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

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Sampling from Unnormalized Densities

Goal. Sample from a D-dimensional target with unnormalized density $\mu(x)$:

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

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.

From sampling to control: reference dynamics

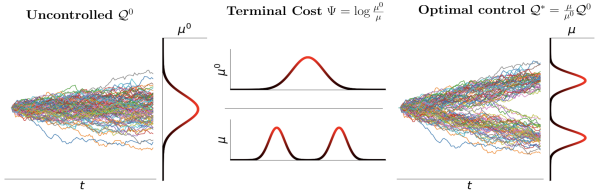
Reference (uncontrolled) diffusion.

$$dx_t = \sigma\, dW_t, \qquad x_0 \sim \nu \text{ (simple, e.g. Gaussian).}$$

More generally, introduce a *feedback control* $u_t = u(x_t, t)$:

$$dx_t = u(x_t, t)\, dt + \sigma\, dW_t, \qquad x_0 \sim \nu.$$

Let Q^{ref} be the path law of the uncontrolled process ($u \equiv 0$), with known terminal marginal p_T^{ref}. Our goal is to *choose a control u so that the terminal law of the controlled process matches the target* $\pi(x) \propto \mu(x)$.



SOC formulation

SOC objective. Choose a control u to minimize

$$\mathbb{E}_{Q^u}\left[\int_0^T \frac{1}{2\sigma^2}\|u(x_t,t)\|^2\,dt \;+\; \Psi(x_T)\right].$$

Pick the terminal cost to encode the target.

$$\Psi(x_T) \;=\; \log\frac{p_T^{\mathrm{ref}}(x_T)}{\mu(x_T)} \quad \big(\text{equivalently } -\log\mu(x_T) \text{ up to } \log p_T^{\mathrm{ref}}\big).$$

Key theorem (path–KL $\Leftrightarrow$ SOC). Define the *target path measure* by terminal reweighting:

$$P(x_{0:T}) \;\propto\; Q^{\mathrm{ref}}(x_{0:T})\;\frac{\mu(x_T)}{p_T^{\mathrm{ref}}(x_T)}.$$

Then, under standard regularity,

$$\boxed{D_{\mathrm{KL}}(Q^u\|P) = \mathbb{E}_{Q^u}\Big[\int_0^T \tfrac{1}{2\sigma^2}\|u\|^2\,dt + \log\tfrac{p_T^{\mathrm{ref}}(x_T)}{\mu(x_T)}\Big] \;+\; \text{const}}$$

Steps 1–2: Build forward & reference diffusions

Step 1 (controlled forward process). Parameterize a sampler as a controlled diffusion:

$$dx_t = f(x_t, t)\,dt + \sigma\,dW_t, \qquad x_0 \sim p_0^{\text{ref}},$$

with drift $f(\cdot,\cdot)$ (the control) to be learned. Let Q denote the path law of this process.

Step 2 (uncontrolled reference). Use the same noise but zero drift:

$$dx_t = \sigma\,dW_t, \qquad x_0 \sim p_0^{\text{ref}},$$

whose marginals p_t^{ref} are known in closed form. Let Q^{ref} be its path law.

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

Step 3: Target path measure via terminal reweighting

Construct a target measure on paths by reweighting only the terminal state:

$$P(x_{0:T}) \;\propto\; Q^{\text{ref}}(x_{0:T})\;\frac{\mu(x_T)}{p_T^{\text{ref}}(x_T)}.$$

Key property (endpoint correctness). By construction, the terminal marginal of P satisfies

$$P(x_T) \;\propto\; \mu(x_T) \quad\Longrightarrow\quad P(x_T) = \pi(x_T) \text{ up to the (unknown) normalizer } Z.$$

Takeaway. We have a principled path-space target P whose endpoint is exactly the desired distribution, without ever using Z along the way.

Step 4: Path–KL equals an SOC objective

Match the target on path space by minimizing a KL divergence:

$$\min_f \; D_{\mathrm{KL}}\big(Q \parallel P\big).$$

KL–control identity (Girsanov + chain rule). Under standard regularity,

$$\boxed{D_{\mathrm{KL}}(Q\|P) = \mathbb{E}_Q\Big[\int_0^T \tfrac{1}{2\sigma^2}\|f(x_t,t)\|^2\,dt \;+\; \log \tfrac{p_T^{\mathrm{ref}}(x_T)}{\mu(x_T)}\Big] \;+\; \text{const}}$$

Interpretation (SOC).

- *Running cost:* $\frac{1}{2\sigma^2}\|f\|^2$ (control effort).
- *Terminal cost:* $\log p_T^{\mathrm{ref}}(x_T) - \log \mu(x_T)$ (rewards high-μ endpoints).
- The additive constant absorbs $+\log Z \Rightarrow Z$ **cancels**.

Therefore: Minimizing $D_{\mathrm{KL}}(Q\|P)$ is *equivalent* to solving a stochastic optimal control problem.

Step 5 & intuition: why this works, what remains hard

Continuous-time view (optional). With T fixed and finer discretization, the discrete sum becomes

$$\min_f \ \mathbb{E}_Q\Big[\int_0^T \tfrac{1}{2\sigma^2}\|f(x_t,t)\|^2\,dt \ + \ \log \tfrac{p_T^{\text{ref}}(x_T)}{\mu(x_T)}\Big],$$

the classic entropy-regularized SOC form.

Intuition (why it works).

- We *steer* a simple diffusion toward regions where μ is large, trading control effort vs. terminal reward.
- The endpoint of the ideal optimizer matches $\pi = \mu/Z$ (calibrated sampling), while never needing Z explicitly.
- Training only requires evaluating $\mu(x_T)$ (and optionally $\nabla \log \mu$), not intermediate-time scores.

What remains hard (motivation for DGFS).

- The loss provides signal *only at terminal time* $\Rightarrow$ poor credit assignment, high-variance gradients.

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* $\nabla_x \log p_t(x)$:

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

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

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

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).

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

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:

$$u_\theta(x,t) \;=\; f_{\text{ref}}(x,t) \;-\; \sigma^2 \, s_\theta(x,t) \quad\Longleftrightarrow\quad s_\theta(x,t) \;=\; \tfrac{f_{\text{ref}}(x,t) - u_\theta(x,t)}{\sigma^2}.$$

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:

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

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

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

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

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

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.)

Why SOC, and what still hurts (motivation for DGFS)

Why SOC/control-as-inference?

- Principled *path-space* objective; Z cancels, so only μ (and optionally $\nabla \log \mu$) is needed.
- Calibrated sampling by *steering* a simple reference process toward the target.

Pain point in prior SOC samplers (PIS/DDS).

- Training signal sits *only at terminal time* N and losses use *full trajectories* $\Rightarrow$ poor credit assignment, high variance, weaker mode coverage.

DGFS in one line.

- Keep the same SOC/path-KL setup, but introduce a learned *flow function* $F_n(x_n)$ and enforce *subtrajectory balance* to inject *intermediate* learning signals and enable *partial-trajectory* training.

Conclusion