# Score-based generative modeling (theory & extensions)

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# Summary of the previous lecture (1/2)

- The previous lecture was an **introduction** to **score-based generative modeling**:
  - **Ancestral sampling** and discrete **time-reversal**.
  - **Efficient** and **stable** implementation.
  - Links with **annealed Langevin**.
  - Connections with **EBMs** and **VAEs**.
- Recall the basics of **SGM**:
  - Sample a **forward trajectory**, noising the distribution.

$$\boxed{X_{k+1} = X_k - \gamma X_k + \sqrt{2\gamma} Z_{k+1} \ .}$$

  - Sample a **backward trajectory** via **ancestral sampling**.

$$\boxed{X_k = X_{k+1} + \gamma\{X_{k+1} + \mathbf{s}_\theta(k\gamma, X_{k+1})\} + \sqrt{2\gamma} Z_{k+1} \ .}$$

  - Backward sampling relies on learning the **score** (**score-matching**)

$$\boxed{\mathbf{s}_{\theta^\star}(k\gamma, \cdot) = \arg\min_\theta \{\mathbb{E}[\|\mathbf{s}_\theta(k\gamma, X_k) - \nabla \log p_{k|0}(X_k|X_0)\|^2] \ : \ f \in \mathrm{L}^2(p_k)\} \ .}$$

# Summary of the previous lecture (2/2)

Videos extracted from an online tutorial blogpost.

# Outline of the course

- We dive further into **score-based generative models**.
- **Goal of the course**:
  - Introduce a **theoretical** framework (continuous-time).
  - Present **extensions** of SGMs and other **interpretations**.
- **Outline of the course**
  - A **continuous** approach to score-based generative modeling.
  - **Likelihood computation** and connection with **normalizing flows**.
  - **Faster** diffusion based models.
  - A **continuous** ELBO.

**Figure 1:** Interpolation with ODE flow. Image extracted from Song et al. (2020b).

# Continuous score-based generative models

# Continuous forward process

- Recall that in classical **score-based generative models**, the forward dynamics is given by the following **Markov chain**

$$\boxed{X_{k+1} = X_k - \gamma X_k + \sqrt{2\gamma} Z_{k+1} \ .}$$

- This is the **Euler-Maruyama** discretization of the **Ornstein-Ulhenbeck** process.

$$\boxed{\mathrm{d}\mathbf{X}_t = -\mathbf{X}_t \mathrm{d}t + \sqrt{2}\mathrm{d}\mathbf{B}_t \ .}$$

  - $(\mathbf{B}_t)_{t\geq 0}$ is a **Brownian motion**.

- A technical point Ikeda and Watanabe (2014): two different definitions.
  - A **strong solution**: given a probability space $(\Omega, \mathcal{F}, \mathbb{P})$ and a Brownian motion $(\mathbf{B}_t)_{t\geq 0}$ with filtration $(\mathcal{F}_t)_{t\geq 0}$ we want to find $(\mathbf{X}_t)_{t\geq 0}$ which is $(\mathcal{F}_t)_{t\geq 0}$ adapted and for any $t \geq 0$

$$\boxed{\mathbf{X}_t = \mathbf{X}_0 + \int_0^t b(s, \mathbf{X}_s)\mathrm{d}s + \int_0^t \sigma(s, \mathbf{X}_s)\mathrm{d}\mathbf{B}_s \ .}$$

  - A **weak solution**: we just need that *there exists* a probability space such that such a process exists.

# Technical point continued

- The weak formulation is equivalent to a **martingale** problem, see (Stroock and Varadhan, 1997, Chapter 6).
- We introduce the **infinitesimal generator** $\mathscr{A} : \mathbb{R}_+ \times \mathrm{C}^2(\mathbb{R}^d) \to \mathcal{F}(\mathbb{R}^d)$ such that for any $f \in \mathrm{C}^2(\mathbb{R}_+ \times \mathbb{R}^d)$ and $t \geq 0$

$$\boxed{\mathscr{A}(t,f)(x) = \langle b(t,x), \nabla f(t,x)\rangle + (1/2)\langle \Sigma(t,x), \nabla^2 f(t,x)\rangle \ .}$$

  - $\Sigma = \sigma^\top \sigma$.
  - Morally, $\mathbb{E}[\mathscr{A}(t,f)(\mathbf{X}_t)] = \lim_{h\to 0}(\mathbb{E}[f(\mathbf{X}_{t+h})] - \mathbb{E}[f(\mathbf{X}_t)])/h$.
- The existence of a weak solution is equivalent to the existence of a process $(\mathbf{X}_t)_{t\geq 0}$ such that for any $f \in \mathrm{C}^2(\mathbb{R}_+ \times \mathbb{R}^d)$, the process $(\mathbf{M}_t^f)_{t\geq 0}$ is a $(\mathcal{F}_t)_{t\geq 0}$-**martingale** where

$$\boxed{f(\mathbf{X}_t) = f(\mathbf{X}_0) + \int_0^t (\partial_s f(s,\mathbf{X}_s) + \mathscr{A}(s,f)(\mathbf{X}_s))\mathrm{d}s \ .}$$

# Analysis of the Ornstein-Ulhenbeck process

- Back to the **Ornstein-Ulhenbeck** (OU) process, **strong solutions** exist. The OU process is the *nicest* process:
  - $(\mathbf{X}_t)_{t\geq 0}$ is a Gaussian process
  - $(\mathbf{X}_t)_{t\geq 0}$ admits a closed form solution

$$\boxed{\mathbf{X}_t = \mathrm{e}^{-t}\mathbf{X}_0 + \mathbf{B}_{1-\mathrm{e}^{-2t}} \ .}$$

  - From the previous equation it is clear that

$$\boxed{\mathbf{W}_2(\mathcal{L}(\mathbf{X}_t), \mathrm{N}(0, \mathrm{Id})) \leq \mathrm{e}^{-t}\{\mathbb{E}^{1/2}[\|\mathbf{X}_0\|^2] + d^{1/2}\} \ .}$$

- We can also control the **Kullback-Leibler** divergence between $\mathcal{L}(\mathbf{X}_t)$ and $\mathrm{N}(0, \mathrm{Id})$ using that $\mathrm{N}(0, \mathrm{Id})$ satisfies a **logarithmic Sobolev** inequality Bakry et al. (2014).
- We can also control the$\chi^2$ divergence between $\mathcal{L}(\mathbf{X}_t)$ and $\mathrm{N}(0, \mathrm{Id})$ using that $\mathrm{N}(0, \mathrm{Id})$ satisfies a **Poincaré** inequality Bakry et al. (2014).
- **Geometric** convergence rates **independent of the dimension**.
- Very fast mixing compared to Langevin dynamics targeting **non-convex** potentials.

# Time reversal (1/5)

- In discrete time we consider the **ancestral sampling** of the discretized **Ornstein-Ulhenbeck**.
- In the continuous-time setting we need to compute the **time-reversal** of the Ornstein-Ulhenbeck.
  - More precisely: does $(\mathbf{Y}_t)_{t\in[0,T]} = (\mathbf{X}_{T-t})_{t\in[0,T]}$ also satisfies a **Stochastic Differential Equation** (SDE)?
- The answer is *yes* under conditions.
  - A **coefficient regularity** approach Haussmann and Pardoux (1986).
  - An **finite entropy** approach Föllmer (1985); Cattiaux et al. (2021).
- **Finite-entropy** conditions are well-suited for our approach.
- In what follows, we present an **informal derivation** of time-reversal following Haussmann and Pardoux (1986).

