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

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Overview

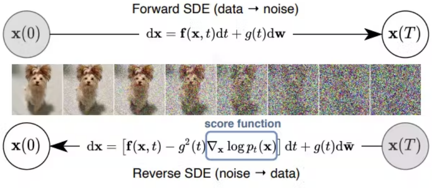
Generative Modeling

Task

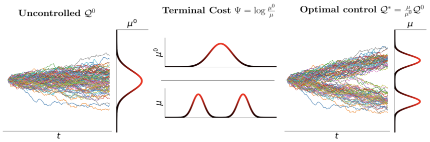
Sample from a complex (high-dimensional and multimodal) distribution D.

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

Context. 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.

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

Chemistry (molecule conformers).

Different 3D conformations have a formation energy from force-field terms (bonds, angles, dihedrals, nonbonded). A low energy means a higher probability of being sampled. A well-calibrated sampler is needed to draw conformers in proportion to these probabilities, which is important in binding-pose ranking, free-energy estimation 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. This means learning a control function that steers a diffusion process so its *terminal marginal* matches π.

Why this helps.

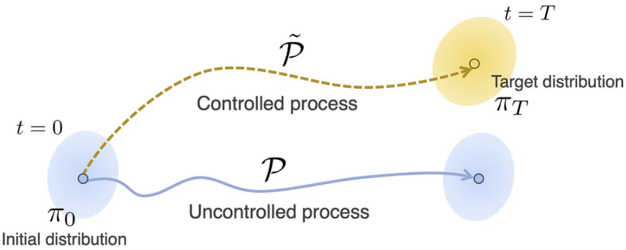
- Gives a *path-space* training objective/metric: a KL on trajectories $\mathrm{KL}(Q \,\|\, P)$ where P is the reference paths reweighted by $\mu(x_T)$.
- The *partition function Z cancels* inside this objective, so we can train using only μ (and optionally $\nabla \log \mu$).
- Lets us optimize *without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

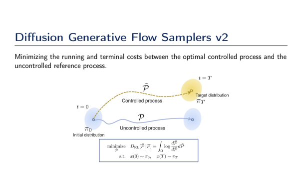
DGFS fix (preview). Inject *intermediate* learning signals via a GFlowNet-inspired *learned flow* and *subtrajectory balance*, enabling partial-trajectory training and more stable learning.

Diffusion Generative Flow Samplers v2

Minimizing the running and terminal costs between the optimal controlled process and the uncontrolled reference process.



$$\begin{aligned} &\underset{\tilde{\mathcal{P}}}{\text{minimize}} \quad D_{\mathrm{KL}}[\tilde{\mathcal{P}} \| \mathcal{P}] = \int_\Omega \log \frac{d\tilde{\mathcal{P}}}{d\mathcal{P}} d\tilde{\mathcal{P}} \\ &\text{s.t.} \quad x(0) \sim \pi_0, \quad x(T) \sim \pi_T \end{aligned}$$



refaire cette illustration avec le controlled, uncontrolled et target (optimal controlled) processus

Controlled and Reference Processes

Controlled forward transition (learned drift).

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

Controlled process.

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

Uncontrolled/Reference forward transition (zero drift).

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

Uncontrolled/Reference process and marginals.

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

$$p_n^{\text{ref}}(x) = \mathcal{N}\left(x; \mu_0, \Sigma_0 + nh\sigma^2 I\right), \text{ is closed form.}$$

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

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Why closed form for uncontrolled but not controlled? The uncontrolled reference process has no drift, so each transition is a simple Gaussian convolution, leading to Gaussian marginals with closed-form means and variances ($e.g., p_n^{ref}(x) = N(x; mu_0, cov_0 + nh\sigma^2 I)$). The controlled process includes a learned drift $f(x_n, n)$, which makes transitions non-Gaussian and dependent on f, preventing a closed-form marginal expression without solving the integral numerically or via simulation.

je dois refaire cette slide, on ne voit meme comment xn est sample (par rapport a la SDE) et aussi d'ou sort sigma mu et la closed form expliquer et c'est une convolution de gaussienne

Path space KL objective

Target path measure via terminal reweighting.

$$P(x_{0:N}) \;\propto\; Q^{\text{ref}}(x_{0:N-1}|x_N)\mu(x_N) \;\propto\; Q^{\text{ref}}(x_{0:N})\,\frac{\mu(x_N)}{p_N^{\text{ref}}(x_N)} \qquad \Longrightarrow \qquad P(x_N) \propto \mu(x_N).$$

KL decomposition.

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

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

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

Terminal cost.

