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

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Overview

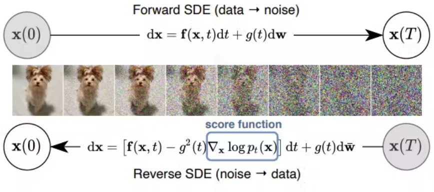
Generative Modeling

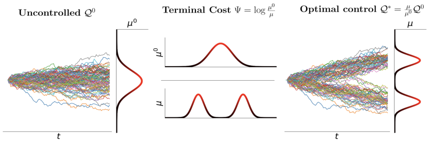
Task

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)


Forward SDE (data → noise)
$\mathbf{x}(0)$
$\mathrm{d}\mathbf{x} = \mathbf{f}(\mathbf{x}, t)\mathrm{d}t + g(t)\mathrm{d}\mathbf{w}$
$\mathbf{x}(T)$
score function
$\mathbf{x}(0)$
$\mathrm{d}\mathbf{x} = \left[\mathbf{f}(\mathbf{x}, t) - g^2(t)\boxed{\nabla_{\mathbf{x}} \log p_t(\mathbf{x})}\right] \mathrm{d}t + g(t)\mathrm{d}\bar{\mathbf{w}}$
$\mathbf{x}(T)$
Reverse SDE (noise → data)



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.

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

Uncontrolled (reference) transition (zero drift).

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

Reference path law and marginals.

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

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.

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

KL decomposition.

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

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

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

Terminal potential from the target Girsanov theorem.

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

SOC objective

SOC objective (discrete-time).

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

we will be using this discrete-time objective as our loss function to optimize the drift f. Thus we can model the drift with a neural network f_θ and optimize the parameters θ backpropagating through time (BPTT) while avoiding to use the stochastic-adjoint method necessary for a neural SDE.

Credit Assignment Problem in Path Space

Current Loss Function

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

Explanation. Since we are guiding our trajectory using the terminal marginal distribution p_N^{ref} and $\mu(x)$, the only signal we have is at the end. Thus, when we do the chain rule for backpropagation through time, it is very hard to know which decision at which time step got the right or wrong action (credit assignment problem).

GFlowNet's perspective on DGFS

Recap of GFlowNets. GFlowNets learn to sample from unnormalized distributions by modeling flows on a DAG.

- **DAG Structure:** Define a DAG $G = (S, A)$ with states S and directed edges $s \to s' \in A$.
- **Trajectories:** Complete trajectories $\tau = s_0 \to s_1 \to \cdots \to s_T$ from start to terminal states.
- **Forward Policy:** $P_F(s'|s)$, the probability of transitioning from s to s'.
- **Terminal Marginal:** $P_T(x) = \sum_{\tau \text{ ending at } x} P_F(\tau)$, the marginal over terminating states.
- **Goal:** Learn P_F such that $P_T(x) \propto R(x)$, where $R(x)$ is the unnormalized reward/density, and $Z = \sum_x R(x)$.

SOC as a GFlowNet

Comparison Table: GFlowNet vs. SOC Framework

Concept	**GFlowNet**	**SOC**
Forward Process	Trajectory sampling on DAG	Controlled diffusion path
Forward Transition Probability	$P_F(s'\|s)$	$P_F(x_{n+1}\|x_n) = \mathcal{N}(x_{n+1}; x_n + hf(x_n), h\sigma^2 I)$
Reward Function	$R(x)$ (unnormalized)	$\mu(x)$ (unnormalized density)
Terminal Marginal Distribution	$P_T(x) \propto R(x)$	$Q(x_N) \propto \mu(x_N)$
Flow State	Flow $F(s)$ at states	Learned flow $F_n(x)$

Insight. Since SOC can be viewed as a GFlowNet, we can apply GFlowNet tools (e.g., detailed balance loss, subtrajectory balance) to solve the credit assignment problem in diffusion sampling.

Insight in solving credit assignment problem

What if we could know or approximate the target distribution at any step n?

$$P(x_0, \dots, x_N) := Q^{\text{ref}}(x_0, \dots, x_N) \frac{\pi(x_N)}{p_N^{\text{ref}}(x_N)}.$$

Using the reference bridge decomposition:

$$Q^{\text{ref}}(x_{0:N}) = Q^{\text{ref}}(x_{0:N-1}|x_N)\, p_N^{\text{ref}}(x_N), \qquad p_N^{\text{ref}}(x_N) = \int Q^{\text{ref}}(x_{0:N})\, dx_{0:N-1}.$$

$$P(x_{0:N}) = \pi(x_N) \prod_{n=0}^{N-1} P_B(x_n|x_{n+1}),$$

Unfortunately, although we know the form of $P_B(\cdot|\cdot)$, for general target distribution there is generally no known analytical expression for it. As a result, we propose to use a deep neural network $F_n(\cdot;\theta)$ with parameter θ as a "helper" to approximate the unnormalized density of the n-th step target $p_n(\cdot)$.

