iterated Denoising Energy Matching

for sampling from Boltzmann densities

Tara Akhound-Sadegh et al

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Chivintar Amenty, June 2025

Introduction

$$\mu_{\text{target}}(x) = \frac{\exp\left(-\mathcal{E}(x)\right)}{\mathcal{Z}}, \; \mathcal{Z} = \int_{\mathbb{R}^d} \exp\left(-\mathcal{E}(x)\right) dx.$$

- Boltzmann Probability Density
- Partition function Z: intractable
- Goal: sample from distribution μ only having access to Boltzmann energy

Motivation

$$\mu_{\text{target}}(x) = \frac{\exp\left(-\mathcal{E}(x)\right)}{\mathcal{Z}}, \ \mathcal{Z} = \int_{\mathbb{R}^d} \exp\left(-\mathcal{E}(x)\right) dx.$$

- Statistical Physics
- Molecular Dynamics
- Protein Modeling
- Material Science
- Bayesian Inference in Astrophysics, Quantum Chromo-Dynamics and *many* more . . .

Related Work

$$\mu_{\text{target}}(x) = \frac{\exp\left(-\mathcal{E}(x)\right)}{\mathcal{Z}}, \ \mathcal{Z} = \int_{\mathbb{R}^d} \exp\left(-\mathcal{E}(x)\right) dx.$$

- MC techniques: AIS, SMC
  - Computationally expensive
  - Slow convergence in HD spaces
- Simulation techniques
  - Scalability issues
- Diffusion Models
  - Need training data

