Modeling and Computation in the Space of Language: Symbolic and LLM-Based Approaches

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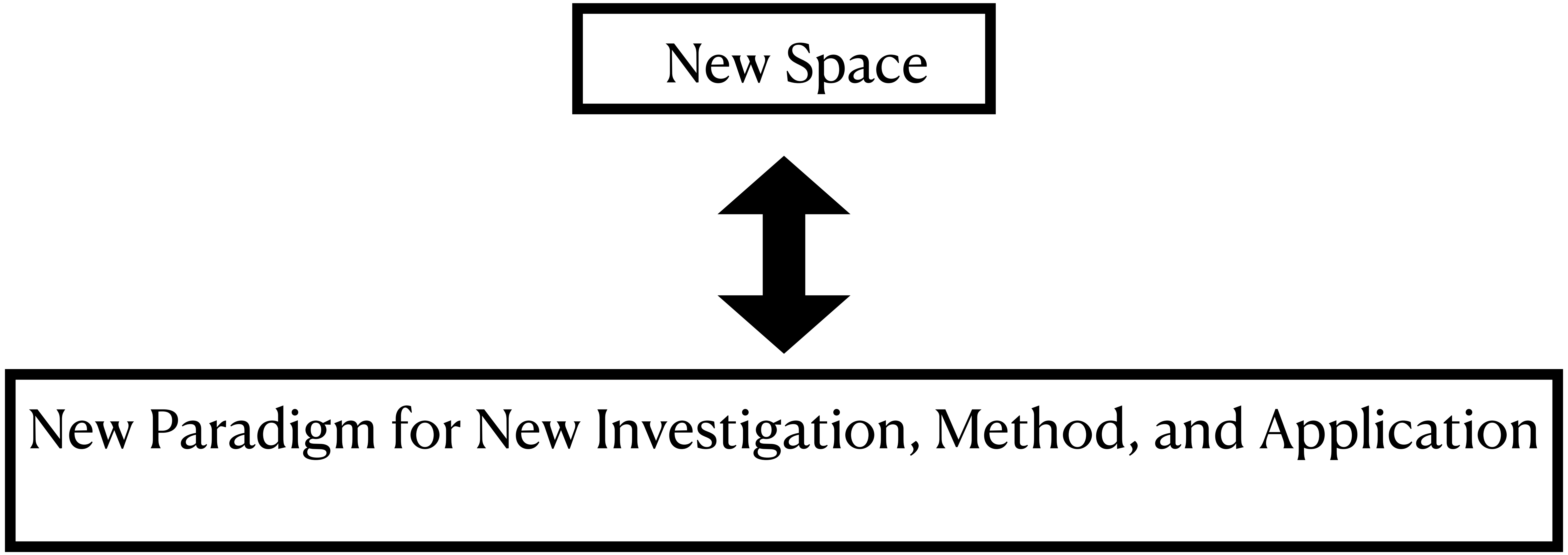
Modeling & Computing in the Right Space

- Sparse Grids
  - "Right Space" - the solution can be approximated well by sparse combinations of basis functions
- Low-Rank Tensor Methods
  - "Right Space" - the solution can be approximated by a sum of products of lower-dimensional functions
- Neural Network Methods
  - "Right Space" - the implicit function space learned by the network during training

Modeling & Computing in the Right Space



Modeling & Computing in the Right Space

The space of language: Example 1. math expression and description

A function $f : \mathbb{R}^d \to \mathbb{R}$ is **permutation symmetric** if it is invariant under any permutation of its input components. That is:

$$f(x_1, x_2, \ldots, x_d) = f(x_{\pi(1)}, x_{\pi(2)}, \ldots, x_{\pi(d)})$$

for any permutation $\pi \in S_d$ (the symmetric group on d elements).

Example: $f(x) = \sum_{i=1}^{d} x_i^2$ is permutation symmetric.

Modeling & Computing in the Right Space

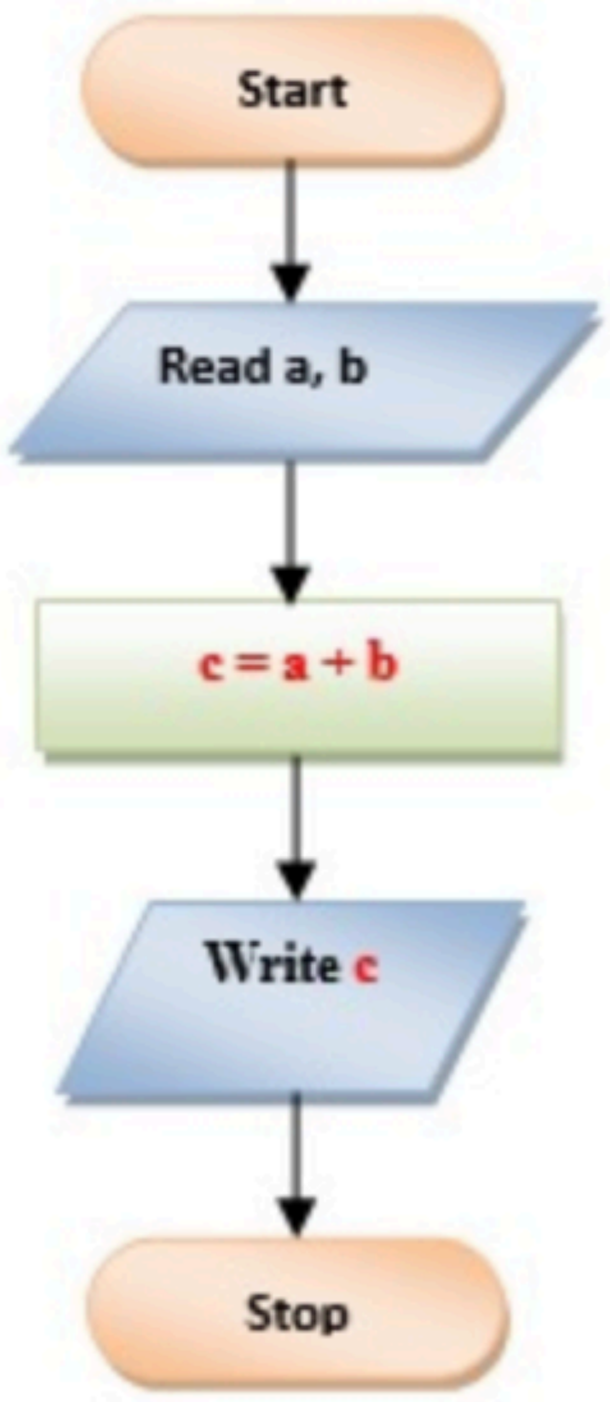
The space of language: Example 2. Algorithm, Flowchart, and code language

