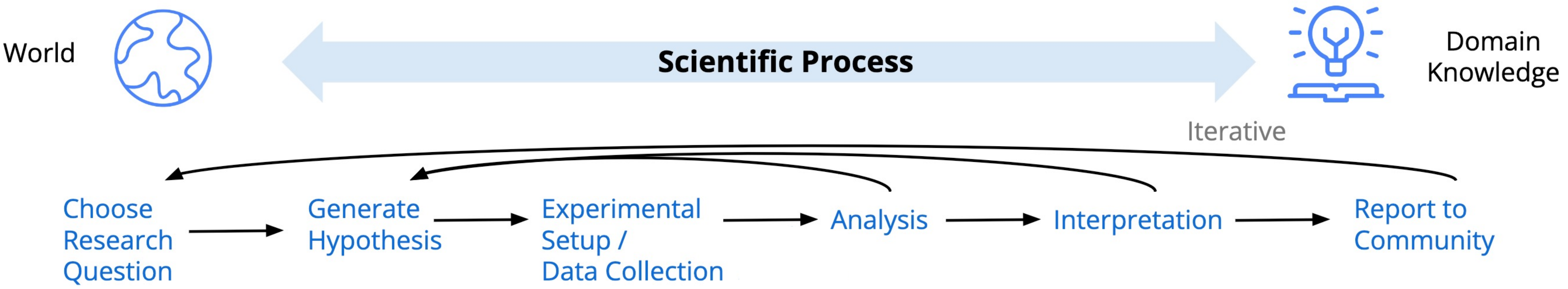

Goal: We want AI to achieve human level performance at *research in the natural sciences*.

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

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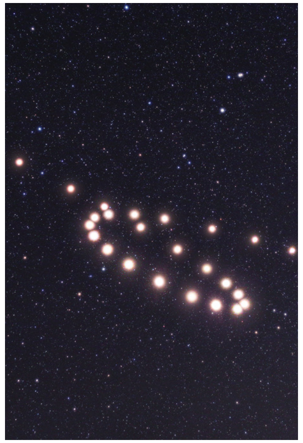

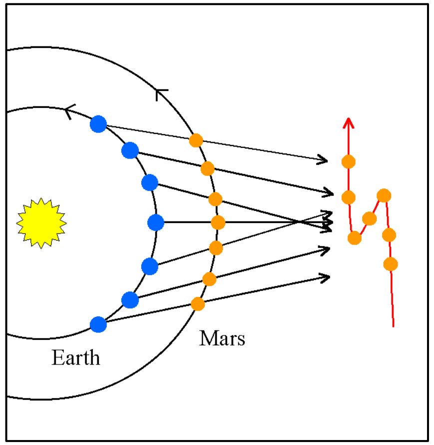

Observation: Apparent Retrograde Planetary Motion
Theory: Heliocentric Model

c.The Astronomical Revolution: Copernicus- Kepler-Borelli

World

Scientific Process

Domain Knowledge

Iterative

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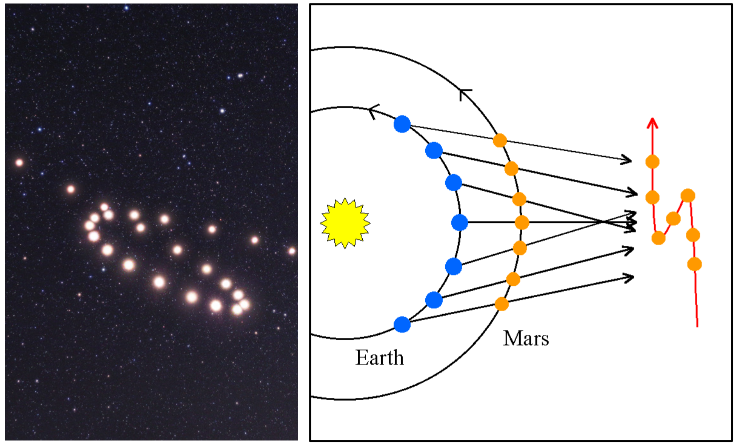
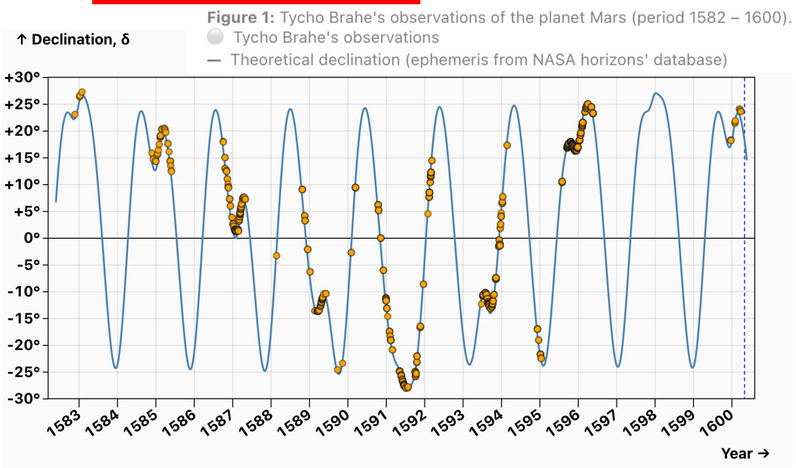


Observation: Apparent Retrograde Planetary Motion
Theory: Heliocentric Model



Data Collection: Sample data in regime of interest.

c.The Astronomical Revolution: Copernicus- Kepler-Borelli

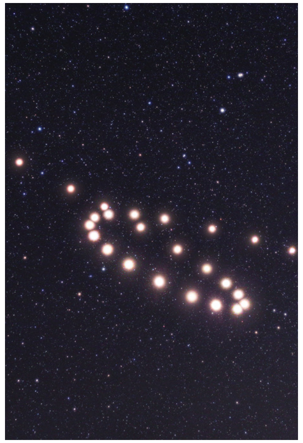
World

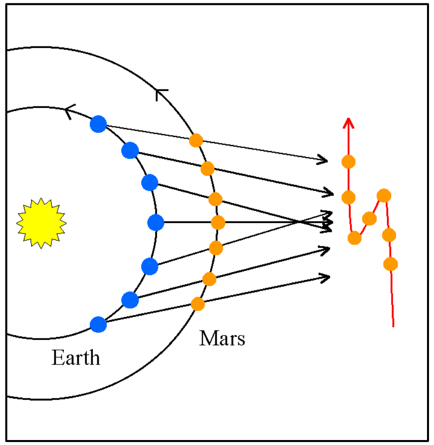
Scientific Process

Domain Knowledge

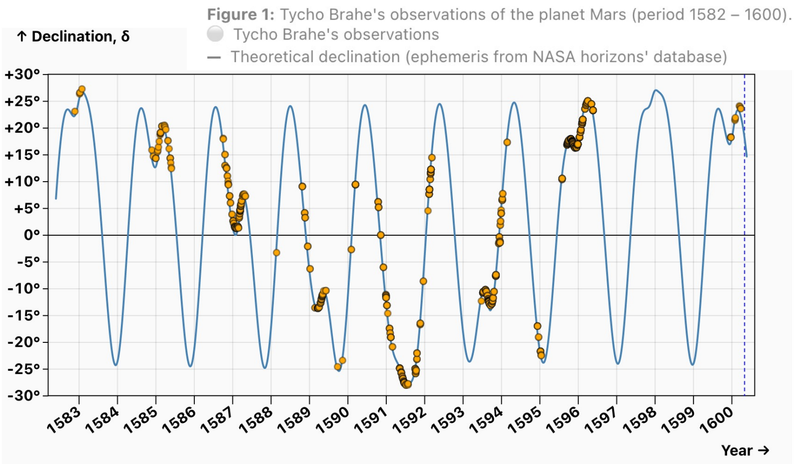
Iterative

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

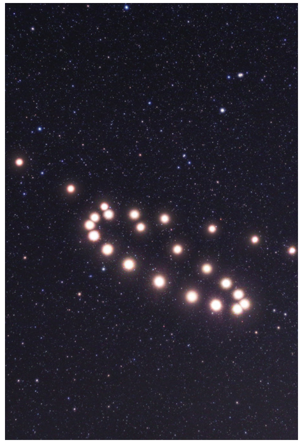
World

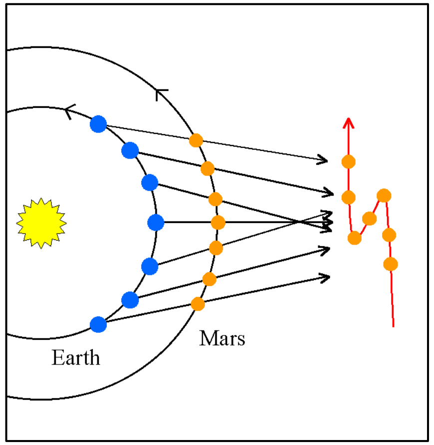
Scientific Process

Domain Knowledge

Iterative

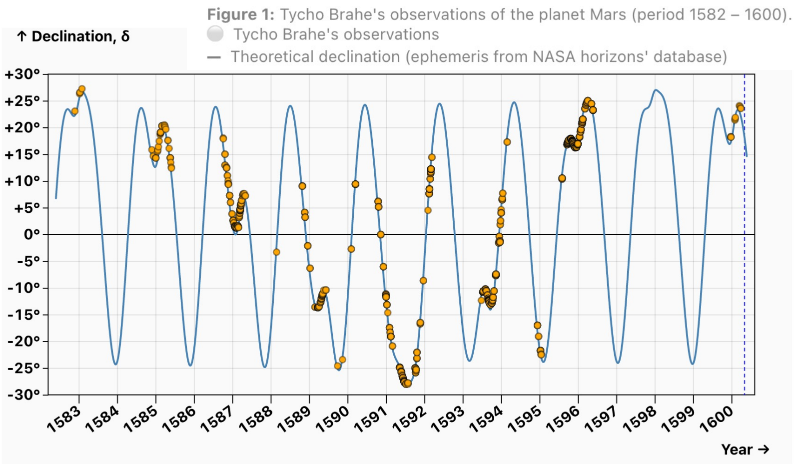
Choose Research Question → Generate Hypothesis → Experimental Setup / Data Collection → Analysis → Interpretation → Report to Community





