UNIVERSITY OF MARYLAND

APPLIED MATHEMATICS & STATISTICS, AND SCIENTIFIC COMPUTATION PROGRAM

Finite EXpression Method (FEX) for Solving High-Dimensional Committor Problems

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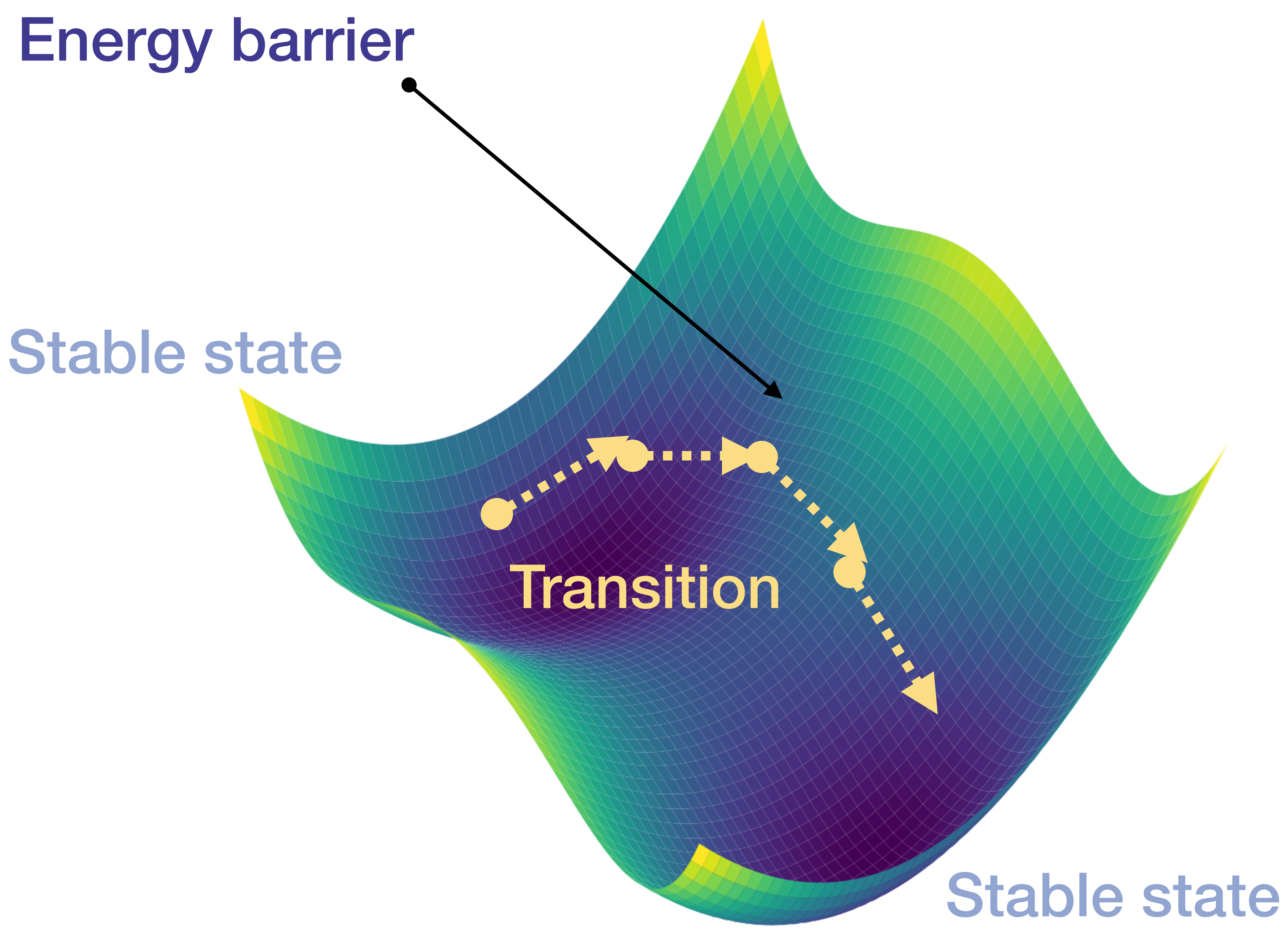
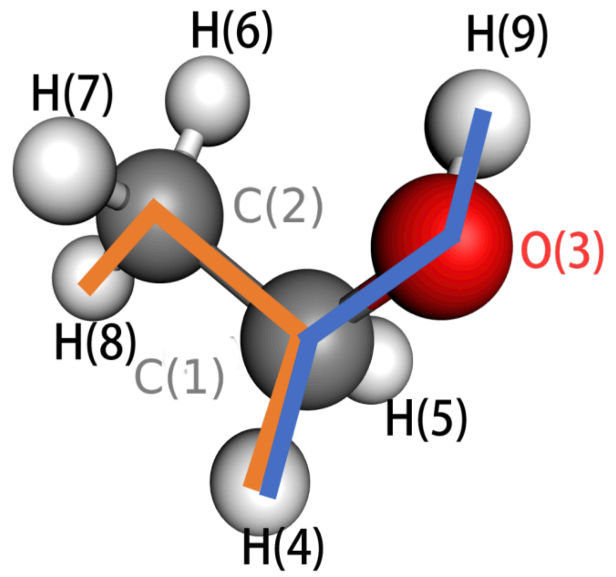
Rare Transitions in Molecular Dynamics

Potential Energy Surface

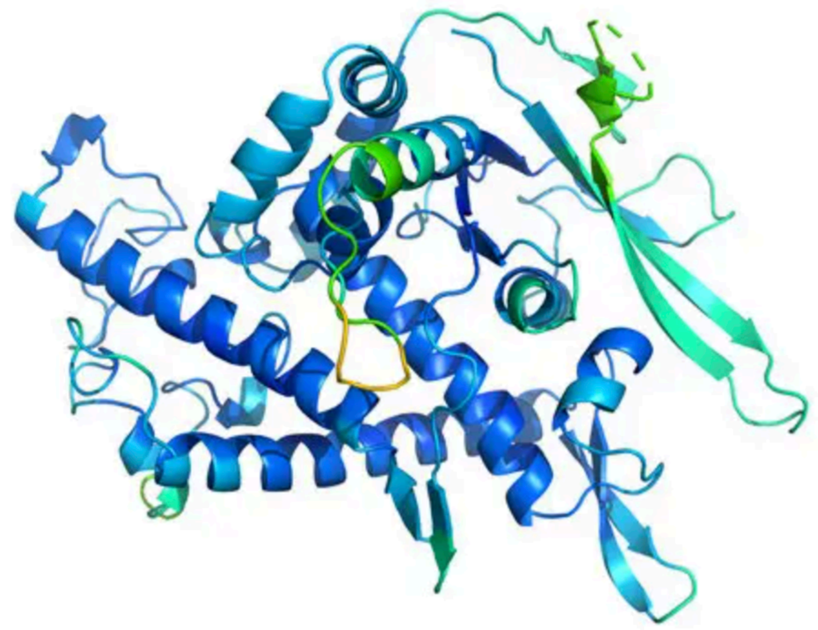


Examples:



Chemical Reaction

Material Sciences

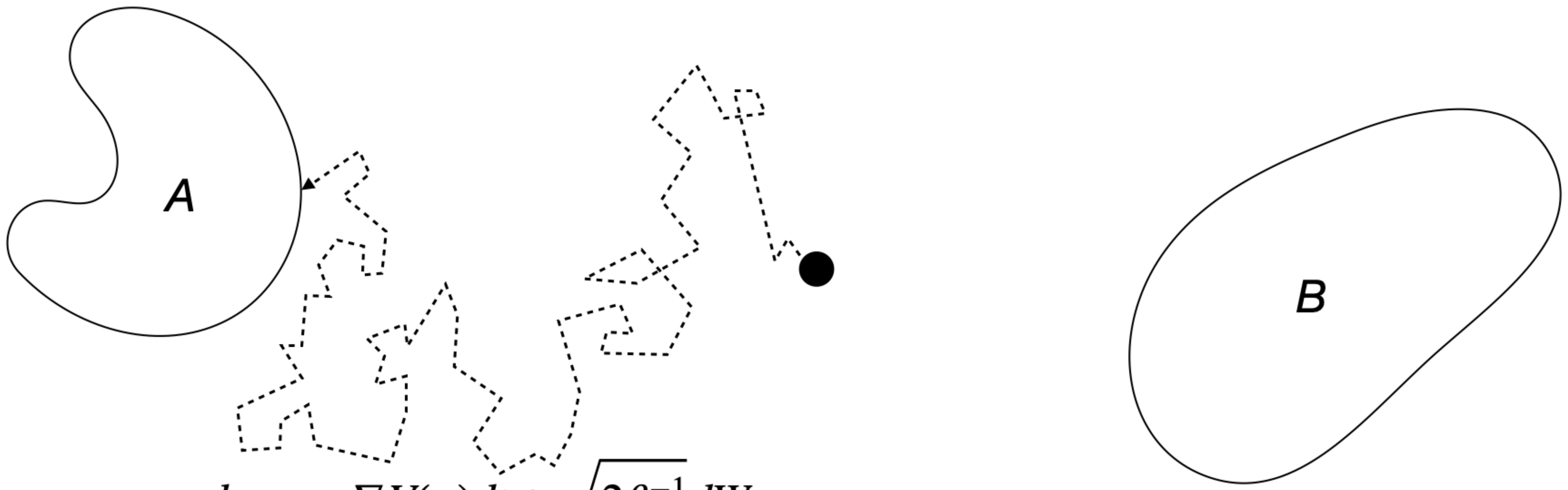


Protein Folding

Rare events are hard to observe yet crucial

Problem Setting

Dynamics governed by an SDE,



$$dx_t = -\nabla V(x_t)dt + \sqrt{2\beta^{-1}}dW_t$$

where:

- $\mathbf{x}_t \in \Omega \subset \mathbb{R}^d$ is the state of the system;
- $V : \mathbb{R}^d \to \mathbb{R}$ is a smooth potential;
- $\beta = 1/T$ is the inverse of temperature;
- $\mathbf{w}_t$ is the standard d-dimensional Brownian motion.

We are interested in the committor

$$q(\mathbf{x}) = \mathbb{P}\left(\tau_B < \tau_A \mid \mathbf{x}_0 = \mathbf{x}\right)$$

Committor Function as a PDE Solution

$$\begin{cases} (Lq)(\mathbf{x}) = 0 & \text{for } x \notin A \cup B \\ q(\mathbf{x}) = 0 & \text{for } \boldsymbol{x} \in A \\ q(\mathbf{x}) = 1 & \text{for } \boldsymbol{x} \in B\,. \end{cases}$$

where L is the infinitesimal generator of the process defined as:

$$Lq = -\beta^{-1}\Delta q + \nabla V \cdot \nabla q$$

Previous work:

- Diffusion map

Coifman, R. R., Kevrekidis, I. G., Lafon, S., Maggioni, M., & Nadler, B. (2008). Diffusion maps, reduction coordinates, and low dimensional representation of stochastic systems. *Multiscale Modeling & Simulation*

Lai, R., & Lu, J. (2018). Point Cloud Discretization of Fokker--Planck Operators for Committor Functions. *Multiscale Modeling & Simulation*

Evans, L., Cameron, M. K., & Tiwary, P. (2023). Computing committors in collective variables via Mahalanobis diffusion maps. *Applied and Computational Harmonic Analysis*

- Neural network

Khoo, Y., Lu, J., & Ying, L. (2019). Solving for high-dimensional committor functions using artificial neural networks. *Research in the Mathematical Sciences*

Li, H., Khoo, Y., Ren, Y., & Ying, L. (2022, April). A semigroup method for high dimensional committor functions based on neural network. In *Mathematical and Scientific Machine Learning*

- Tensor network

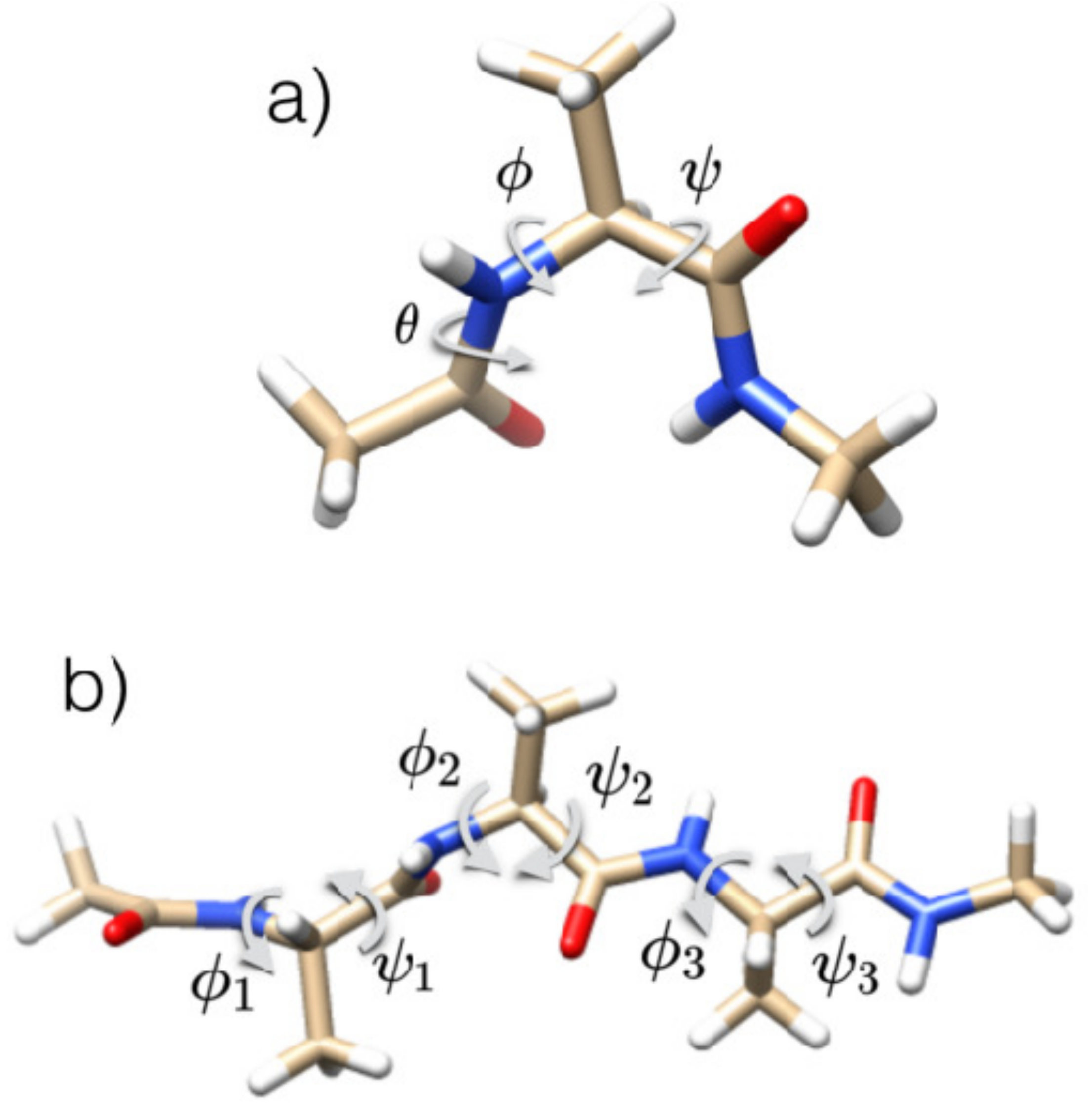
Chen, Y., Hoskins, J., Khoo, Y., & Lindsey, M. (2023). Committor functions via tensor networks. *Journal of Computational Physics*

Lessen Curse of Dimensionality with FEX

Challenge:

High-dimensional configuration space!