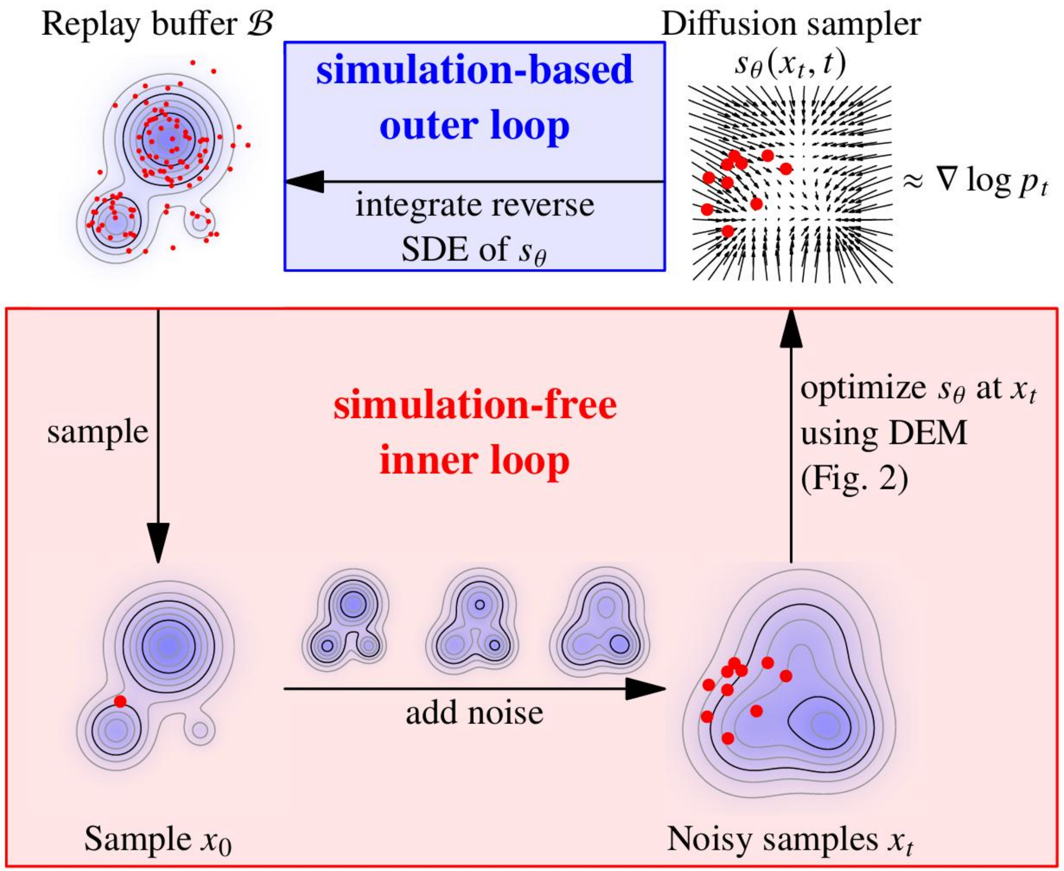
iDEM

iDEM introduction

- Neural sampler
- Diffusion-style
- Simulation-free (in inner loop)
- Computationally tractable
- Stochastic regression objective

- Diffusion sampled data

- Good coverage of all modes
- Imbues symmetries (SE(3) group)



iDEM introduction

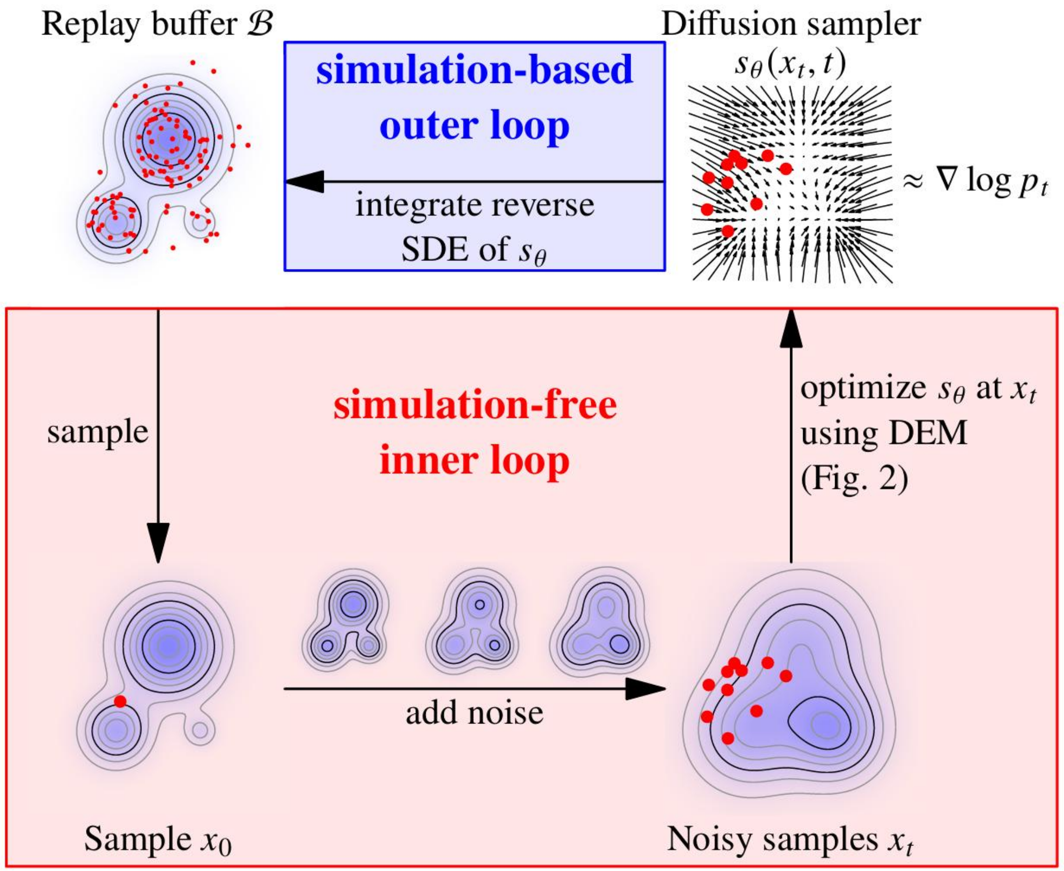
Bi-Level algorithm

Inner loop

- Optimizes score function
  1. How, when we do not have samples from the distribution?

Outer loop

- Reverse SDE of score function
- Actual samples are generated
  2. Where to get good samples?