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

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Je devrais avoir une slide complete a explier d’ou vient le foward target process P parce que c’est le coeur de mon algorithme

Target Path Measure via Importance Sampling

Importance Sampling Basics. Importance sampling is a technique to estimate expectations under a hard-to-sample target distribution P using samples from an easy-to-sample proposal distribution Q. The key formula is:

$$\mathbb{E}_{x\sim Q}[f(x)\cdot w(x)] = \mathbb{E}_{x\sim P}[f(x)],$$

where the *importance weight* $w(x) = \frac{P(x)}{Q(x)}$ corrects the samples from Q to behave as if they were from P.
Intuition. Q provides "biased" samples; $w(x)$ upweights samples that are likely under P and downweights those that aren't, effectively resampling from P without directly sampling it.
Application to Path Measures. In our case, the "samples" are entire trajectories $x_{0:N}$, and we want the path measure P to have the correct terminal marginal $\pi(x_N) \propto \mu(x_N)$. We use the reference path measure Q^{ref} (easy to sample, e.g., Gaussian paths) as the proposal. The reweighted path measure is:

$$P(x_{0:N}) \propto Q^{\text{ref}}(x_{0:N}) \cdot w(x_{0:N}),$$

where the weight $w(x_{0:N}) = \frac{\pi(x_N)}{p_N^{\text{ref}}(x_N)}$. This ensures $P(x_N) \propto \mu(x_N)$, as the weight depends only on the endpoint.

Credit Assignment Problem in SOC objective

SOC Discrete-time objective

$$\min_{f_\theta} \mathbb{E}_Q\Big[\underbrace{\sum_{n=0}^{N-1} \tfrac{h}{2\sigma^2}\|f_\theta(x_n, n)\|^2}_{\text{Running cost}} + \underbrace{\log p_N^{\text{ref}}(x_N) - \log \mu(x_N)}_{\text{Terminal cost}}\Big]$$

This objective is used on the seminar paper *Path Integral Sampler: Diffusion-based Sampling for Unnormalized Densities* by Dinghuai Zhang et al which presented the sampling from unnormalized densities as a stochastic optimal control problem.

Explanation. The SOC objective provides feedback signal only at the terminal step, making credit assignment difficult via backpropagation through time. This causes high-variance gradients, weak feedback for early actions, poor mode discovery, and inefficient optimization of the drift f without intermediate signals.

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	$P_F(s'\|s)$	$P_F(x_{n+1}\|x_n) = \mathcal{N}(x_{n+1}; x_n + hf(x_n), h\sigma^2 I)$
Backward Transition Probability	$P_B(s\|s')$	$P_B^{\text{ref}}(x_n\|x_{n+1})$ (known)
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.

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make a mental note to comeback to professor hernandez comment on Tristan's Deleu presentation when someone asked: "The if GFlowNets are just Reinfrocement Learning, then why keep doing research on this framework?" Professor Hernandez reponded by proving the felxibility of GFN, he said that it was en entery point between RL, Diffusion models, Energy-based models and in this case we prove that it can also be used in Stochastic Optimal Control problems.

Decomposition of the Target Process

Target Process Decomposition. The target path measure can be decomposed into a product of conditional distributions:

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

Conditional Form. Since the reweighting only affects the terminal state, the joint can be written as:

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

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conditional form is exactly like the RHS of the trajectory balance equation in gfn. Lire le paper de Nikolay sur Trajectory Balance pour bien comprendre cette equation et comment elle se relie a DGFS

Rewriting the Target Process with Marginal

If We Had Access to $p_n(x_n)$ we could write the partial joint which would allow training on subtrajectories and thus have better credit assignment:

$$P(x_{0:n}) = p_n(x_n) \prod_{k=0}^{n-1} P_B(x_k | x_{k+1}),$$

But There's No Closed Form for $p_n(x_n)$. To calculate $p_n(x_n)$, we would need to compute the integral:

$$p_n(x_n) = \int \pi(x_N) \prod_{n}^{N-1} P_B(x_n | x_{n+1}) \, dx_{n+1:N}.$$

Why Is $p_n(x_n)$ Hard to Compute? The reference marginal at step N is a simple Gaussian formula. But for the target marginal at earlier steps $n < N$, there's no easy formula because the target process depends on the terminal state $\pi(x_N)$, making it complex. Computing it needs integrating over many future states, which can't be done analytically for general targets. At $n = N$, it's just $\pi(x_N)$, but earlier steps are harder.
Solution: Learn an Approximation $F_n \approx p_n$. We introduce a learned flow function $F_n(x_n; \theta)$ parameterized by a neural network to approximate $p_n(x_n)$. This avoids computing the intractable integral at every training step.

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ne pas oublier de parler des MC quadrature method pour approximer l'integral mais c'est couteux en temps de calcul et pas scalable du tout

Trajectory Balance with Learned Flow

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

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

Details.