N atoms $\propto$ 3N-dim config. space

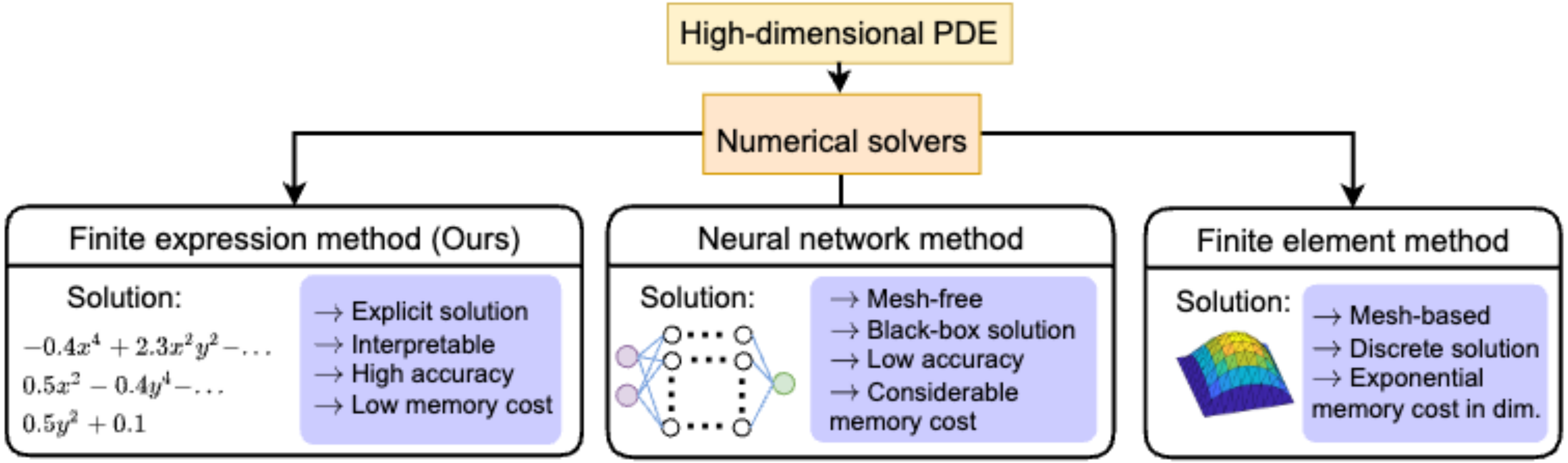


Collective variables

However, they usually possess a low-dimensional structure, e.g collective variables.

Our work: FEX can identify the low-dimensional structure.

Overview of PDE Solvers



- Q: Why finite expression?
- A: Low-dimensional structure of high-dimensional problem

- Mathematical expressions: combination of symbols with rules to form a valid function

Finite Expression Method (FEX)

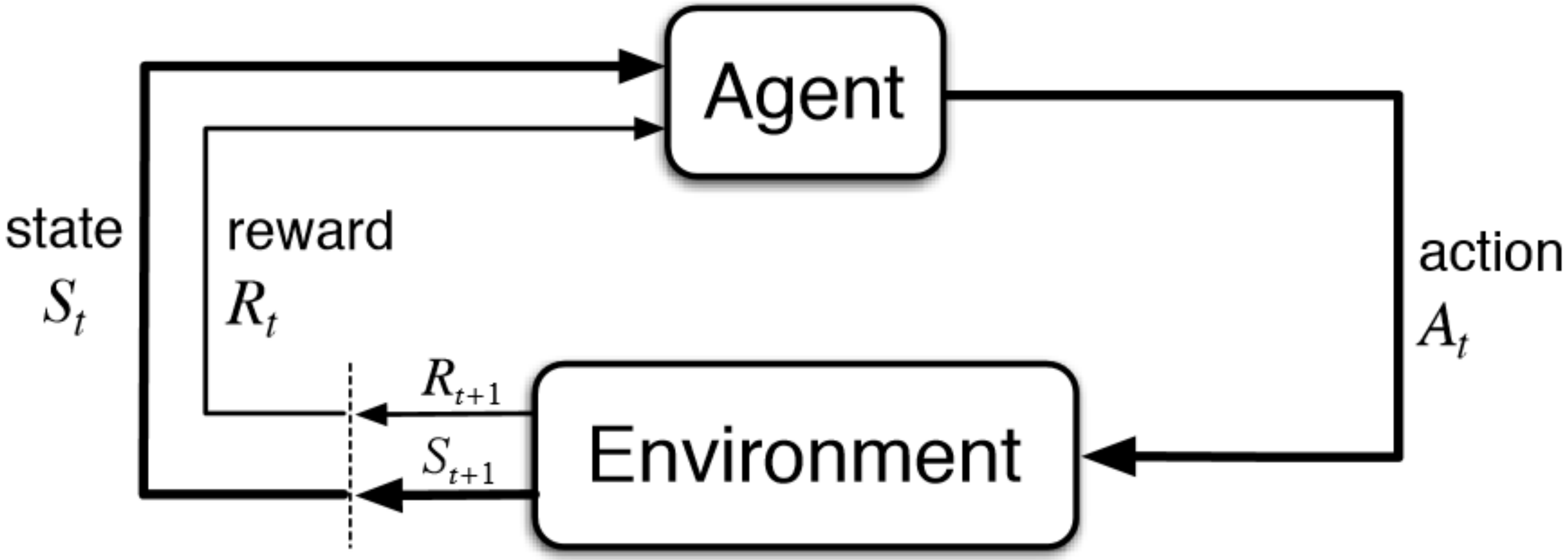
Advantages: No curse of dimensionality in approximation

- 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 $s < k$

- **Theorem** (Liang and Yang, 2022) Suppose the function space $\mathbb{S}_k$ is generated with operators including $''+'', ''-'', ''\times'', ''/'', ''max\{0,x\}'', ''sin(x)'', ''2^x''$. Let $p \in [1, +\infty)$, for any f in the Holder function class $\mathscr{H}_\mu^\alpha([0,1]^d)$ and $\epsilon > 0$, there exists a k-finite expression $\phi \in \mathbb{S}_k$ such that $\|f - \phi\|_{L^p} \le \epsilon$, if $k \ge \mathcal{O}(d^2(\log d + \log \frac{1}{\epsilon})^2)$.

- Q: How to numerically identify such finite expression?
- A: Combinatorial optimization.

Reinforcement Learning for Combinatorial Optimization



By Richard S. Sutton and Andrew G. Barto.

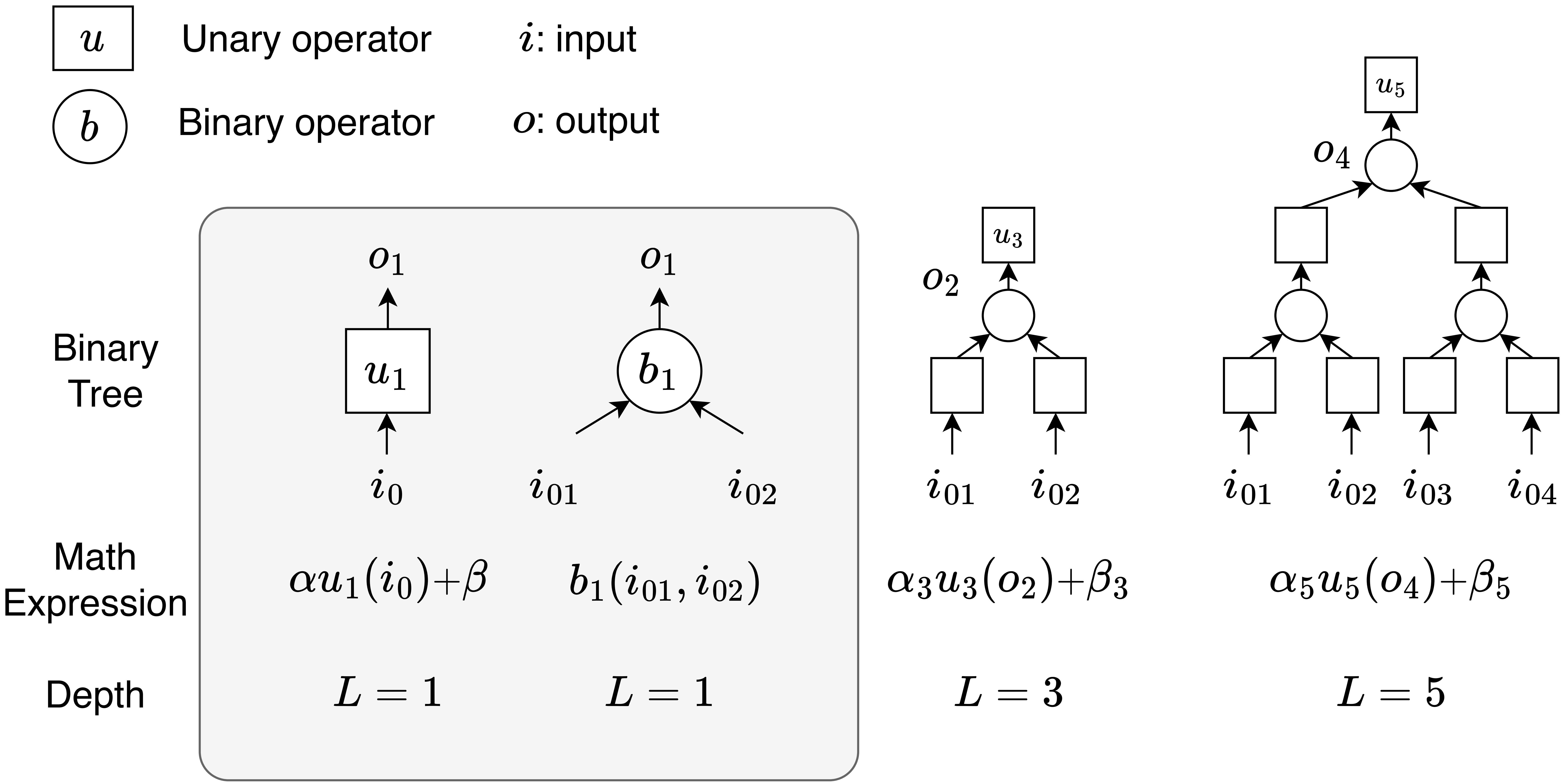
- Goal: Apply RL to implement the combinatorial optimization to find the expression