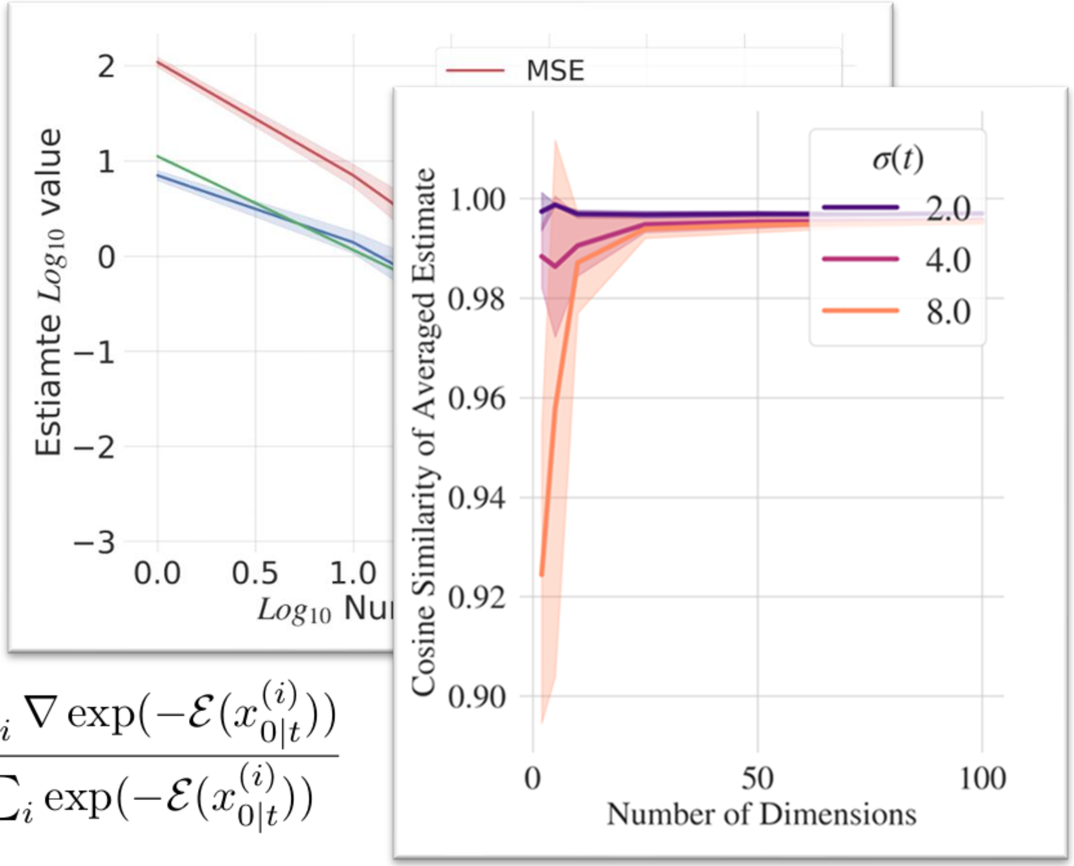


C1 – Inner Loop

$$\nabla \log p_t(x_t) = \frac{((\nabla p_0) * \mathcal{N}(0, \sigma_t^2))(x_t)}{p_t(x_t)}$$

$$= \frac{\mathbb{E}_{x_{0|t} \sim \mathcal{N}(x_t, \sigma_t^2)}[\nabla p_0(x_{0|t})]}{\mathbb{E}_{x_{0|t} \sim \mathcal{N}(x_t, \sigma_t^2)}[p_0(x_{0|t})]}$$

$$= \frac{\mathbb{E}_{x_{0|t} \sim \mathcal{N}(x_t, \sigma_t^2)}[\nabla \exp(-\mathcal{E}(x_{0|t}))]}{\mathbb{E}_{x_{0|t} \sim \mathcal{N}(x_t, \sigma_t^2)}[\exp(-\mathcal{E}(x_{0|t}))]}, \quad \approx \frac{\frac{1}{K}\sum_i \nabla \exp(-\mathcal{E}(x_{0|t}^{(i)}))}{\frac{1}{K}\sum_i \exp(-\mathcal{E}(x_{0|t}^{(i)}))}$$