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

World

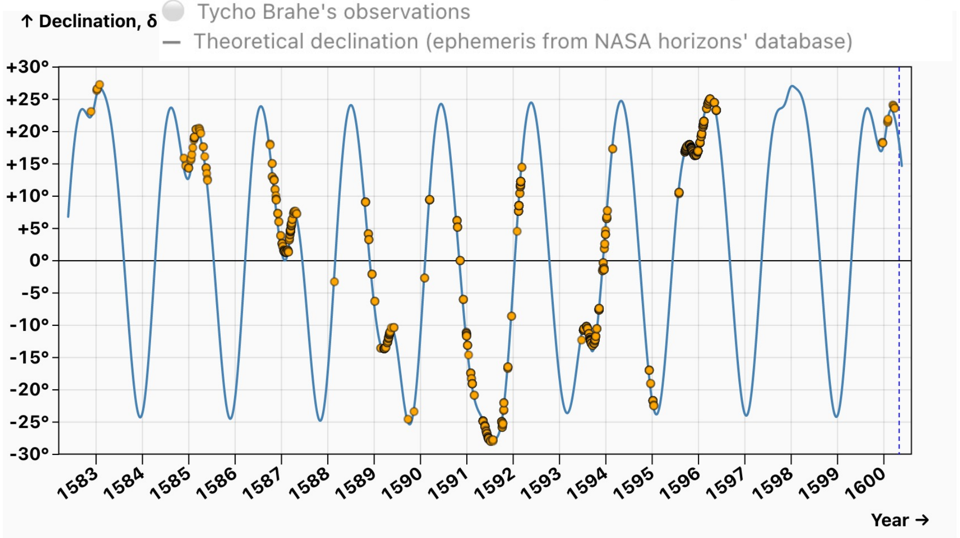
Scientific Process

Domain Knowledge

Iterative

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

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

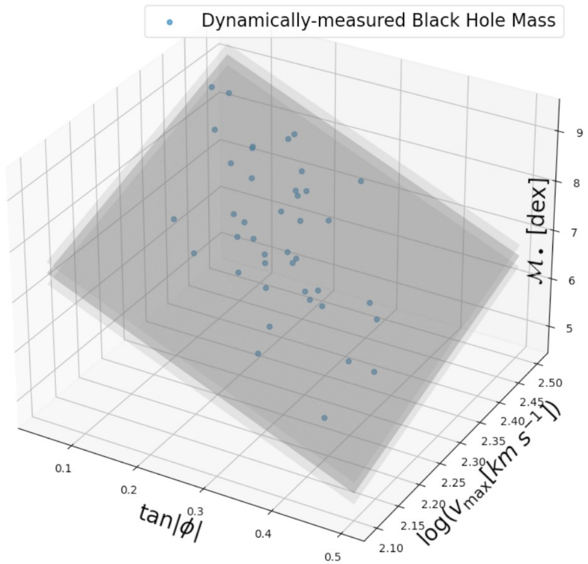
Symbolic Regression Algorithms

c. PySR. Miles Cranmer

Symbolic Regression Algorithms

c. PySR. Miles Cranmer

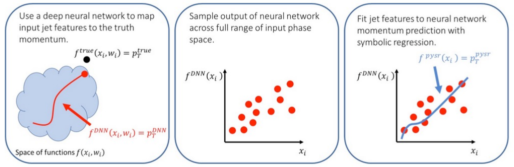
PySR's impact



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

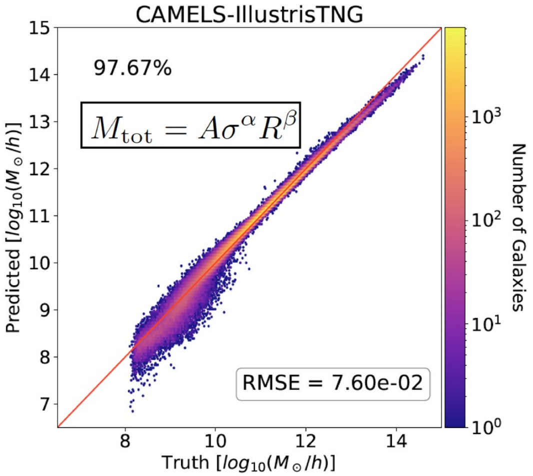
Tanner Mengel [1], Patrick Steffanic [1], Charles Hughes [1,2], Antonio Carlos Oliveira da Silva [1,2], Christine Nattrass [1]

[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

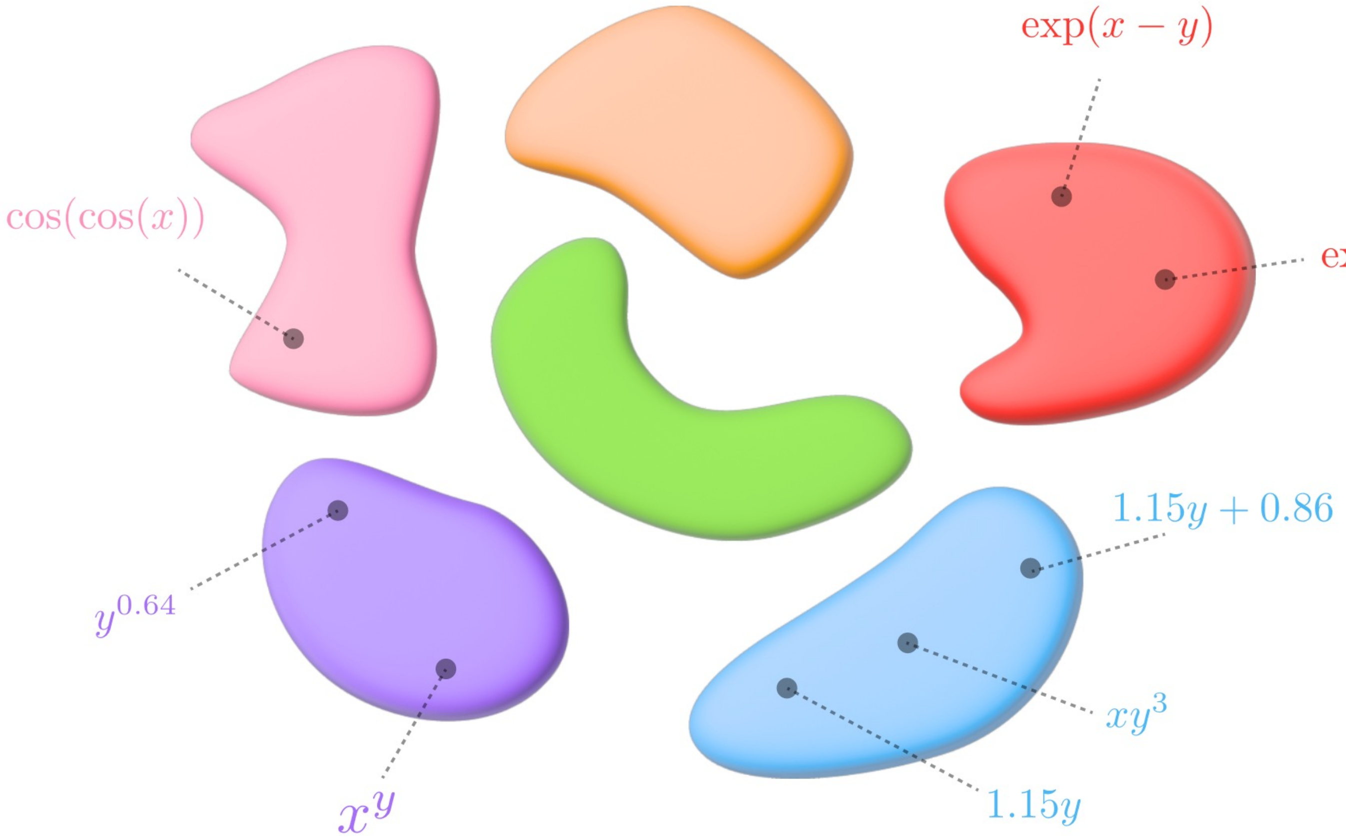


Finding universal relations in subhalo properties with artificial intelligence

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]