To find sum of two numbers

Algorithm

1. Start
2. Read a, b
3. c = a + b
4. Print or display c
5. Stop

Flowchart



Program

```
#include<stdio.h>

int main()
{
    int a, b, c;

    printf("Enter value of a: ");
    scanf("%d", &a);

    printf("Enter value of b: ");
    scanf("%d", &b);
    c = a+b;

    printf("Sum of given two numbers is: %d", c);

return 0;
}
```

Modeling & Computing in the Space of Natural Language

Question:

- How to model and compute in the space of natural language?

Two Complementary Approaches:

- Symbolic learning (Finite Expression Method)
- Large language model (LLM)

Applications:

- Search for a solution
- Search for a mathematical model
- Search for a computational algorithm
- Search for executable code
- ...

- **Symbolic learning (Finite Expression Method)**
- Large language model (LLM) for modeling and computing assistant

Finite Expression Method (FEX) Methodology

Liang and Y. arXiv:2206.10121

Motivating Problem:

- A **structured** high-dimensional Poisson equation

$$-\Delta u = f \quad \text{for } x \in \Omega, \quad u = g \text{ for } x \in \partial\Omega$$

  with a solution $u(x) = \frac{1}{2}\sum_{i=1}^{d} x_i^2$ of low complexity $O(d)$, i.e., $O(d)$ operators in this expression

Idea:

- Find an explicit expression that approximates the solution of a PDE
- Function space with finite expressions
  - **Mathematical expressions**: a combination of symbols with rules to form a valid function, e.g., $\sin(2x) + 5$
  - k**-finite expression**: a mathematical expression with at most k operators
  - Function space in FEX: $\mathbb{S}_k$ as the set of s-finite expressions with $s \leq k$

Finite Expression Method (FEX) Theory

Liang and Y. arXiv:2206.10121

Advantages in Real Analysis: "No" curse of dimensionality in approximation

Theorem (Liang and Y. 2022) Suppose the function space is $\mathbb{S}_k$ generated with operators including ``+", ``-", ``$\times$", ``/", ``$\max\{0,x\}$", ``sin(x)", and ``2^x". Let $p \in [1, +\infty)$. For any f in the Holder function class $\mathscr{H}_\mu^\alpha([0,1]^d)$ and $\varepsilon > 0$, there exists a k-finite expression ϕ in $\mathbb{S}_k$ such that

$$\|f - \phi\|_{L^p} \leq \varepsilon,$$

if

$$k \geq \mathcal{O}(d^2(\log d + \log \frac{1}{\varepsilon})^2).$$

Finite Expression Method (FEX) Practice

Advantages in Practice:

- Leverage the power of descriptive structures of problems

Question:

- How to do computation with description?

Answers:

- Reinforcement learning
- In-context learning
- Bayesian approach

Finite Expression Method for Solving PDEs

Liang and Y. arXiv:2206.10121

Least square based FEX

- e.g., $\mathscr{D}(u) = f$ in Ω and $\mathscr{B}(u) = g$ on $\partial\Omega$
- A mathematical expression u^* to approximate the PDE solution via

$$u^* = \arg\min_{u \in \mathbb{S}_k} \mathscr{L}(u) := \arg\min_{u \in \mathbb{S}_k} \|\mathscr{D}u - f\|_2^2 + \lambda \|\mathscr{B}u - g\|_2^2$$

- Or numerically

$$u^* = \arg\min_{u \in \mathbb{S}_k} \mathscr{L}(u) := \arg\min_{u \in \mathbb{S}_k} \frac{1}{n} \sum_{i=1}^{n} |\mathscr{D}u(x_i) - f(x_i)|^2 + \lambda \frac{1}{m} \sum_{j=1}^{m} |\mathscr{B}u(x_j) - g(x_j)|^2$$

- Question: how to solve this combinatorial optimization problem? Reinforcement learning

Numerical Comparison

Liang and Y. arXiv:2206.10121

- NN method:
  - Neural networks with a ReLU^2-activation function
  - ResNet with depth 7 and width 50

- FEX method:
  - Depth 3 binary tree
  - Binary set $\mathbb{B} = \{+, -, \times\}$
  - Unary set $\mathbb{U} = \{0, 1, \text{Id}, (\cdot)^2, (\cdot)^3, (\cdot)^4, \exp, \sin, \cos\}$