Selection → Action → Operators sampled from policy network

Realization → State → Mathematical expression

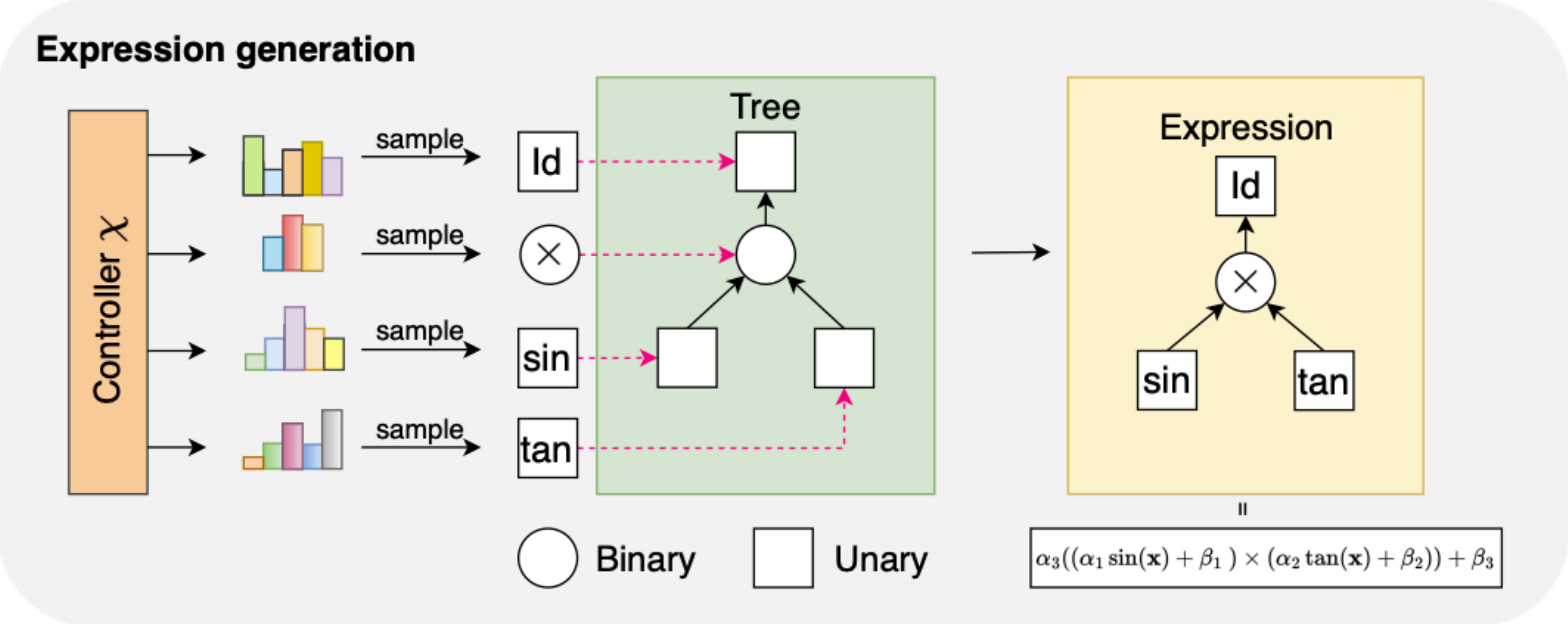
Evaluation → Reward → **PDE regression quality**

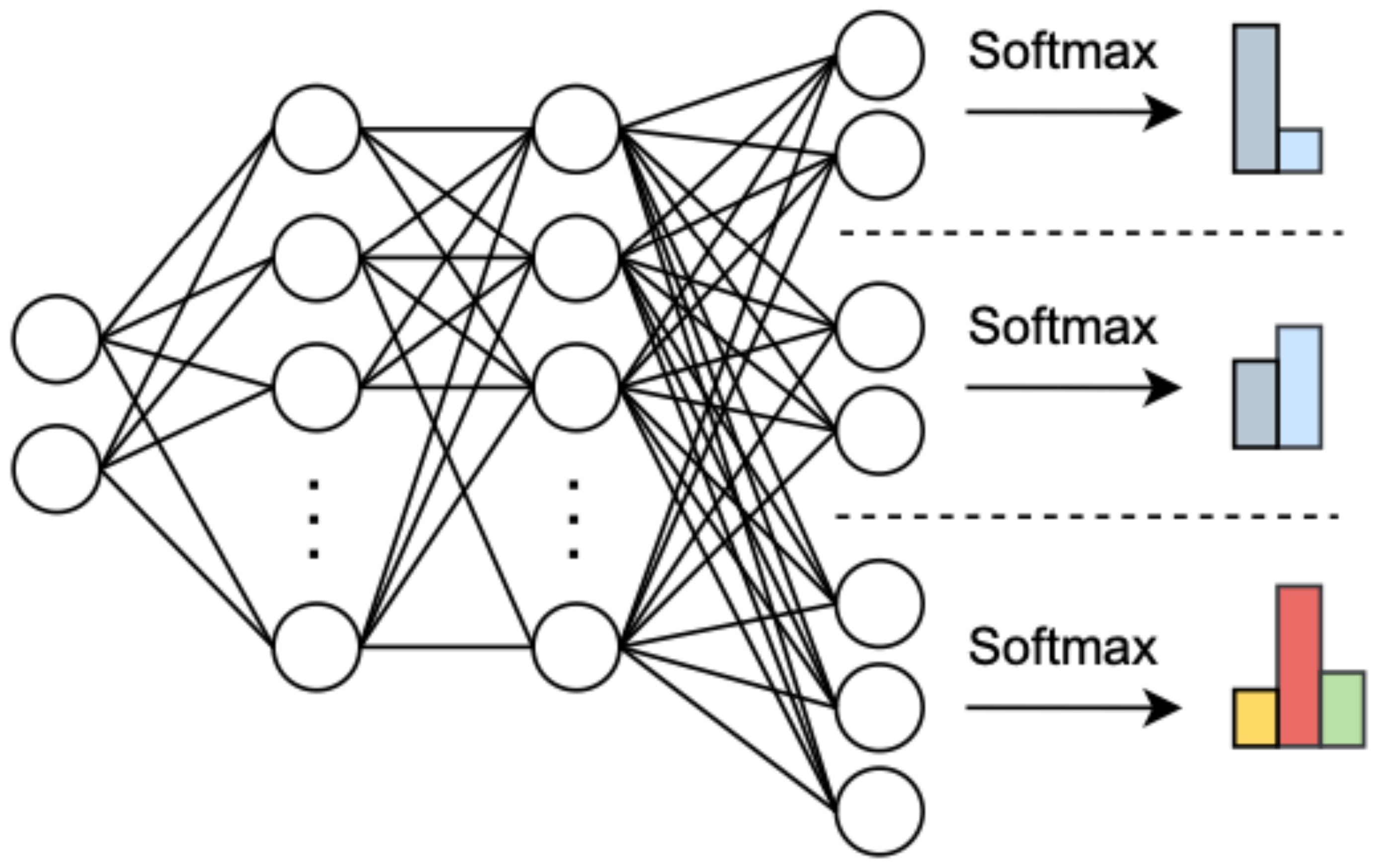
FEX Expression Tree



Pre-order traversal of the tree generates a finite expression, e.g., $\exp(\cos(3x_1)) + x_2$.

