PySR. Miles Cranmer

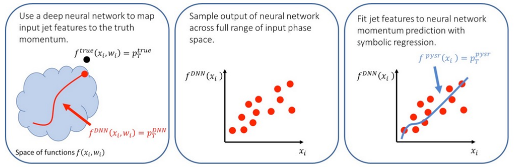
PySR’s impact



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

Benjamin L. Davis [1], Zehao Jin [1]

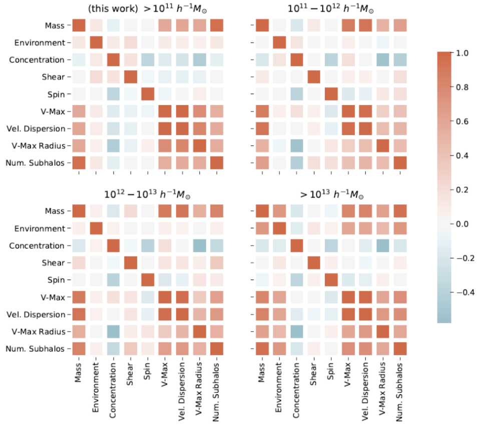
[1]Center for Astrophysics and Space Science, New York University Abu Dhabi



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 Nattrass [1]

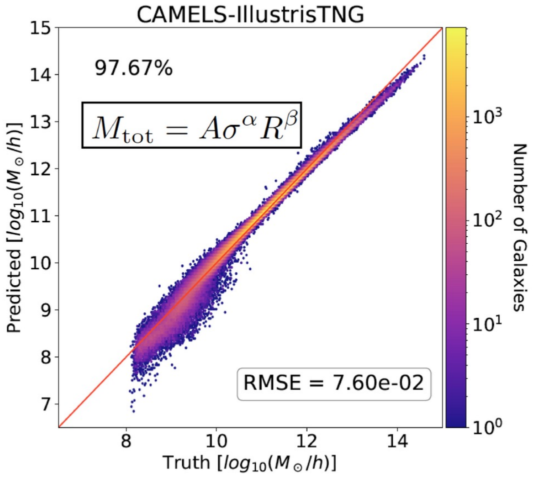
[1]University of Tennessee, Knoxville, [2]Iowa State University of Science and Technology



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]

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

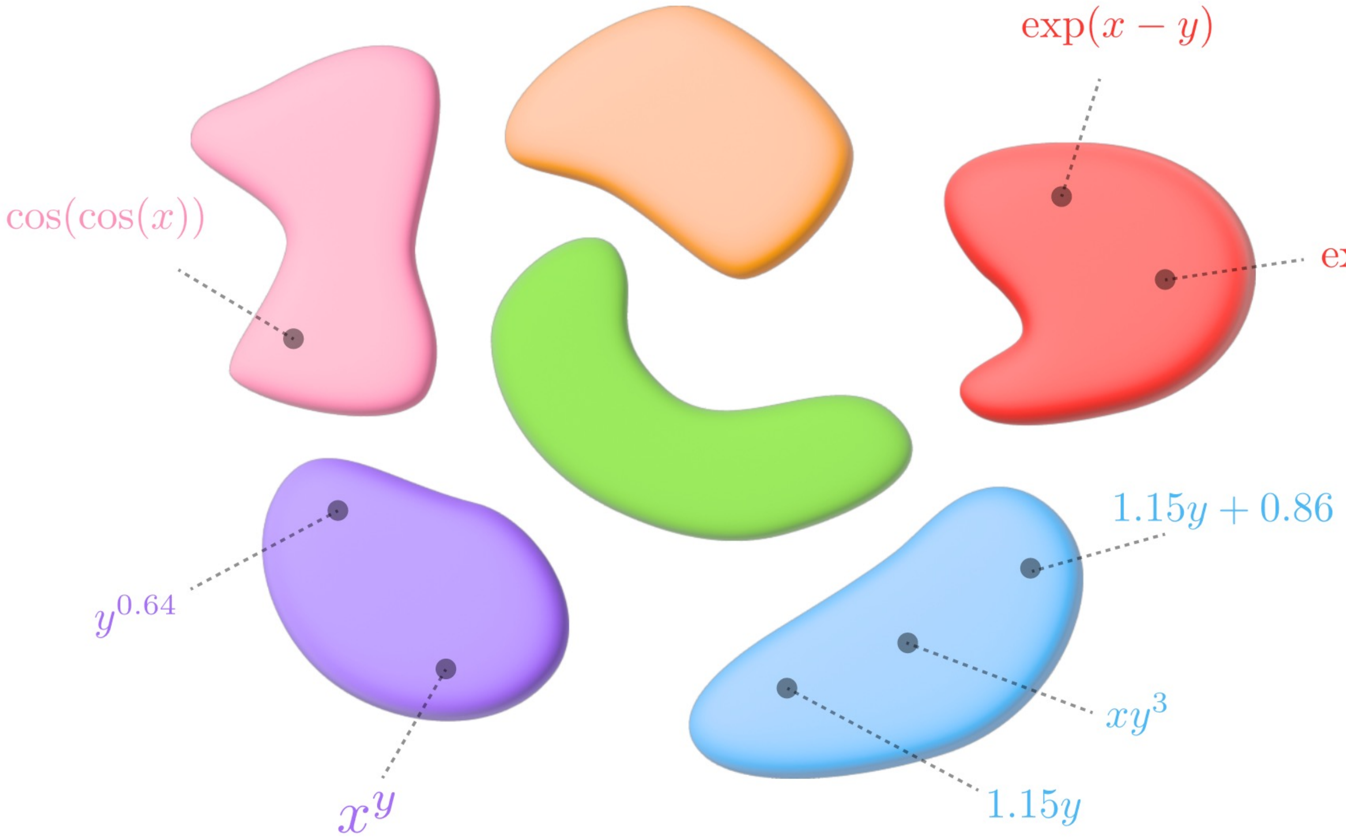


Finding universal relations in subhalo properties with artificial intelligence

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]