# Time reversal (2/5)

- In order to show that $(\mathbf{Y}_t)_{t\in[0,T]}$ satisfies a SDE (weakly) we need to show that for any $f \in \mathrm{C}^2(\mathbb{R}^d)$, $(\mathbf{M}_t^f)_{t\in[0,T]}$ is a martingale where for any $t \in [0, T]$

$$\boxed{\mathbf{M}_t^f = f(\mathbf{Y}_t) - f(\mathbf{Y}_0) - \int_0^t \bar{\mathscr{A}}_s f(\mathbf{Y}_s)\mathrm{d}s.}$$

- This is equivalent to show that for any $s, t \in [0, T]$ with $t \geq s$ and any $f, g \in \mathrm{C}^2(\mathbb{R}^d)$ we have

$$\mathbb{E}[\{f(\mathbf{Y}_t) - f(\mathbf{Y}_s) - \int_s^t \bar{\mathscr{A}}_u f(\mathbf{Y}_u)\mathrm{d}u\}g(\mathbf{Y}_s)] = 0 \ .$$

- This is again equivalent to show that for any $s, t \in [0, T]$ with $t \geq s$ and any $f, g \in \mathrm{C}^2(\mathbb{R}^d)$ we have

$$\mathbb{E}[\{f(\mathbf{X}_{T-t}) - f(\mathbf{X}_{T-s}) - \int_{T-t}^{T-s} \bar{\mathscr{A}}_{T-u} f(\mathbf{X}_u)\mathrm{d}u\}g(\mathbf{X}_{T-s})] = 0 \ .$$

- Finally, this is equivalent to show that for any $s, t \in [0, T]$ with $t \geq s$ and any $f, g \in \mathrm{C}^2(\mathbb{R}^d)$ we have

$$\boxed{\mathbb{E}[\{f(\mathbf{X}_s) - f(\mathbf{X}_t) - \int_s^t \bar{\mathscr{A}}_{T-u} f(\mathbf{X}_u)\mathrm{d}u\}g(\mathbf{X}_t)] = 0 \ .}$$

# Time reversal (3/5)

- Let $h(s,x) = \mathbb{E}[g(\mathbf{X}_t)\,|\mathbf{X}_s = x]$. $h$ satisfies the **backward Kolmogorov** equation

$$\boxed{\partial_t h(t,x) = -\mathscr{A} h(t,x)\ ,}$$

- where $\mathscr{A}$ is the infinitesimal generator of the Ornstein-Ulhenbeck.
- We have that

$$\boxed{\mathbb{E}[f(\mathbf{X}_t)h(t,\mathbf{X}_t)] - \mathbb{E}[f(\mathbf{X}_s)h(s,\mathbf{X}_s)] = \int_s^t \{f(\mathbf{X}_u)\partial_u h(u,\mathbf{X}_u) + \mathscr{A} f(\mathbf{X}_u)h(u,\mathbf{X}_u)\}\mathrm{d}u\ .}$$

- For the Ornstein-Ulhenbeck infinitesimal generator, we have

$$\mathscr{A} fg = f\mathscr{A} g + g\mathscr{A} f + 2\langle \nabla f, \nabla g\rangle\ .$$

- Therefore, we get that

$$\begin{aligned} &f(x)\partial_u h(u,x) + \mathscr{A} fh(x) \\ &\qquad = -f(x)\mathscr{A} h(u,x) + f(x)\mathscr{A} h(u,x) + h(u,x)\mathscr{A} f(x) + 2\langle \nabla f(x), \nabla g(x)\rangle \\ &\qquad = h(u,x)\mathscr{A} f(x) + 2\langle \nabla f(x), \nabla h(u,x)\rangle\ . \end{aligned}$$

# Time reversal (4/5)

- Therefore we have

$$f(x)\partial_u h(u,x) + \mathscr{A} f h(x) = h(u,x)\mathscr{A} f(x) + 2\langle \nabla f(x), \nabla h(u,x)\rangle \ .$$

- Using this result and the **divergence theorem** we get that

$$\begin{aligned}
\mathbb{E}[f(\mathbf{X}_t)h(t,\mathbf{X}_t)] - \mathbb{E}[f(\mathbf{X}_s)h(s,\mathbf{X}_s)] &= \int_s^t \{f(\mathbf{X}_u)\partial_u h(u,\mathbf{X}_u) + \mathscr{A} f(\mathbf{X}_u)h(u,\mathbf{X}_u)\}\mathrm{d}u \\
&= \int_s^t \mathbb{E}[\mathscr{A} f(\mathbf{X}_u)h(u,\mathbf{X}_u) + 2\langle \nabla f(\mathbf{X}_u), \nabla h(u,\mathbf{X}_u)\rangle]\mathrm{d}u \\
&= \int_s^t \{\mathbb{E}[\mathscr{A} f(\mathbf{X}_u)h(u,\mathbf{X}_u)] + 2\int_{\mathbb{R}^d} \langle \nabla f(x)p_u(x), \nabla h(u,x)\rangle \mathrm{d}x\}\mathrm{d}u \\
&= \int_s^t \mathbb{E}[\{\mathscr{A} f(\mathbf{X}_u) - 2\Delta f(\mathbf{X}_u) - 2\langle \nabla \log(p_u)(\mathbf{X}_u), \nabla f(\mathbf{X}_u)\rangle\}h(u,\mathbf{X}_u)]\mathrm{d}u \\
&= \int_s^t \mathbb{E}[\{\mathscr{A} f(\mathbf{X}_u) - 2\Delta f(\mathbf{X}_u) - 2\langle \nabla \log(p_u)(\mathbf{X}_u), \nabla f(\mathbf{X}_u)\rangle\}h(u,\mathbf{X}_u)]\mathrm{d}u \\
&= \int_s^t \mathbb{E}[\{\langle \nabla f(\mathbf{X}_u), -\mathbf{X}_u - 2\nabla \log p_u(\mathbf{X}_u)\rangle - \Delta f(\mathbf{X}_u)\}h(u,\mathbf{X}_u)]\mathrm{d}u \\
&= \mathbb{E}[g(\mathbf{X}_t)\int_s^t \langle \nabla f(\mathbf{X}_u), -\mathbf{X}_u - 2\nabla \log p_u(\mathbf{X}_u)\rangle - \Delta f(\mathbf{X}_u)]\mathrm{d}u \ .
\end{aligned}$$

- Therefore, we get that

$$\boxed{\mathbb{E}[\{f(\mathbf{X}_t) - f(\mathbf{X}_s) - \int_s^t \langle \nabla f(\mathbf{X}_u), -\mathbf{X}_u - 2\nabla \log p_u(\mathbf{X}_u)\rangle - \Delta f(\mathbf{X}_u)\mathrm{d}u\}g(\mathbf{X}_t)] = 0 \ .}$$

# Time reversal (5/5)

- Therefore, we get that

$$\mathbb{E}[\{f(\mathbf{Y}_t) - f(\mathbf{Y}_s) - \int_s^t \bar{\mathscr{A}}_u f(\mathbf{Y}_u)\mathrm{d}u\}g(\mathbf{Y}_s)] = 0 \ ,$$