FEX: A generative model for math expression





NN Controller (policy) χ

Training Objective: $\mathcal{J}(\Phi) := \mathbb{E}_{\mathbf{e}\sim\chi_\Phi} S(\mathbf{e})$. ← Reward

$$\nabla_\Phi \mathcal{J}(\Phi) = \mathbb{E}_{\mathbf{e}\sim\chi_\Phi} \left\{ S(\mathbf{e}) \sum_{i=1}^{s} \nabla_\Phi \log \left(\mathbf{p}_\Phi^i(e_i)\right) \right\}$$

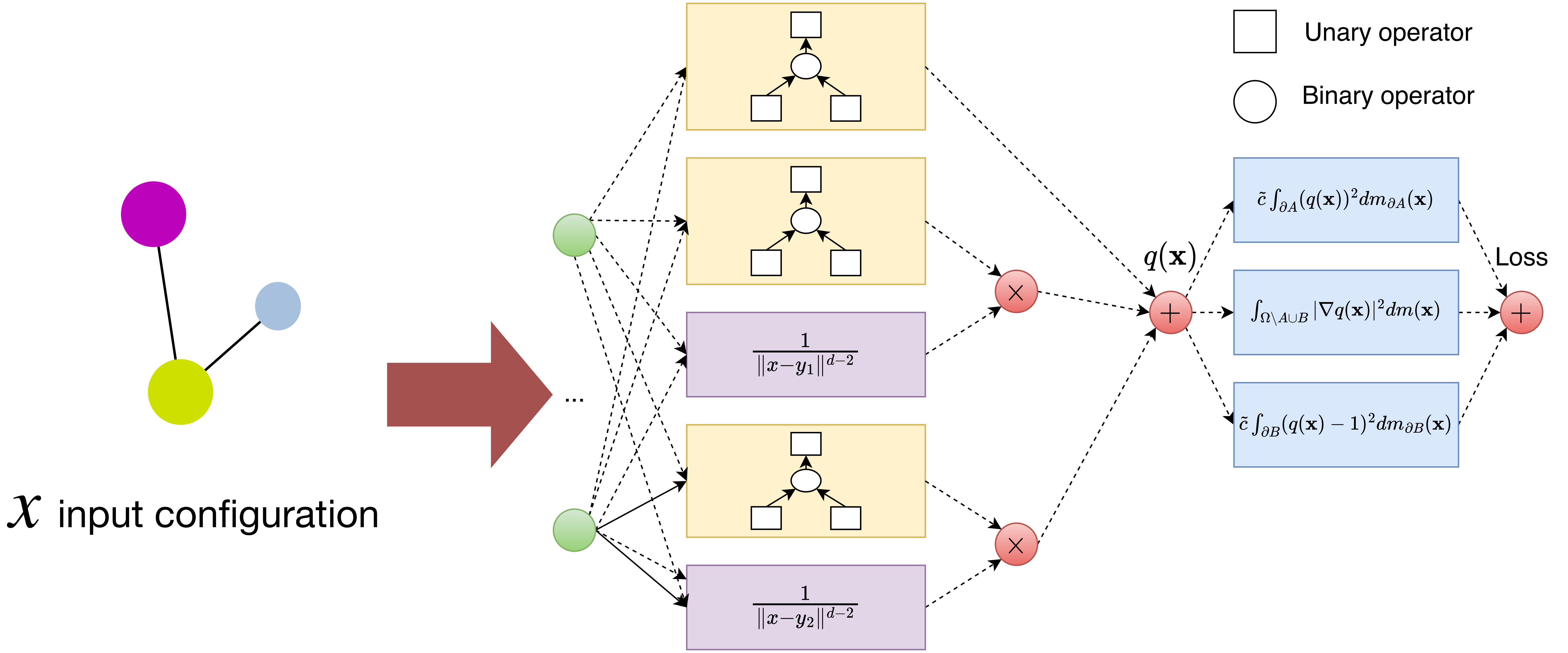
Parameterization of committer by FEX

Variational formulation:

$$C(q) = \int_{\Omega_{AB}} \| \nabla q(\mathbf{x}) \|^2 d\rho(\mathbf{x}) + \tilde{c}\left(\int_{\partial A} q(\mathbf{x})^2 dm_{\partial A}(\mathbf{x}) + \int_{\partial B} \left(q(\mathbf{x}) - 1\right)^2 dm_{\partial B}(\mathbf{x}) \right)$$

and parameterize $q(\mathbf{x})$ with FEX binary trees.

with $d\rho(\mathbf{x}) = \mathbf{Z}^{-1} \exp^{-\beta \mathbf{V}(\mathbf{x})} \mathbf{dx}$