- The right space: solutions with simple descriptive structures

Solving High-Dimensional PDEs with FEX

Poisson equation

$\Omega = [0,1]^d$

$-\Delta u = f$ for $x \in \Omega$ and $u = g$ on $\partial\Omega$

True solution: $u(\boldsymbol{x}) = \frac{1}{2}\sum_{i=1}^{d} x_i^2$

Linear conservation law

$T\times\Omega = [0,1]\times[-1,1]^d$

$\frac{\pi d}{4} u_t - \sum_{i=1}^{d} u_{x_i} = 0$ and $u(0,x) = \sin\left(\frac{\pi}{4}\sum_{i=1}^{d} x_i\right)$

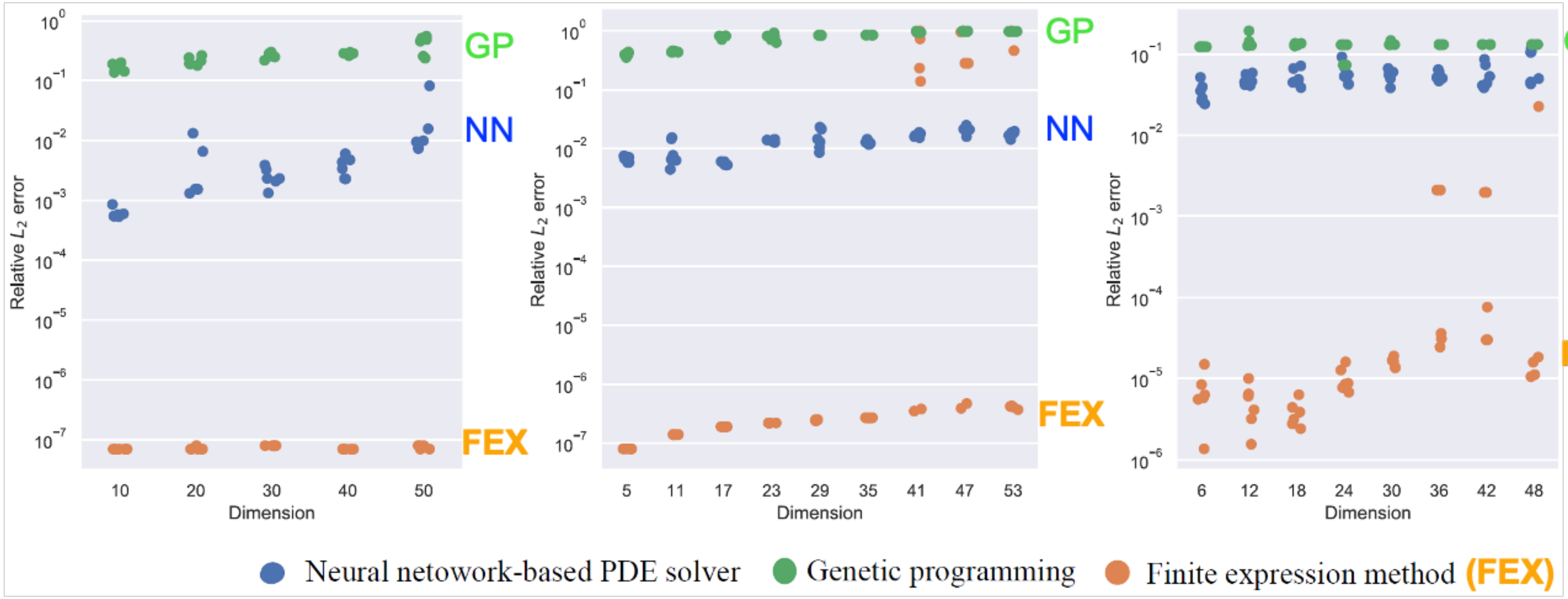
True solution: $u(\boldsymbol{x}) = \sin(t + \frac{\pi}{4}\sum_{i=1}^{d} x_i)$

Nonlinear Schrödinger equation

$\Omega = [-1,1]^d$

$-\Delta u + u^3 + Vu = f$ for $x \in \Omega$

True solution: $u(\boldsymbol{x}) = \exp(\sum_{i=1}^{d} \cos(x_i)/d)$



Liang and Y. arXiv:2206.10121

FEX for Partial Integral Differential Equations

Hardwick, Liang, Y., arxiv:2410.00835

$$\frac{\partial u}{\partial t} + b \cdot \nabla u + \frac{1}{2}\mathrm{Tr}(\sigma\sigma^T H(u)) + \mathrm{A}u + f = 0$$

$$u(T, \cdot\,) = g(\,\cdot\,)$$

$$\mathrm{A}u(t,x) = \int_{\mathbb{R}^n} (u(t, x + G(x,z)) - u(t,x) - G(x,z)\cdot \nabla u(t,x))\nu(dz)$$

$G(x,z) \in \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}^d$, and ν is a Levy measure associated with a Poisson random measure.

Dimension	2	4	6	8	10	20	30
FEX-PG	2.99e-7	3.17e-7	5.16e-7	7.26e-7	2.05e-7	8.02e-7	4.49e-7
TD-NN [23]	0.00954	0.00251	0.00025	0.00671	0.01895	0.00702	0.01221

Dimension	40	50	60	70	80	90	100
FEX-PG	9.05e-7	4.27e-7	4.55e-7	3.54e-7	5.89e-7	6.44e-7	5.64e-7
TD-NN [23]	0.00956	0.00219	0.00944	0.00044	0.00277	0.00460	0.00548

