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

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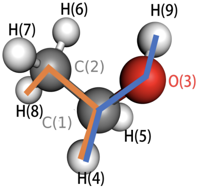
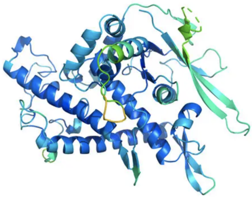
Rare Transitions in Molecular Dynamics

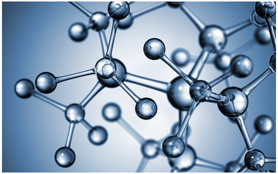
Examples:



(a) Chemical Reaction



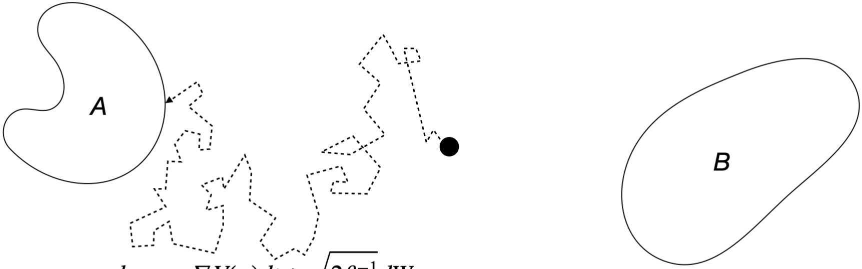
(b) Protein Folding



(c) Material Science

Phenomena: Long residence times in stable states, quick transitions between stable states

Problem Setting



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

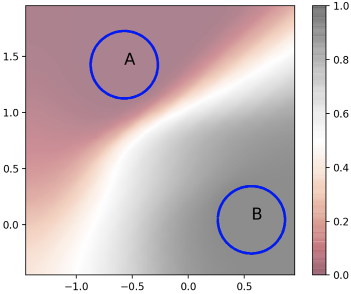
where

- $\mathbf{x}_t \in \Omega \subset \mathbb{R}^d$ 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 T,
- $\mathbf{w}_t$ is the standard d-dimensional Brownian motion.

We are interested in

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

Committor Function as a PDE Solution



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

$$\begin{aligned} &\beta^{-1}\Delta q - \nabla V \cdot \nabla q = 0, \quad \mathbf{x} \in \Omega_{AB} := \Omega \backslash (\bar{A} \cup \bar{B}), \\ &q(\mathbf{x})|_{\partial A} = 0, \quad q(\mathbf{x})|_{\partial B} = 1. \end{aligned} \tag{1}$$

Lessen Curse of Dimensionality with FEX

The major difficulty in solving (1) is the curse of dimensionality.

Example: configuration spaces of dimension $\propto$ number of atoms.

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

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

The Solution Model for the Committor Problem

- We minimize the variational formulation $\int_{\Omega_{AB}} \|\nabla q(\mathbf{x})\|^2 \rho(d\mathbf{x}) + \tilde{c}(\int_{\partial A} q(\mathbf{x})^2 dm_{\partial A}(\mathbf{x}) + \int_{\partial B} (q(\mathbf{x})-1)^2 dm_{\partial B}(\mathbf{x}))$.

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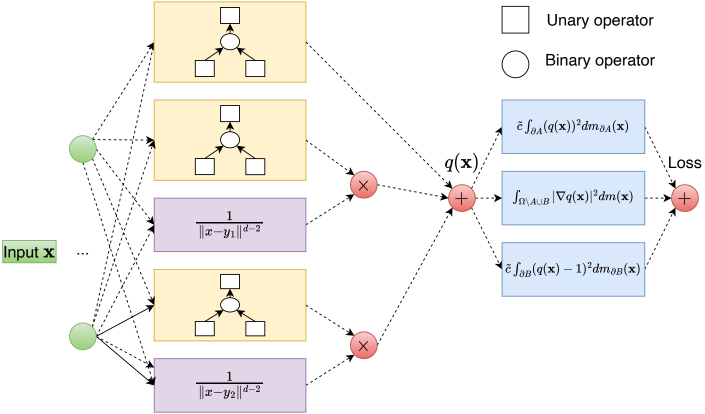
- We model the committor $q(\mathbf{x})$ as FEX binary trees



