Adaptive denoising diffusion modelling via random time reversal

MFO Mini-Workshop on *Probabilistic Perspectives in Neural Network-Based Machine Learning*

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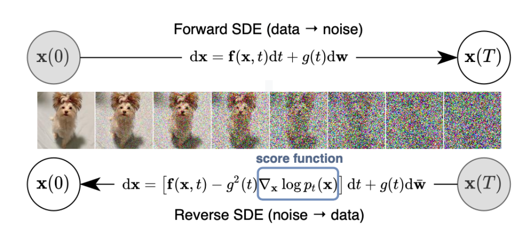
Denoising diffusion models

- provide an iterative generative algorithm to create new samples that approximately match the target distribution p_0, given a finite number of samples corresponding to an unknown p_0
- general idea: find a stochastic process that perturbs p_0 to a new distribution p_T such that
  1) p_T or a good approximation thereof is easy to sample from, and
  2) the perturbation is reversible in the sense that we know how to simulate the time-reversed process



Source: Song et al. (2021). Score based generative modeling through stochastic differential equations. *ICLR*.

Denoising Diffusion Models

- for some fixed time $T > 0$ consider the forward model

$$\mathrm{d}X_t = b(t, X_t)\,\mathrm{d}t + \sigma(t, X_t)\,\mathrm{d}W_t, \quad t \in [0, T], X_0 \sim p_0$$

- under sufficient regularity conditions, the forward model has a solution $X = (X_t)_{t\in[0,T]}$ with marginal densities $p_t(x) = \int p_{0,t}(y, x)\,p_0(\mathrm{d}y)$ such that the time reversal $\overleftarrow{X}_t = X_{T-t}$ solves

$$\mathrm{d}\overleftarrow{X}_t = -\overline{b}(T - t, \overleftarrow{X}_t)\,\mathrm{d}t + \sigma(T - t, \overleftarrow{X}_t)\,\mathrm{d}\overline{W}_t, \quad t \in [0, T], \overleftarrow{X}_0 \sim p_T,$$

  where

$$\begin{aligned}\overline{b}_i(t, x) &= b_i(t, x) - \frac{1}{p_t(x)} \sum_{j,k=1}^{d} \frac{\partial}{\partial x_j}\big(p_t(x)\sigma_{ik}(t, x)\sigma_{jk}(t, x)\big) \\ &= b_i(t, x) - (\nabla \cdot \Sigma(t, x))_i - (\nabla \log p_t(x))_i, \quad i = 1, \ldots, d, \Sigma = \sigma\sigma^\top\end{aligned}$$

⇝ time-reversed process solves a time-inhomogeneous SDE, now with drift $-\overline{b}(T - \cdot, \cdot)$ involving the score $\nabla \log p_t$, which depends on the unknown data distribution p_0

⇝ score needs to be estimated from the data

Denoising score matching

- denoising score matching:

$$\nabla \log p_t(x) = \frac{\int \nabla_x p_{0,t}(y,x)\, p_0(\mathrm{d}y)}{p_t(x)} = \int \nabla_x \log p_{0,t}(y,x) \underbrace{\frac{p_{0,t}(y,x)\, p_0(\mathrm{d}y)}{p_t(x)}}_{=\mathbb{P}(X_0 \in \mathrm{d}y | X_t = x)}$$

$$= \mathbb{E}[\nabla_2 \log p_{0,t}(X_0, X_t) \mid X_t = x]$$

and thus

$$\mathfrak{s} := \nabla \log p_t \in \operatorname*{arg\,min}_{s \text{ meas.}} \mathbb{E}\Big[\|s(X_t) - \nabla_2 \log p_{0,t}(X_0, X_t)\|^2\Big]$$

$\rightsquigarrow$ given data $(X_0^i)_{i \in [n]} \overset{\text{iid}}{\sim} p_0$ define the denoising score estimator

$$\hat{\mathfrak{s}} \in \operatorname*{arg\,min}_{s \in \mathcal{S}} \frac{1}{n} \sum_{i=1}^{n} \int_{\underline{T}}^{T} \|s(t, X_t^i) - \nabla_2 \log p_{0,t}(X_0^i, X_t^i)\|^2 \, \mathrm{d}t,$$

where $0 < \underline{T} \ll T$ and $\mathcal{S}$ is an approximating function class, e.g. space-time neural networks