- P_F (forward policy) and F_n are parameterized by deep neural networks, with parameters θ and ϕ respectively.
- We can view F_n as an approximation to the unknown marginal $p_n(x_n)$ thus an amortized way to estimate the intractable integral.
- We use only $\mu(\cdot)$ (no Z), so the unknown normalization is absorbed into F_n.

Detailed Balance with Learned Flow

Detailed Balance from Trajectory Balance condition. Comparing the constraint for n and $n+1$ gives a formula independent of μ which now only involves local transitions (signal subtrajectories instead of full trajectories)

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

Subtrajectories Loss

Subtrajectory Balance Loss for Partial Trajectories.

$$\ell_{\mathrm{SubTB}}(x_{m:n};\theta,\phi) = \left(\log \frac{F_m(x_m;\phi)\prod_{k=m}^{n-1} P_F(x_{k+1}|x_k;\theta)}{F_n(x_n;\phi)\prod_{k=m}^{n-1} P_B(x_k|x_{k+1})}\right)^2$$

Forward Process (Controlled). The learned forward transition depends on θ:

$$P_F(x_{n+1}|x_n;\theta) = \mathcal{N}\left(x_{n+1}; x_n + hf_\theta(x_n,n), h\sigma^2 I\right),$$

where $f(x_n,n)$ is the learned drift parameterized by θ.

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a voir si je voudrais pas mettre une schema sur l'une des 3 derniers slides pour faire un recap de scrap la SOC objective, now we build DB loss with learned flow to solve credit assignment problem

Overall Training Objective

Recall SubTB Loss

$$\ell_{\text{SubTB}}(x_{m:n};\theta,\phi)=\left(\log\frac{F_m(x_m;\phi)\prod_{k=m}^{n-1}P_F(x_{k+1}|x_k;\theta)}{F_n(x_n;\phi)\prod_{k=m}^{n-1}P_B(x_k|x_{k+1})}\right)^2$$

Diffusion Generative Flow Sampler (DGFS) Loss

$$L(\tau;\theta;\phi)=\frac{\sum_{0\leq m<n\leq N}\lambda^{n-m}\ell_{\text{SubTB}}(x_{m:n})}{\sum_{0\leq m<n\leq N}\lambda^{n-m}},\quad \tau=(x_0,\ldots,x_N)$$

This combines signals from all subtrajectory lengths, reducing variance and improving credit assignment

- τ: Full trajectory $(x_0,\ldots,x_N)$.
- λ: Positive scalar weighting different subtrajectory lengths (e.g., shorter subtrajectories get higher weight if $\lambda<1$).
- The numerator sums SubTB losses over all subtrajectories $x_{m:n}$, weighted by λ^{n-m} (length-based weighting).
- The denominator normalizes to average the losses..

Algorithm 1 DGFS Training

Require: $\mu(\cdot)$, $\bar{\sigma}$, N, λ, B, η

Init $\theta = (\theta_f, \phi)$
repeat
    Sample trajectories:
    for $b = 1$ to B **do**
        $\tau^{(b)} = (x_0^{(b)}, \ldots, x_N^{(b)})$ under $x_{n+1} = x_n + hf_{\theta_f}(x_n, n) + \sqrt{h}\bar{\sigma}\varepsilon_n$, $\varepsilon_n \sim \mathcal{N}(0, I)$
    end for
    Build subtrajectories: $\mathcal{S}(\tau^{(b)})$ of (m, n) with $0 \le m < n \le N$
    Compute SubTB loss:

$$\mathcal{L}(\tau^{(b)}; \theta) = \sum_{(m,n)\in\mathcal{S}(\tau^{(b)})} \lambda^{n-m} \left[\log \frac{F_\phi(x_m) \prod_{l=m}^{n-1} P_F(x_{l+1} \mid x_l; \theta_f)}{F_\phi(x_n) \prod_{l=m}^{n-1} P_B^{\mathrm{ref}}(x_l \mid x_{l+1})}\right]^2$$

    $g \leftarrow \nabla_\theta \frac{1}{B} \sum_{b=1}^{B} \mathcal{L}(\tau^{(b)}; \theta)$
    $\theta \leftarrow \mathrm{Adam}(\theta, g, \eta)$
until convergence

Reduction of gradient variance

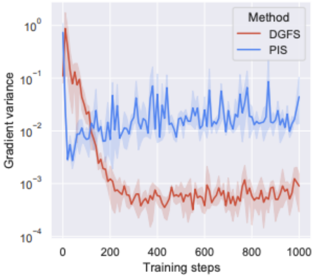

Figure: Gradient variance comparison between DGFS and PIS. DGFS shows significantly