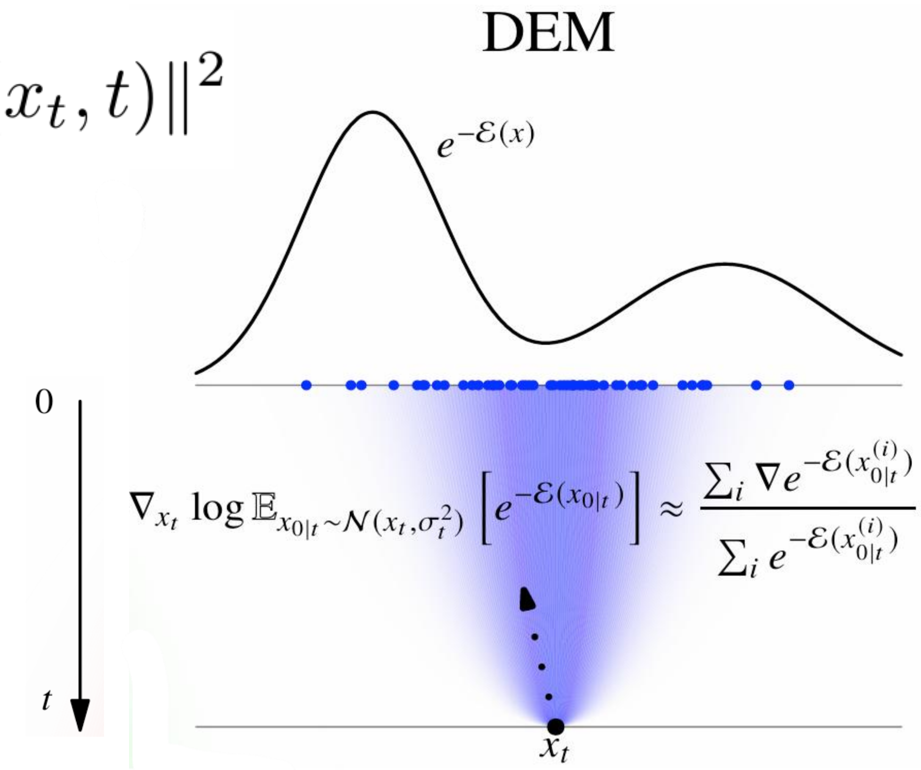
$= \mathcal{S}_K(x_t, t)$

$$x_{0|t}^{(1)}, \ldots, x_{0|t}^{(K)} \sim \mathcal{N}(x_t, \sigma_t^2)$$

C1 – Inner Loop

$$\mathcal{S}_K(x_t, t) \Leftarrow s_\theta(x_t, t)$$

$$\mathcal{L}_{\mathrm{DEM}}(x_t, t) := \|\mathcal{S}_K(x_t, t) - s_\theta(x_t, t)\|^2$$



inner loop summary:

- Estimate the smoothed score function using noisy samples
- Train a neural network with DEM loss
- Use network in outer loop

C2 – Outer Loop

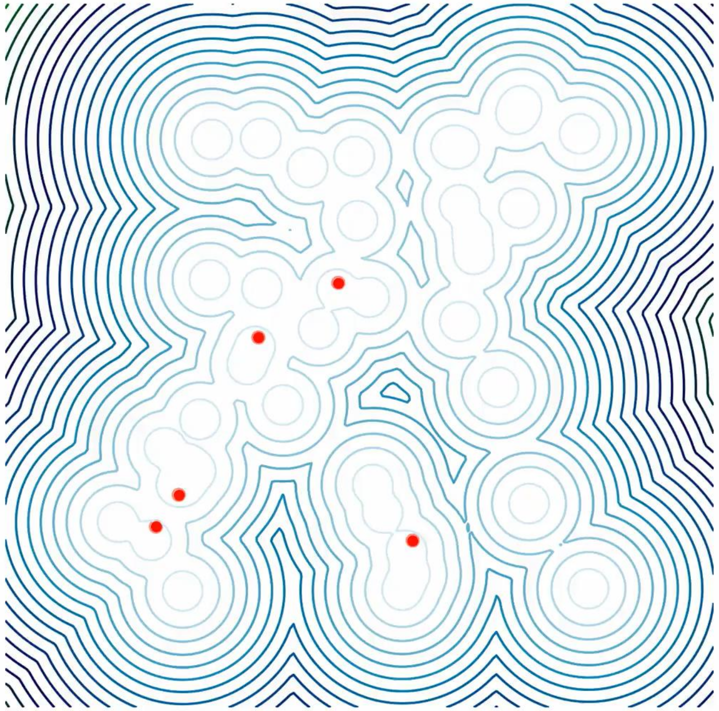
- With $s_\theta(x_t, t)$ frozen:
- Reverse time SDE
- Generate samples
- Store in replay buffer