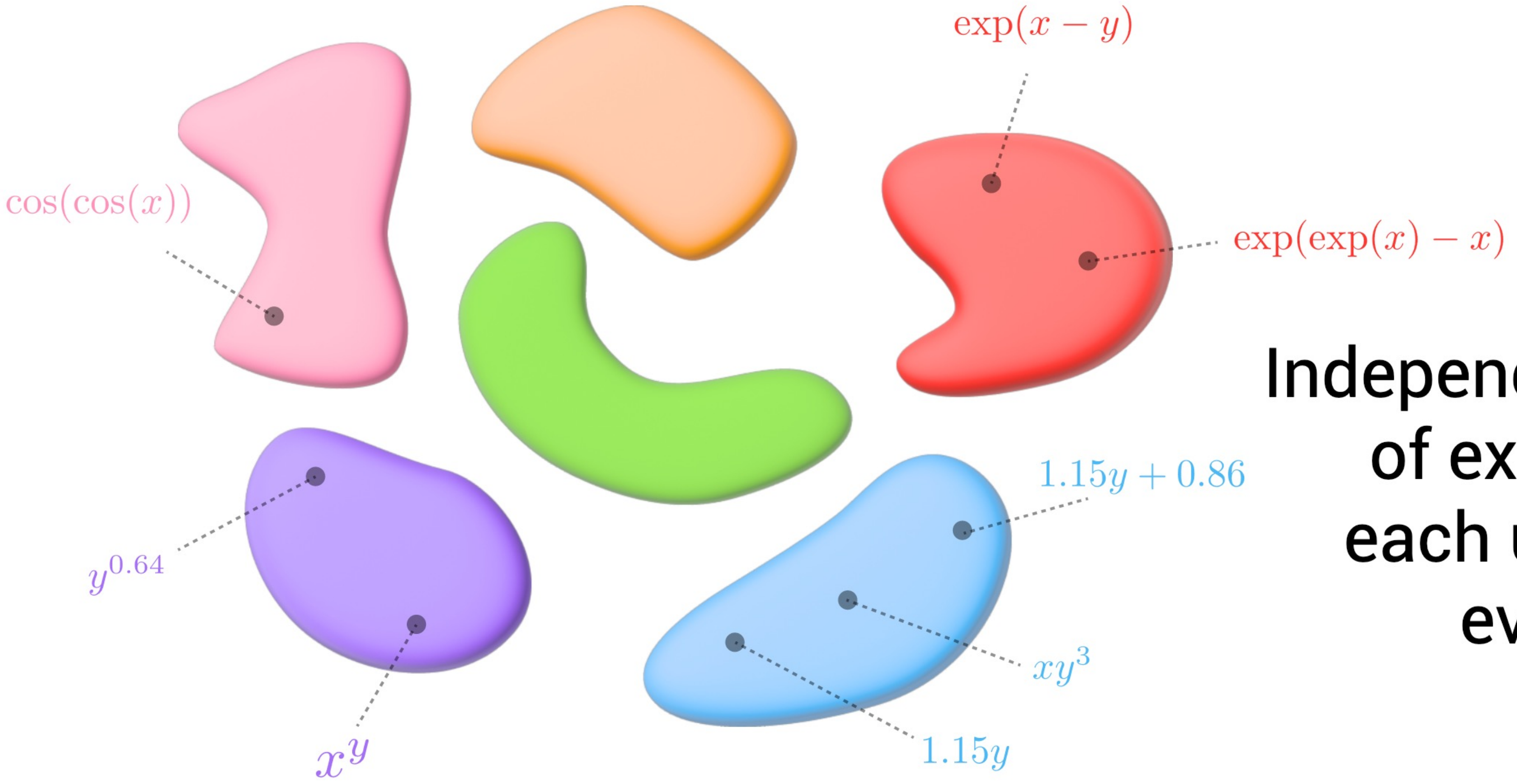
[1]Princeton University, [2]Flatiron Institute, [3]Columbia University, [4]University of Connecticut, [5]Center for Astrophysics | Harvard & Smithsonian, [6]University of Edinburgh, [7]University of the Western Cape, [8]South African Astronomical Observatories, [9]University of Florida, [10]University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

c. PySR. Miles Cranmer



Independent "islands" of expressions, each undergoing evolution

c. PySR. Miles Cranmer



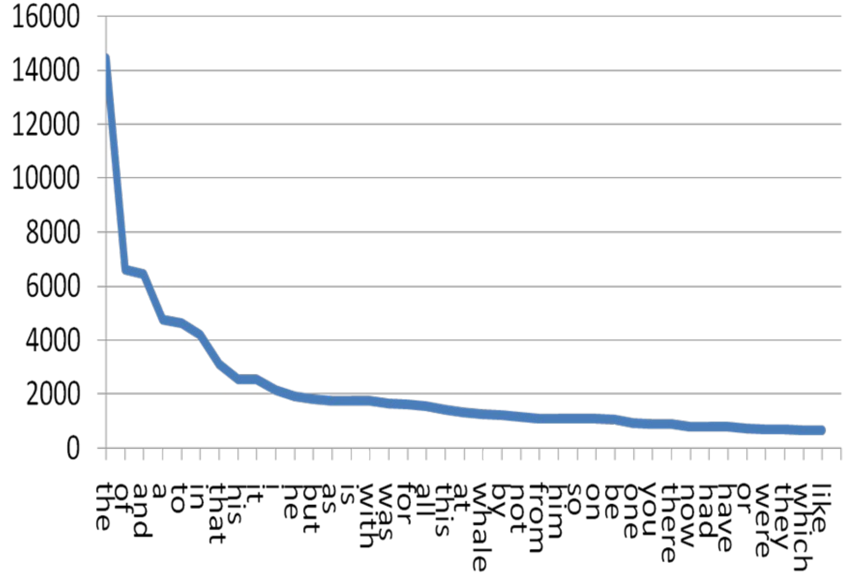
Independent "islands" of expressions, each undergoing evolution

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

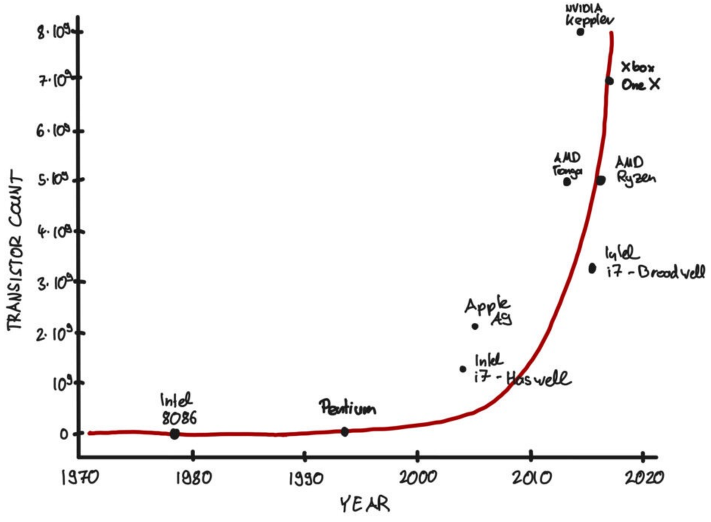
LaSR: Symbolic Regression with a Learned Concept Library

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

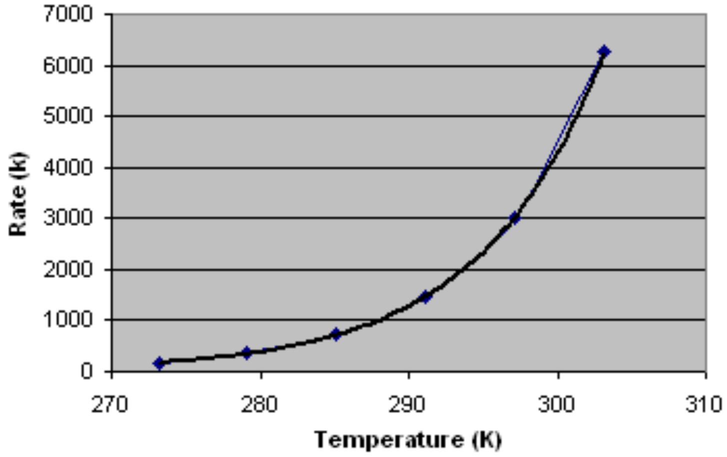
Zipf's Law



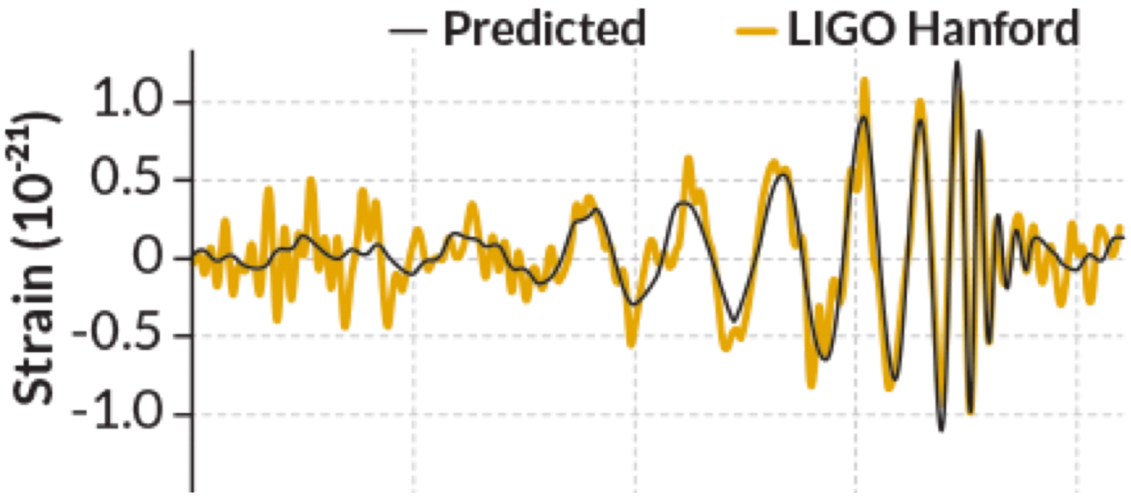
Moore's Law



Arrhenius' Equation



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



Concepts (by Physicist or LLM)