Example 1: Double-Well Potential

Consider the potential

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

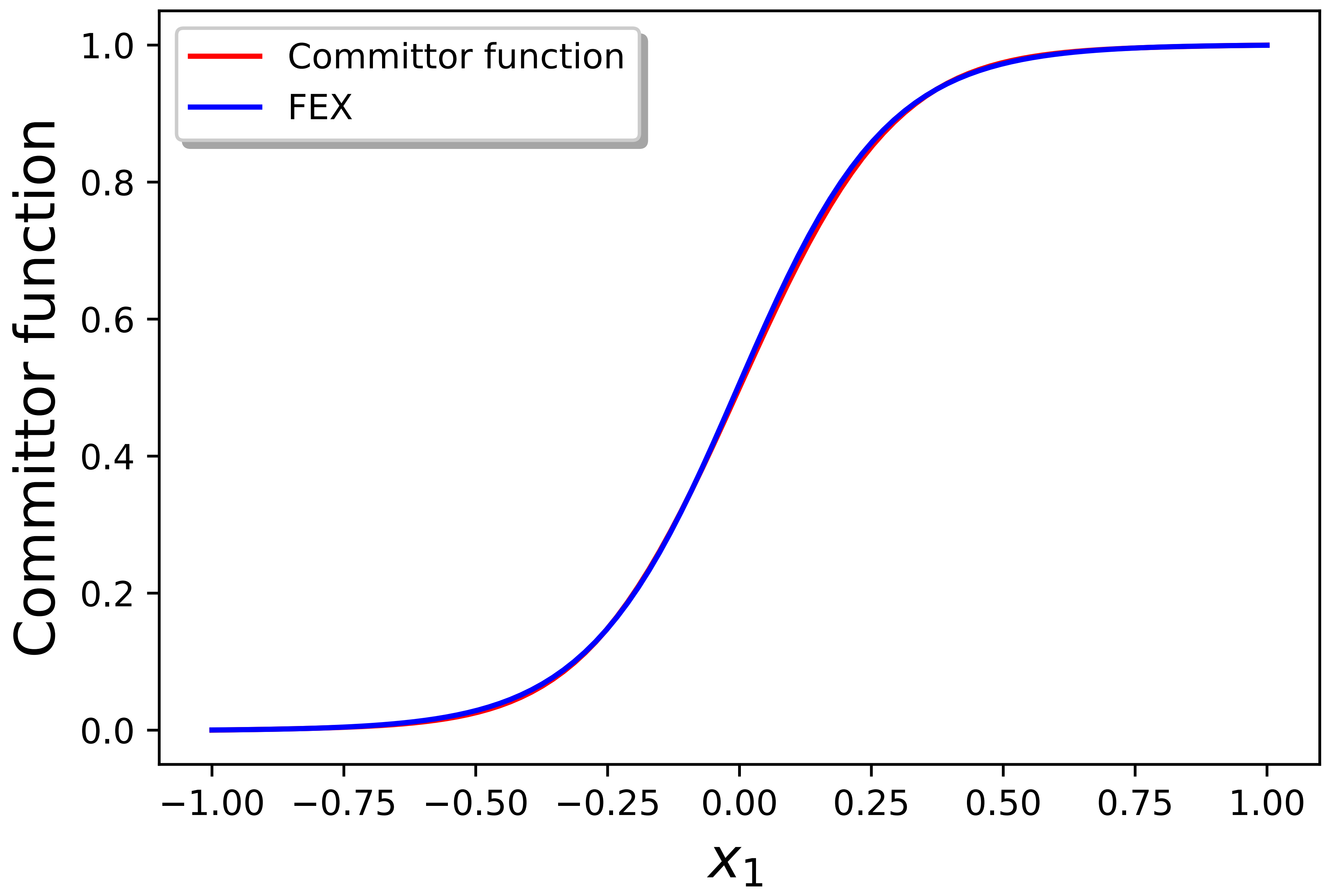
with

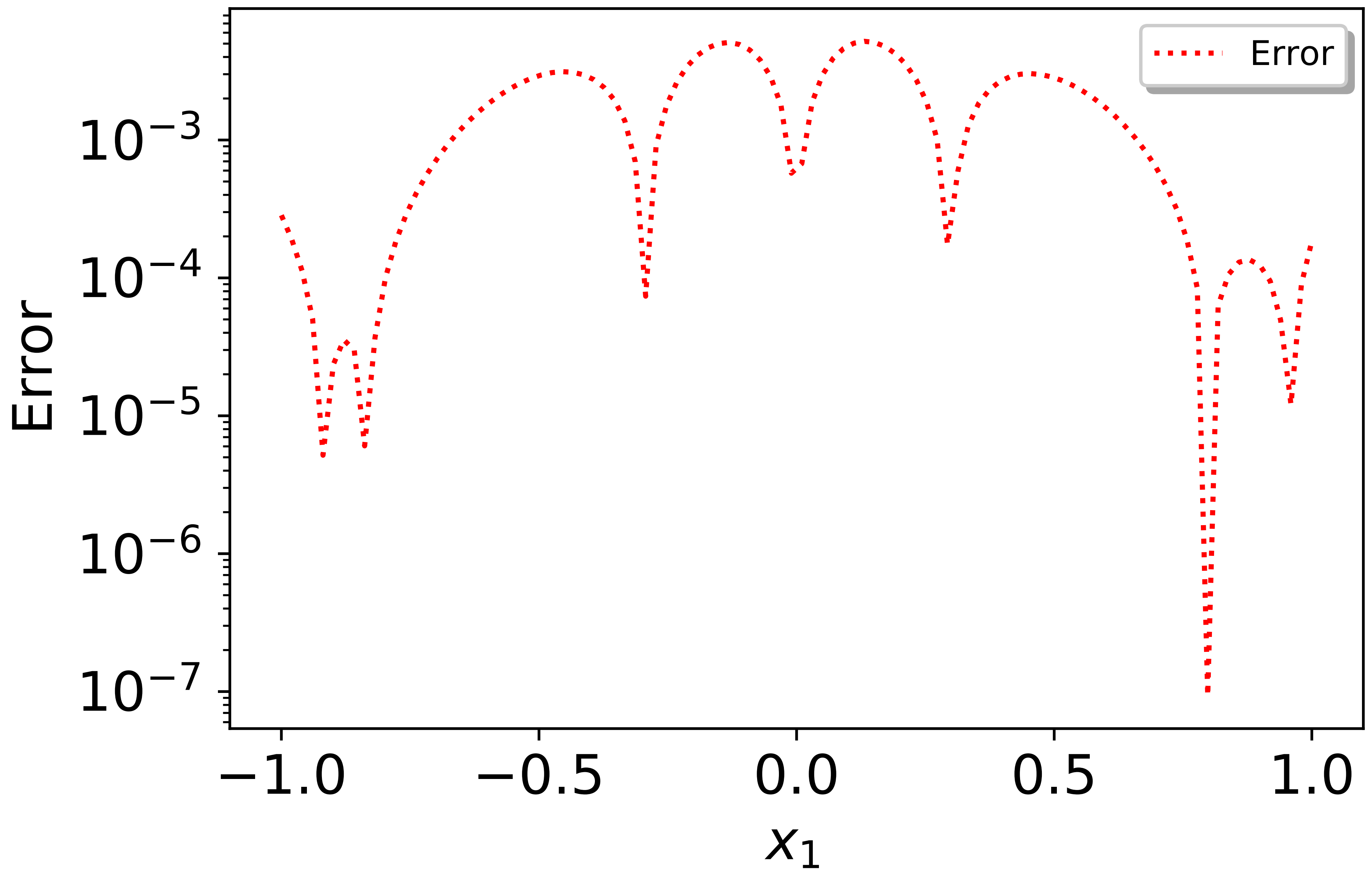
$$A = \left\{x \in \mathbb{R}^d \mid x_1 \le -1\right\}, \quad B = \left\{x \in \mathbb{R}^d \mid x_1 \ge 1\right\}$$

The ground truth solution is $q(\mathbf{x}) = f(x_1)$

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

Example 1: Double-Well Potential





Example 1: Double-Well Potential

FEX identifies the following representation

leaf 1: Id $\rightarrow \alpha_{1,1}x_1 + \ldots + \alpha_{1,10}x_{10} + \beta_1$

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

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

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

node	α_1	α_2	α_3	α_4	α_5	α_6	α_7	α_8	α_9	α_{10}	β
leaf 1: Id	**1.6798**	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
leaf 2: `tanh`	**1.9039**	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Therefore, we can use spectral method to solve the ODE to achieve spectral accuracy.

Example 2: Concentric Spheres

Consider the potential

$$V(\mathbf{x}) = 10\,|\,\mathbf{x}\,|^2$$

with

$$A = \left\{x \in \mathbb{R}^d \mid \mathbf{x} \geq a\right\}, \quad B = \left\{x \in \mathbb{R}^d \mid \mathbf{x} \leq b\right\} \qquad \text{where } d = 6, \quad a = 1, \quad b = 0.25$$

The ground truth solution is $q(\mathbf{x}) = q(r)$, where $r^2 = \sum_{i=1}^{d} x_i^2$

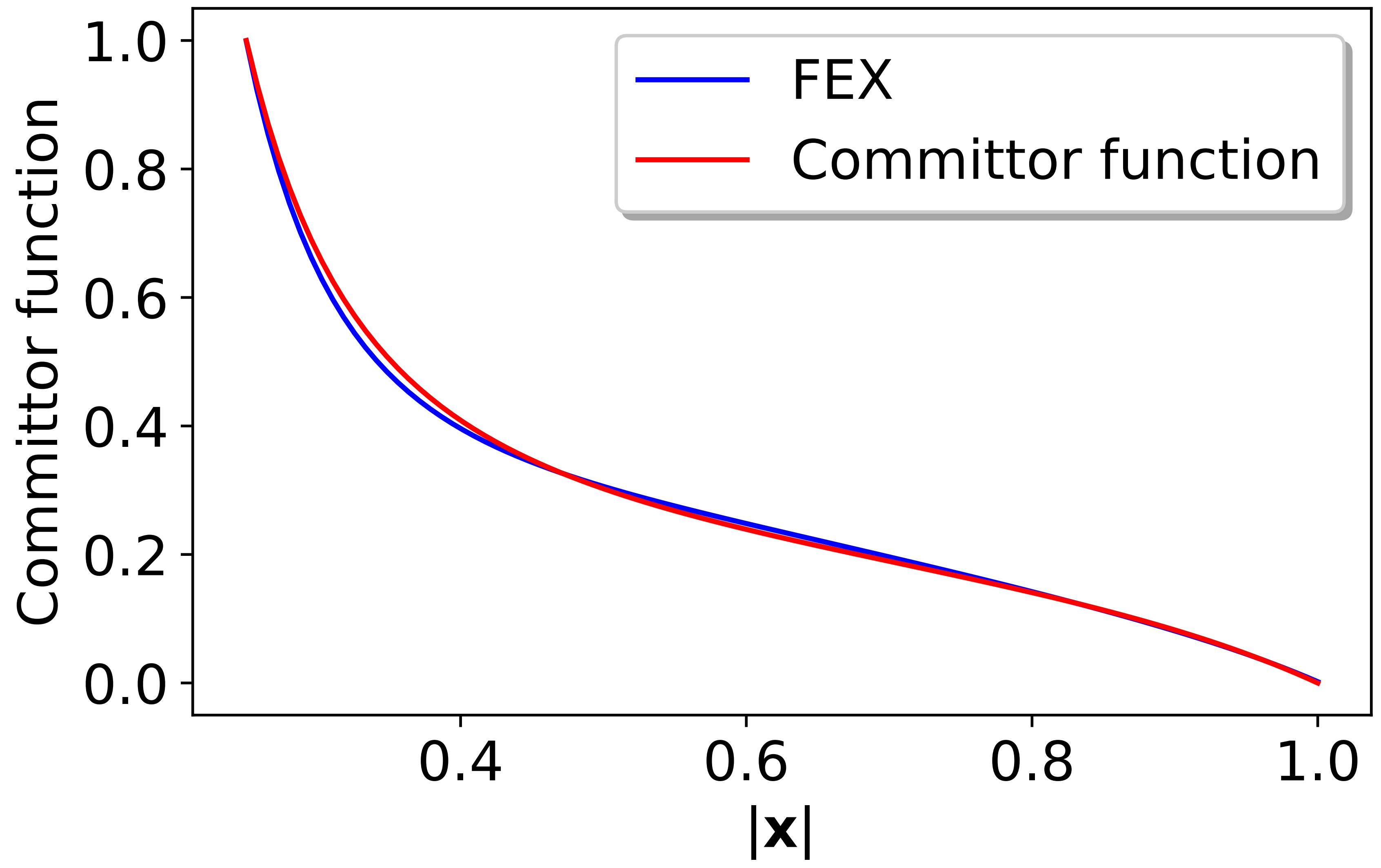
$$\frac{d^2q(r)}{dr^2} + \frac{d-1}{r}\frac{dq(r)}{dr} - \beta\frac{dq}{dr}\frac{dV}{dr} = 0$$