Algorithm 1 ITERATED DENOISING ENERGY MATCHING

Input: Network s_θ, Batch size b, Noise schedule σ_t^2, Prior p_1, Num. integration steps L, Replay buffer $\mathcal{B}$, Max Buffer Size $|\mathcal{B}|$, Num. MC samples K.

while Outer-Loop **do**
  $\{x_1\}_{i=1}^b \sim p_1(x_1)$
  $\{x_0\}_{i=1}^b \leftarrow \texttt{sde\_int}(\{x_1\}_{i=1}^b, s_\theta, L)$ {Sample}
  $\mathcal{B} = (\mathcal{B} \cup \{x_0\}_{i=1}^b)$ {Update Buffer $\mathcal{B}$}
  while Inner-Loop **do**
    $x_0 \leftarrow \mathcal{B}.\texttt{sample()}$ {Uniform sampling from $\mathcal{B}$}
    $t \sim \mathcal{U}(0,1)$, $x_t \sim \mathcal{N}(x_0, \sigma_t^2)$
    $\mathcal{L}_{\text{DEM}}(x_t, t) = \|\mathcal{S}_K(x_t, t) - s_\theta(x_t, t)\|^2$
    $\theta \leftarrow \texttt{Update}(\theta, \nabla_\theta \mathcal{L}_{\text{DEM}})$
  end while
end while
output s_θ

iDEM algorithm



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end while

output s_θ

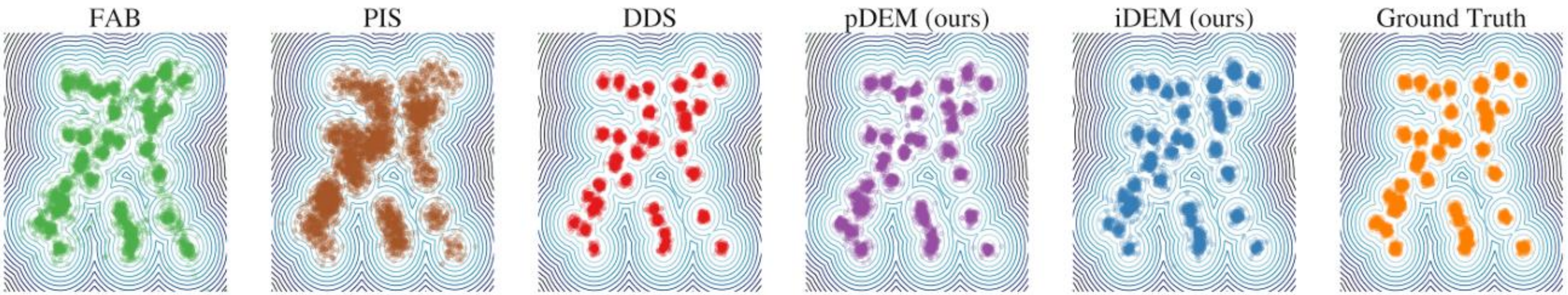
Evaluation on 4 tasks, 5 benchmarks

- 40-mode GMM
- Lennard-Jones 13
- Lennard-Jones 55
- 4-particle double-well potential

