Diffusion Generative Flow Samplers: Improving Learning Signals Through Partial Trajectory Optimization

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Overview

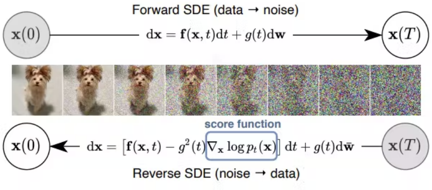
Generative Modeling

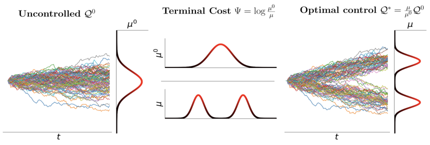
Task

Sample from a complex (high-dimensional and multimodal) distribution D

D can be given under the form of:

- A dataset of samples $\{x_i\}_{i=1}^N \sim D$ (e.g., images, text, audio)
- An unnormalized density $\mu(x)$ where D has density $\pi(x) \propto \mu(x)$ (e.g., energy-based models, physics/chemistry)





Sampling from Unnormalized Densities

Goal. Sample from a D-dimensional target with unnormalized density $\mu(x)$ where $\mathbb{R}^D \to \mathbb{R}^+$.

$$\pi(x) = \frac{\mu(x)}{Z}, \qquad Z = \int_{\mathbb{R}^D} \mu(x)\, dx \text{ (unknown)}.$$

We assume we can evaluate $\mu(x)$, but we have no samples from π and do not know Z.

Context. We seek a *sampler* (similar to MCMC/VI) that produces calibrated samples and, ideally, estimates of $\log Z$, *without* any dataset from π.

Chemistry (small-molecule conformers). Different 3D conformations have a formation energy from force-field terms (bonds, angles, dihedrals, nonbonded); lower energy $\Rightarrow$ higher Boltzmann probability. A well-calibrated sampler is needed to draw conformers in proportion to these probabilities, which is important in binding-pose ranking/free-energy estimation, Boltzmann-weighted property prediction (e.g., NMR shifts), and generating diverse realistic 3D conformers for screening.

Diffusion Generative Flow Samplers

Idea. We will *reframe sampling* from an unnormalized target $\pi(x) \propto \mu(x)$ as a *stochastic optimal control (SOC)* problem: learn a control that steers a simple reference diffusion so its *terminal marginal* matches π.

Why this helps.

- Gives a *path-space* training objective/metric: a KL on trajectories $\mathrm{KL}(Q \,\|\, P)$ where P is the reference paths reweighted by $\mu(x_T)$.
- The *partition function Z cancels* inside this objective, so we can train using only μ (and optionally $\nabla \log \mu$).
- Lets us optimize *without samples from* π and still measure closeness to the true normalized endpoint.

Caveat (sets up DGFS). This path-KL places supervision *only at the terminal time* $\Rightarrow$ poor *credit assignment* and high-variance gradients.

DGFS fix (preview). Inject *intermediate* learning signals via a GFlowNet-inspired *learned flow* and *subtrajectory balance*, enabling partial-trajectory training and more stable learning.

Steps 1–2: Forward & Reference in discrete time

Controlled forward transition (learned drift).

$$P_F(x_{n+1} \mid x_n) \;=\; \mathcal{N}\big(x_{n+1};\; x_n + h\,f(x_n, n),\; h\sigma^2 I\big)$$

Controlled path law.

$$Q(x_{0:N}) \;=\; p_0^{\mathrm{ref}}(x_0)\,\prod_{n=0}^{N-1} P_F(x_{n+1} \mid x_n)$$

Uncontrolled (reference) transition (zero drift).

$$P_F^{\mathrm{ref}}(x_{n+1} \mid x_n) \;=\; \mathcal{N}\big(x_{n+1};\; x_n,\; h\sigma^2 I\big)$$

Reference path law and marginals.

$$Q^{\mathrm{ref}}(x_{0:N}) \;=\; p_0^{\mathrm{ref}}(x_0)\,\prod_{n=0}^{N-1} P_F^{\mathrm{ref}}(x_{n+1} \mid x_n), \qquad p_n^{\mathrm{ref}}(x) \text{ is closed form.}$$

Goal. Learn f so that the terminal marginal $Q(x_N)$ matches $\pi(x) = \mu(x)/Z$ (no data, Z unknown).

Step 3: Path target & KL $\Rightarrow$ SOC objective

Target path measure via terminal reweighting.

$$P(x_{0:N}) \;\propto\; Q^{\mathrm{ref}}(x_{0:N})\,\frac{\mu(x_N)}{p_N^{\mathrm{ref}}(x_N)} \qquad \Longrightarrow \qquad P(x_N) \propto \mu(x_N).$$

KL decomposition.

$$\mathrm{KL}(Q\|P) = \mathbb{E}_Q\left[\log\frac{Q}{Q^{\mathrm{ref}}}\right] + \mathbb{E}_Q\left[\log\frac{p_N^{\mathrm{ref}}(x_N)}{\pi(x_N)}\right].$$

Running control cost (Gaussian mean-shift) Girsanov theorem.