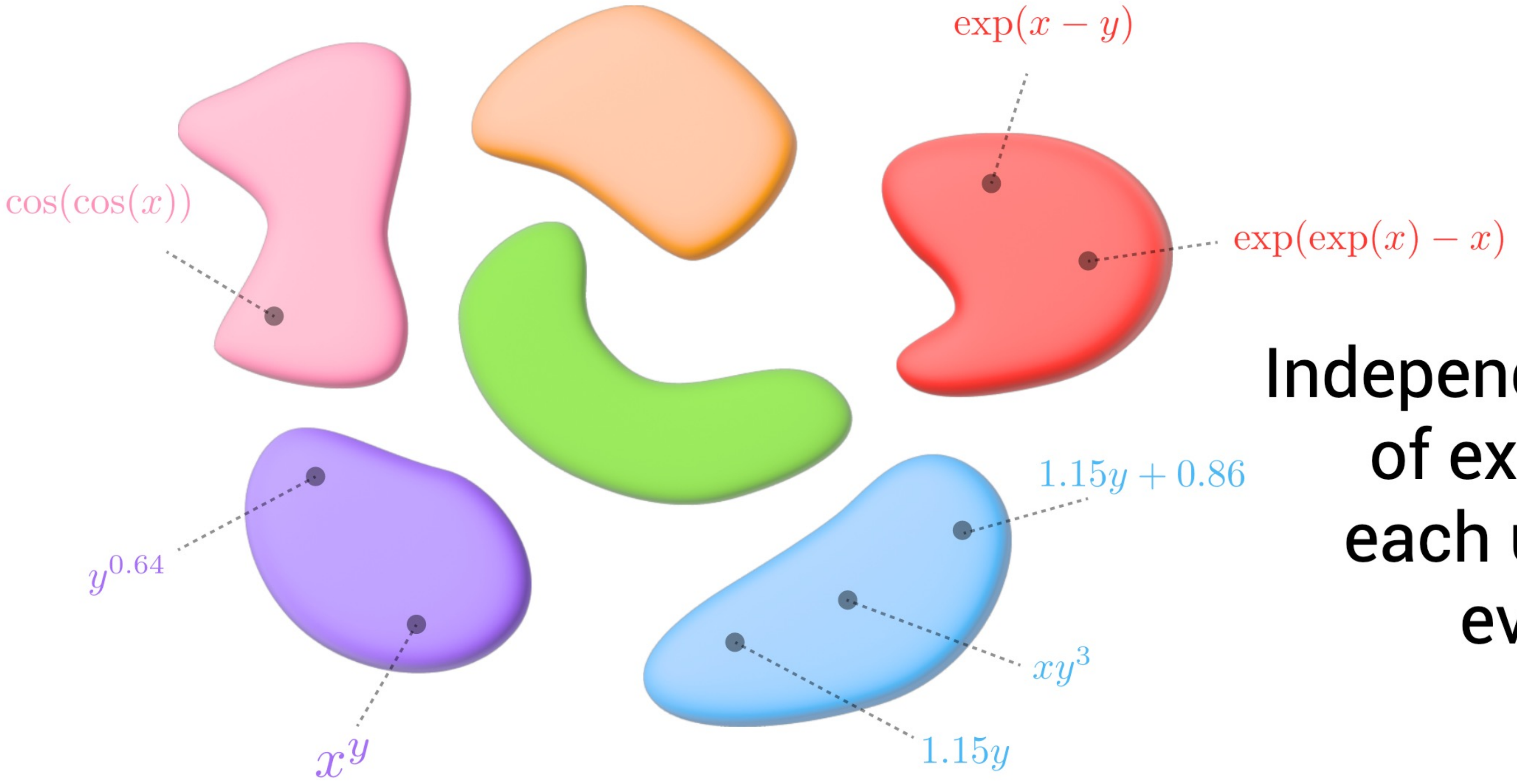
[1]Princeton University, [2]Flatiron Institute, [3]Columbia University, [4]University of Connecticut, [5]Center for Astrophysics | Harvard & Smithsonian, [6]University of Edinburgh, [7]University of the Western Cape, [8]South African Astronomical Observatories, [9]University of Florida, [10]University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

c. PySR. Miles Cranmer



Independent “islands” of expressions, each undergoing evolution

c. PySR. Miles Cranmer



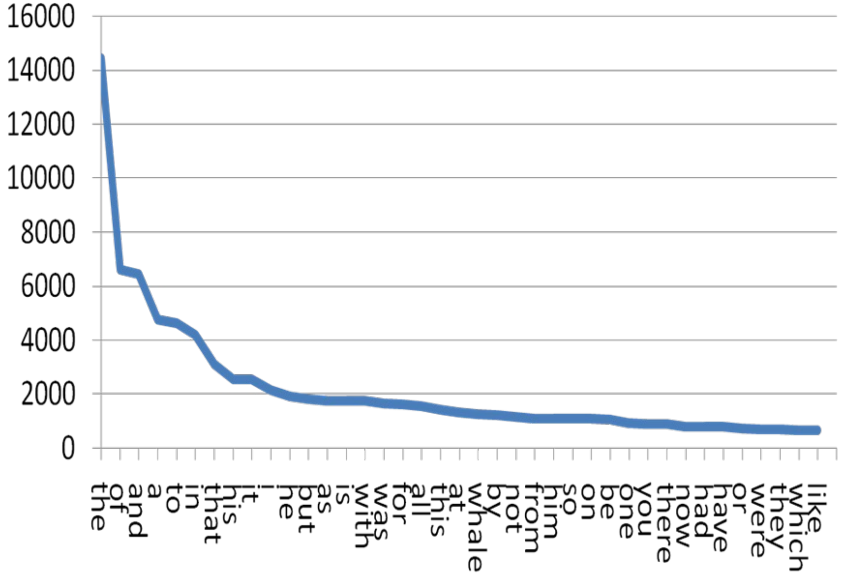
Independent "islands" of expressions, each undergoing evolution

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

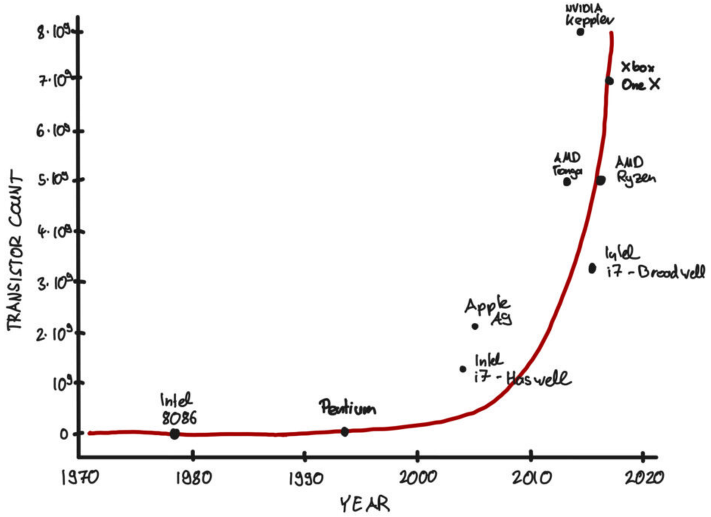
LaSR: Symbolic Regression with a Learned Concept Library

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

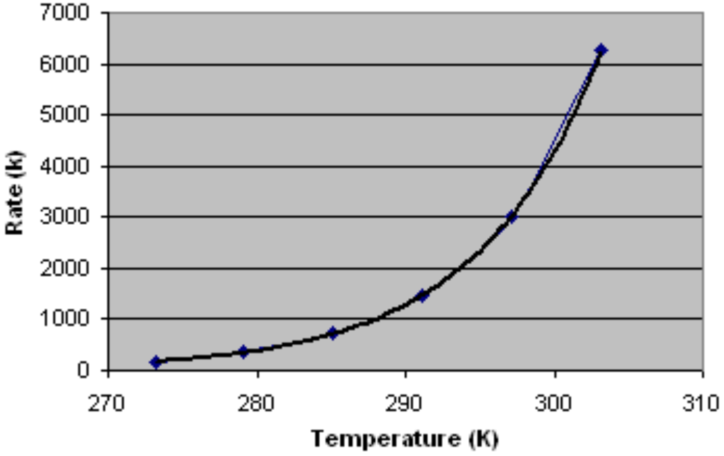
Zipf's Law



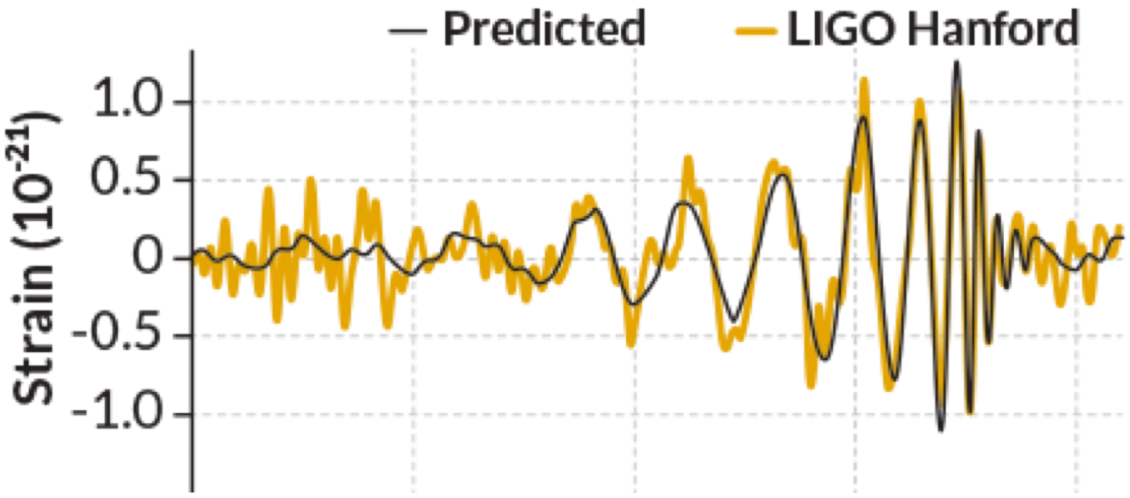
Moore's Law



Arrhenius' Equation



$$y = ax^k + \epsilon \Leftrightarrow$$ *"Power Law Trend"*



Concepts (by Physicist or LLM)