"Wave strain diminishes as distance increases"

"Wave strain has extraordinarily small magnitude"

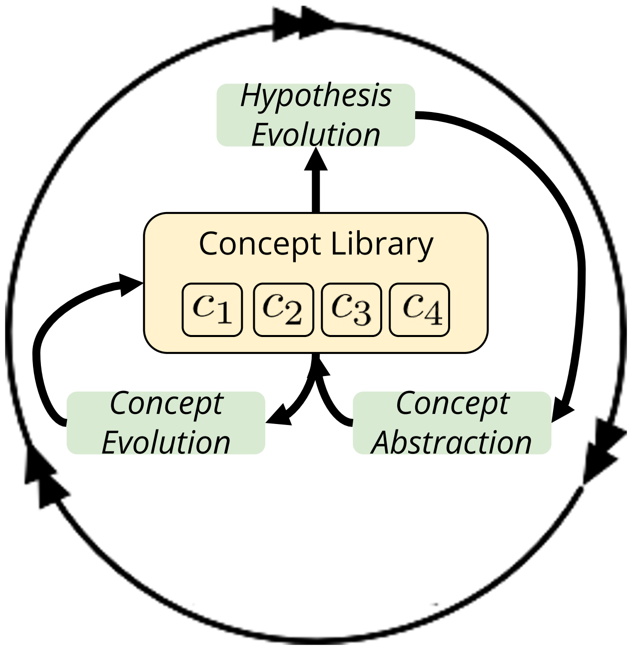
Guide the search for

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

LaSR

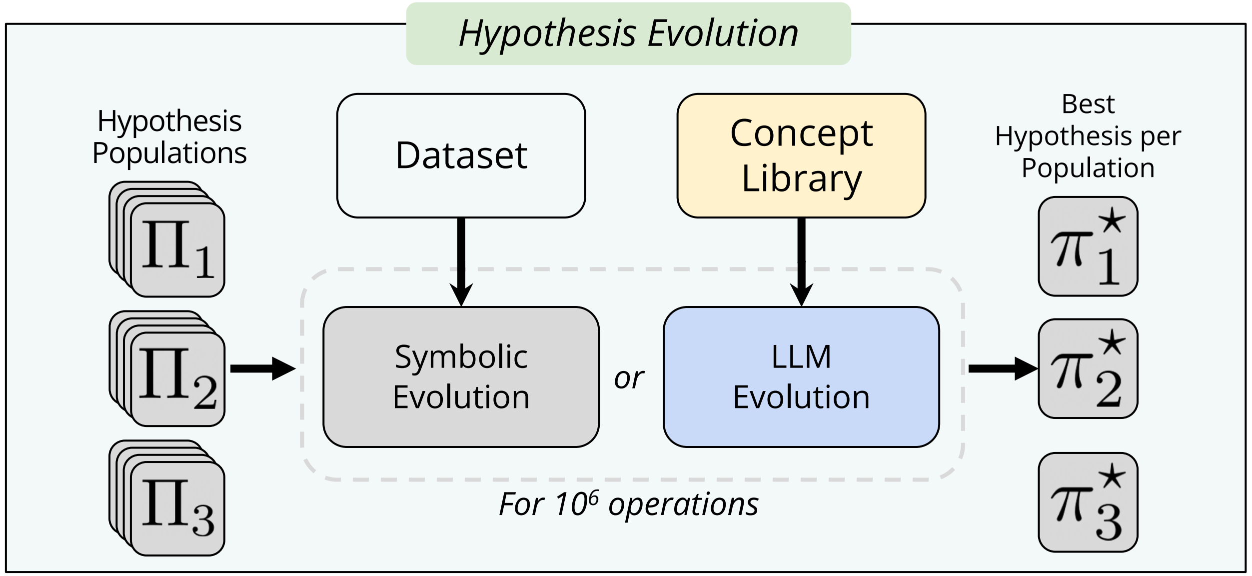
Hypothesis Evolution