$$\mathbb{E}_Q\left[\log\frac{Q}{Q^{\mathrm{ref}}}\right] = \mathbb{E}_Q\sum_{n=0}^{N-1}\frac{h}{2\sigma^2}\,\|f(x_n,n)\|^2.$$

Terminal potential from the target Girsanov theorem.

$$\mathbb{E}_Q\left[\log\frac{p_N^{\mathrm{ref}}(x_N)}{\pi(x_N)}\right] = \mathbb{E}_Q\big[\log p_N^{\mathrm{ref}}(x_N) - \log\mu(x_N)\big] \;+\; \log Z.$$

SOC objective

SOC objective (discrete-time).

$$\boxed{\min_f \ \mathbb{E}_Q\Big[\sum_{n=0}^{N-1} \tfrac{h}{2\sigma^2}\|f(x_n,n)\|^2 \ + \ \log p_N^{\text{ref}}(x_N) - \log \mu(x_N)\Big]}$$

Diffusion Process

Idea. Let the target "diffuse to Gaussian" via a reference process (VP/VE SDE). The *reverse-time* dynamics can, in principle, generate target samples if we know the *score* $\nabla_x \log p_t(x)$:

$$\underbrace{dx_t = \sigma\, dW_t}_{\text{forward/noising}} \quad \Longleftrightarrow \quad \underbrace{dx_t = \left[f_{\text{ref}}(x,t) - \sigma^2 \nabla_x \log p_t(x)\right] dt + \sigma\, d\bar{W}_t}_{\text{reverse/generative}}.$$

What is score matching? Learn a network $s_\theta(x,t) \approx \nabla_x \log p_t(x)$ by regressing on *noised data*:

$$\min_\theta \ \mathbb{E}_t\, \mathbb{E}_{x_0 \sim p_{\text{data}}}\, \mathbb{E}_\varepsilon \left\| s_\theta(x_t, t) - \nabla_x \log p_t(x_t) \right\|^2,$$

which is equivalent to denoising a corrupted sample x_t back toward x_0.

Why Denoising Score Matching is *not* applicable here

- We have *no dataset* from π, only the unnormalized $\mu(x)$ (and maybe $\nabla \log \mu$).

Alternative to DSM: learn the vector field (control)

Reverse SDE drift (generative side).

$$dx_t = \left[f_{\mathrm{ref}}(x,t) - \sigma^2 \nabla_x \log p_t(x)\right] dt + \sigma\, d\bar{W}_t.$$

DSM route (data world). Learn the *score* $s_\theta(x,t) \approx \nabla_x \log p_t(x)$ from noised *data*, then plug it into the reverse drift.
Vector-field route (our setting). Directly learn the *control/drift* $u_\theta(x,t)$ instead of the score. The two are *equivalent* via:

$$u_\theta(x,t) = f_{\mathrm{ref}}(x,t) - \sigma^2 s_\theta(x,t) \iff s_\theta(x,t) = \frac{f_{\mathrm{ref}}(x,t) - u_\theta(x,t)}{\sigma^2}.$$

Why do this here?

- We have no dataset from π, so DSM can't form expectations over p_t; scores $\nabla \log p_t$ are unavailable.
- Instead, treat u_θ as a *control* and *learn it* by minimizing a Z-free *path-space* KL that uses only the given $\mu(\cdot)$.
- This sets up diffusion samplers à la PIS/DDS and enables DGFS's improvements (intermediate, subtrajectory credit).

Notation tip. Use u_θ (or f) for the vector field to avoid clashing with $\mu(\cdot)$, which denotes the unnormalized density.

Sampling as a Stochastic Optimal Control problem

Forward (controlled) process Q. A Markov chain with Gaussian transitions:

$$Q(x_{0:N}): \quad x_0 \sim p_0^{\mathrm{ref}}, \quad x_{n+1} \sim P_F(\cdot \mid x_n) = \mathcal{N}\big(x_n + h\, f(x_n, n),\; h\sigma^2 I\big).$$

Reference process Q^{ref}. Same covariance, zero drift:

$$x_{n+1} \sim P_F^{\mathrm{ref}}(\cdot \mid x_n) = \mathcal{N}\big(x_n,\; h\sigma^2 I\big), \qquad x_0 \sim p_0^{\mathrm{ref}}, \quad p_n^{\mathrm{ref}} \text{ known.}$$

Target process P. Tie the terminal marginal to π via the reference:

$$P(x_{0:N}) \;:=\; Q^{\mathrm{ref}}(x_{0:N})\, \frac{\pi(x_N)}{p_N^{\mathrm{ref}}(x_N)}.$$

Then $P(x_N) \propto \mu(x_N)$, making P a valid path-space target.

Sampling as a Stochastic Optimal Control problem

Learning objective (discrete-time SOC). Learn f by minimizing the path KL:

$$\min_f \; D_{\mathrm{KL}}(Q \parallel P) \iff \min_f \; \mathbb{E}_Q\Big[\sum_{n=0}^{N-1} \frac{h}{2\sigma^2} \|f(x_n, n)\|^2 + \log \Psi(x_N)\Big],$$

with $\Psi(x_N) = \dfrac{p_N^{\mathrm{ref}}(x_N)}{\mu(x_N)}$. (Continuous-time limit recovers the classic VE-SDE SOC formulation.)

Conclusion