"Wave strain diminishes as distance increases"
"Wave strain has extraordinarily small magnitude"

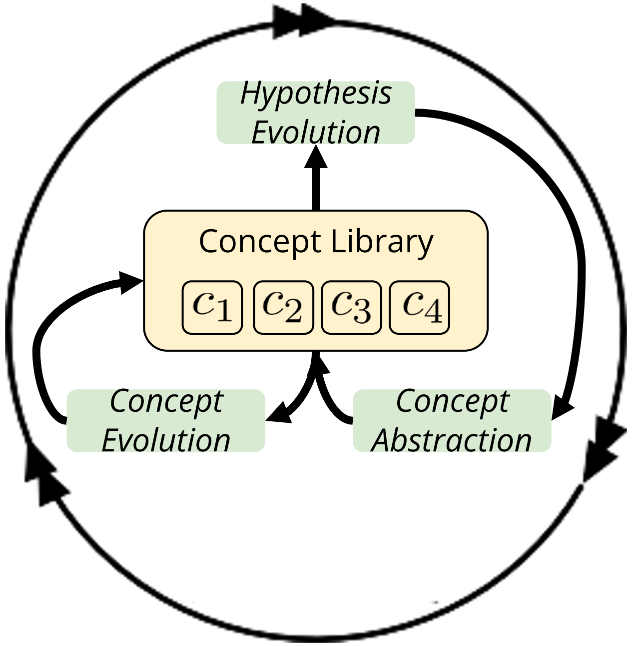
Guide the search for

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

LaSR

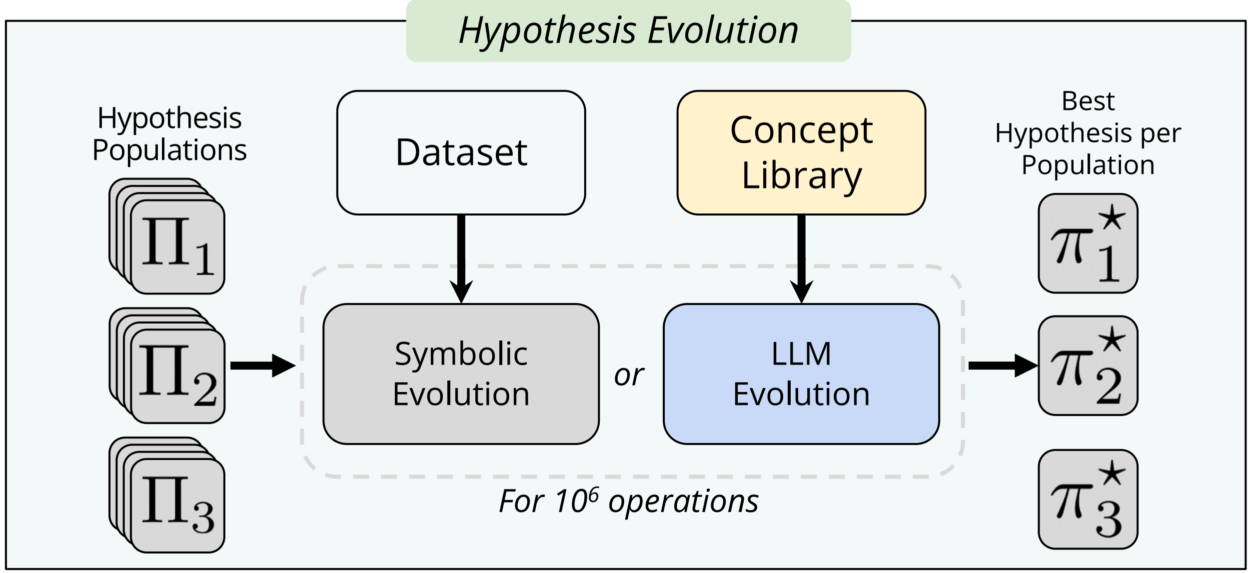
Hypothesis Evolution

Concept Evolution



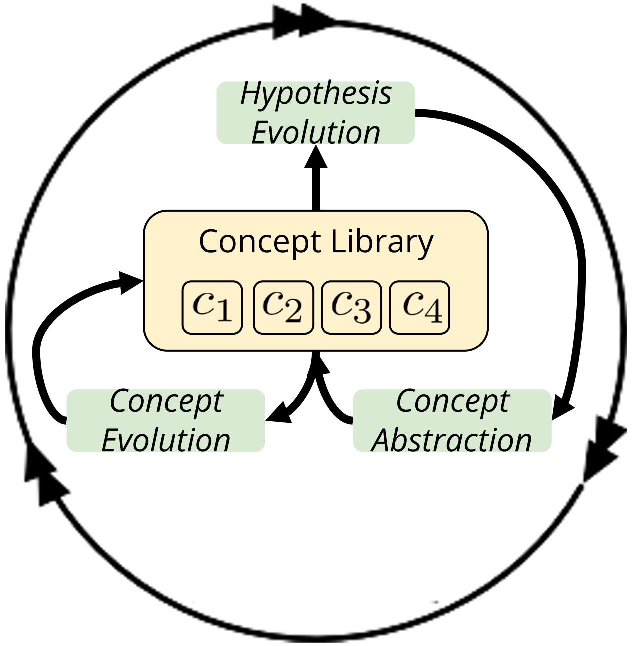
Concept Abstraction

LaSR

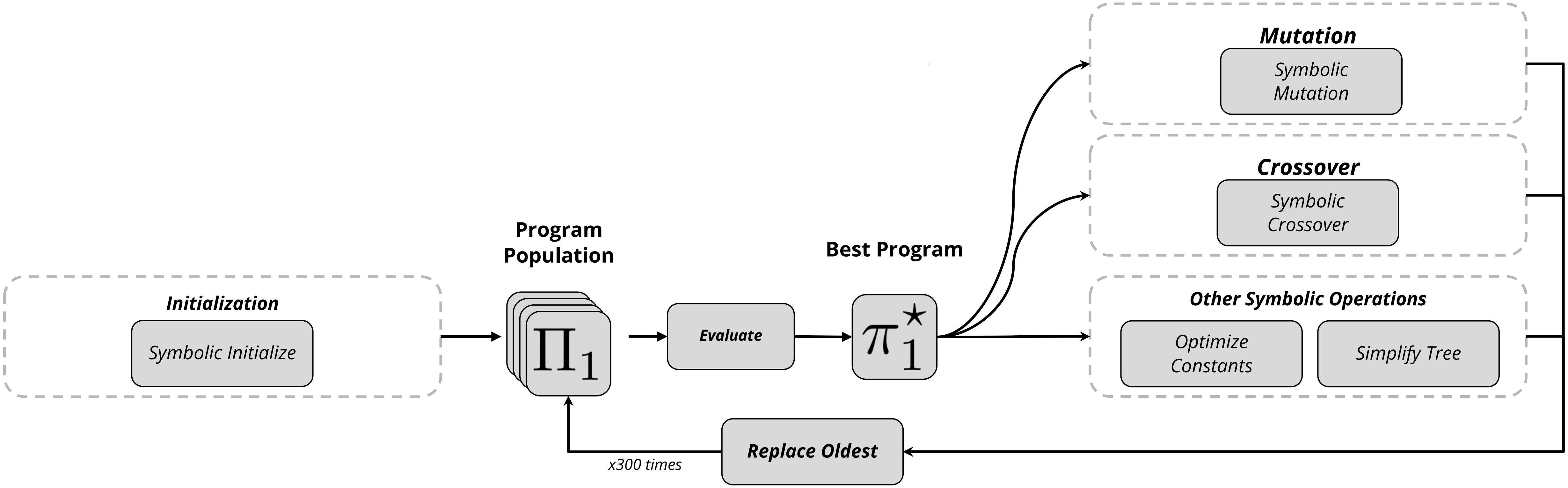


LLM Evolution provides *neural guidance* (over a language prior)