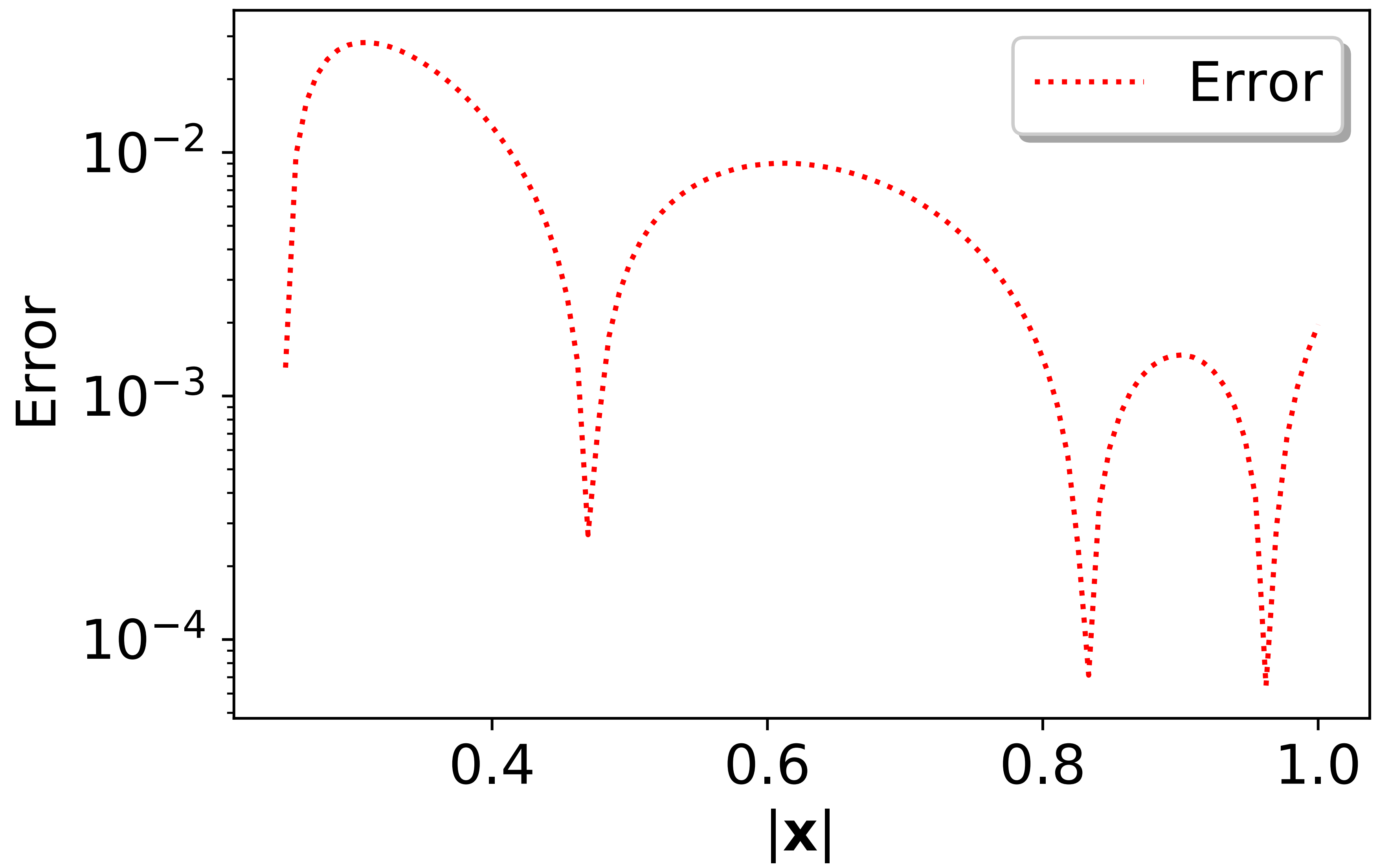
$$q(r)\Big|_{r=a} = 0, \quad q(r)\Big|_{r=b} = 1$$

Example 2: Concentric Spheres

FEX identifies the following representation

$$q(r) := \frac{0.0020}{r^{0.5d-1}} + 0.6016\left(0.6054 - 0.5800r^2\right) - 0.0340$$





Again, we can use spectral method to solve the ODE to achieve spectral accuracy.

Example 3: Rugged-Mueller's Potential

Consider the committer corresponding to the following potential:

$$V(\mathbf{x}) = \underbrace{\tilde{V}\left(x_1, x_2\right)}_{\text{collective variables}} + \frac{1}{2\sigma^2}\sum_{i=3}^{10} x_i^2$$

where

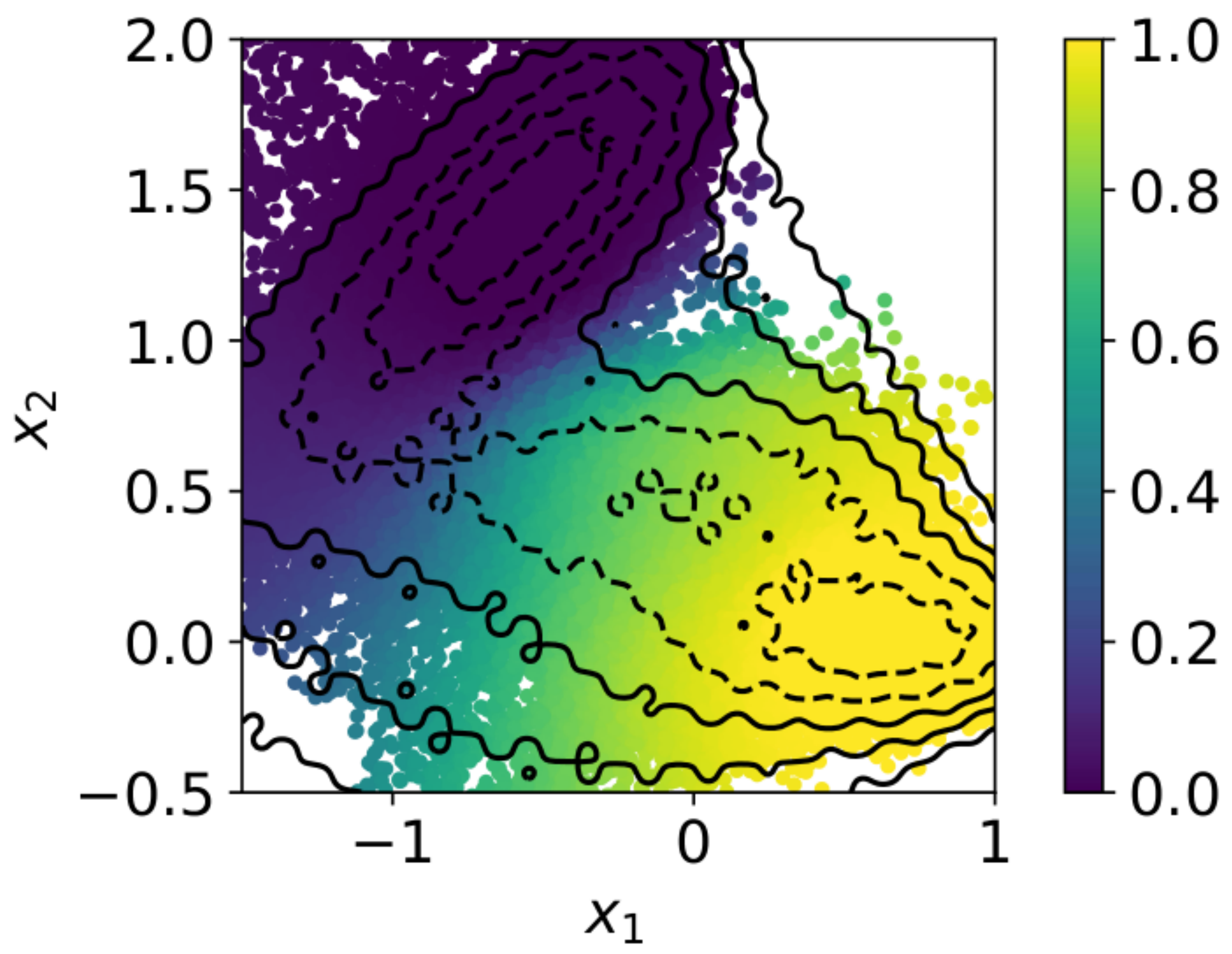
$$\tilde{V}\left(x_1, x_2\right) = \sum_{i=1}^{4} D_i e^{a_i\left(x_1 - X_i\right)^2 + b_i\left(x_1 - X_i\right)\left(x_2 - Y_i\right) + c_i\left(x_2 - Y_i\right)^2} + \gamma \sin\left(2k\pi x_1\right)\sin\left(2k\pi x_2\right)$$