Concept Evolution

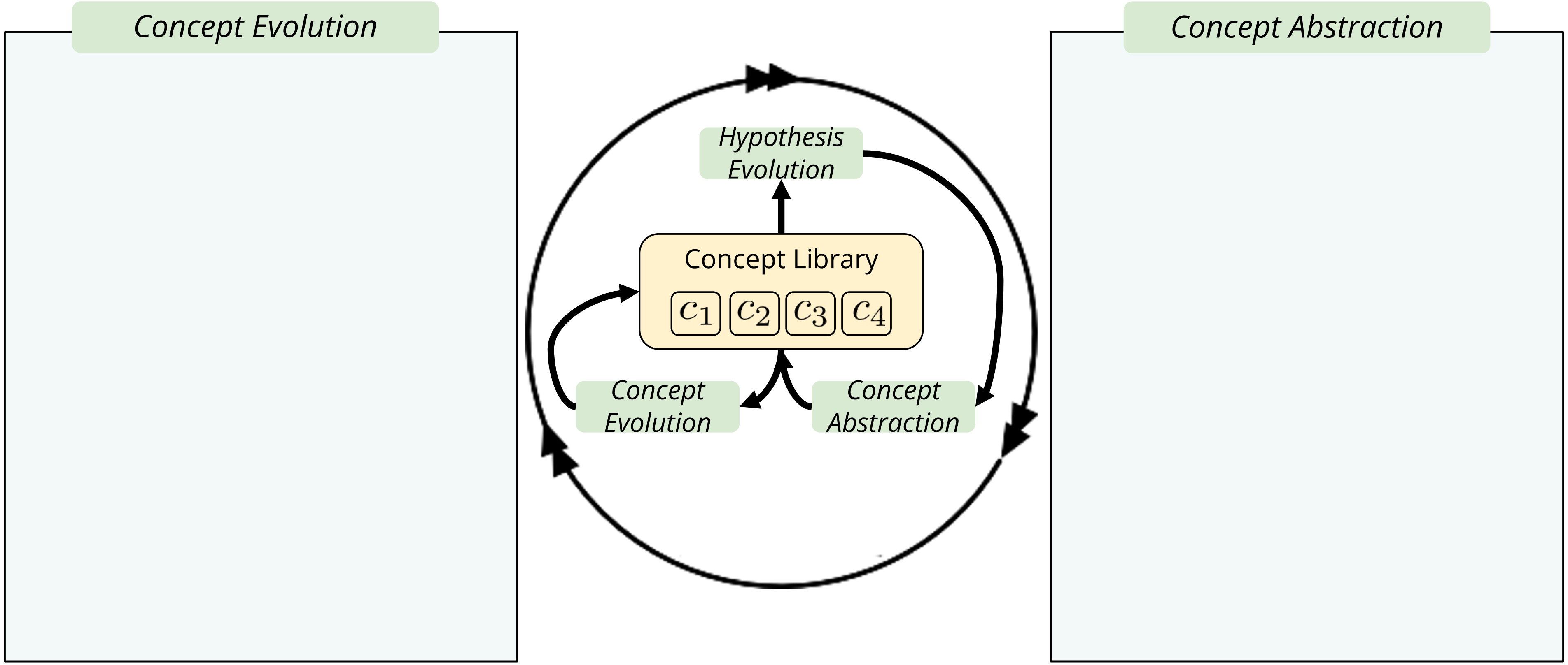


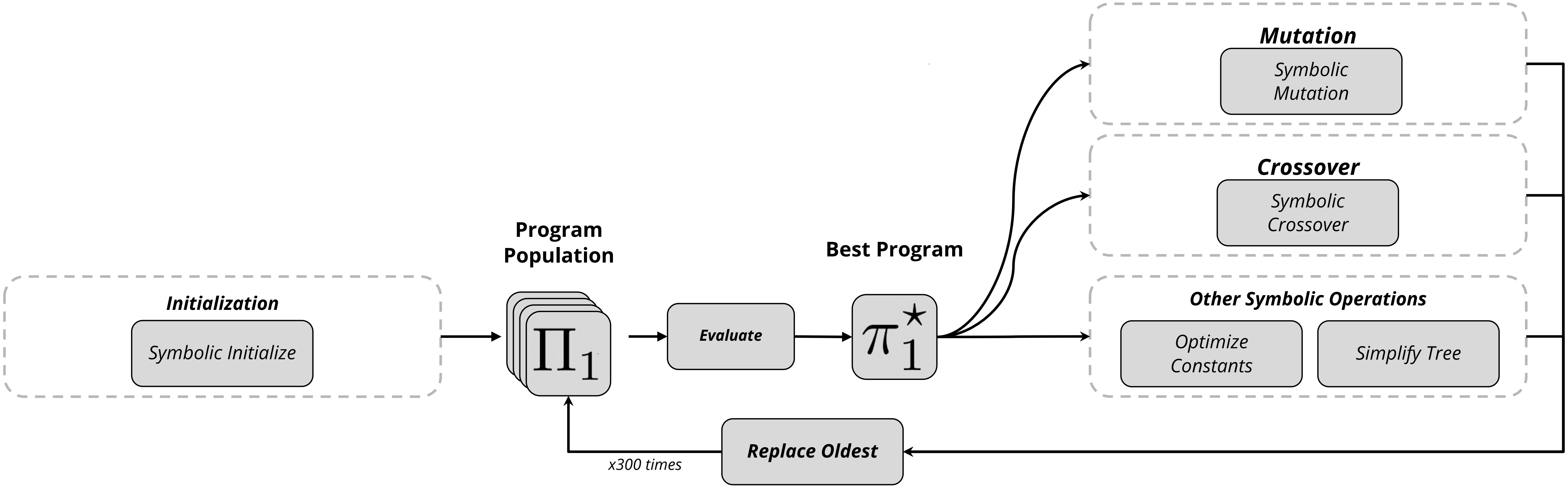
Concept Abstraction

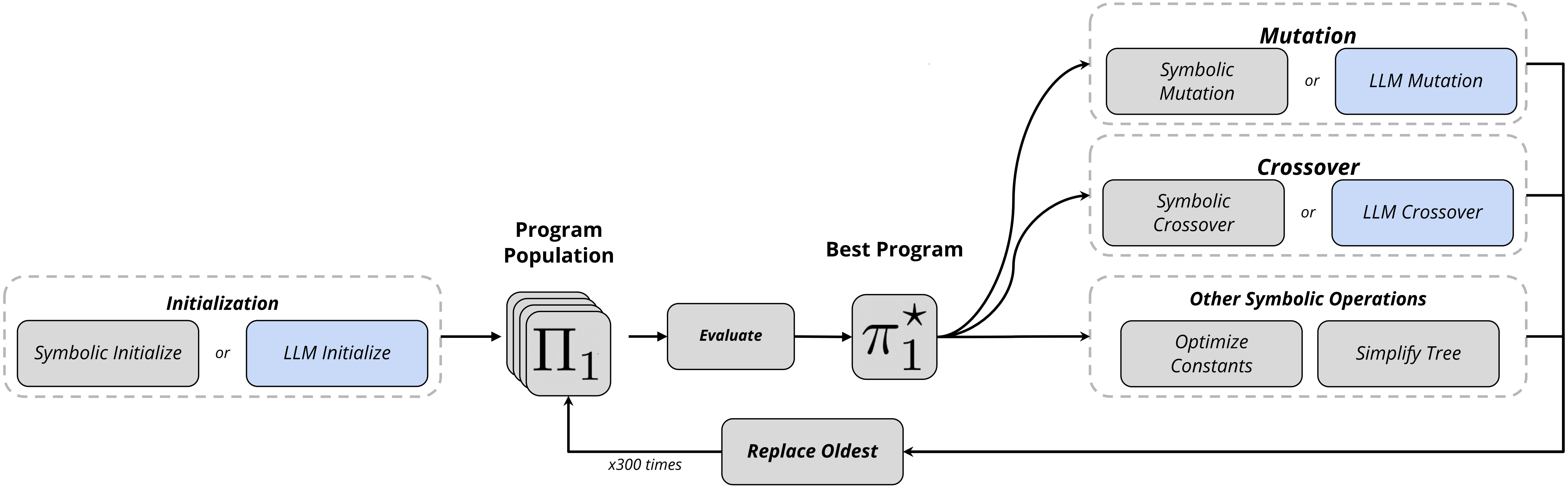
LaSR



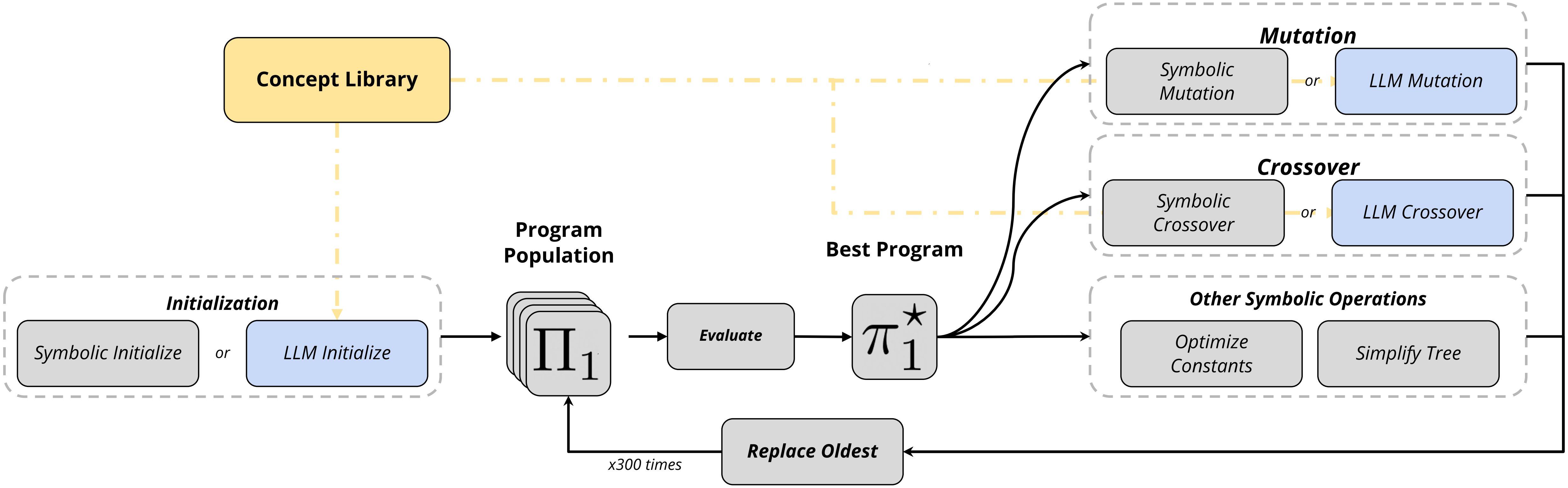
LLM Evolution provides *neural guidance* (over a language prior)



