Efficient and Unbiased Sampling of Boltzmann Distributions via Consistency Models

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Background

Diffusion-based Boltzmann generator:
amortized sampling from
$p(x) \propto \exp(-U(x)/kT)$

Limitations:
(1) ODE solver is slow
(2) no tractable model density

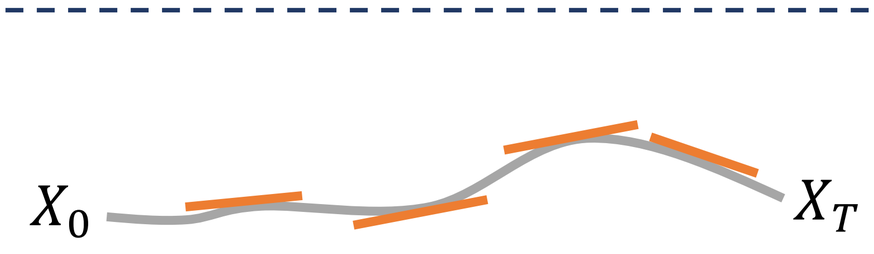
Methods

(1) ODE solver is slow

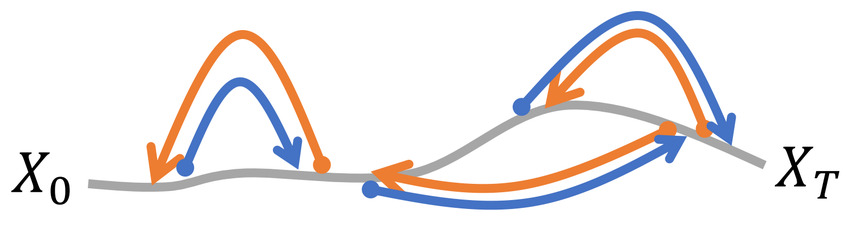
👉 distillation with **Bidirectional consistency trajectory model** (BCTM)

(2) no tractable model density

👉 alternate between ODE and SDE, define **density in the joint space**



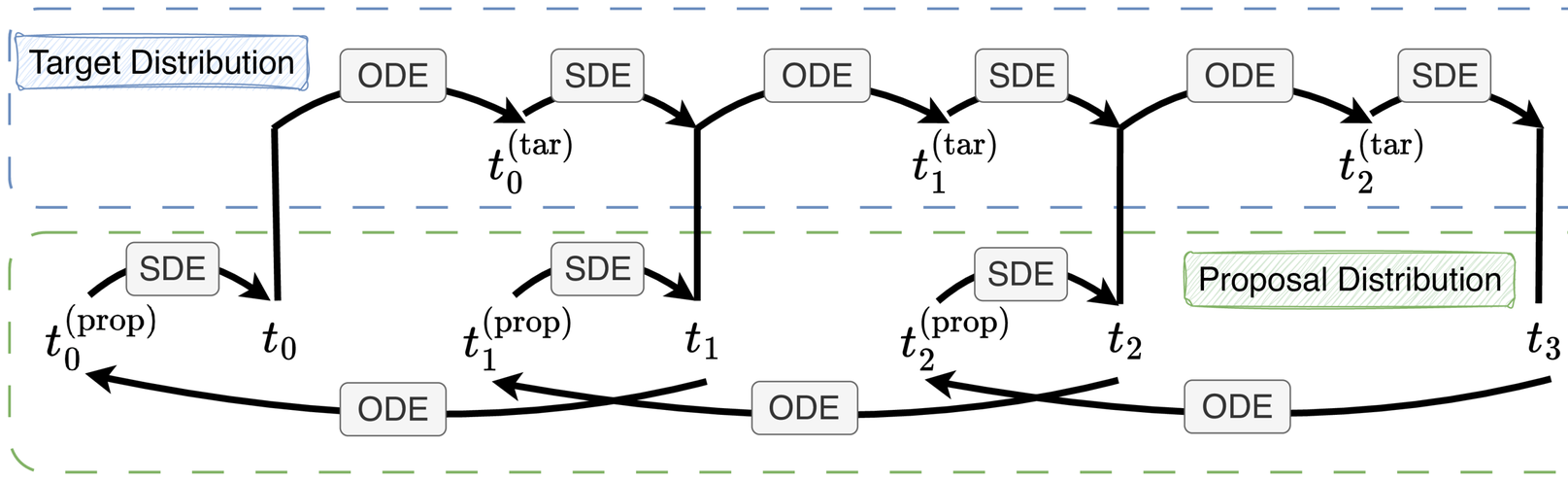
Diffusion estimates **scores** along the PF ODE