The domain of interest $\Omega : [-1.5,1] \times [-0.5,2] \times \mathbb{R}^8$, and

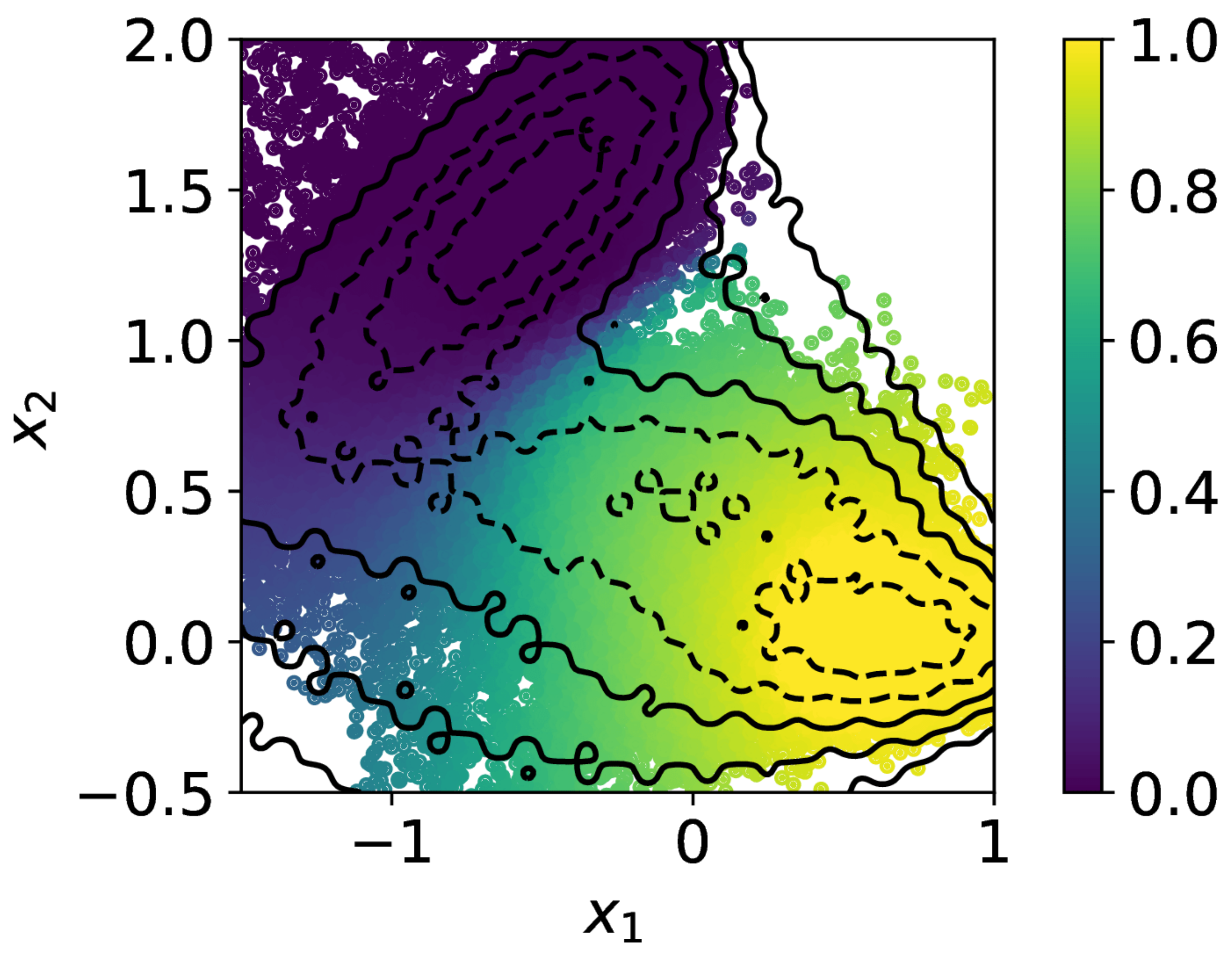
$$A = \left\{\mathbf{x} \in \mathbb{R}^{10} \mid \sqrt{\left(x_1 + 0.57\right)^2 + \left(x_2 - 1.43\right)^2} \leq 0.3\right\}$$

$$B = \left\{\mathbf{x} \in \mathbb{R}^{10} \mid \sqrt{\left(x_1 - 0.56\right)^2 + \left(x_2 - 0.044\right)^2} \leq 0.3\right\}$$

Example 3: Rugged-Mueller's Potential



(a) T = 22 committer (FEM)



(b) T = 22 committer (FEX)

Example 3: Rugged-Mueller's Potential

leaf 1: $(\cdot)^4 \rightarrow \alpha_{1_1} x_1^4 + \ldots + \alpha_{1_{10}} x_{10}^4 + \beta_1$

leaf 2: $(\cdot)^4 \rightarrow \alpha_{2_1} x_1^4 + \ldots + \alpha_{2_{10}} x_{10}^4 + \beta_2$

leaf 3: $(\cdot)^4 \rightarrow \alpha_{3_1} x_1^4 + \ldots + \alpha_{3_{10}} x_{10}^4 + \beta_3$

leaf 4: $(\cdot)^2 \rightarrow \alpha_{4_1} x_1^2 + \ldots + \alpha_{4_{10}} x_{10}^2 + \beta_4,$

$$\mathcal{J}_1(\mathbf{x}) = \alpha_7 \tanh((\alpha_5 \cos(\text{leaf 1} \times \text{leaf 2}) + \beta_5) - (\alpha_6 \text{sigmoid}(\text{leaf 3} \times \text{leaf 4}) + \beta_6)) + \beta_7$$

Furthermore, FEX identifies the low-dimensional structure of the problem

node	α_1	α_2	α_3	α_4	α_5	α_6	α_7	α_8	α_9	α_{10}	β
leaf 1: $(\cdot)^4$	**0.0893**	**−0.0217**	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.9460
leaf 2: $(\cdot)^4$	**−0.0660**	**0.2018**	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.8938
leaf 3: $(\cdot)^4$	**−0.4211**	**0.1263**	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	−3.3150
leaf 4: $(\cdot)^2$	**0.9242**	**1.1818**	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	−1.6088

- FEX is a new methodology to solve high-dimensional committers (PDEs), demonstrating higher or comparable accuracy than the neural network method (PINN).
- FEX can identify the low-dimensional structure inherent in the problem.
- Once FEX successfully identifies the low-dimensional structure, we can achieve arbitrary accuracy by solving the reduced low-dimensional problem with classical methods, e.g. finite element method.

Thank you!

Link to paper

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