- with

$$\boxed{\bar{\mathscr{A}}(u, f) = \langle \nabla f(x), x + 2\nabla \log p_{T-u}(x)\rangle + \Delta f(x) \ .}$$

- This means that $(\mathbf{Y}_t)_{t\in[0,T]}$ is a (weak) solution of the following SDE

$$\boxed{\mathrm{d}\mathbf{Y}_t = \{\mathbf{Y}_t + 2\nabla \log p_{T-t}(\mathbf{Y}_t)\}\mathrm{d}t + \sqrt{2}\mathrm{d}\mathbf{B}_t \ .}$$

- Note that for any $t \in [0, T]$, $p_t$ is the density of $\mathcal{L}(\mathbf{X}_t)$ w.r.t. the Lebesgue measure, where we recall that $(\mathbf{X}_t)_{t\in[0,T]}$ is the **forward** noising process, here a **Ornstein-Ulhenbeck** process.
- A few remarks:
  - The previous derivation is informal, there are conditions on the **data distribution** to make it rigorous.
  - The time-reversal formula is valid for **more complicated diffusions**.
  - Previous formula is valid in an **abstract setting** Cattiaux et al. (2021).

# Comparison with ancestral sampling

- Recall that in the **discrete-time** setting we have (denoting $\{Y_k\}_{k=0}^N = \{X_{N-k}\}_{k=0}^N$

$$\boxed{Y_{k+1} = Y_k + \gamma\{Y_k + 2\nabla \log p_{N-k}(Y_k)\} + \sqrt{2\gamma} Z_{k+1} \ .}$$

- In the **continuous-time** setting we have

$$\boxed{\mathrm{d}\mathbf{Y}_t = \{\mathbf{Y}_t + 2\nabla \log p_{T-t}(\mathbf{Y}_t)\}\mathrm{d}t + \sqrt{2}\mathrm{d}\mathbf{B}_t \ .}$$

- There is a clear link between the two formulations with **Euler-Maruyama** discretization.
- Note that $p_{N-k}$ is the density of $\mathcal{L}(X_{N-k})$ while $p_{T-t}$ is the density of $\mathcal{L}(\mathbf{X}_{T-t})$ but these two densities are close if the **stepsize is small**.
- In practice the **Stein score** is approximated using **score-matching**.
  - **DSM** and **ISM** losses can be defined in continuous-time.
  - Continuous losses can be used in practice because we can **exactly** sample from the **Ornstein-Ulhenbeck** process.

# A first theoretical result (setting)

- We want to know how close the generative model is to the true **data distribution**.
- In order to do so we consider the **total variation** distance between $\mathcal{L}(Y_N)$ and $p$ (the data distribution).
  - Recall that $\|\mu - \nu\|_{\mathrm{TV}} = \sup\{\mu(\mathsf{A}) - \nu(\mathsf{A}) \ : \ \mathsf{A} \in \mathcal{B}(\mathbb{R}^d)\}$
  - If $\mu, \nu$ admit densities $f, g$ w.r.t the Lebesgue measure we have that $\|\mu - \nu\|_{\mathrm{TV}} = \|f - g\|_1$.
  - This distance is stronger than the **weak convergence**.
  - This distance can be seen as a Wasserstein distance with cost $\ell_0$.
- We are going to consider the **Markov chain**

$$\boxed{Y_{k+1} = Y_k + \gamma\{Y_k + 2\mathbf{s}_{\theta^\star}((N-k)\gamma, Y_k)\} + \sqrt{2\gamma} Z_{k+1} \ .}$$

- This Markov chain is initialized with $Y_0 \sim \mathrm{N}(0, \mathrm{Id})$.
- The **data distribution** is denoted by $\pi$.

# Theoretical result

## Convergence of diffusion models (De Bortoli et al., 2021)

- Assume there exists $M \geq 0$ such that for any $t \in [0, T]$ and $x \in \mathbb{R}^d$

$$||\mathbf{s}_{\theta^\star}(t, x) - \nabla \log p_t(x)|| \leq M \ ,$$

  with $\mathbf{s}_{\theta^\star} \in C([0, T] \times \mathbb{R}^d, \mathbb{R}^d)$ and regularity conditions on the density of $\pi$ w.r.t. the Lebesgue measure and its gradients.

- Then there exist $B, C, D \geq 0$ s.t. for any $N \in \mathbb{N}$ and $\{\gamma_k\}_{k=1}^N$ the following hold:

$$\boxed{\|\mathcal{L}(Y_N) - \pi\|_{\mathrm{TV}} \leq B \exp[-T] + C(M + \gamma^{1/2}) \exp[DT] \ .}$$

  where $T = N\gamma$.

- **A few remarks**:
  - The assumption on $\pi$ is *not* satisfied if $\pi$ defined on a **manifold** of $\mathbb{R}^d$ with dimension $p < d$.
  - The approximation assumption is strong and could be **relaxed**.
  - The term $\exp[DT]$ can be improved and turned into a **polynomial dependency**.

# Sketch of the proof

- The central decomposition

$$\begin{aligned}\|\mathcal{L}(Y_N) - \pi\|_{\mathrm{TV}} &= \|\pi_0 \hat{\mathrm{R}}_N - \pi\|_{\mathrm{TV}} \\ &= \|\pi_0 \hat{\mathrm{R}}_N - p_T \mathrm{Q}_T\|_{\mathrm{TV}} \\ &\leq \|\pi_0 \hat{\mathrm{R}}_N - \pi_0 \mathrm{Q}_T\|_{\mathrm{TV}} + \|p_T \mathrm{Q}_T - \pi_0 \mathrm{Q}_T\|_{\mathrm{TV}} \\ &\leq \|\pi_0 \hat{\mathrm{R}}_N - \pi_0 \mathrm{Q}_T\|_{\mathrm{TV}} + \|\pi \mathrm{P}_T - \pi_0\|_{\mathrm{TV}} \ ,\end{aligned}$$

  where
  - $\pi_0 = \mathrm{N}(0, \mathrm{Id})$, $\pi$ is the data distribution.
  - $(\mathrm{P}_t)_{t \in [0,T]}$ is the **forward** Ornstein-Ulhenbeck semi-group.
  - $(\mathrm{Q}_t)_{t \in [0,T]}$ is the **backward** Ornstein-Ulhenbeck semi-group.
  - $(\hat{\mathrm{R}}_n)_{n \in \{1,\dots,N\}}$ is the iterated kernel associated with the backward Markov chain.
- $\|\pi_0 \hat{\mathrm{R}}_N - \pi_0 \mathrm{Q}_T\|_{\mathrm{TV}}$ is the **approximation error**.
  - We first use the **Pinsker theorem** and control $\mathrm{KL}(\pi_0 \hat{\mathrm{R}}_N | \pi_0 \mathrm{Q}_T)$.
  - Then we use the **transfer theorem** and **Girsanov theory**, similarly to Durmus and Moulines (2017); Dalalyan (2017).
- $\|\pi \mathrm{P}_T - \pi_0\|_{\mathrm{TV}}$ is the **mixing time**.
  - This is simply the **geometric ergodicity** of the **Ornstein-Ulhenbeck**.