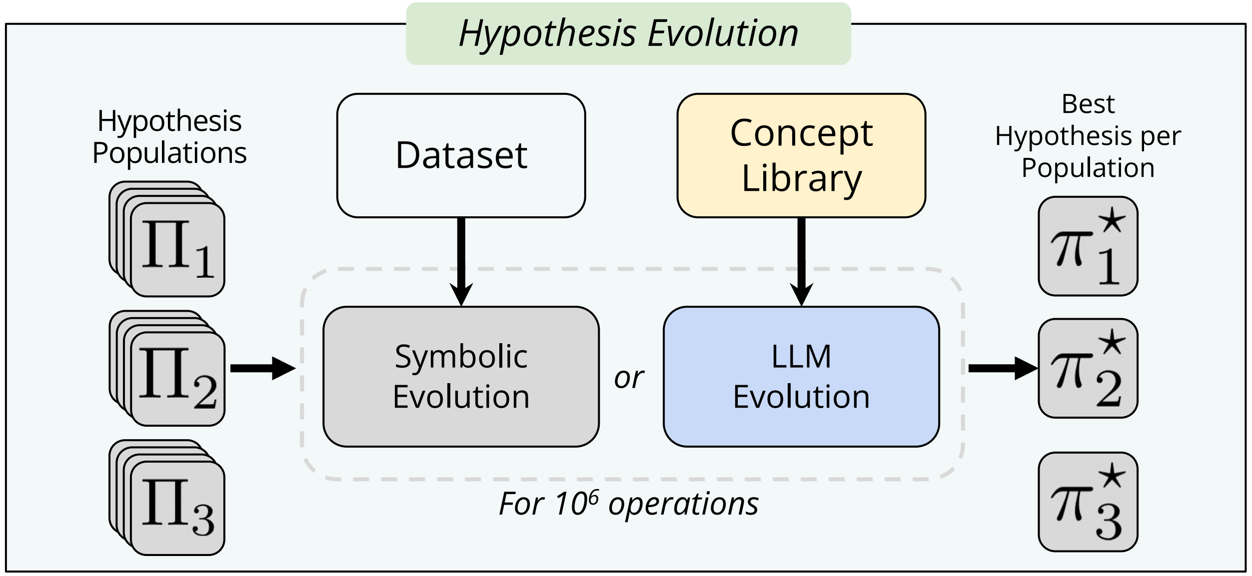

Initialization
Symbolic Initialize
Program
Population
Π_1
Evaluate
Best Program
$\pi_1^\star$
Mutation
Symbolic
Mutation
Crossover
Symbolic
Crossover
Other Symbolic Operations
Optimize
Constants
Simplify Tree
Replace Oldest
x300 times



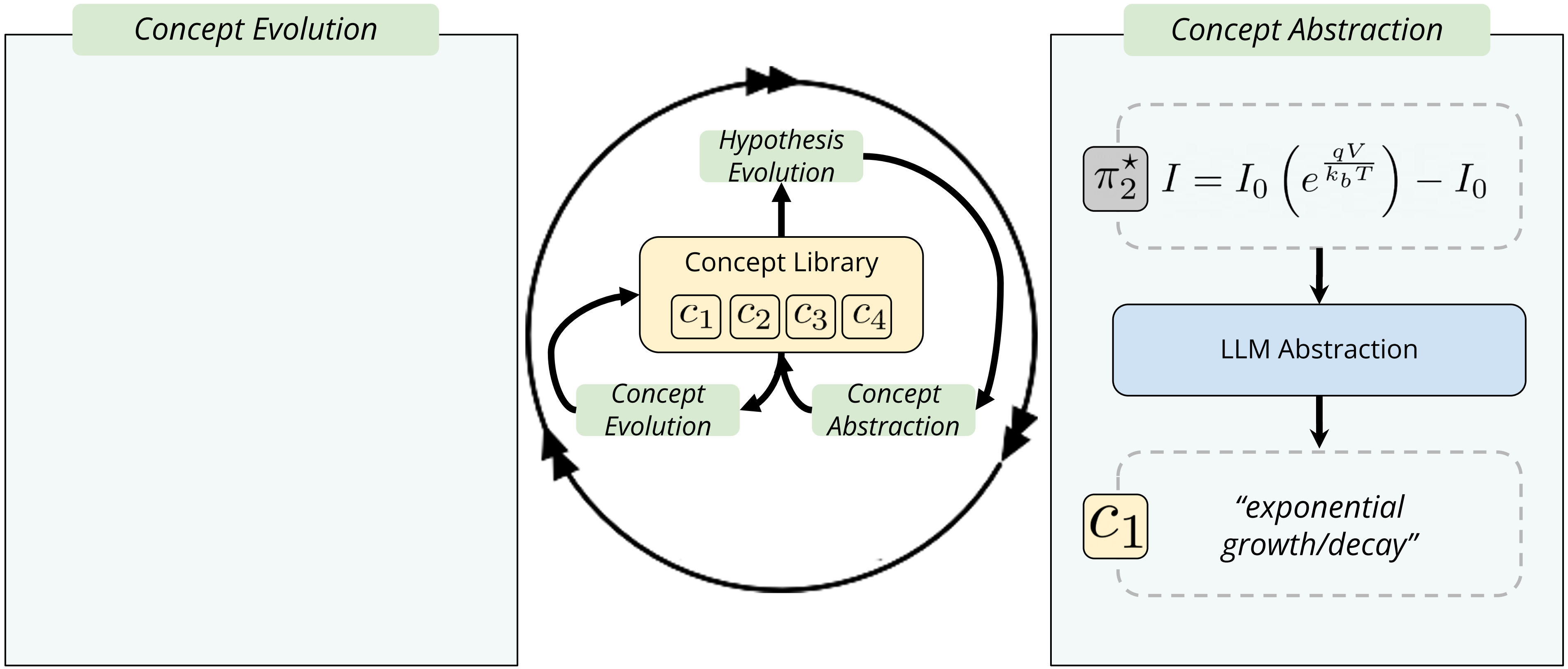
Mutation
Symbolic Mutation
or
LLM Mutation
Crossover
Symbolic Crossover
or
LLM Crossover
Other Symbolic Operations
Optimize Constants
Simplify Tree
Program Population
Π_1
Best Program
$\pi_1^\star$
Evaluate
Initialization
Symbolic Initialize
or
LLM Initialize
Replace Oldest
x300 times


Concept Library
Mutation
Symbolic Mutation
or
LLM Mutation
Crossover
Symbolic Crossover
or
LLM Crossover
Program Population
Best Program
Other Symbolic Operations
Optimize Constants
Simplify Tree
Initialization
Symbolic Initialize
or
LLM Initialize
Π_1
Evaluate
$\pi_1^\star$
Replace Oldest
x300 times