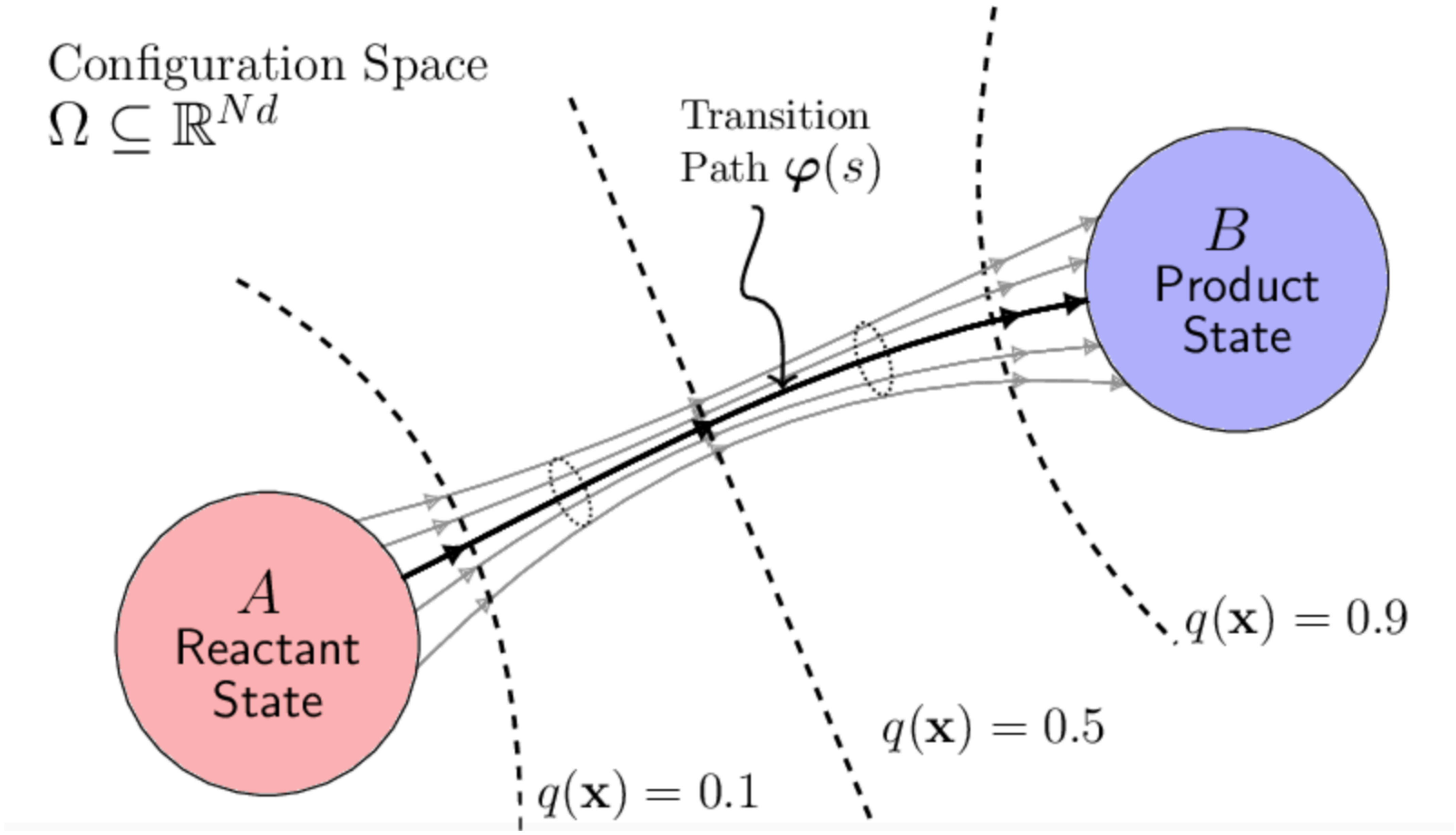
Committor Function for Rare Events

Song, Cameron, Yang arXiv:2306.12268, SISC, 2025

$$\begin{cases} \beta^{-1}\Delta q + \nabla V \cdot \nabla q = 0 & \text{for } \boldsymbol{x} \notin A \cup B \\ q(\mathbf{x}) = 0 & \text{for } \boldsymbol{x} \in A \\ q(\mathbf{x}) = 1 & \text{for } \boldsymbol{x} \in B\,. \end{cases}$$

where β is temperature and $q(\boldsymbol{x})$ is the probability

for starting from $\boldsymbol{x}$, visiting B before visiting A.



Committor Function for Rare Events

Song, Cameron, Yang arXiv:2306.12268, SISC, 2025

Difficulty

- dimension $\propto$ number of atoms

Physical Structure

- Low-dimensional structure: a small number of collective variables

Machine Learning

- Identify a low-dimensional structure
- High-dimension $\rightarrow$ low-dimension

Committor Function for Rare Events

Song, Cameron, Yang arXiv:2306.12268, SISC, 2025

Example: Double-Well potential

$$V(\mathbf{x}) = \underbrace{\left(x_1{}^2 - 1\right)^2}_{\text{collective variable}} + 0.3 \sum_{i=2}^{d} x_i^2$$

with $$A = \left\{x \in \mathbb{R}^d \mid x_1 \le -1\right\}, \quad B = \left\{x \in \mathbb{R}^d \mid x_1 \ge 1\right\}$$

The ground truth solution is

$$q(\mathbf{x}) = f(x_1)$$

where $f(x_1)$ solves a 1D BVP:

$$\frac{d^2 f\left(x_1\right)}{dx_1^2} - 4x_1\left(x_1^2 - 1\right)\frac{df\left(x_1\right)}{dx_1} = 0, \quad f(-1) = 0, \quad f(1) = 1$$