# Bottleneck of score-matching methods

- We end up with

$$\boxed{\|\mathcal{L}(Y_N) - \pi\|_{\mathrm{TV}} \leq B\exp[-T] + C(M + \gamma^{1/2})\exp[DT]\ .}$$

- **A few remarks:**
  - The mixing time of the **reverse** is the same as the mixing time of the **forward**. This is a remarkable property because the **backward** targets a potentially complicated distribution.
  - Where is the trick? The **bottleneck** is in the **computation of the drift**.
  - To compare it with the **Unadjusted Langevin Algorithm** (ULA) (statistical sampling). The mixing time depends on the **convexity** of the target but the drift is **tractable**.
  - Here the mixing time is independent of the **convexity** of the target but the drift is **approximated**.
  - Note that the two algorithms *do not* solve the same problem. ULA addresses the **statistical sampling** problem while SGM addresses the **generative modeling** problem.

# Likelihood computation and connection with continuous normalizing flows

# Outline of the section

- In this section:
  - We present a link with **Normalizing Flows**.
  - We highlight the **training differences** with normalizing flows.
  - We present **likelihood computation** results.
  - We show the advantages of a **deterministic** transform.

**Figure 2:** Interpolation with ODE flow. Image extracted from Song et al. (2020b).

# Recap on Continuous Normalizing Flows

- One **problem** of **normalizing flows**: the set of valid transformation is restricted by the **tractability of the log-Jacobian**.

- Moving from the **discrete** time setting to the **continuous** time setting allows **greater flexibility** (Chen et al. (2018); Grathwohl et al. (2018)).
  - Normalizing flow: $\mathcal{O}(d^3)$ computation.
  - **C**ontinuous **N**ormalizing **F**low (CNF): $\mathcal{O}(d^2)$ computation Chen et al. (2018).
  - CNF with trace estimator: $\mathcal{O}(d)$ computation Grathwohl et al. (2018).

- We introduce a **continuous** evolution:
  - A (stochastic) **dynamics** $\mathrm{d}\mathbf{X}_t = b(t, \mathbf{X}_t)\mathrm{d}t + \sigma(t, \mathbf{X}_t)\mathrm{d}\mathbf{B}_t$ with $\mathbf{X}_0 \sim \pi_0$.
  - $(\mathbf{B}_t)_{t \geq 0}$ is a $d$-dimensional Brownian motion.
  - $b : \mathbb{R}_+ \times \mathbb{R}^d \to \mathbb{R}^d$, $\sigma : \mathbb{R}_+ \times \mathbb{R}^d \to \mathbb{R}^{d \times d}$ smooth, $\pi_0$ has density $p_0$.
  - What is the evolution of $t \mapsto \log(p(\mathbf{X}_t))$?

- This is equivalent to a continuous **change of variable**.

# Recap on the Fokker-Planck equation

- We have the **Fokker-Planck** equation

$$\boxed{\partial_t p_t(x) = -\mathrm{div}(b(t,\cdot)p_t)(x) + (1/2)\sum_{i,j=1}^{d} \partial_{i,j}\{\Sigma_{i,j}(t,\cdot)p_t\}(x)\ .}$$

- This equation describes the **evolution of the density**.
- Some special cases:

- Case $\sigma = 0$ (**deterministic dynamics**)

$$\boxed{\partial_t p_t(x) = -\mathrm{div}(b(t,\cdot)p_t)(x)\ .}$$

- Case $\sigma = c^{1/2}\,\mathrm{Id}$ $(c > 0)$ (**Langevin dynamics**)

$$\boxed{\partial_t p_t(x) = -\mathrm{div}(b(t,\cdot)p_t)(x) + (c/2)\Delta p_t(x) = -\mathrm{div}(\{b(t,\cdot) - (c/2)\nabla \log p_t\}p_t)(x)\ .}$$

- As a consequence the two following dynamics have the **same** marginal densities.

- $\mathrm{d}\mathbf{X}_t = b(t,\mathbf{X}_t)\mathrm{d}t + c^{1/2}\mathrm{d}\mathbf{B}_t$
- $\mathrm{d}\mathbf{X}_t = \{b(t,\mathbf{X}_t) - (c/2)\nabla \log p_t(\mathbf{X}_t)\}\mathrm{d}t$.
- One is **deterministic**, the other is **stochastic**.

# Log-likelihood evolution

- Assume that the **deterministic** process $(\mathbf{X}_t)_{t\in[0,T]}$ satisfies

$$\boxed{\mathrm{d}\mathbf{X}_t = b(t, \mathbf{X}_t)\mathrm{d}t \ .}$$

- The associated **Fokker-Planck** equation is

$$\boxed{\partial_t p_t(x) = -\mathrm{div}(b(t,\cdot)p_t)(x) \ .}$$

- **Evolution of the logarithm**

$$\partial_t \log p_t(x) = -\mathrm{div}(b(t,\cdot))(x) - \langle b(t,x), \nabla \log p_t(x)\rangle \ .$$

- Combining the two dynamics

$$\begin{aligned}\partial_t \log p_t(\mathbf{X}_t) &= -\mathrm{div}(b(t,\cdot))(\mathbf{X}_t) - \langle b(t,\mathbf{X}_t), \nabla \log p_t(\mathbf{X}_t) + \langle b(t,\mathbf{X}_t), \nabla \log p_t(\mathbf{X}_t) \\ &= -\mathrm{div}(b(t,\cdot))(\mathbf{X}_t) \ .\end{aligned}$$

- Hence, we have the following **log-likelihood** computation

$$\boxed{\log(p_0(\mathbf{X}_0)) = \log p_T(\mathbf{X}_T) + \int_0^T \mathrm{div}(b(t,\cdot))(\mathbf{X}_t)\mathrm{d}t \ .}$$

# From score-based models to normalizing flows

- Recall that the **continuous**-time version of **SGM** is given by

$$\boxed{\mathrm{d}\mathbf{Y}_t = \{\mathbf{Y}_t + 2\nabla \log p_{T-t}(\mathbf{Y}_t)\}\mathrm{d}t + \sqrt{2}\mathrm{d}\mathbf{B}_t \ .}$$

- It is the **backward** dynamics associated with the **forward Ornstein-Ulhenbeck**

$$\boxed{\mathrm{d}\mathbf{X}_t = -\mathbf{X}_t + \sqrt{2}\mathrm{d}\mathbf{B}_t \ .}$$

- For any $t \geq 0$, $\mathcal{L}(\mathbf{X}_t)$ has the same distribution as $\mathcal{L}(\hat{\mathbf{X}}_t)$ where for any $t \geq 0$

$$\boxed{\mathrm{d}\hat{\mathbf{X}}_t = \{-\hat{\mathbf{X}}_t - \nabla \log p_t(\hat{\mathbf{X}}_t)\}\mathrm{d}t \ .}$$

- The **backward** of this **deterministic** dynamics is $(\hat{\mathbf{Y}}_t)_{t\in[0,T]}$ given by

$$\boxed{\mathrm{d}\hat{\mathbf{Y}}_t = \{\hat{\mathbf{Y}}_t + \nabla \log p_{T-t}(\hat{\mathbf{Y}}_t)\}\mathrm{d}t \ .}$$

- Comparing $(\mathbf{Y}_t)_{t\in[0,T]}$ and $(\hat{\mathbf{Y}}_t)_{t\in[0,T]}$
  - $(\mathbf{Y}_t)_{t\in[0,T]}$ is **stochastic** and $(\hat{\mathbf{Y}}_t)_{t\in[0,T]}$ is **deterministic**.
  - Both are given by the **time-reversal** of a **forward dynamics**.
  - They both approximate the **data distribution** at time $t = T$.