LaSR

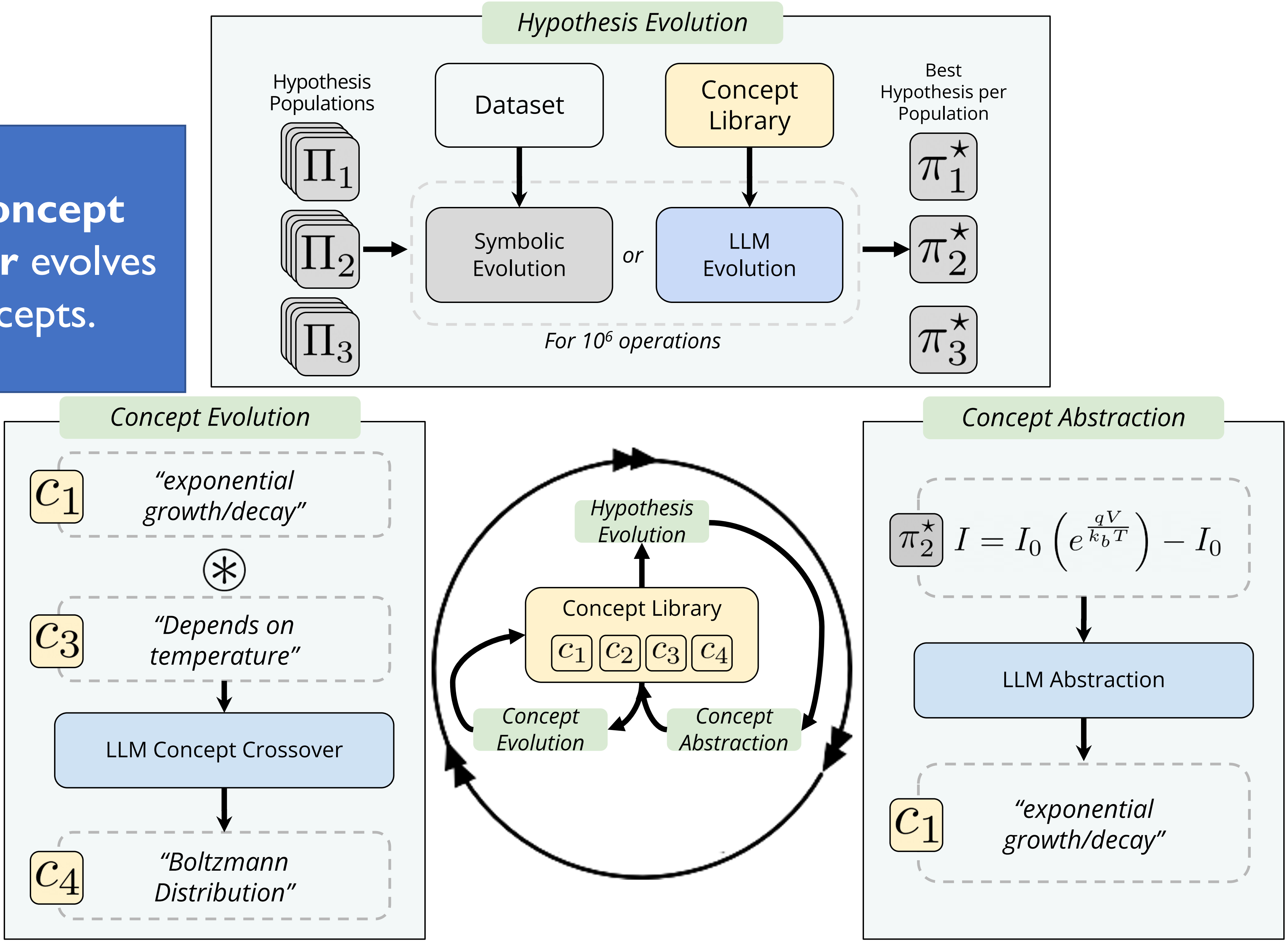


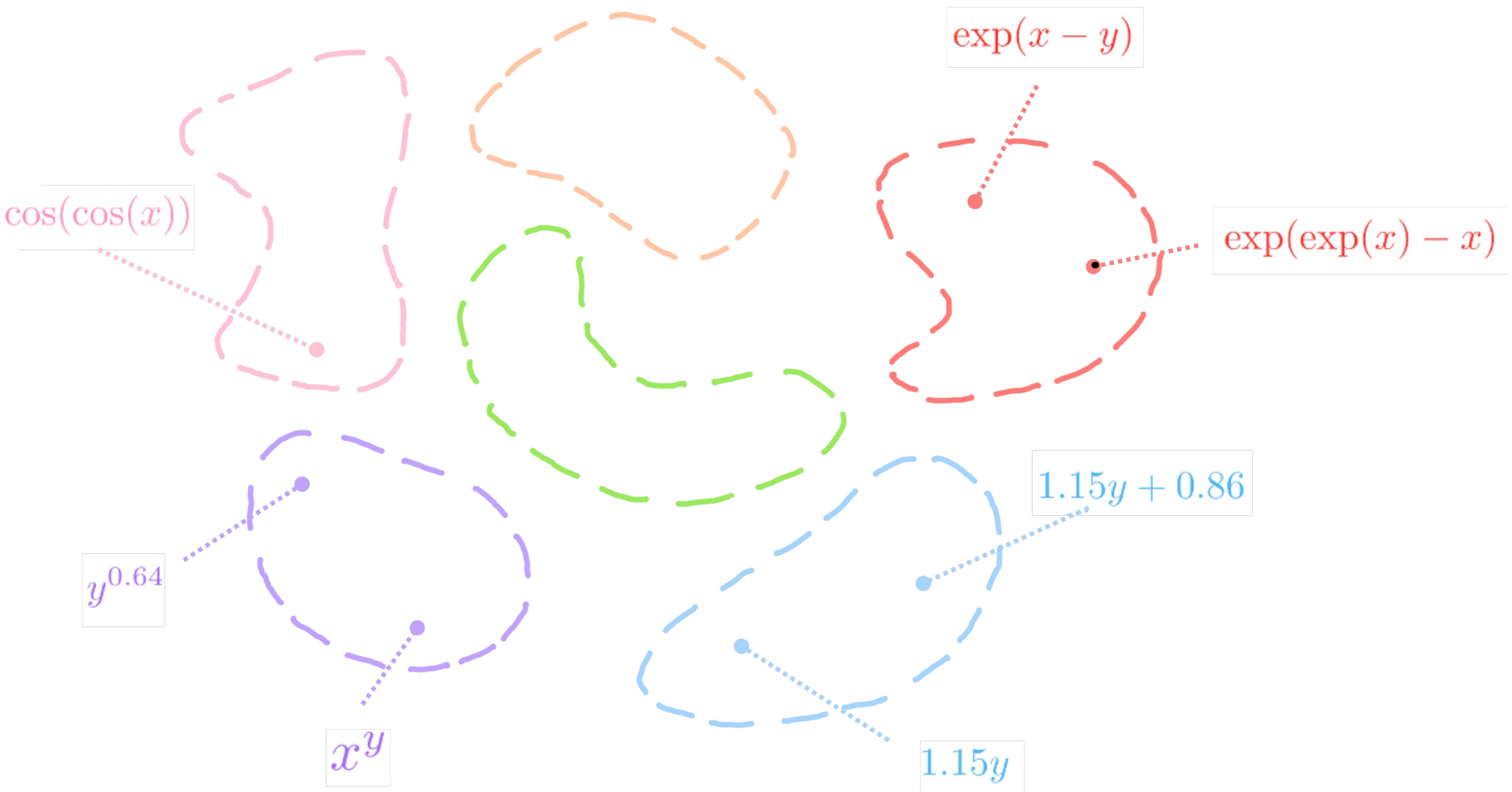
LLM Abstraction induces *useful** abstractions.