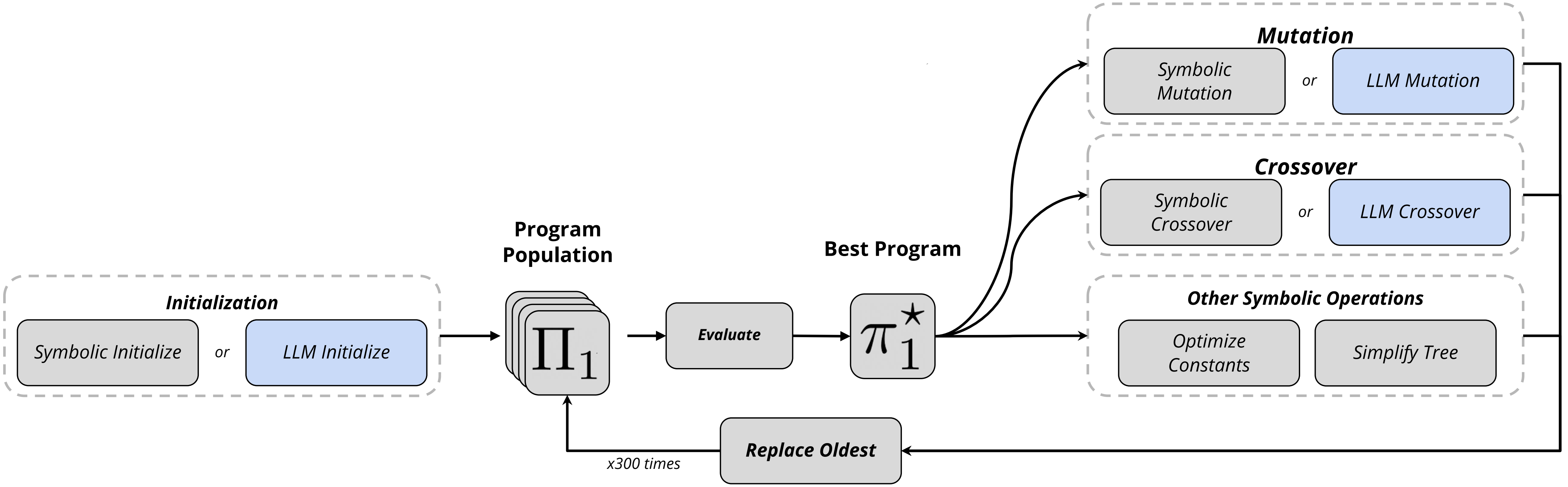
Concept Evolution



Concept Abstraction



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


Program
Population
Best Program
Mutation
Symbolic
Mutation
or
LLM Mutation
Crossover
Symbolic
Crossover
or
LLM Crossover
Initialization
Symbolic Initialize
or
LLM Initialize
Π_1
Evaluate
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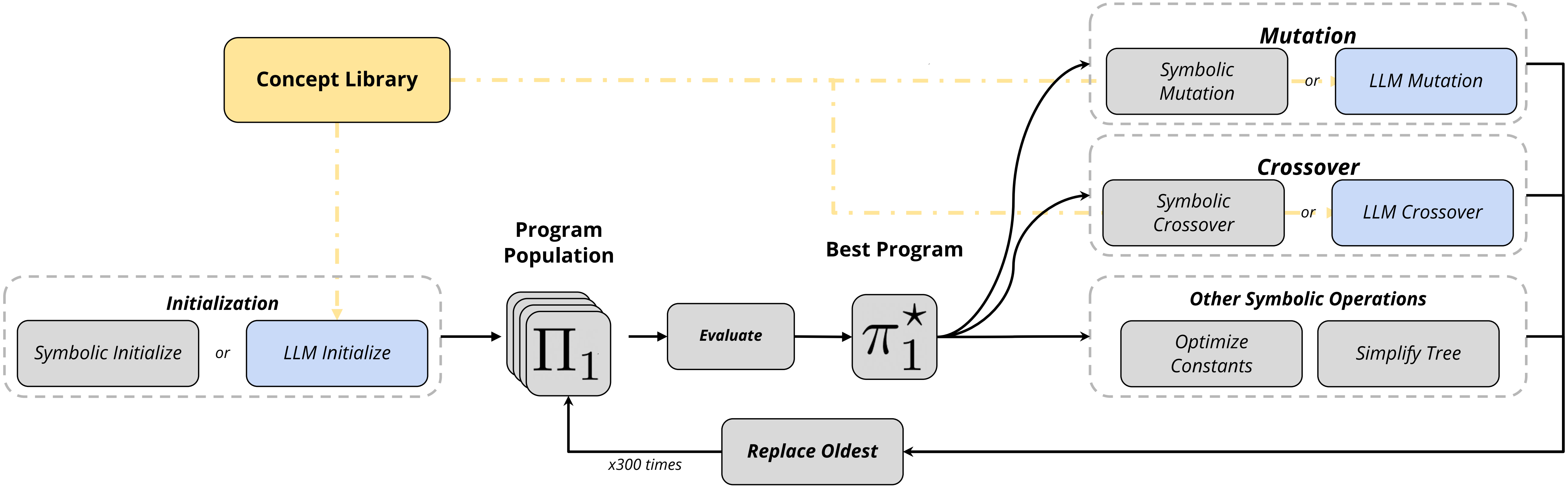
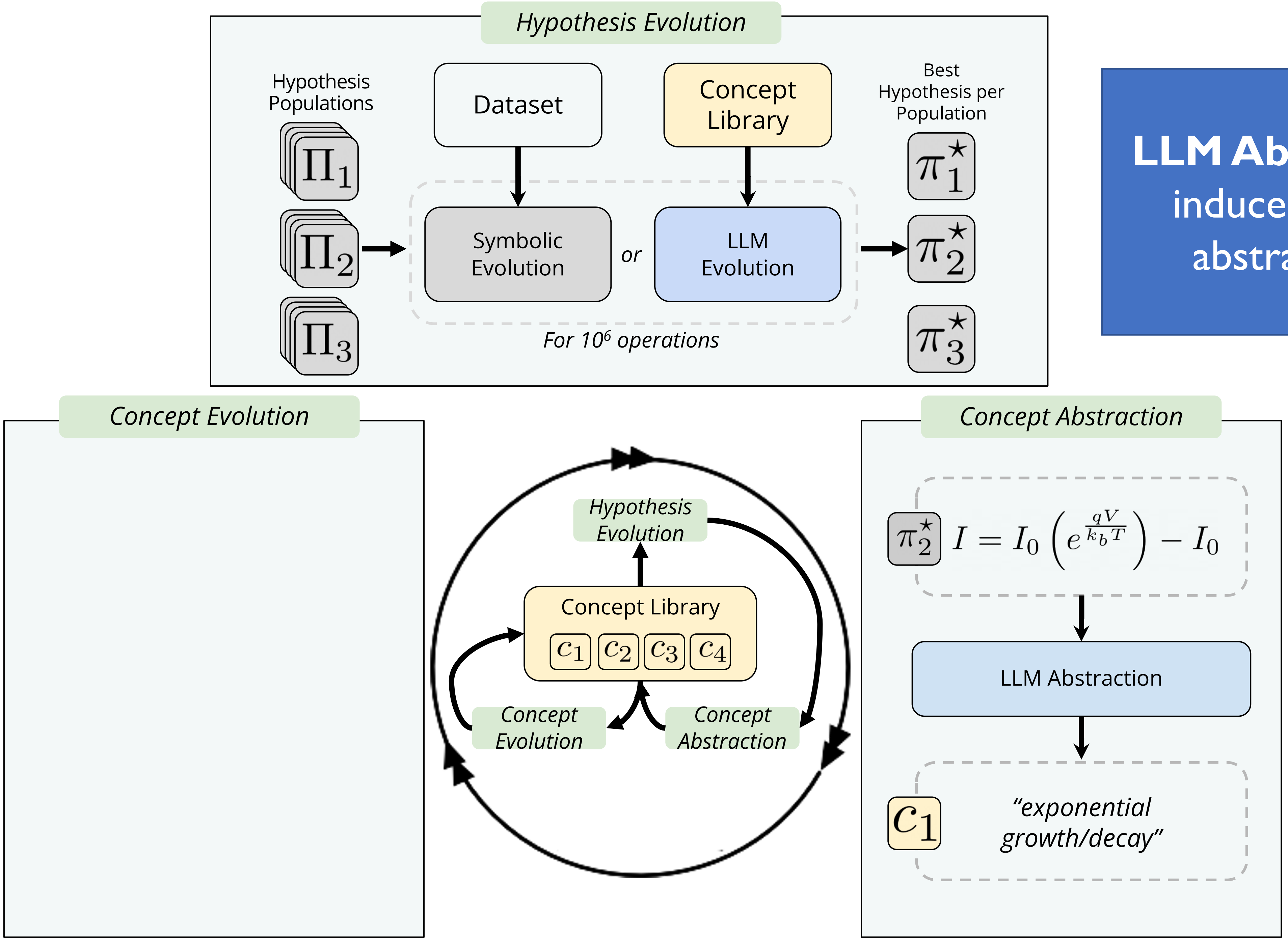


Concept Library
Mutation
Symbolic Mutation
or
LLM Mutation
Crossover
Symbolic Crossover
or
LLM Crossover
Other Symbolic Operations
Optimize Constants
Simplify Tree
Initialization
Symbolic Initialize
or
LLM Initialize
Program Population
Π_1
Evaluate
Best Program
$\pi_1^\star$
Replace Oldest
x300 times