BCTM estimates integral of PF ODE
between any two point along any direction

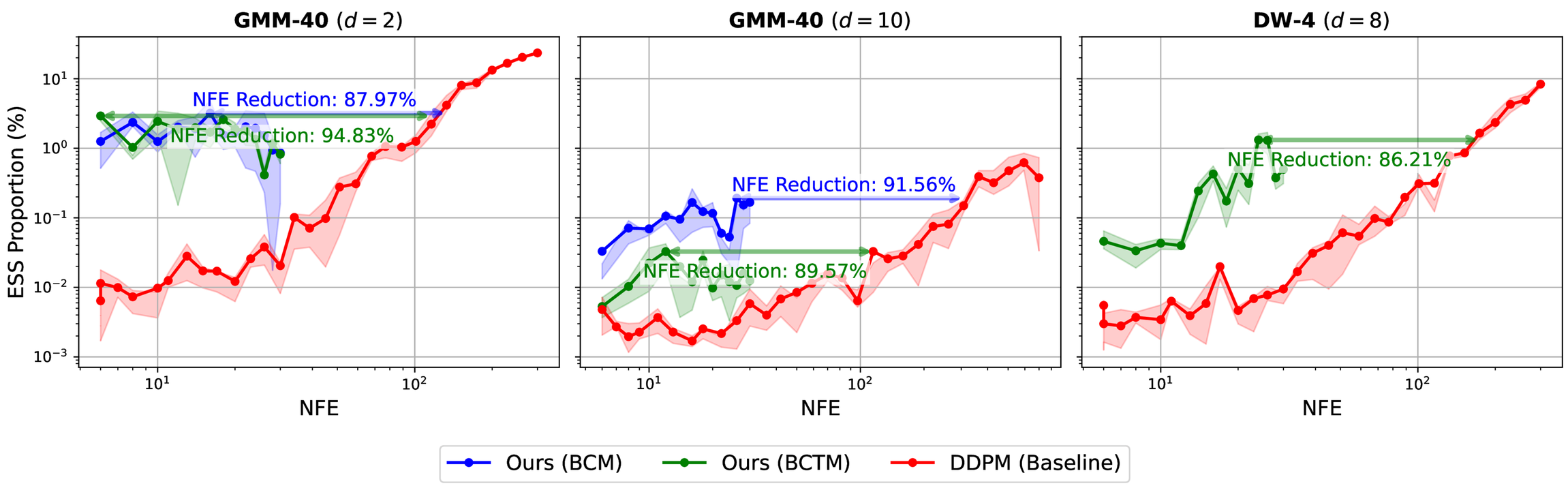
Target from t_n to t_{n+1}:
$\mathcal{N}(\mathrm{BCTM}(t_n \to t_n^{(\mathrm{tar})}), \sigma_n^2)$

Proposal from t_{n+1} to t_n:
$\mathcal{N}(\mathrm{BCTM}(t_{n+1} \to t_n^{(\mathrm{prop})}), \sigma_n'^2)$



Hyperparameters are tuned with forward KL divergence.

Results



Limitations

- Performance plateaus when NFEs exceed 10–20
- Tuning hyperparameters requires great effort in high-dimensional spaces