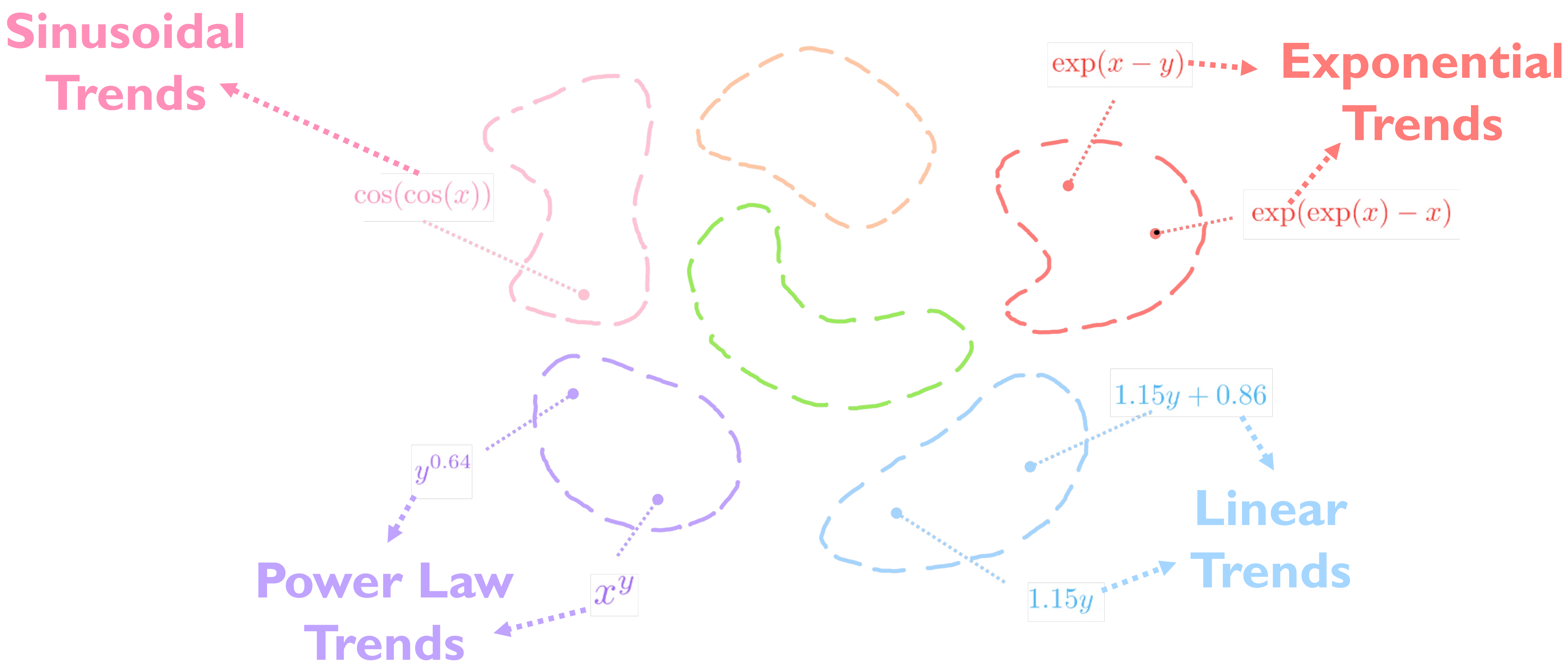
LaSR

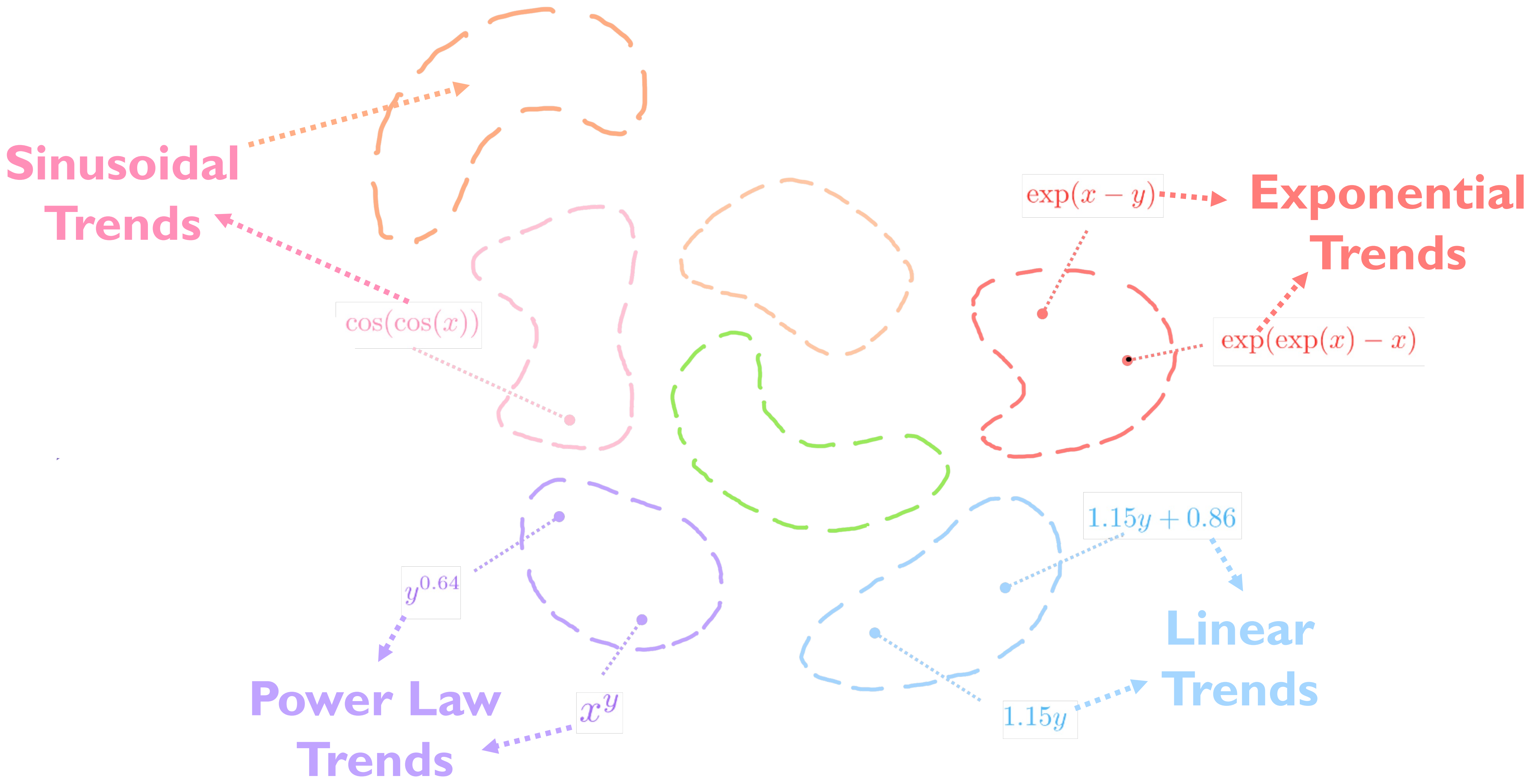
LLM Concept Crossover evolves all concepts.