- PIS
- DDS
- FAB
- pDEM
- iDEM

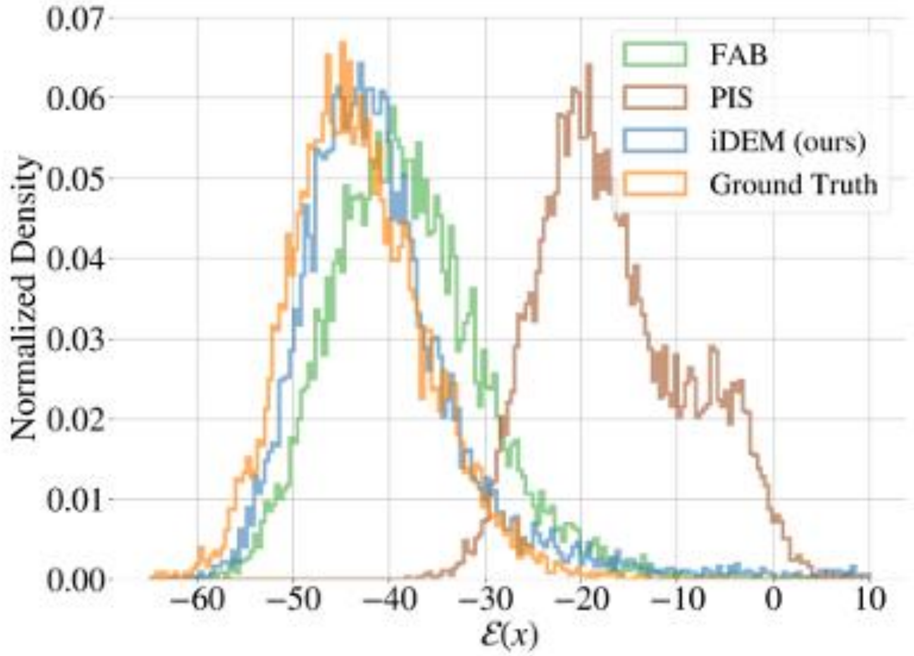
Evaluation on 4 tasks, 5 benchmarks

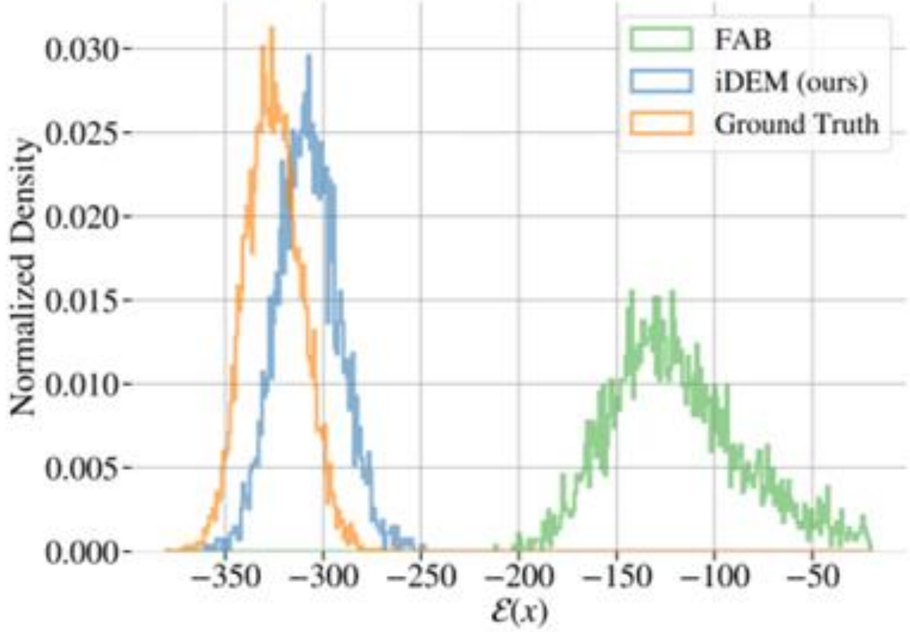
40-mode GMM



Evaluation on 4 tasks, 5 benchmarks

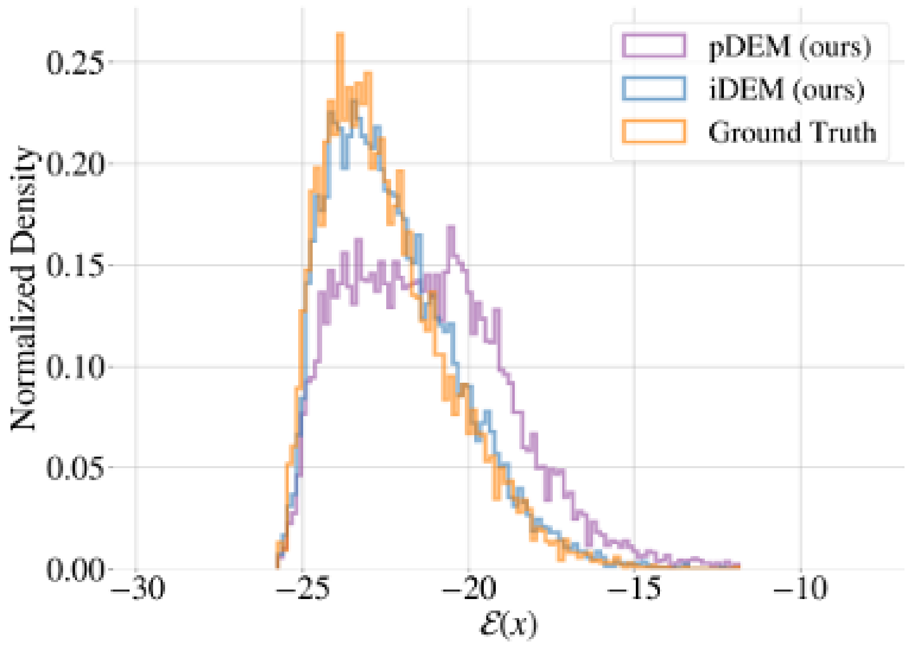
Lennard-Jones 13 , Lennard-Jones 55

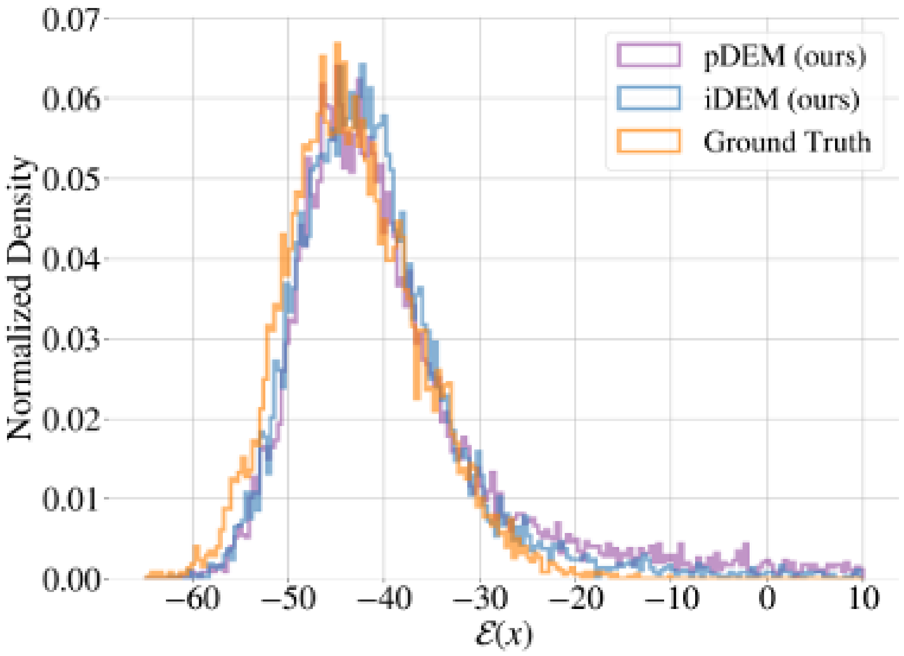




Evaluation on 4 tasks, 5 benchmarks

4-particle double-well potential , LJ-13





Performance Results

- Negative Log Likelihood
- Effective Sample Size
- Wasserstein distance

- Efficient
- High quality samples

Algorithm ↓ Dataset →	GMM	DW-4	LJ-13	LJ-55
FAB (Midgley et al., 2023b)	1.71	6.87	21.78	40.35
PIS (Zhang & Chen, 2022)	4.11	11.29	17.36	*
DDS (Vargas et al., 2023)	1.81	5.65	*	*
pDEM (ours)	0.36	1.40	1.79	*
iDEM (ours)	0.87	4.30	6.55	7.75