# Stochastic and deterministic trajectories

- Recall that the **forward Ornstein-Ulhenbeck** is given by

$$\boxed{\mathrm{d}\mathbf{X}_t = -\mathbf{X}_t + \sqrt{2}\mathrm{d}\mathbf{B}_t \ .}$$

- Its **deterministic** counterpart is given by

$$\boxed{\mathrm{d}\hat{\mathbf{X}}_t = \{-\hat{\mathbf{X}}_t - \nabla \log p_t(\hat{\mathbf{X}}_t)\}\mathrm{d}t \ .}$$

- By the **Fokker-Planck** equation (and its uniqueness) we have that for any $t \geq 0$, $\mathcal{L}(\mathbf{X}_t) = \mathcal{L}(\hat{\mathbf{X}}_t)$.
- Is this property still true for the **backward** dynamics $(\mathbf{Y}_t)_{t\in[0,T]}$ and $(\hat{\mathbf{Y}}_t)_{t\in[0,T]}$?
- Both dynamics are started at $\mathcal{L}(\mathbf{Y}_T) = \mathcal{L}(\hat{\mathbf{Y}}_T)$. The question is then: do the distributions $(\mathcal{L}(\mathbf{Y}_t))_{t\in[0,T]}$ and $(\mathcal{L}(\hat{\mathbf{Y}}_t))_{t\in[0,T]}$ follow the same dynamics?
- We are going to compute the associated **Fokker-Planck** evolution equations.

# Fokker-Planck of the stochastic backward dynamics

- Recall that the **stochastic** time-reversal is given by

$$\boxed{\mathrm{d}\mathbf{Y}_t = \{\mathbf{Y}_t + 2\nabla \log p_{T-t}(\mathbf{Y}_t)\}\mathrm{d}t + \sqrt{2}\mathrm{d}\mathbf{B}_t \ .}$$

- Denote $(q_t)_{t\in[0,T]}$ the distribution of $(\mathbf{Y}_t)_{t\in[0,T]}$.
- We have the following evolution equation

$$\begin{aligned}\partial_t q_t(x) &= -\mathrm{div}(q_t(x)\{x + 2\nabla \log p_{T-t}(x)\}) + \Delta q_t \\ &= -\mathrm{div}(q_t(x)\{x + 2\nabla \log p_{T-t}(x) - \nabla \log q_t(x)\}) \ .\end{aligned}$$

- Recall that the **deterministic** time-reversal is given by

$$\boxed{\mathrm{d}\hat{\mathbf{Y}}_t = \{\hat{\mathbf{Y}}_t + \nabla \log p_{T-t}(\hat{\mathbf{Y}}_t)\}\mathrm{d}t \ .}$$

- Denote $(\hat{q}_t)_{t\in[0,T]}$ the distribution of $(\hat{\mathbf{Y}}_t)_{t\in[0,T]}$.
- We have the following evolution equation

$$\partial_t \hat{q}_t = -\mathrm{div}(\hat{q}_t(x)\{x + \nabla \log p_{T-t}(x)\}) \ .$$

- The **evolutions are equal** if $p_{T-t} = q_t = \hat{q}_t$, i.e. $\mathcal{L}(\mathbf{Y}_0) = \mathcal{L}(\hat{\mathbf{Y}}_0) = \mathcal{L}(\mathbf{X}_T)$.
- Hence as $T \to +\infty$ the two dynamics get **closer**, see De Bortoli et al. (2022).

# Difference between stochastic and deterministic dynamics

- We have a **stochastic** and a **deterministic** representation of $\mathcal{L}(\mathbf{X}_t)$ where for any $t \geq 0$

$$\boxed{\mathrm{d}\mathbf{X}_t = -\mathbf{X}_t + \sqrt{2}\mathrm{d}\mathbf{B}_t \ .}$$

- Are the **dynamics** the same? The answer is **no**. They can be really different.
- An example:

- $\mathcal{L}(\mathbf{X}_0) = \mathrm{N}(m, \mathrm{Id})$ with $m \in \mathbb{R}^d$.
- $\mathbf{X}_t = \mathrm{e}^{-t}\mathbf{X}_0 + \mathbf{B}_{1-\mathrm{e}^{-2t}}$, $p_t = \mathrm{N}(\mathrm{e}^{-t}m, \mathrm{Id})$
- Recall that the **deterministic** dynamics is given by

$$\boxed{\mathrm{d}\hat{\mathbf{X}}_t = \{-\hat{\mathbf{X}}_t - \nabla \log p_t(\hat{\mathbf{X}}_t)\}\mathrm{d}t = \{-\hat{\mathbf{X}}_t + \hat{\mathbf{X}}_t - m\mathrm{e}^{-t}\}\mathrm{d}t = -m\mathrm{e}^{-t}\mathrm{d}t \ .}$$

- $\hat{\mathbf{X}}_t = \mathbf{X}_0 - m(1 - \mathrm{e}^{-t})$.
- No **forgetting of the initial condition** with the **deterministic** dynamics.
- Khrulkov and Oseledets (2022) show that the deterministic dynamics yield the **optimal transport** between the Gaussian distributions.

# Back to normalizing flows

- We have a **deterministic** model $(\hat{\mathbf{X}}_t)_{t\in[0,T]}$

$$\boxed{\mathrm{d}\hat{\mathbf{X}}_t = \{-\hat{\mathbf{X}}_t - \nabla \log p_t(\hat{\mathbf{X}}_t)\}\mathrm{d}t \ .}$$

- The initialization is given by $\hat{\mathbf{X}}_0 \sim \pi$ (the **data distribution**).
- We want to maximize $\mathbb{E}[\log q_T(\hat{\mathbf{X}}_0)]$ where $q_T = \mathrm{N}(0, \mathrm{Id})$ and

$$\boxed{\partial_t q_t(x) = -\mathrm{div}(\{x + \nabla \log p_{T-t}(x)\} q_t(x)) \ .}$$

  - $(\mathcal{L}(\hat{\mathbf{X}}_{T-t}))_{t\in[0,T]}$ and $(q_t)_{t\in[0,T]}$ have the same dynamics.
  - **Difference:** $\mathcal{L}(\hat{\mathbf{X}}_T) \neq q_0 = \mathrm{N}(0, \mathrm{Id})$ (approximately true when $T \to +\infty$).
  - We still have that

$$\boxed{\mathrm{d} \log q_t(\hat{\mathbf{X}}_{T-t}) = -\mathrm{div}\{\hat{\mathbf{X}}_{\mathrm{T-t}} + \nabla \log \mathrm{p}_{\mathrm{T-t}}(\hat{\mathbf{X}}_{\mathrm{T-t}})\}\mathrm{d}t \ .}$$

- Hence, we have

$$\mathbb{E}[\log q_T(\hat{\mathbf{X}}_0)] = \mathbb{E}[\log q_0(\hat{\mathbf{X}}_T) - \int_0^T \mathrm{div}\{\hat{\mathbf{X}}_{\mathrm{T-t}} + \nabla \log \mathrm{p}_{\mathrm{T-t}}(\hat{\mathbf{X}}_{\mathrm{T-t}})\}\mathrm{d}t] \ .$$

# Interpolation with normalizing flows

- Having a **deterministic** model is useful for:
  - **Likelihood computation**
  - **Interpolation**
  - **Temperature scaling**
- We can explore the **latent structure**.