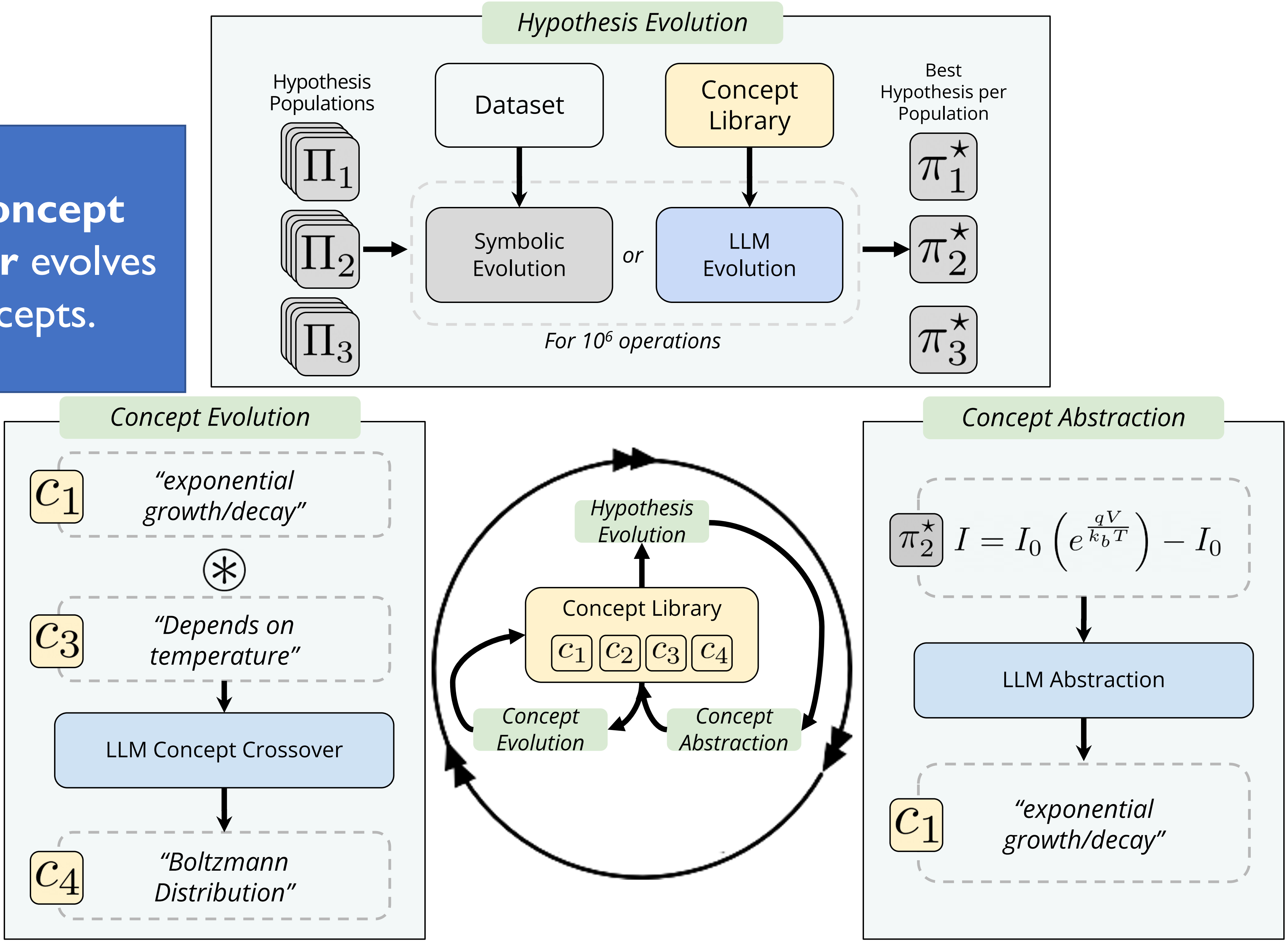
LaSR

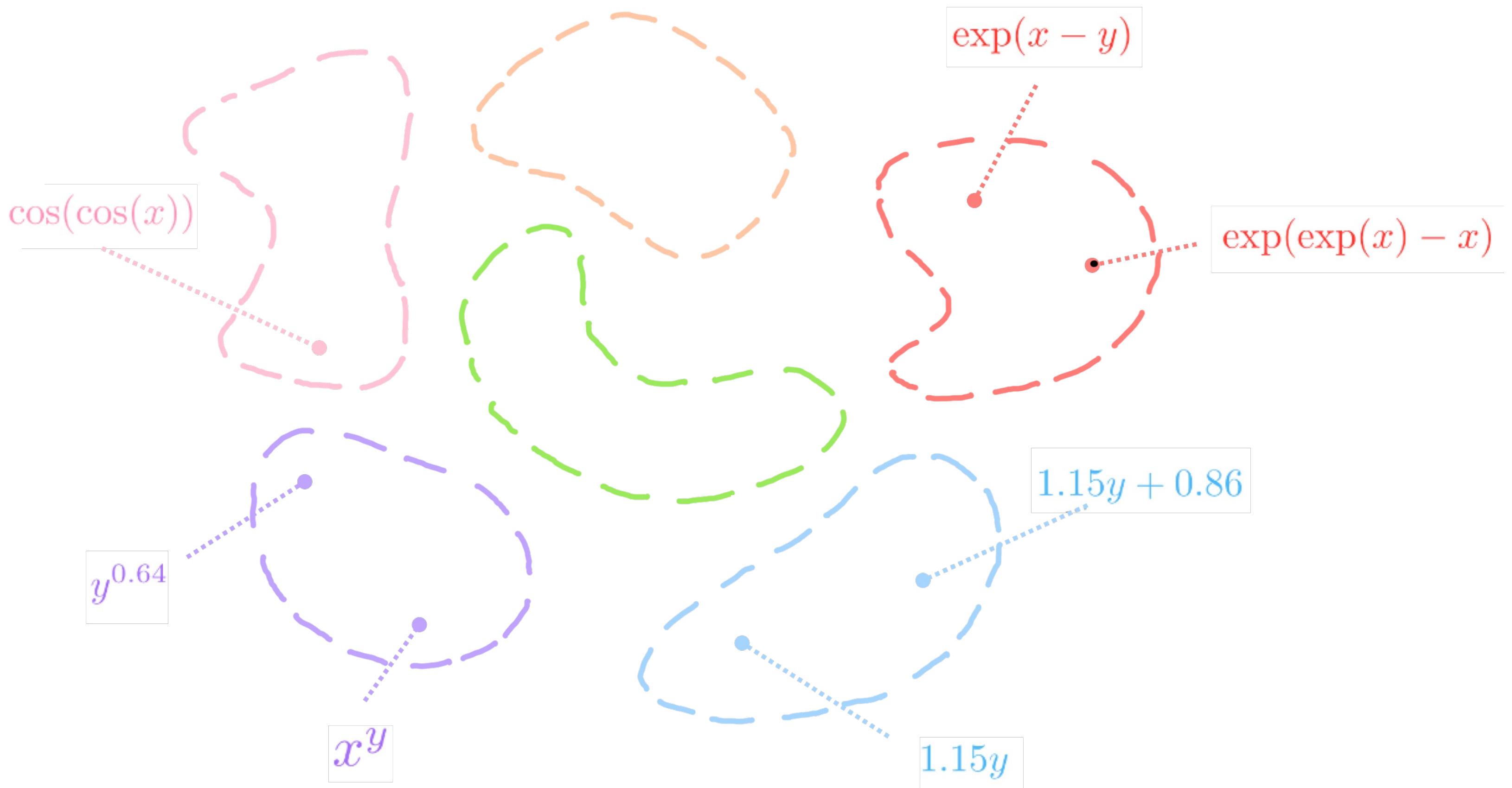


LLM Abstraction induces *useful** abstractions.

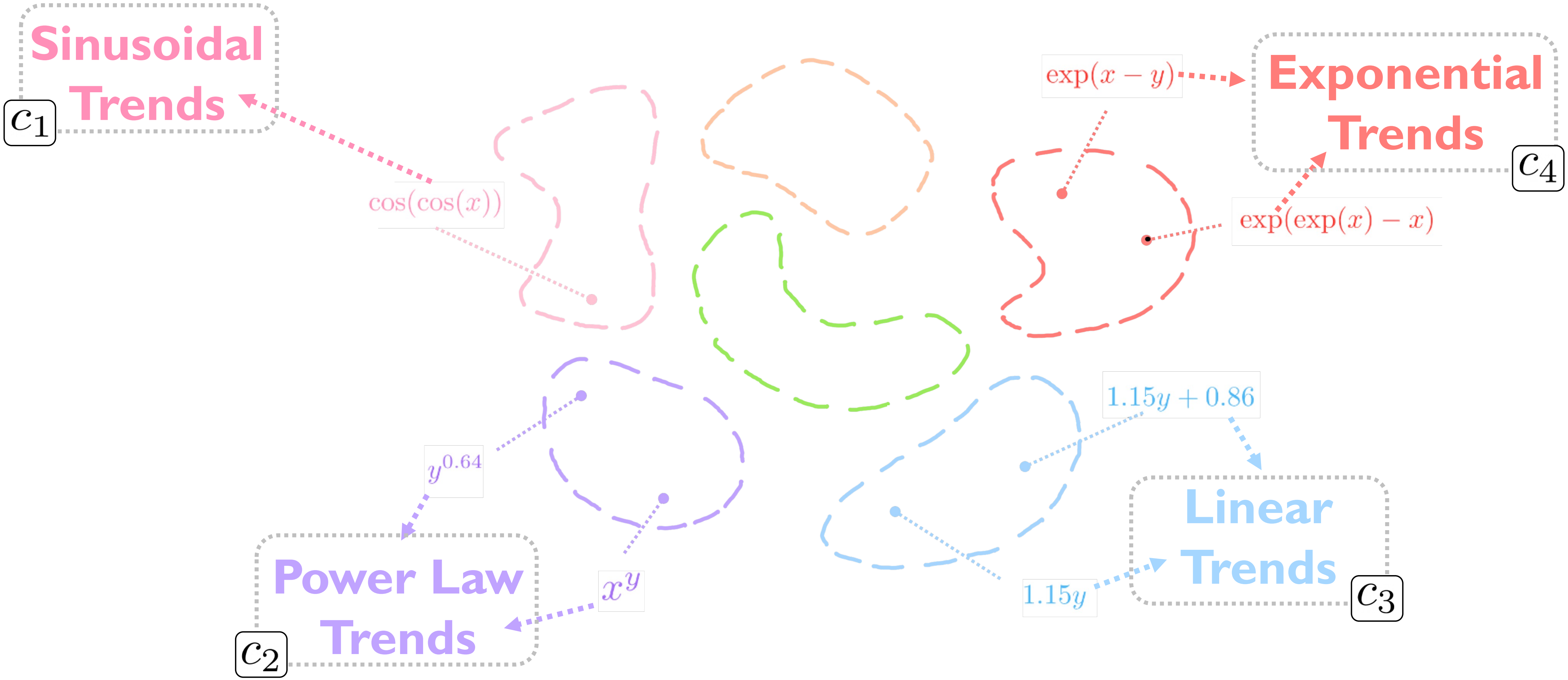
LaSR

LLM Concept Crossover evolves all concepts.