Double-Well Potential

Consider the potential

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

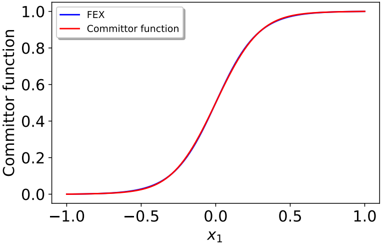
with

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

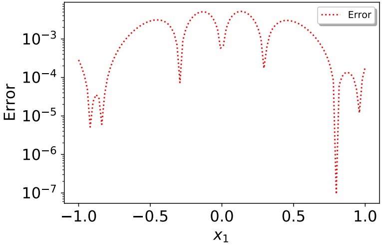
The ground truth solution is $q(\mathbf{x}) = f(x_1)$,

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

Numerical Results



(a) Committor function and FEX



(b) Error of FEX

Figure: The committor function for the double-well potential along x_1 dimension when $\beta^{-1} = 0.2$ for an arbitrary $(x_2, \cdots, x_d)$ with $d = 10$.

Identification of Low-Dimensional Structure by FEX

FEX identifies the following expression

$$\begin{aligned}
&\text{leaf 1: } \texttt{Id} \to \alpha_{1,1}x_1 + \ldots + \alpha_{1,10}x_{10} + \beta_1 \\
&\text{leaf 2: } \texttt{tanh} \to \alpha_{2,1}\tanh(x_1) + \ldots + \alpha_{2,10}\tanh(x_{10}) + \beta_2 \\
&\mathcal{J}(\mathbf{x}) = \alpha_3 \tanh(\text{leaf 1} + \text{leaf 2}) + \beta_3,
\end{aligned}$$

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

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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	$\mathbf{1.6798}$	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
leaf 2: `tanh`	$\mathbf{1.9039}$	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 (2) to achieve spectral accuracy.

Rugged-Mueller's Potential

Consider the committor function corresponding to the following rugged-Mueller's 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

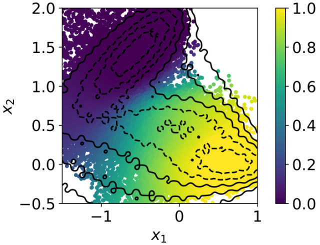
$$\tilde{V}\left(x_1, x_2\right) = \sum_{i=1}^{4} D_i e^{a_i(x_1-X_i)^2+b_i(x_1-X_i)(x_2-Y_i)+c_i(x_2-Y_i)^2} + \gamma\sin\left(2k\pi x_1\right)\sin\left(2k\pi x_2\right)$$

The domain of interest Ω is $[-1.5, 1] \times [-0.5, 2] \times \mathbb{R}^8$ and the regions A and B are two cylinders:

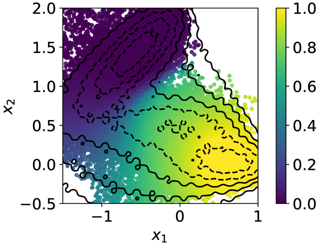
$$A = \left\{\mathbf{x} \in \mathbb{R}^{10} \mid \sqrt{\left(x_1 + 0.57\right)^2 + \left(x_2 - 1.43\right)^2} \leq 0.3\right\}$$

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

Numerical Results



(a) $T = 22$ committor function (FEM)



(b) $T = 22$ committor function (FEX)

T	Method	E	$\tilde{c}$	No. of samples in Ω_{AB}	No. of testing samples
22	NN	3.70×10^{-2}	1.3×10^2	1.0×10^5	1.5×10^5
22	FEX	2.90×10^{-2}	1.3×10^2	1.0×10^5	1.5×10^5

Identification of Low-Dimensional Structure by FEX

The FEX formula for $\mathcal{J}_1$ is

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

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

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

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

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

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Furthurmore, FEX can identify 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: $(\cdot)^4$	$\mathbf{0.0893}$	$\mathbf{-0.0217}$	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.9460
leaf 2: $(\cdot)^4$	$\mathbf{-0.0660}$	$\mathbf{0.2018}$	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.8938
leaf 3: $(\cdot)^4$	$\mathbf{-0.4211}$	$\mathbf{0.1263}$	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-3.3150
leaf 4: $(\cdot)^2$	$\mathbf{0.9242}$	$\mathbf{1.1818}$	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-1.6088

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- 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 (1) with the finite element method.

Thank you!

https://arxiv.org/pdf/2306.12268.pdf