Committor Function for Rare Events

Song, Cameron, Yang arXiv:2306.12268, SISC, 2025

FEX identifies the following representation

Eqn 1: $\alpha_{1,1}x_1 + \ldots + \alpha_{1,10}x_{10} + \beta_1$

Eqn 2: $\alpha_{2,1}\tanh(x_1) + \ldots + \alpha_{2,10}\tanh(x_{10}) + \beta_2$

$\mathcal{J}(\mathbf{x}) = \alpha_3 \tanh(\text{Eqn 1} + \text{Eqn 2}) + \beta_3$

where $\alpha_3 = 0.5,\ \beta_3 = 0.5$

	α_1	α_2	α_3	α_4	α_5	α_6	α_7	α_8	α_9	α_{10}	β
Eqn 1	**1.6798**	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Eqn 2	**1.9039**	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

FEX discovers $q(\mathbf{x}) = f(x_1)$ and high-dimensional → low-dimension

FEX for Learning Physical Laws

2D Burgers equation with periodic boundary conditions on $(x, y, t) \in [0,2\pi]^2 \times [0,10]$:

$$\frac{\partial u}{\partial t} = -u\frac{\partial u}{\partial x} - v\frac{\partial u}{\partial y} + \nu(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2})$$

$$\frac{\partial v}{\partial t} = -u\frac{\partial v}{\partial x} - v\frac{\partial v}{\partial y} + \nu(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2})$$

$$u(x, y, 0) = u_0(x, y)$$

$$v(x, y, 0) = v_0(x, y)$$

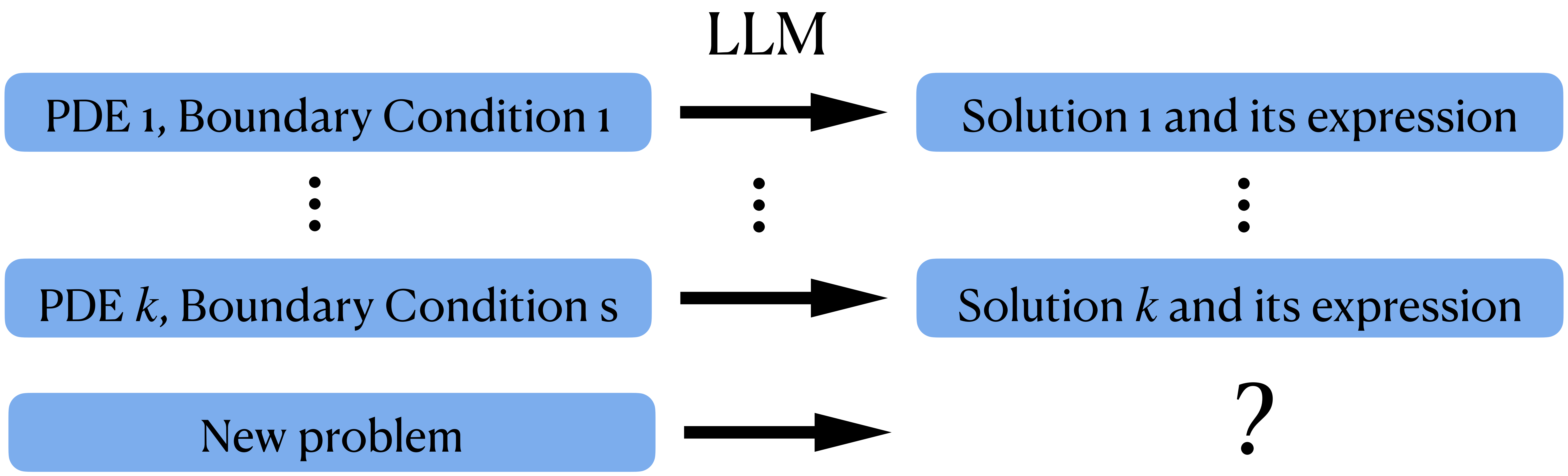
$$\nu = 0.1$$

	PDE-Net 2.0	SINDy	GP	SPL	FEX
Mean Absolute Error	1.086×10^{-3}	3.239×10^{-1}	4.973×10^{-1}	2.1×10^{-1}	2.021×10^{-4}

Unraveling Symbolic Structures in FEX with LLMs

Bhatnagar, Liang, Patel, Y., arXiv:2503.09986

- Methodology: Fine-tune LLM & in-context learning



- Advantages: faster convergence & higher accuracy

Unraveling Symbolic Structures in FEX with LLMs

Bhatnagar, Liang, Patel, Y., arXiv:2503.09986

Operator information preserved in solution from condition

Theorem $-\Delta u = f$ in Ω and $u = g$ on $\partial\Omega$. Reasonable smoothness for f and g. $\forall \delta \in (0,1)$, $\exists \bar{u} : \mathbb{R}^d \to \mathbb{R}$ such that

- $\|u - \bar{u}\|_{L^2(\Omega)} \leq \delta$
- $\bar{u}$ only has operators $+$, $\times$, $(\,\cdot\,)^2$, and those in f, g, and $\mathrm{dist}(x, \partial\Omega)$
- $\#\mathrm{ops}(\bar{u}) = (\#\mathrm{ops}(f) + \#\mathrm{ops}(g)) \times \mathrm{poly}(\frac{1}{\delta})$

Results generalize to time-dependent problems.