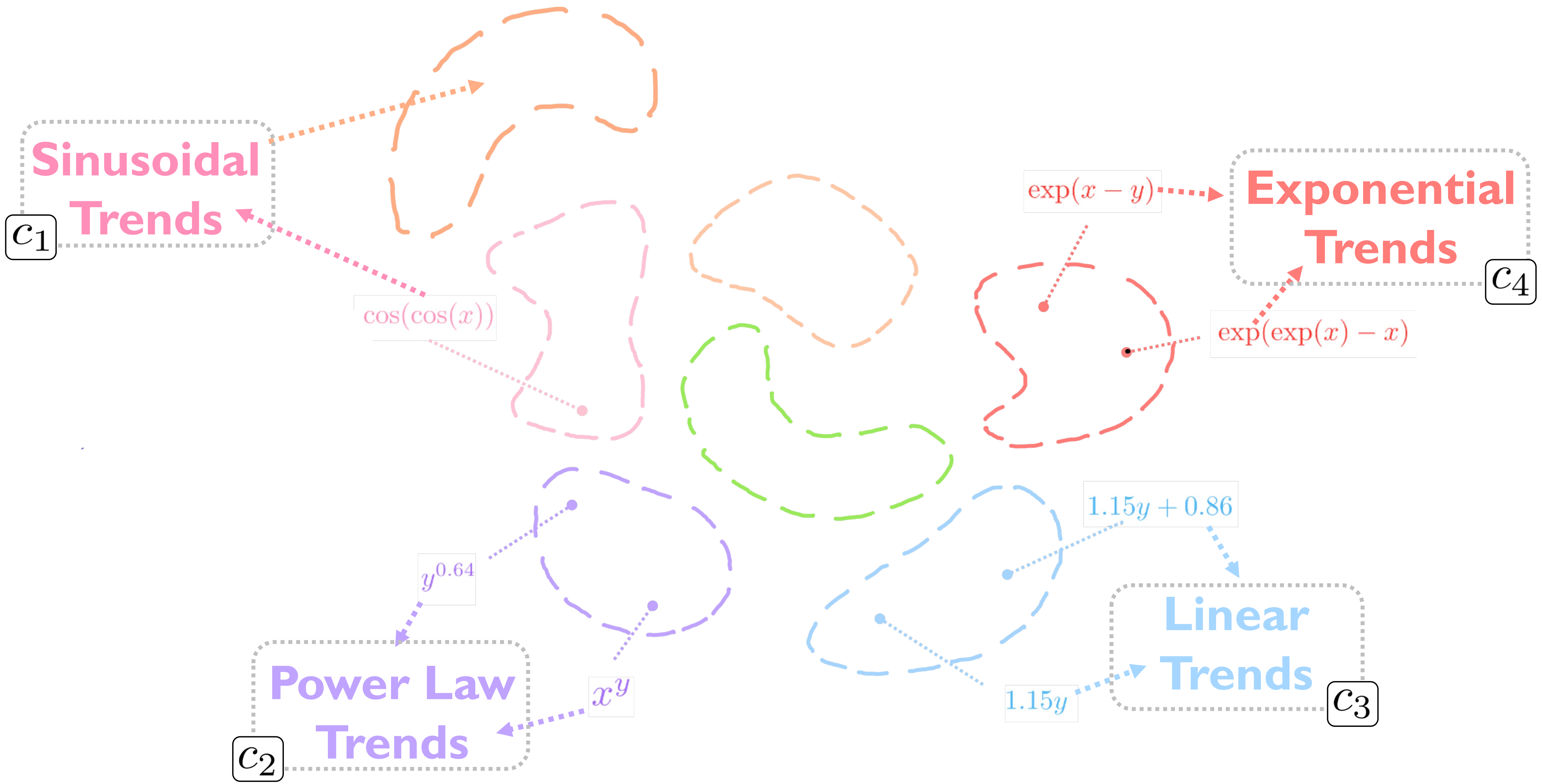




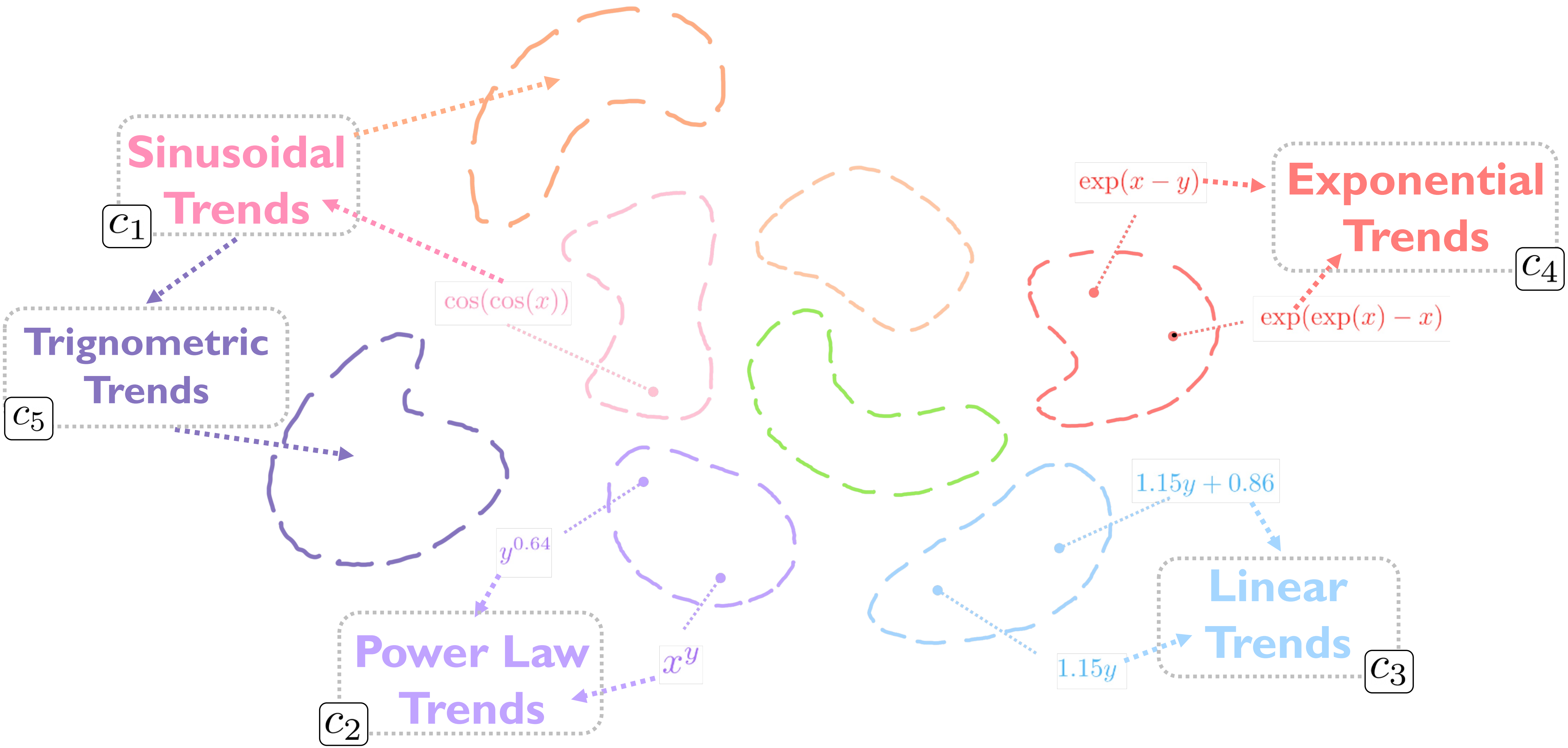
$\exp(x - y)$
$\cos(\cos(x))$
$\exp(\exp(x) - x)$
$1.15y + 0.86$
$y^{0.64}$
x^y
$1.15y$



Sinusoidal Trends
c_1
$\cos(\cos(x))$
$\exp(x-y)$
Exponential Trends
c_4
$\exp(\exp(x)-x)$
$1.15y+0.86$
$y^{0.64}$
Linear Trends
c_3
x^y
$1.15y$
Power Law Trends
c_2



Sinusoidal Trends
c_1
$\cos(\cos(x))$
Exponential Trends
$\exp(x-y)$
$\exp(\exp(x)-x)$
c_4
Linear Trends
$1.15y+0.86$
$1.15y$
c_3
Power Law Trends
$y^{0.64}$
x^y
c_2



Sinusoidal Trends
c_1
$\cos(\cos(x))$
Trignometric Trends
c_5
$y^{0.64}$
Power Law Trends
c_2
x^y
$\exp(x-y)$
Exponential Trends
c_4
$\exp(\exp(x)-x)$
$1.15y+0.86$
Linear Trends
$1.15y$
c_3

- Concept Guidance accelerates scientific discovery.