Generative process

On $[0, T - \underline{T}]$, simulate

$$\mathrm{d}Y_t = \big(-b(T-t, Y_t) + \nabla\cdot\Sigma(T-t, Y_t) + \Sigma(T-t, Y_t)\hat{\mathfrak{s}}(T-t, Y_t)\big)\,\mathrm{d}t + \sigma(T-t, Y_t)\,\mathrm{d}W_t, \quad \mathbb{P}^{Y_0}(\mathrm{d}y) \approx p_T(y)\,\mathrm{d}y$$

Output:

$$Y_{T-\underline{T}} \overset{d}{\approx} \overleftarrow{X}_{T-\underline{T}} = X_{\underline{T}} \overset{d}{\approx} X_0$$

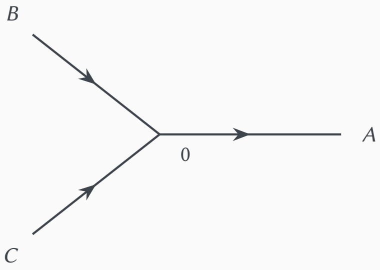
Basic observations

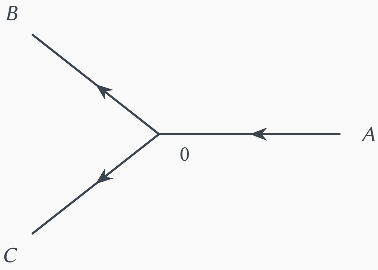
- time reversal at deterministic time T forces the backward process to be time-inhomogeneous
- if p_0 has low-dimensional support $\mathscr{M}$, for small t and x close to $\mathscr{M}$, $\nabla \log p_t(x)$ is approximately orthogonal to $\mathscr{M}$ (Stanczuk et al., 2024)[1]
- initialising the generative process in a distribution that is not close to $\mathbb{P}^{X_T}$ and simulating for $T - \underline{T}$ time units will not give useful results $\rightsquigarrow$ algorithm is not adaptive to the noise level in the data

[1] Stanczuk et al. (2024). Your diffusion model secretely knows the dimension of the data manifold. *ICML*.

Homogeneous time reversal

- Markov property: “the past and future of a Markov process are conditionally independent given the present” $\rightsquigarrow$ time-reversed Markov processes are Markov
- to ensure that a homogeneous Markov process remains homogeneous under time reversal, we need to reverse at a suitable random (life)time ζ. This can be
  - a randomised stopping time such as an independent exponential time;
  - a last exit time;
  - a first hitting time;
  - any terminal time, that is, any stopping time T such that $T = t + T \circ \theta_t$ on $\{T > t\}$
- retaining the strong Markov property under time reversal is a bit more tricky:





h-transforms and time reversal

h-transform

For a possibly killed, homogeneous strong Markov process X with state space S, let h be an excessive function, that is

$$\mathbb{E}_x[h(X_t)] \leq h(x) \quad \text{and} \quad \lim_{t\to 0} \mathbb{E}_x[h(X_t)] = h(x).$$

Then,

$$P_t^h f(x) = \mathbb{E}_x\left[\frac{h(X_t)}{h(x)} f(X_t) \mathbf{1}_{\{X_t \in S\}}\right] \mathbf{1}_{(0,\infty)}(h(x)), \quad f \in \mathcal{B}_b(\mathbb{R}^d),$$

defines a sub-Markov semigroup. The corresponding Markov process X^h is strong Markov and is called h-transform of X.

- suppose that X is a continuous and self-dual Feller process (i.e., its generator satisfies $A = A^*$)
- if X^h has a finite killing time ζ, then the time-reversed process $\overleftarrow{X}_t^h = X_{\zeta-t}^h$ is homogeneous, strong Markov and is a $\overleftarrow{h}$-transform of X.

h-transforming a killed diffusion

- consider a symmetric diffusion process

$$\mathrm{d}X_t = b(X_t)\,\mathrm{d}t + \sigma(X_t)\,\mathrm{d}W_t$$

  with invariant measure m and let Z be its version killed at an independent exponential time with parameter $r > 0$

- as an excessive function for Z use

$$h(x) = \int G_r(x, y)\,\kappa(\mathrm{d}y)$$

  for the Green kernel $G_r(x, y) = \int_0^\infty e^{-rt} p_t(x, y)\,\mathrm{d}y$ and a representing measure κ