Unraveling Symbolic Structures in FEX with LLMs

Bhatnagar, Liang, Patel, Y., arXiv:2503.09986

PDE Type	Metric	Uninformed FEX	LLM-Informed FEX	Speedup
Conservation	Avg. Iter	28.52	5.23	5.45×
	Avg. Time (m)	23.67	3.95	6.00×
Poisson	Avg. Iter	28.73	6.47	4.44×
	Avg. Time (m)	62.07	14.09	4.41×

$u(x)$	Method	Binary Size	Unary Size	Iters	Time [m]	Error
$4\cos\big(4x^2\cos(x_0)\big)$	**LLM-informed**	1	2	4.25	8.25	0
	Uninformed	3	9	167	340	0
$4\,x_1^3+4\,x_1^2+2\cos\big(4\,x_1^3\cos(x_0)\big)$	**LLM-informed**	2	4	102	286	10^{-8}
	Uninformed[6]	3	9	2000+	2400+	N/A

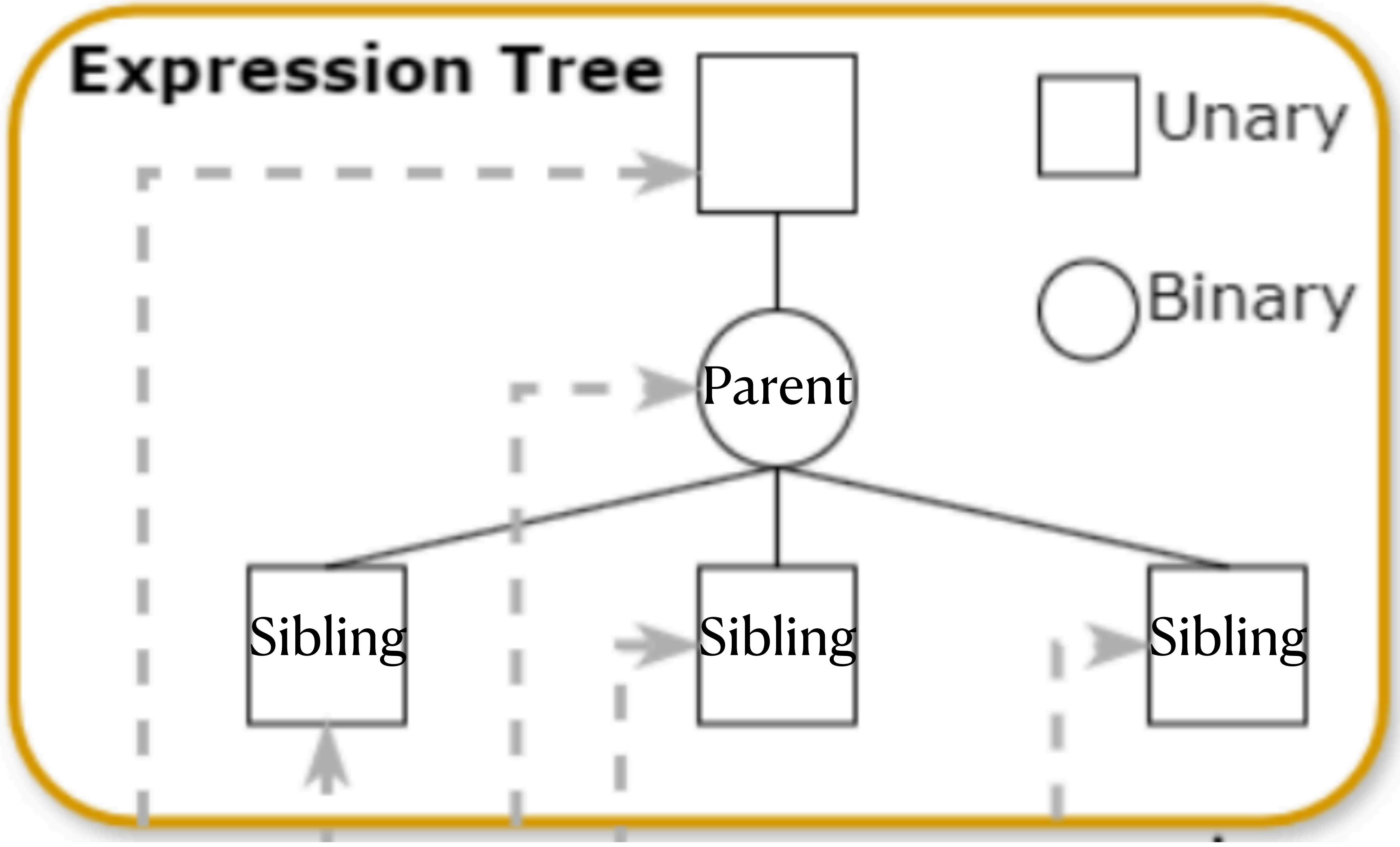
Bayesian Symbolic Learning

Huang, Wen, Adusumilli, Choudhary, Y., arXiv:2503.09592

Scientific Paper → Domain Specific Expressions → Domain Specific Priors → Optimization

Domain Specific Priors
- Pr(·| Parent)
- Pr(·| Parent, siblings)
- Formulation rules