**Figure 3:** Interpolation with ODE. Image extracted from Song et al. (2020b).

# Temperature scaling with normalizing flows

**Figure 4:** Temperature scaling with ODE Image extracted from Song et al. (2020b).

# Faster diffusion models

# Few-step sampling: a well-known problem

- For **high-quality** image sampling **vanilla** SGMs are notably **slow**.

A critical drawback of these models is that they require many iterations to produce a high quality sample. For DDPMs, this is because that the generative process (from noise to data) approximates the reverse of the forward *diffusion process* (from data to noise), which could have thousands of steps; iterating over all the steps is required to produce a single sample, which is much slower compared to GANs, which only needs one pass through a network. For example, it takes around 20

control the generation sample. To obtain high-quality synthesis, a large number of denoising steps is used (i.e. 1000 steps). A notable property of the diffusion process is a closed-form formulation of

network). Although very powerful, score-based models generate data through an undesirably long iterative process; meanwhile, other state-of-the-art methods such as GANs generate data from a single forward pass of a neural network. Increasing the speed of the generative process is thus an active area of research.

denoises the samples under the fixed noise schedule. However, DDPMs often need hundreds-to-thousands of denoising steps (each involving a feedforward pass of a large neural network) to achieve

However, GANs are typically much more efficient than DDPMs at generation time, often requiring a single forward pass through the generator network, whereas DDPMs require hundreds of forward passes through a U-Net model. Instead of learning a generator directly, DDPMs learn to convert

A major downside to score-based generative models is that they require performing expensive MCMC sampling, often with a thousand steps or more. As a result, they can be up to three orders of magnitude slower than GANs, which only require a single network evaluation. To address this issue, Denoising Diffusion Implicit Models, or DDIMs, have been

# A myriad of methods

- A bunch of **approaches** have been proposed to solve this problem:
  - **D**enoising **D**iffusion **I**mplicit **M**odels (**DDIM**) Song et al. (2020a).
  - **Discovering the stepsizes** Watson et al. (2022, 2021).
  - Knowledge **distillation** Luhman and Luhman (2021); Salimans and Ho (2022).
  - Improved **SDE solvers** Jolicoeur-Martineau et al. (2021); Liu et al. (2022).
  - **Non-Gaussian** diffusions Nachmani et al. (2021).
  - **Multiscale** denoising Saharia et al. (2021).
  - **GAN jumps** Xiao et al. (2021).

- We present two of these approaches:
  - DDIM and **subsampling** Song et al. (2020a).
  - Discovering the stepsize and **dynamic programming** Watson et al. (2021).

# Non-Markov models and subsampling

# From DDPM to DDIM

- **DDIM** (**D**enoising **D**iffusion **I**mplicit **M**odel) is based on **DDPM** (**D**enoising **D**iffusion **P**robabilistic **M**odel).
- Both are based on the **variational approach** to recover **score-based generative models**.
- The contributions of **DDIM**:
  - A **non-Markov** noising process (interpolating between **deterministic** and **stochastic** dynamics).
  - An **accelerated** variational formulation.
  - **Combining** these techniques lead to high-quality accelerated models.

**Figure 5:** DDPM/DDIM comparison. Image extracted from Song et al. (2020a).

# Recap on DDPM (1/2)

- We start by deriving an **ELBO** for the **score-based generative models**. Note that such a derivation was already obtained by Sohl-Dickstein et al. (2015).
- Similar to VAE we maximize the **log-likelihood**

$$\begin{aligned}\log(p_{\theta,0}(x_0)) &= \log(\int_{(\mathbb{R}^d)^N} \prod_{k=0}^{N-1} p_{\theta,k|k+1}(x_k|x_{k+1}) p_N(x_N) \mathrm{d}x_{1:N}) \\ &= \log(\int_{(\mathbb{R}^d)^N} \prod_{k=0}^{N-1} p_{\theta,k|k+1}(x_k|x_{k+1}) p_N(x_N) / q(x_{1:N}|x_0) q(x_{1:N}|x_0) \mathrm{d}x_{1:N}) \\ &\geq \int_{(\mathbb{R}^d)^N} \log(\prod_{k=0}^{N-1} p_{\theta,k|k+1}(x_k|x_{k+1}) p_N(x_N) / q(x_{1:N}|x_0)) q(x_{1:N}|x_0) \mathrm{d}x_{1:N} \ .\end{aligned}$$

- The last inequality is obtained the **concavity** of the logarithm.
- We now choose the **variational distribution** $q(x_{1:N}|x_0)$:
  - **Factorization** $q(x_{1:N}|x_0) = q_{N|0}(x_N|X_0) \prod_{k=1}^{N-1} q_{k|k+1,0}(x_k|x_{k+1}, x_0)$.
  - **Tractability** of $q_{k|k+1,0}$.
  - We choose a tractable (Gaussian) decomposition

  $q(x_{1:N}|x_0) = \prod_{k=0}^{N-1} q_{k+1|k}(x_{k+1}|x_k)$.
- Here, we consider

$$\boxed{q_{k+1|k}(x_{k+1}|x_k) = (4\pi\gamma)^{-d/2} \exp[-\|x_{k+1} - x_k + \gamma x_k\|^2/(4\gamma)] \ .}$$

- This is a slightly different discretization from the one of Ho et al. (2020).

# Recap on DDPM (2/2)

- Recall that we have $\log(p_{\theta,0}(x_0)) \geq \mathcal{L}$ with

$$\boxed{\mathcal{L} = \int_{(\mathbb{R}^d)^N} \log\left(\prod_{k=0}^{N-1} p_{\theta,k|k+1}(x_k|x_{k+1}) p_N(x_N) / q(x_{1:N}|x_0)\right) q(x_{1:N}|x_0) \mathrm{d}x_{1:N} \ .}$$

- We use the **backward decomposition** of $q(x_{1:N}|x_0)$ and we get

$$\boxed{\mathcal{L} = \mathcal{L}_N + \sum_{k=1}^{N-1} \mathcal{L}_k + \mathcal{L}_0 \ ,}$$

- with:
  - $\mathcal{L}_N = \int_{\mathbb{R}^d} \log(p_N(x_N)/q(x_N|x_0)) q_{N|0}(x_N|x_0) \mathrm{d}x_N$.
  - $\mathcal{L}_k = \int_{\mathbb{R}^d} \log(p_{\theta,k|k+1}(x_k|x_{k+1}) / q_{k|k+1,0}(x_k|x_{k+1}, x_0)) q_{k,k+1|0}(x_k, x_{k+1}|x_0) \mathrm{d}x_k$.
  - $\mathcal{L}_0 = \int_{\mathbb{R}^d} \log(p_{\theta,0|1}(x_0|x_1)) q_{1|0}(x_1|x_0) \mathrm{d}x_1$.
- **The different terms**:
  - $\mathcal{L}_N$ does not depend on $\theta$.
  - $\mathcal{L}_k$ is related to **score-matching**.
  - $\mathcal{L}_0$ is a **reconstruction** term.