Energy →	GMM ($d=2$)			DW-4 ($d=8$)			LJ-13 ($d=39$)			LJ-55 ($d=165$)		
Algorithm ↓	NLL	ESS	$\mathcal{W}_2$	NLL	ESS	$\mathcal{W}_2$	NLL	ESS	$\mathcal{W}_2$	NLL	ESS	$\mathcal{W}_2$
FAB (Midgley et al., 2023b)	$7.14_{\pm 0.01}$	$0.653_{\pm 0.017}$	$12.0_{\pm 5.73}$	$\mathbf{7.16}_{\pm 0.01}$	$\mathbf{0.947}_{\pm 0.007}$	$2.15_{\pm 0.02}$	$\mathbf{17.52}_{\pm 0.17}$	$0.101_{\pm 0.059}$	$4.35_{\pm 0.01}$	$200.32_{\pm 62.3}$	$0.063_{\pm 0.001}$	$18.03_{\pm 1.21}$
PIS (Zhang & Chen, 2022)	$7.72_{\pm 0.03}$	$0.295_{\pm 0.018}$	$\mathbf{7.64}_{\pm 0.92}$	$7.19_{\pm 0.01}$	$0.901_{\pm 0.003}$	$\mathbf{2.13}_{\pm 0.02}$	$47.05_{\pm 12.46}$	$0.004_{\pm 0.002}$	$4.67_{\pm 0.11}$	*	*	*
DDS (Vargas et al., 2023)	$7.43_{\pm 0.46}$	$0.687_{\pm 0.208}$	$9.31_{\pm 0.82}$	$11.27_{\pm 1.24}$	$0.408_{\pm 0.001}$	$2.15_{\pm 0.04}$	*	*	*	*	*	*
pDEM (ours)	$7.10_{\pm 0.02}$	$0.634_{\pm 0.084}$	$12.20_{\pm 0.14}$	$7.44_{\pm 0.05}$	$0.547_{\pm 0.010}$	$\mathbf{2.11}_{\pm 0.03}$	$18.80_{\pm 0.48}$	$0.044_{\pm 0.013}$	$\mathbf{4.21}_{\pm 0.06}$	*	*	*
iDEM (ours)	$\mathbf{6.96}_{\pm 0.07}$	$\mathbf{0.734}_{\pm 0.092}$	$\mathbf{7.42}_{\pm 3.44}$	$\mathbf{7.17}_{\pm 0.00}$	$0.825_{\pm 0.002}$	$\mathbf{2.13}_{\pm 0.04}$	$\mathbf{17.68}_{\pm 0.14}$	$\mathbf{0.231}_{\pm 0.005}$	$\mathbf{4.26}_{\pm 0.03}$	$\mathbf{125.86}_{\pm 18.03}$	$\mathbf{0.106}_{\pm 0.022}$	$\mathbf{16.128}_{\pm 0.071}$

Discussion & Future Work

- Consistent DEM objective
  - can it be biased still?

- reverse SDE: simulation step still
  - can it be replaced by a learned policy? RL-like or GFlowNets inspired methods?

- Molecule's energy is *really* complex (low temperatures, huge variations)
  - maybe flatten a little the energy landscape with more energy?
    - collect samples and then somehow simulate the trained model at lower temperature progressively until we reach the target temperature?

Conclusion & Acknowledgements

paper

code

iDEM strong step forward:

- scalable
- symmetry-aware
- simulation-efficient sampling
- general
- extensible
  - Feynman-Kac Correctors, Schrodinger Bridges, Transition Matching . . .

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