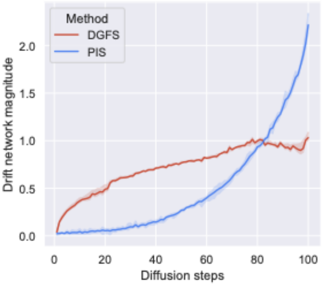

Figure: Caption for drift.png

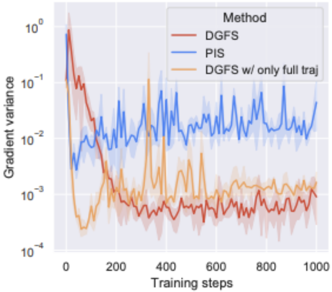

Figure: Caption for

Mode coverage results

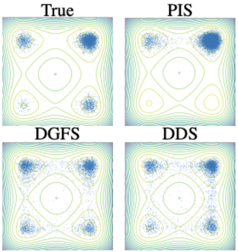

Figure: Manywell plots. DGFS and DDS but not PIS recover all modes

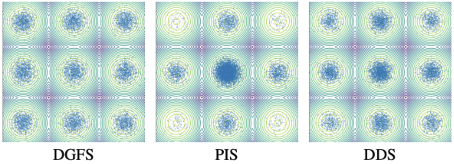

Figure: MoG visualization of DGFS and other diffusion-based samplers shows that DGFS could capture the diverse modes well. The contours display the landscape of the target density

Accurate partition function Z estimation

How to Estimate Z. The partition function $Z = \int \mu(x)\, dx$ normalizes the density. Since we sample trajectories from the learned process Q, we estimate Z using importance sampling on the terminal states.
Log-partition function estimator:

$$\log \sum_{b=1}^{B} \exp(S(\tau^{(b)}; \theta)) - \log B \leq \log Z, \quad \tau^{(b)} \sim Q(\cdot; \theta).$$

Intuition (Simple).

- $S(\tau; \theta)$: Weight showing how well the trajectory matches the target (higher if it ends in high-μ regions).
- Sample many trajectories from Q, compute their weights, and average in log space.
- This gives a lower bound on $\log Z$ because Q approximates the target, providing an estimate without direct π samples.

Partition function estimation results

	MoG	Funnel	Manywell	VAE	Cox
SMC	$0.289_{\pm 0.112}$	$0.307_{\pm 0.076}$	$22.36_{\pm 7.536}$	$14.34_{\pm 2.604}$	$99.61_{\pm 8.382}$
VI-NF	$1.354_{\pm 0.473}$	$0.272_{\pm 0.048}$	$2.677_{\pm 0.016}$	$6.961_{\pm 2.501}$	$83.49_{\pm 2.434}$
CRAFT	$0.348_{\pm 0.210}$	$0.454_{\pm 0.485}$	$0.987_{\pm 0.599}$	$0.521_{\pm 0.239}$	$13.79_{\pm 2.351}$
FAB w/ Buffer[5]	$0.003_{\pm 0.0005}$	$0.0022_{\pm 0.0005}$	$0.032_{\pm 0.004}$	N/A	$0.19_{\pm 0.04}$
PIS	$0.036_{\pm 0.007}$	$0.305_{\pm 0.013}$	$1.391_{\pm 1.014}$	$2.049_{\pm 2.826}$	$11.28_{\pm 1.365}$
DDS	$0.028_{\pm 0.013}$	$0.416_{\pm 0.094}$	$1.154_{\pm 0.626}$	$1.740_{\pm 1.158}$	N/A[6]
DGFS	$0.019_{\pm 0.008}$	$0.274_{\pm 0.014}$	$0.904_{\pm 0.067}$	$0.180_{\pm 0.083}$	$8.974_{\pm 1.169}$

Figure: The lower the better, DGFS achieves the lowest bias in estimating the partition function across various benchmarks compared to PIS and DDS.

Convergence Theorem

Convergence Guarantees for DGFS.

- Previous studies (Bortoli, 2022; Chen et al., 2022; Lee et al., 2022) show that the terminal sample distribution of a diffusion model converges to the target under mild assumptions if the control term is well learned. These apply to DGFS since proofs are independent of training method.
- Zhang et al. (2022a) prove that a perfectly learned score corresponds to zero GFlowNet training loss (Bengio et al., 2021; 2023), ensuring a well-trained DGFS accurately samples from the target distribution.

Off-policy training capability

Conclusion

Summary of DGFS. We propose the Diffusion Generative Flow Sampler (DGFS), a novel algorithm that trains diffusion models to sample from given unnormalized target densities. Different from prior works that could only learn from complete diffusion chains, DGFS can update its parameters with only partial specification of the stochastic process trajectory; moreover, DGFS can receive intermediate signals before completing the entire path. These features help DGFS benefit from efficient credit assignment and thus achieve better partition function estimation bias in the sampling benchmarks.

Questions and hopefully answers :)

Questions?