  - $\kappa(\mathrm{d}y) = r\,\mathrm{d}y \rightsquigarrow h = 1$ and $Z^h = Z$
  - $\kappa(\mathrm{d}y) = \frac{1}{G_r(x_0, y)}\,\beta(\mathrm{d}y) \rightsquigarrow Z$ conditioned to have distribution β before killing if started in x_0
  - Z is a killed Brownian motion and $\kappa(\mathrm{d}y) = \sigma_R(\mathrm{d}y)$ for the surface measure σ_R of an R-sphere $\mathbb{S}^{d-1}(R) \rightsquigarrow Z^h$ is killed at last exit from $\mathbb{S}^{d-1}(R)$

A time-homogeneous generative process

Proposition

1. Z^h is an Itô-diffusion with dynamics

$$\mathrm{d}Z_t^h = \big(b(Z_t^h) + \Sigma(X_t)\nabla \log h(X_t)\big)\,\mathrm{d}t + \sigma(Z_t^h)\,\mathrm{d}W_t$$

   outside $\operatorname{supp}\kappa$ and its distribution at the lifetime is given by

$$\mathbb{P}_x(Z_{\zeta-}^h \in \mathrm{d}y) = \frac{G_r(x,y)}{h(x)}\kappa(\mathrm{d}y)$$

2. Let $\alpha = \mathbb{P}^{Z_0^h}$. Then $\overleftarrow{Z}_t^h$ is an $\overleftarrow{h}$-transform of Z with initial distribution $\mathbb{P}_\alpha(Z_{\zeta-}^h \in \mathrm{d}y)$ and

$$\overleftarrow{h}(x) := \int \frac{G_r(x,y)}{h(y)}\,\alpha(\mathrm{d}y).$$

   In particular, $\overleftarrow{Z}^h$ has dynamics

$$\mathrm{d}\overleftarrow{Z}_t^h = \big(b(\overleftarrow{Z}_t^h) + \Sigma(\overleftarrow{Z}_t^h)\nabla \log \overleftarrow{h}(\overleftarrow{Z}_t^h)\big)\,\mathrm{d}t + \sigma(\overleftarrow{Z}_t^h)\,\mathrm{d}\overline{W}_t,$$

   outside $\operatorname{supp}\alpha =: \mathscr{M}$ and $\mathbb{P}_\alpha(\overleftarrow{Z}_{\zeta-}^h \in \mathrm{d}y \mid \overleftarrow{Z}_0^h = x) = \frac{G_r(x,y)}{\overleftarrow{h}(x)h(y)}\alpha(\mathrm{d}y)$ for $\mathbb{P}_\alpha(Z_{\zeta-}^h \in \cdot)$-a.e. x.

A time-homogeneous generative process

Idealised algorithm:

1. Initialise $Z_0^{\overleftarrow{h}} \sim \tilde{\beta} \approx \mathbb{P}_\alpha(Z^h_{\zeta-})$
   - for ergodic forward process with stationary distribution μ and small exponential killing rate $r > 0$, choose $\tilde{\beta} = \mu$ [$\leftrightsquigarrow$ ergodic diffusion model]
   - for exponentially killed BM with small killing rate $r > 0$, choose $\tilde{\beta} = \text{Laplace}(0, (2r)^{-1/2}\mathbb{I}_d)$ [$\leftrightsquigarrow$ variance exploding diffusion model]
   - for $\kappa(\mathrm{d}y) = \frac{1}{G_r(x_0,y)}\delta_z$, choose $\tilde{\beta} = \delta_z$
2. Simulate diffusion $Z^{\overleftarrow{h}}$ until killing time and output $Z^{\overleftarrow{h}}_{\zeta-}$

Requirements for implementation

1. learn $\nabla \log \overleftarrow{h}$ (only a function in space – no time component);
2. learn killing time ζ of $Z^{\overleftarrow{h}}$

Learning to kill

Polarity hypothesis

Assume that $\mathscr{M} = \operatorname{supp}\alpha$ is polar for X, i.e., for any $x \in \mathbb{R}^d$, $\mathbb{P}_x(\inf\{t > 0 : X_t \in \mathscr{M}\} < \infty) = 0$.