# Minimal requirements on the noising distribution

- We have $\log(p_{\theta,0}(x_0)) \geq \mathcal{L}$ with

$$\boxed{\mathcal{L} = \int_{(\mathbb{R}^d)^N} \log(\prod_{k=0}^{N-1} p_{\theta,k|k+1}(x_k|x_{k+1}) p_N(x_N)/q(x_{1:N}|x_0)) q(x_{1:N}|x_0) \mathrm{d}x_{1:N} \ .}$$

- We use the **backward decomposition** of $q(x_{1:N}|x_0)$ and we get

$$\boxed{\mathcal{L} = \mathcal{L}_N + \sum_{k=1}^{N-1} \mathcal{L}_k + \mathcal{L}_0 \ ,}$$

- with:
  - $\mathcal{L}_N = \int_{\mathbb{R}^d} \log(p_N(x_N)/q(x_N|x_0)) q_{N|0}(x_N|x_0) \mathrm{d}x_N$.
  - $\mathcal{L}_k = \int_{\mathbb{R}^d} \log(p_{\theta,k|k+1}(x_k|x_{k+1})/q_{k|k+1,0}(x_k|x_{k+1}, x_0)) q_{k,k+1|0}(x_k, x_{k+1}|x_0) \mathrm{d}x_k$.
  - $\mathcal{L}_0 = \int_{\mathbb{R}^d} \log(p_{\theta,0|1}(x_0|x_1)) q_{1|0}(x_1|x_0) \mathrm{d}x_1$.
- What do we need on the **variational distribution** $q(x_{1:N}|x_0)$?
  - **Sampling**: $q(x_k|x_0)$ is an **easy-to-sample** distribution.
  - **Tractability** of $q_{k|k+1,0}$.
- In **DDPM** we choose $q$ by specifying **Gaussian transition** (discretization of the Ornstein-Ulhenbeck process) for $q_{k+1|k}$.

# From DDPM to DDIM

- In **DDPM** we choose $q$ by specifying **Gaussian transition** (discretization of the Ornstein-Ulhenbeck process) for $q_{k+1|k}$.
- This choice specifies $q_{k|0}$ (because $q_{k+1|k}$ is Gaussian with **linear** mean).
- Therefore we have
  $q_{k|k+1,0}(x_k|x_{k+1}, x_0) = q_{k+1|k}(x_{k+1}|x_k)q_{k|0}(x_k|x_0)/q_{k+1|0}(x_{k+1}|x_0)$.
- In **DDIM** we choose a different approach.
  - We specify $q_{k|k+1,0}(x_k|x_{k+1}, x_0) = \mathrm{N}(C_k x_{k+1} + D_k x_0, \bar{\sigma}_k^2)$.
  - $\{\bar{\sigma}_k\}_{k=1}^{N-1}$ will be **fixed by the user**.
  - The parameters $\{C_k\}_{k=1}^{N-1}$, $\{D_k\}_{k=1}^{N-1}$ are chosen such that $q_{k|0} = \mathrm{N}(\alpha_k x_0, \sigma_k^2)$.
- The **parameters** $\{\alpha_k\}_{k=0}^{N-1}$ and $\{\sigma_k\}_{k=0}^{N-1}$ match the ones of **DPPM**.
- We present here a derivation of **DDIM** inspired from Song et al. (2020a).

# DDIM derivation (1/2)

- We assume that there exist $C_k, D_k \geq 0$ such that

$$\boxed{q_{k|k+1,0}(x_k|x_{k+1}, x_0) \propto \exp[-\|x_k - (C_k x_{k+1} + D_k x_0)\|^2/(2\bar{\sigma}_k^2)] \ .}$$

- We assume that $q_{N|0}(x_N|x_0) = \mathrm{N}(\alpha_N x_0, \sigma_N^2)$.
- We are going to proceed by recursion. We assume that for any $j \in \{k+1, \ldots, N\}$, $q_{j|0}(x_j|x_0) = \mathrm{N}(\alpha_j x_0, \sigma_j^2)$.
- **Question**: what **conditions** on $C_k, D_k, \bar{\sigma}_k$ should we impose so that $q_{k|0} = \mathrm{N}(\alpha_k x_0, \sigma_k^2)$?
- We are going to use that for any $x_k \in \mathbb{R}^d$

$$\boxed{q_{k|0}(x_k|x_0) = \int_{\mathbb{R}^d} q_{k|k+1,0}(x_k|x_{k+1}, x_0) q_{k+1|0}(x_{k+1}|x_0) \mathrm{d}x_{k+1} \ .}$$

  - **Computing** the integral.
  - **Finding** the parameter of the resulting Gaussian.

# DDIM derivation (2/2)

- We have the following:
  - $X_k = C_k X_{k+1} + D_k X_0 + \bar{\sigma}_k \bar{Z}_k$,
  - $X_{k+1} = \alpha_{k+1} X_0 + \sigma_{k+1} Z_{k+1}$.
  - With $\bar{Z}_k, Z_{k+1} \sim \mathrm{N}(0, \mathrm{Id})$.
- Hence, we get that

$$\begin{aligned} X_k &= (C_k \alpha_{k+1} + D_k) X_0 + \bar{\sigma}_k \bar{Z}_k + C_k \sigma_{k+1} Z_{k+1} \\ &= (C_k \alpha_{k+1} + D_k) X_0 + (\bar{\sigma}_k^2 + C_k^2 \sigma_{k+1}^2)^{1/2} Z_k \ . \end{aligned}$$

- Therefore, we obtain the following **parameters**:
  - $\alpha_k = C_k \alpha_{k+1} + D_k$.
  - $\sigma_k^2 = \bar{\sigma}_k^2 + C_k^2 \sigma_{k+1}^2$.
  - **Solving the system**: setting $\bar{\sigma}_k$ implies setting $C_k$ implies setting $D_k$.
  - Choosing $\bar{\sigma}_k = (\alpha_{k+1|k}^2 / \sigma_{k+1|k}^2 + (1/\sigma_k^2))^{-1}$ gives **DDPM**.
- Recall that the **discretized Ornstein-Ulhenbeck** gives
  - $\alpha_k = (1-\gamma)^k$.
  - $\sigma_k^2 = (1 - (1-\gamma)^{2k})/(1-\gamma/2)$.

# Choice of the parameters

- Recall that we have:
  - $\alpha_k = C_k \alpha_{k+1} + D_k$.
  - $\sigma_k^2 = \bar{\sigma}_k^2 + C_k^2 \sigma_{k+1}^2$.
  - **Solving the system**: setting $\bar{\sigma}_k$ implies setting $C_k$ implies setting $D_k$.
  - Choosing $\bar{\sigma}_k = (\alpha_{k+1|k}^2 / \sigma_{k+1|k}^2 + (1/\sigma_k^2))^{-1}$ gives **DDPM**.
- We can choose $\bar{\sigma}_k$ **arbitrary small**.
- Choosing $\bar{\sigma}_k \to 0$, we get **D**enoising **D**iffusion **I**implicit **M**odels (**DDIM**).
- We end up with a **deterministic** model.
  - Recall that when we train the model we estimate $X_0$, i.e. $\mathbf{t}_\theta(k+1, X_{k+1}) \approx X_0$.
  - The recursion is then given by

$$\boxed{X_k = C_k X_{k+1} + \mathbf{t}_\theta(k+1, X_{k+1}) + \bar{\sigma}_k \bar{Z}_k \ .}$$

# Interpolation with DDIM

- An alternative to **normalizing flows**.
- Like any **deterministic** we can **interpolate**.