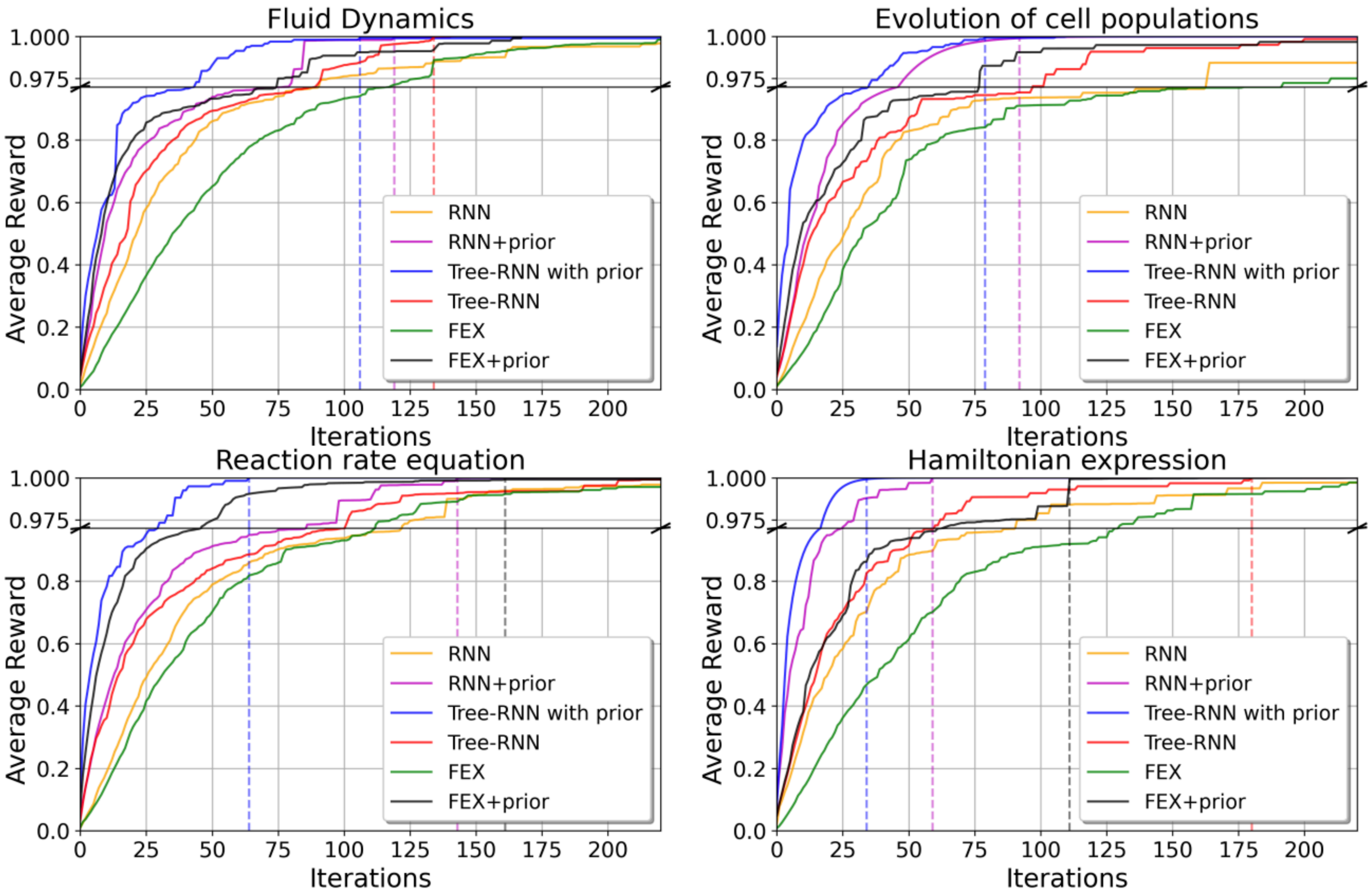
Optimization
- Better samples
- Faster convergence
- Eliminate artifacts