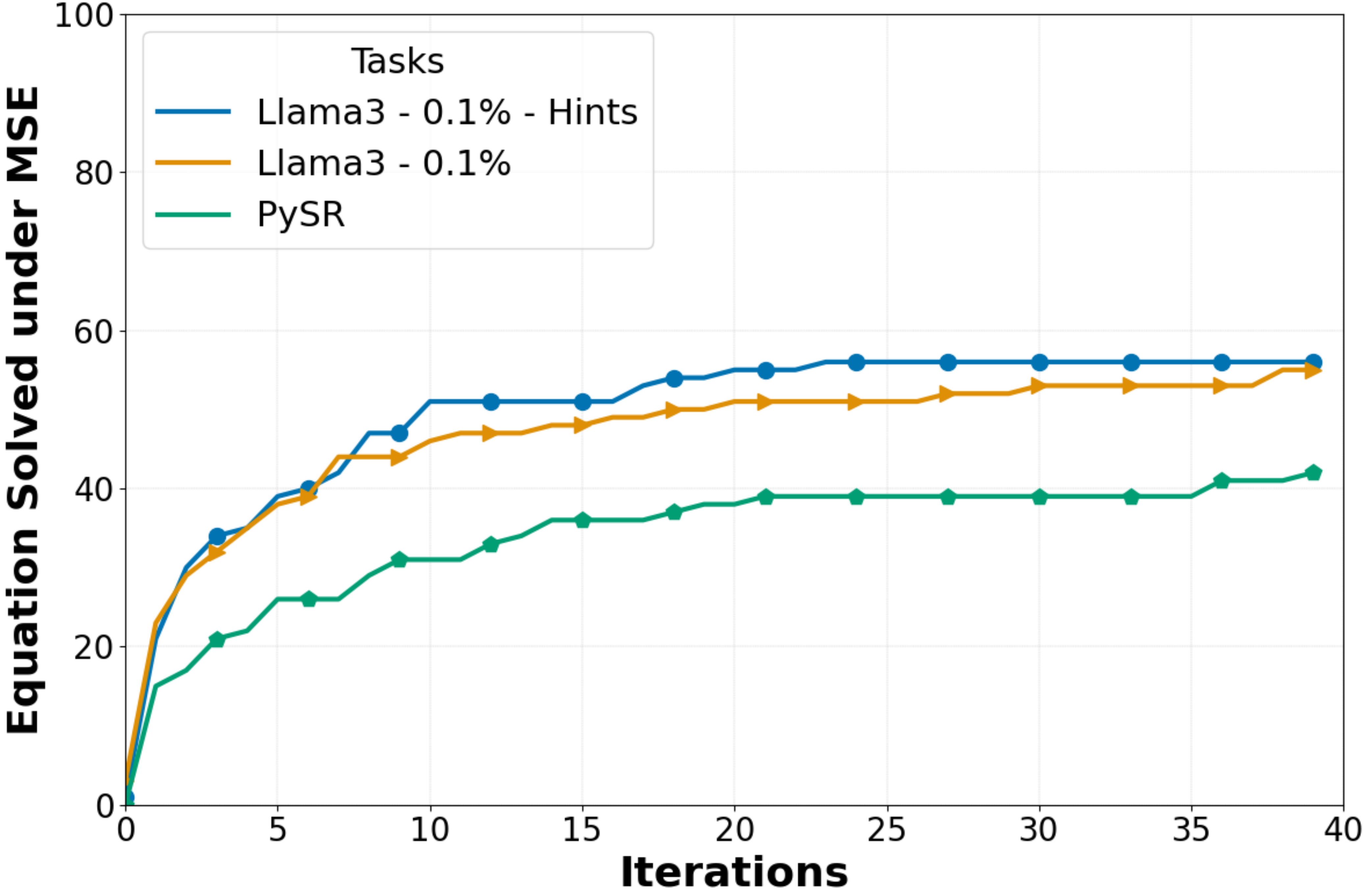
GPlearn	AFP	AFP-FE	DSR	uDSR	AIFeynman	PySR	LaSR
20/100	24/100	26/100	23/100	40/100	38/100	59/100	**72/100**

Table 1: Results on 100 Feynman equations from [49]. We report exact match solve rate for all models. LASR achieves the best exact match solve rate using the same hyperparameters as PySR.

- 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	67/100	69/100	71/100	72/100
Almost Solve	7/100	5/100	6/100	2/100	3/100
Close	16/100	9/100	12/100	12/100	10/100
Not Close	18/100	19/100	13/100	16/100	15/100

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

$$\begin{aligned}
F &= \frac{q_1}{\left(\frac{r}{q_2}\right)\left(r + \frac{1.9181636\times10^{-5}}{q_2}\right)\epsilon} \cdot 0.07957782 \\
&= \frac{q_1}{\left(\frac{r}{q_2}\right)\left(r + \frac{1.9181636\times10^{-5}}{q_2}\right)\epsilon} \cdot \frac{1}{4\pi} && \text{(Substitute constant)} \\
&= \frac{q_1 q_2}{r\left(r + \frac{1.9181636\times10^{-5}}{q_2}\right)\epsilon} \cdot \frac{1}{4\pi} && \text{(Simplify denominator)} \\
&\approx \frac{q_1 q_2}{r\,(r)\,\epsilon} \cdot \frac{1}{4\pi} && \text{(Negligible. } \tfrac{1.9181636\times10^{-5}}{q_2} \approx 0\text{)}
\end{aligned}$$

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.

Step 1: Postulate Scaling Law

$$L(N, D) = \underbrace{\frac{A}{N^{\alpha}}}_{\text{finite model}} + \underbrace{\frac{B}{D^{\beta}}}_{\text{finite data}} + \underbrace{E}_{\text{irreducible}}$$

Step 2: Measure model loss w.r.t hyper parameters.

Google DeepMind MassiveText

Step 3: Fit scaling law to dataset.

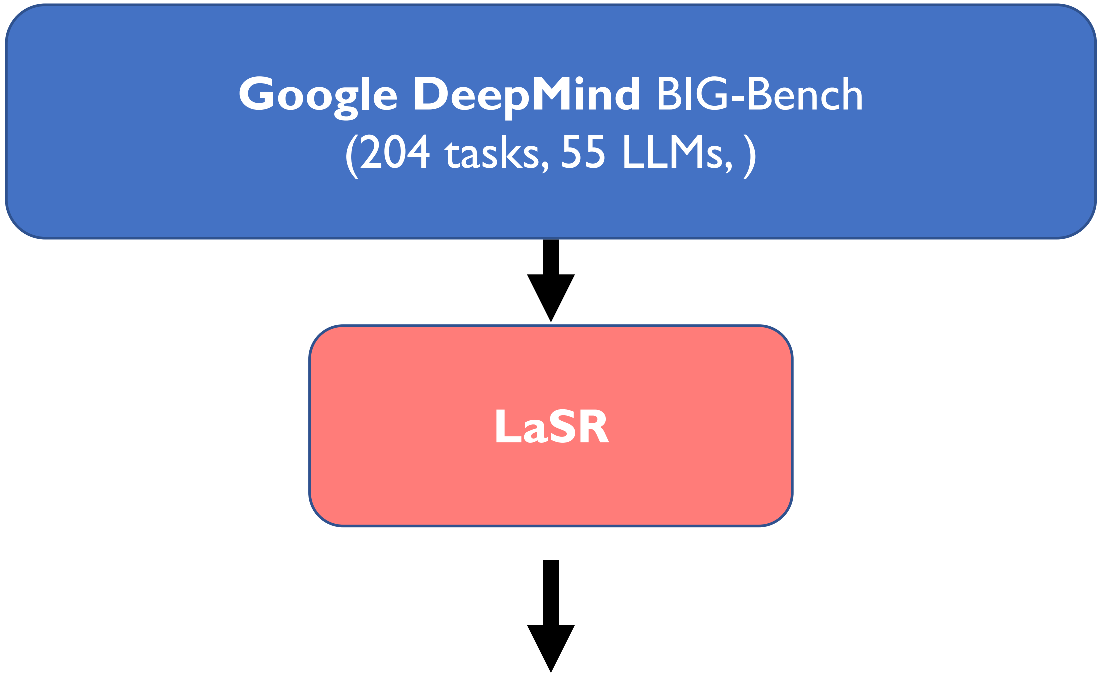
$$L(N, D) = \underbrace{\frac{406.4}{N^{0.34}}}_{\text{finite model}} + \underbrace{\frac{410.7}{D^{0.28}}}_{\text{finite data}} + \underbrace{1.69}_{\text{irreducible}}$$

Training Compute-Optimal Large Language Models, Hoffman et. al

Step 1: Measure model loss w.r.t hyper parameters.

Step 2: Use symbolic regression to postulate and fit scaling laws

Step 3: Choose the scaling law that fits the data the best while using the least parameters.



$$\texttt{score} = \frac{-0.0248235}{\left(\frac{\texttt{train\_steps}}{116050.999}\right)^{\texttt{\#shots}}} + 0.366991$$