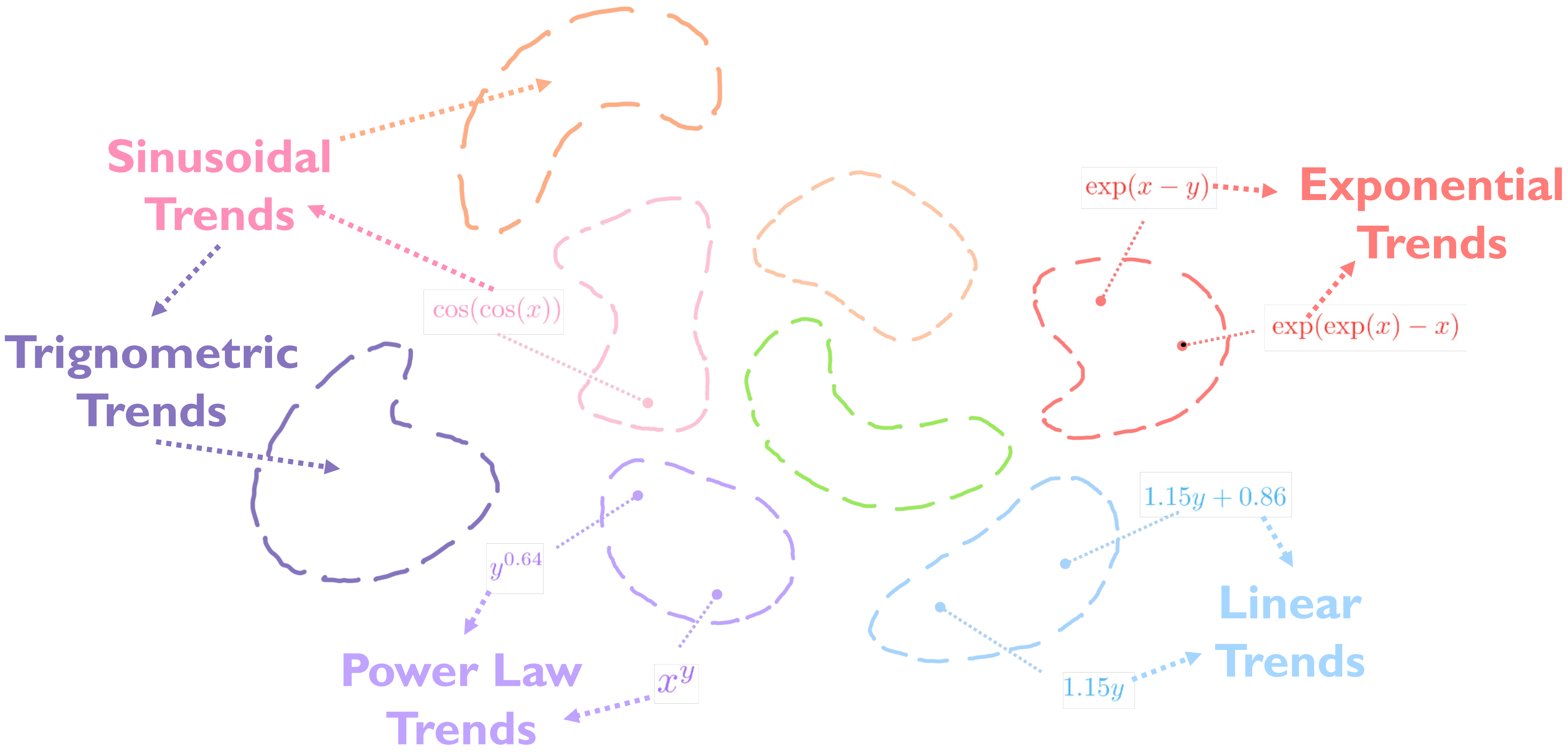


exp(x − y)
cos(cos(x))
exp(exp(x) − x)
1.15y + 0.86
y^0.64
x^y
1.15y


Sinusoidal Trends
$\cos(\cos(x))$
Exponential Trends
$\exp(x-y)$
$\exp(\exp(x)-x)$
Power Law Trends
$y^{0.64}$
x^y
Linear Trends
$1.15y+0.86$
$1.15y$



Sinusoidal Trends
$\cos(\cos(x))$
$\exp(x-y)$
Exponential Trends
$\exp(\exp(x)-x)$
$1.15y+0.86$
$y^{0.64}$
Linear Trends
Power Law Trends
x^y
$1.15y$



Sinusoidal Trends
cos(cos(x))
Trignometric Trends
exp(x − y)
Exponential Trends
exp(exp(x) − x)
1.15y + 0.86
Linear Trends
1.15y
$y^{0.64}$
Power Law Trends
x^y

- Concept Guidance accelerates scientific discovery.

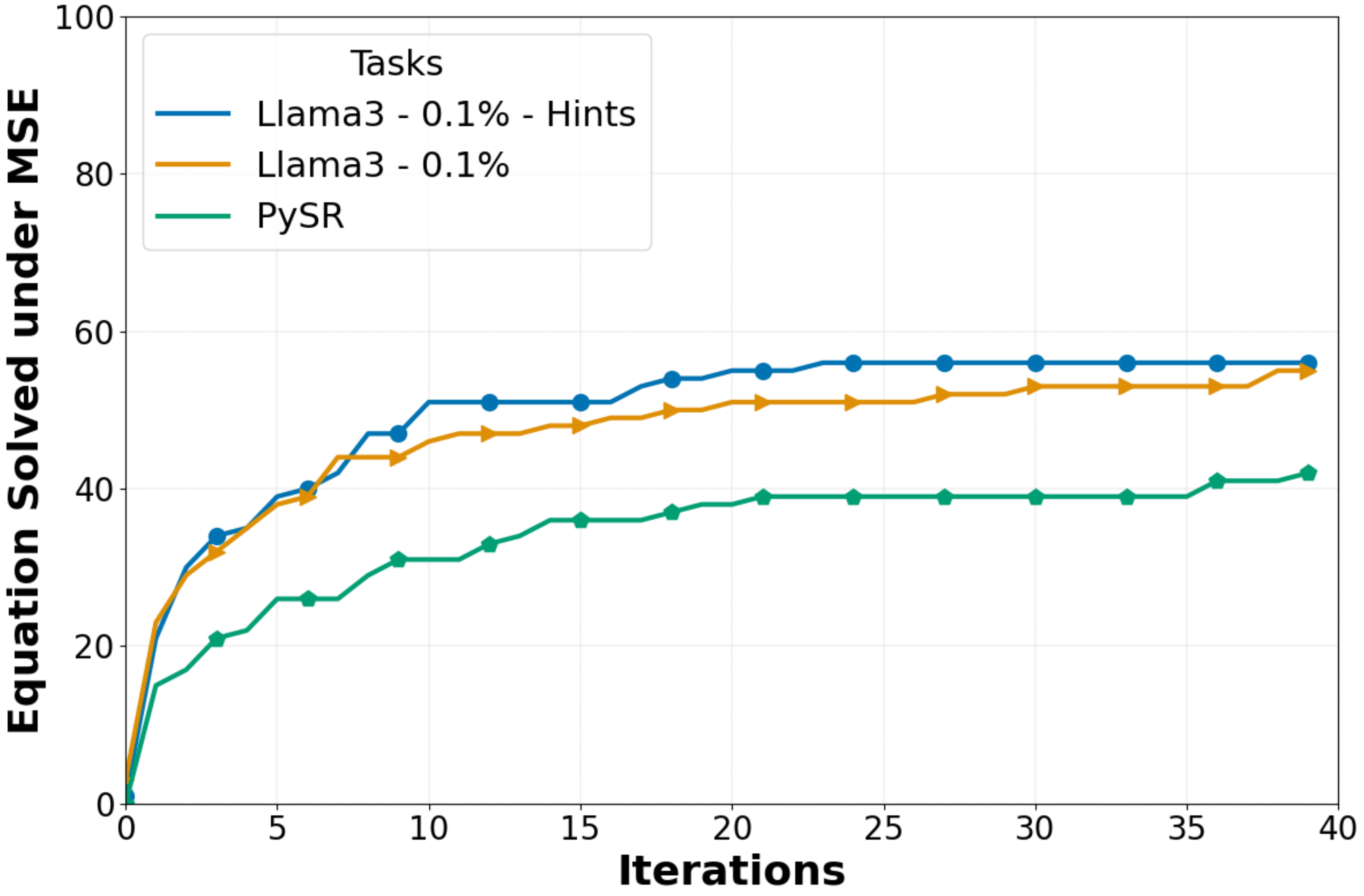
GPlearn	AFP	AFP-FE	DSR	uDSR	AIFeynman	PySR	LaSR
20/100	24/100	26/100	23/100	40/100	38/100	59/100	**59 + 7/100**

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].

- LaSR outperforms PySR even with local language models (llama-3-7b, 1%)

		LaSR (Llama3-8B)			LaSR (GPT-3.5)
Type of Solve	**PySR**	$p = 1\%$	$p = 5\%$	$p = 10\%$	$p = 1\%$
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.


Tasks
Llama3 - 0.1% - Hints
Llama3 - 0.1%
PySR
Equation Solved under MSE
Iterations
0
20
40
60
80
100
0
5
10
15
20
25
30
35
40

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

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

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.
- Unwieldly
- Fitting more constants => more optimization errors

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

Eq 10: Coulomb's Law

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

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

LaSR's Solution

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

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

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.