Fill in Operators

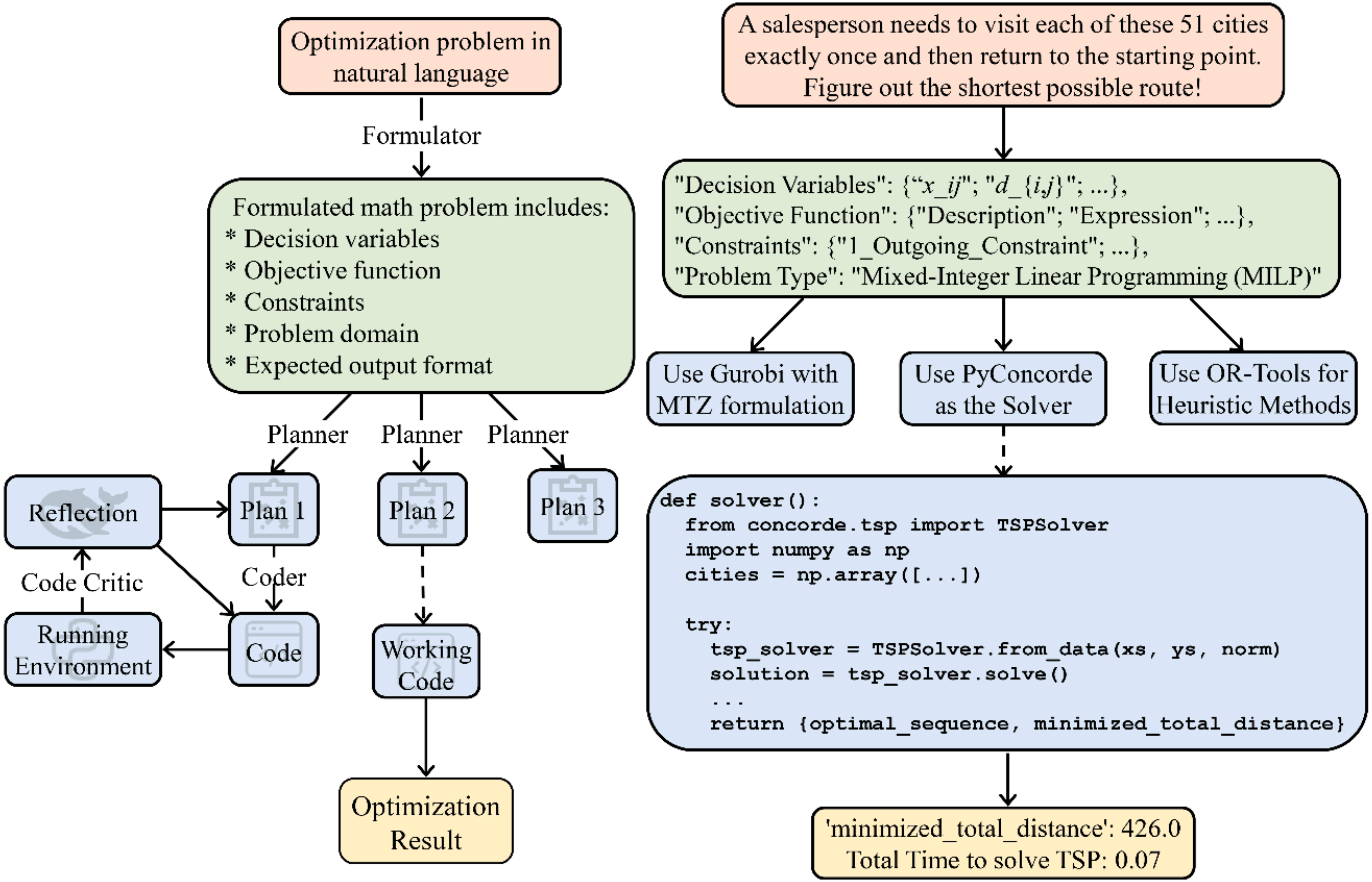
Bayesian Symbolic Learning

Huang, Wen, Adusumilli, Choudhary, Y., arXiv:2503.09592



- Symbolic learning (Finite Expression Method)
- **Large language model (LLM) for modeling and computing assistant**
  - **Example**: automatic optimization modeling, solving, and testing

Overview and New Features of OptimAI



LLM Agents for Modeling & Computing from Natural Language

OptimAI: Thind, Sun, Liang, Y., arXiv:2504.16918

Table 1: Comparison of Functional Capabilities between OptimAI and Prior Methods.

Functional Capabilities	OptiMUS	Optibench	CoE	OptimAI
Natural language input	✗	✓	✓	✓
Planning before coding	✗	✗	✓	✓
Multi-solver support	✗	✗	✗	✓
Switching between plans	✗	✗	✗	✓
Code generation	✓	✓	✓	✓
Distinct LLM collaboration	✗	✗	✗	✓

LLM Agents for Modeling & Computing from Natural Language

OptimAI: Thind, Sun, Liang, Y., arXiv:2504.16918

Table 2: Previous work on using LLMs for optimization.

Work	Dataset Proposed	Size	Problem Type(s)
NL4Opt Competition [8]	NL4Opt	289	LP
Chain-of-Experts (CoE) [9]	ComplexOR	37	LP, MILP
OptiMUS [10, 11, 12]	NLP4LP	67	LP, MILP
Optibench [13]	Optibench	605	LP, NLP, MILP, MINLP
OR-LLM-Agent[14]	OR-LLM-Agent	83	LP, MILP

Abbreviations: LP - Linear Programming, NLP - Nonlinear Programming, MI - Mixed-Integer.

LLM Agents for Modeling & Computing from Natural Language

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Table 3: Accuracy comparison between OptimAI and state-of-the-art methods.

Agent \ Dataset	NLP4LP	Optibench Linear w/o Tab.	Optibench Linear w/ Tab.	Optibench Nonlin. w/o Tab.	Optibench Nonlin. w/ Tab.
OptiMUS [11]	71.6%	-	-	-	-
Optibench [13]	-	75.4%	62.5%	42.1%	32.0%
Ours w/ GPT-4o	79.1%	81.2%	73.8%	72.0%	48.0%
Ours w/ GPT-4o+o1-mini	**88.1%**	84.2%	**80.0%**	77.3%	56.0%
Ours w/ QwQ (by Qwen)	79.1%	86.2%	77.5%	**81.6%**	50.0%
Ours w/ DeepSeek-R1	82.1%	**87.4%**	78.8%	79.5%	**60.0%**

All evaluations were conducted under a zero-shot prompting setting. GPT-4o+o1-mini refers to using o1-mini as the planner while employing GPT-4o for all other roles.

LLM Agents for Modeling & Computing from Natural Language

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Table 4: Generalization of OptimAI across NP-hard combinatorial optimization problems.

	Math Programming	TSP	JSP	Set Covering
OptimAI	✓	✓	✓	✓
OptiMUS	✓	✗	✗	✗
Optibench	✓	✗	✗	✗

Traveling salesman problem (TSP), job shop scheduling problem (JSP), and set covering problem.

LLM Agents for Modeling & Computing from Natural Language

OptimAI: Thind, Sun, Liang, Y., arXiv:2504.16918

Table 5: Synergistic effects of combining heterogeneous LLMs.

Planner \ Remaining Roles	Llama 3.3 70B	DeepSeek-R1 14B	Gemma 2 27B
Llama 3.3 70B	59%	54%	54%
DeepSeek-R1 14B	**68%**	50%	41%
Gemma 2 27B	**77%**	**59%**	54%

LLM Agents for Modeling & Computing from Natural Language

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Table 6: Ablation study of OptimAI design.

Formulator	Planner	Code Critic	Revisions	Executability	Productivity
✓	✓	✓	**1.7**	**3.6**	**6.8**
✗	✓	✓	2.0	3.2	6.3
✓	✗	✓	7.8	3.1	1.2
✓	✓	✗	6.2	3.3	2.2

Take Home Messages

- Modeling and Computing **in the language space**
- **Descriptive structures** ease challenges and form a right space
- Language space admits **automatic big** search