Theorem

Under the polarity hypothesis, the backward process $\overleftarrow{Z}^h$ is killed at first entrance into $\mathscr{M}$.

Possible strategies to estimate a δ-fattening $\mathscr{M}_\delta = \{x : \operatorname{dist}(x, \mathscr{M}) \leq \delta\}$ given data $X^1, \dots, X^n \overset{\text{iid}}{\sim} \alpha$ and an estimator $\hat{\mathfrak{s}}$ of $\mathfrak{s} := \nabla \log \overleftarrow{h}$:

- plug-in approach: estimate $\mathscr{M}_\delta$ directly or indirectly by setting $\widehat{\mathscr{M}}_\delta = (\widehat{\mathscr{M}})_\delta$; then set $\hat{\zeta} := \inf\{t \geq 0 : Z_t^{\hat{\mathfrak{s}}} \in \widehat{\mathscr{M}}_\delta\}$
- use explosive behaviour of $\mathfrak{s}$ as $x \to \mathscr{M}$:

Theorem

Suppose that $\mathscr{M}$ is polar for X and Y solving $\mathrm{d}Y_t = \sigma(Y_t)\,\mathrm{d}B_t$. Then, it a.s. holds that

$$\zeta = \inf\Big\{t \geq 0 : \sup_{s \leq t} |\mathfrak{s}(\overleftarrow{Z}_s^h)| = \infty\Big\} = \inf\Big\{t \geq 0 : \|\mathfrak{s}(\overleftarrow{Z}^h)\|_{L^2([0,t])} = \infty\Big\}.$$

Denoising score matching

- for $\mathbb{P}_\alpha(Z^h_{\zeta_-} \in \cdot)$-a.e. x

$$\mathfrak{s}(x) = \nabla \log \overleftarrow{h}(x) = \frac{1}{\overleftarrow{h}(x)} \int \nabla_x G_r(x,y) \frac{1}{h(y)}\, \alpha(\mathrm{d}y) = \int \nabla_x \log G_r(x,y) \frac{G_r(x,y)}{\overleftarrow{h}(x) h(y)}\, \alpha(\mathrm{d}y)$$
$$= \mathbb{E}\big[\nabla_x \log G_r(x, Z^{\overleftarrow{h}}_{\zeta_-}) \mid Z^{\overleftarrow{h}}_0 = x\big]$$
$$= \mathbb{E}_\alpha\big[\nabla_x \log G_r(x, Z^h_0) \mid Z^h_{\zeta_-} = x\big]$$

- this implies that on $\mathbb{R}^d \setminus \mathscr{M}_\delta$, $\mathfrak{s}$ agrees $\mathbb{P}_\alpha(Z^h_{\zeta_-} \in \cdot)$-a.e. with the minimiser of

$$\mathcal{B}(\mathbb{R}^d; \mathbb{R}^d) \ni s \mapsto \mathbb{E}_\alpha\Big[\big\|s(Z^h_{\zeta_-}) - \nabla \log G_r(Z^h_0, Z^h_{\zeta_-})\big\|^2 \mathbf{1}_{\{\|Z^h_{\zeta_-} - Z^h_0\| > \delta\}}\Big]$$

- note that if $Z^h = Z$, then $\zeta \sim \mathrm{Exp}(r)$ independent of X, $Z_{\zeta_-} = X_\zeta$ has full support and we have

$$\mathbb{E}_\alpha\Big[\big\|s(Z^h_{\zeta_-}) - \nabla \log G_r(Z^h_0, Z^h_{\zeta_-})\big\|^2 \mathbf{1}_{\{\|Z^h_{\zeta_-} - Z^h_0\| > \delta\}}\Big] = r\mathbb{E}_\alpha\Big[\int_0^\zeta \big\|s(Z^h_t) - \nabla \log G_r(Z^h_0, Z^h_t)\big\|^2 \mathbf{1}_{\{\|Z^h_t - Z^h_0\| > \delta\}}\, \mathrm{d}t\Big]$$

Projection learning

- we don't have to start the backward process approximately in $\mathbb{P}_\alpha(Z^h_{\zeta_-} \in \mathrm{d}y)$: it will always be killed on the data support $\mathscr{M}$ and different initialisations will yield different output distributions supported on $\mathscr{M}$ $\rightsquigarrow$ natural conditioning
- a natural question is therefore what happens if we don't start the generative process from pure noise but something more informative, say a masked or moderately noised picture