Training the Flow Network: Naive Approach

Naive Way to Train $F_n(\cdot;\theta)$. One simple method is to fit F_n to a Monte Carlo (MC) quadrature estimate of the integral in Equation 11 (which approximates the unnormalized density at step n).
Why Not? Every training step requires a computationally expensive quadrature calculation (e.g., sampling many trajectories to estimate the integral). This makes the algorithm extremely inefficient, as MC quadrature is slow and scales poorly with dimensionality.
Decision. Instead of direct quadrature per step, amortize the computation by turning it into an optimization problem that learns F_n end-to-end.

Amortized Training: The Subtrajectory Constraint

Proposed Amortized Approach. Train $F_n(\cdot;\theta)$ to satisfy the following constraint for all partial trajectories $x_{n:N}$:

$$F_n(x_n;\theta)\prod_{l=n}^{N-1} P_F(x_{l+1}|x_l;\theta) = \mu(x_N)\prod_{l=n}^{N-1} P_B(x_l|x_{l+1}).$$

Details.

- P_F (forward policy) and F_n are parameterized by deep neural networks.
- Once this constraint holds, $F_n(x_n;\theta)$ equals the integral in Equation 11, amortizing the integration into the learning of θ.
- We use only $\mu(\cdot)$ (no Z), so the unknown normalization is absorbed into F_n.

Decision. This avoids per-step quadrature by enforcing a global constraint on partial trajectories, making training efficient and scalable.

Training Objective and Implementation

Training Objective. Regress the left-hand side (LHS) of the constraint to the right-hand side (RHS). For stability, perform this in log space:

$$\min_{\theta} \left|\log(\mathrm{LHS}) - \log(\mathrm{RHS})\right| .$$

Details.

- This is a regression loss that minimizes the difference between the learned flow products and the target products involving μ.
- Log space prevents numerical issues from large or small values.

Shared Parameters. The flow function at different steps shares the same parameters; achieved by adding a step embedding input to the network $F(\cdot, n; \theta)$.
Decision. Sharing parameters reduces model complexity and ensures consistency across time steps, while embeddings allow step-specific behavior.

Derived Subtrajectory Balance (SubTB)

Deriving SubTB. Comparing the constraint for n and $n+1$ gives a formula independent of μ:

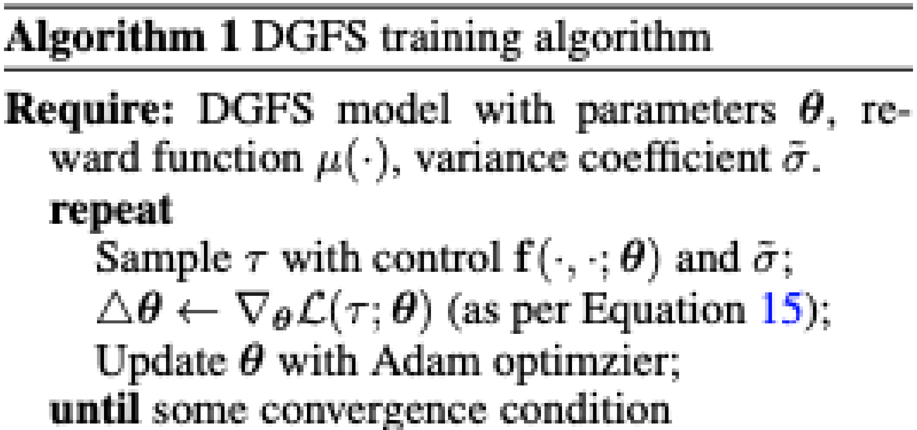
$$F_n(x_n;\theta)P_F(x_{n+1}|x_n;\theta) = F_{n+1}(x_{n+1};\theta)P_B(x_n|x_{n+1}).$$

Details.

- This is the Subtrajectory Balance (SubTB) constraint, a generalization of detailed balance for partial trajectories.
- It provides intermediate learning signals without needing μ directly, improving credit assignment.

Overall Decision. The method learns two neural networks: the flow $F(\cdot, n; \theta)$ and the forward policy P_F. This setup enables efficient, stable training with intermediate supervision.

DGFS algorithm



Algorithm 1 DGFS training algorithm

```
Require: DGFS model with parameters $\theta$, reward function $\mu(\cdot)$, variance coefficient $\bar{\sigma}$.
  repeat
    Sample $\tau$ with control $\mathbf{f}(\cdot, \cdot; \theta)$ and $\bar{\sigma}$;
    $\triangle\theta \leftarrow \nabla_\theta \mathcal{L}(\tau; \theta)$ (as per Equation 15);
    Update $\theta$ with Adam optimzier;
  until some convergence condition
```

Conclusion