- it turns out that the natural conditioning aspect entails a blessing of dimensionality

Projection learning

Let Z be an exponentially killed Brownian motion. Then,

$$\overleftarrow{h}(x) = \int G_r(x,y)\,\alpha(\mathrm{d}y), \quad G_r(x,y) = 2(2\pi)^{-d/2} r \left(\frac{\sqrt{2r}}{|x-y|}\right)^{\frac{d-2}{2}} K_{\frac{d-2}{2}}\left(\frac{\sqrt{2r}}{|x-y|}\right).$$

For large d,

$$\nabla \log \overleftarrow{h}(x) \approx d\,\frac{\int \frac{x-y}{|x-y|^d}\,\alpha(\mathrm{d}y)}{\int |x-y|^{2-d}\,\alpha(\mathrm{d}y)}$$

and thus, if there is a unique projection $x^* \in \arg\min_{y\in\mathscr{M}} |x-y|$ of x onto $\mathscr{M}$, then

$$\nabla \log \overleftarrow{h}(x) \approx d\,\frac{x^*-x}{|x^*-x|^2} = d\,\frac{\operatorname{sign}(x^*-x)}{|x^*-x|}$$

Theorem

Let $\delta, \varepsilon > 0$ and fix an observation $x \in \mathbb{R}^d$. If $\alpha(B(x,r)) > \varepsilon$ for some ball $B(x,r)$ with radius $r > 0$ around y, then

$$\mathbb{P}\left(Z^{\overleftarrow{h}}_{\zeta_-} \in \mathscr{M} \cap B(x,(1+\delta)r) \mid Z^{\overleftarrow{h}}_0 = x\right) \geq 1 - \frac{1}{\varepsilon}(1+\delta)^{2-d}.$$

Projection learning

Consider now estimators $\hat{\mathfrak{s}}_n$, an independent Brownian motion W and let $\widehat{Z}^{\hat{\mathfrak{s}}_n}$ be the process solving

$$\mathrm{d}\widehat{Z}_t^{\hat{\mathfrak{s}}_n} = \hat{\mathfrak{s}}_n(\widehat{Z}_t^{\hat{\mathfrak{s}}_n})\mathbf{1}_{\{t\le\hat{\zeta}\}}\,\mathrm{d}t + \mathbf{1}_{\{t\le\hat{\zeta}\}}\,\mathrm{d}W_t, \quad \hat{\zeta} := \inf\Big\{t \ge 0 \,:\, \|\widehat{Z}^{\hat{\mathfrak{s}}_n}\|_{L^2[0,t]} > M\Big\}.$$

Theorem

Fix an observation $x \in \mathbb{R}^d$. Suppose that

- for any $\tilde{\delta}, \delta, \varepsilon > 0$ it holds for sufficiently large n that
$$\mathbb{P}\Big(\Big\|(\hat{\mathfrak{s}}_n(Z^{\overleftarrow{h}}) - \mathfrak{s}(Z^{\overleftarrow{h}}))\mathbf{1}_{\{Z^{\overleftarrow{h}}\notin\mathcal{M}_{\tilde{\delta}}\}}\Big\|_{L^2(\zeta)} > \delta \,\Big|\, Z_0^{\overleftarrow{h}} = x\Big) < \varepsilon$$
- for any $n \in \mathbb{N}$ and $\tilde{\delta} > 0$, the function $\hat{\mathfrak{s}}_n$ is $L_{\tilde{\delta}}$-Lipschitz on $\mathcal{M}_{\tilde{\delta}}^{c}$

Let $\delta, \varepsilon, \tilde{\delta}, \tilde{\varepsilon} > 0$. If $\alpha(B(x, r)) > \varepsilon$, then, for sufficiently large $M > 0$ and $n \in \mathbb{N}$,

$$\mathbb{P}\big(\widehat{Z}_{\hat{\zeta}}^{\hat{\mathfrak{s}}_n} \in \mathcal{M}_{\tilde{\delta}} \cap B(x, (1+\delta)r) \,\big|\, \widehat{Z}_0^{\hat{\mathfrak{s}}_n} = x\big) \;>\; 1 - \frac{1}{\varepsilon}(1+\delta)^{2-d} - \tilde{\varepsilon}.$$

Thank you for your attention!