**Figure 6:** DDIM interpolation. Image extracted from Song et al. (2020a).

# Subsampling with DDIM

- **Chain model**: (classical **DDIM**/**DDPM**)

- **Star graph model**: (multiple **encoder**/**decoder**)

- **Subsampled model**:

# Subsampled model

- In the **chain model** we parameterize $q(x_{1:N}|x_0)$ by

$$\boxed{q(x_{1:N}|x_0) = q_N(x_N|x_0) \prod_{k=1}^{N-1} q_{k|k+1,0}(x_k|x_{k+1}, x_0) \ .}$$

- The **backward chain** $p_\theta(x_{0:N})$ is then given by

$$\boxed{p_\theta(x_{0:N}) = p(x_N) \prod_{k=0}^{N-1} p_{\theta,k|k+1}(x_k|x_{k+1}) \ .}$$

- In the **subsampled model** we parameterize $q(x_{1:N}|x_0)$ by

$$\boxed{q(x_{1:N}|x_0) = \prod_{i=1}^{M-1} q_{k_i|k_{i+1},0}(x_{k_i}|x_{k_{i+1}}, x_0) \prod_{k\in\mathcal{N}\setminus\mathcal{M}} q_{k|0}(x_k|x_0) \ ,}$$

- where $\mathcal{N} = \{0, \ldots, N-1\}$ and $\mathcal{M} = \{k_1, \ldots, k_{M-1}\}$ with $k_M = N$
- The **backward chain** $p_\theta(x_{0:N})$ is then given by

$$\boxed{p_\theta(x_{0:N}) = p(x_N) \prod_{i=1}^{M-1} p_{\theta,k_i|k_{i+1}}(x_{k_i}|x_{k_{i+1}}) \prod_{k\in\mathcal{N}\setminus\mathcal{M}} \tilde{p}_{\theta,0|k}(x_0|x_k) \ .}$$

# Susbsampled ELBO

- The **backward chain** $p_\theta(x_{0:N})$ is then given by

$$\boxed{p_\theta(x_{0:N}) = p(x_N) \prod_{i=1}^{M-1} p_{\theta,k_i|k_{i+1}}(x_{k_i}|x_{k_{i+1}}) \prod_{k\in\mathcal{N}\setminus\mathcal{M}} \tilde{p}_{\theta,0|k}(x_0|x_k)\ .}$$

- Recall that $\log(p_\theta(x_0)) \geq \mathcal{L} = \int_{(\mathbb{R}^d)^N} \log(q(x_{1:N}|x_0)/p_\theta(x_{0:N}))q(x_{1:N}|x_0)\mathrm{d}x_{1:N}$.
- We use the **backward decomposition** of $q(x_{1:N}|x_0)$ and we get

$$\boxed{\mathcal{L} = \mathcal{L}_N + \sum_{i=1}^{M-1} \mathcal{L}_i + \sum_{k\in\mathcal{N}\setminus\mathcal{M}} \mathcal{L}_k\ ,}$$

- with:

- $\mathcal{L}_N = \int_{\mathbb{R}^d} \log(p_N(x_N)/q(x_N|x_0))q_{N|0}(x_N|x_0)\mathrm{d}x_N$.
- The **backward terms**:

$\mathcal{L}_i = \int_{\mathbb{R}^d} \log(p_{\theta,k_i|k_{i+1}}(x_{k_i}|x_{k_i+1})/q_{k_i|k_{i+1},0}(x_{k_i}|x_{k_{i+1}}, x_0))q_{k_i,k_{i+1}|0}(x_{k_i}, x_{k_{i+1}}|x_0)\mathrm{d}x_{k_i}$.

- The **decoder terms**: $\mathcal{L}_k = \int_{\mathbb{R}^d} \log(\tilde{p}_{\theta,0|k}(x_0|x_k))q_{k|0}(x_k|x_0)\mathrm{d}x_k$.

# DDIM results

| | | CIFAR10 ($32 \times 32$) | | | | | CelebA ($64 \times 64$) | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | $S$ | 10 | 20 | 50 | 100 | 1000 | 10 | 20 | 50 | 100 | 1000 |
| $\eta$ | 0.0 | **13.36** | **6.84** | **4.67** | **4.16** | 4.04 | **17.33** | **13.73** | **9.17** | **6.53** | 3.51 |
| | 0.2 | 14.04 | 7.11 | 4.77 | 4.25 | 4.09 | 17.66 | 14.11 | 9.51 | 6.79 | 3.64 |
| | 0.5 | 16.66 | 8.35 | 5.25 | 4.46 | 4.29 | 19.86 | 16.06 | 11.01 | 8.09 | 4.28 |
| | 1.0 | 41.07 | 18.36 | 8.01 | 5.78 | 4.73 | 33.12 | 26.03 | 18.48 | 13.93 | 5.98 |
| | $\hat{\sigma}$ | 367.43 | 133.37 | 32.72 | 9.99 | **3.17** | 299.71 | 183.83 | 71.71 | 45.20 | **3.26** |

**Figure 7:** DDIM results. Image extracted from Song et al. (2020a).

# Dynamic programming and stepsize selection

# Choosing the stepsizes

- Given a sequence of steps $\mathcal{T} = \{t_0 = 0, t_1, \ldots, t_N = T\}$ and a budget of $K$ steps which **subsampled** sequence is the **best**?
- The "best" in a **variational sense**.
- We recall that in the variational setting we set $p_{\theta^\star, t_i|t_{i+1}}(x_{t_i}|x_{t_{i+1}}) = q_{t_i|t_{i+1},0}(x_{t_i}|x_{t_{i+1}}, \mathbf{t}_{\theta^\star}(t_{i+1}, x_{t_{i+1}}))$.
- $\mathbf{t}_{\theta^\star}(t_{i+1}, \cdot)$ is trained with the loss

$$\boxed{\ell_{t_{i+1}}(\theta) = \mathbb{E}[\|\mathbf{t}_\theta(t_{i+1}, X_{t_{i+1}}) - X_0\|^2]\ .}$$

- **Take-home** message: *all* $p_{\theta^\star, t_i|t_{i+1}}(x_{t_i}|x_{t_{i+1}})$ with $t_i < t_{i+1}$ can be computed using $\mathbf{t}_{\theta^\star}(t_{i+1}, x_{t_{i+1}})$.

# Choosing the best subsample

- Given a **subsample** $t_{k_0} = 0 < t_{k_1} < \cdot < t_{k_K} = T$ ($\mathcal{K} = \{t_{k_0}, \ldots, t_{k_K}\}$) we have a **variational lower bound**

$$\boxed{\mathcal{L}_{\mathcal{K}} = \mathcal{L}_T + \sum_{i=1}^{K-1} \mathcal{L}_{t_{k_{i+1}}, t_{k_i}} + \mathcal{L}_{t_{k_1}, 0} \ .}$$

- where:

- $\mathcal{L}_T = \int_{\mathbb{R}^d} \log(p_T(x_T)/q_{T|0}(x_T|x_0)) q(x_T|x_0) \mathrm{d}x_T$.
- $\mathcal{L}_{t_{k_{i+1}}, t_{k_i}} = \int_{\mathbb{R}^d} \log(p_{\theta, t_{k_i}|t_{k_{i+1}}}(x_{t_{k_i}}|x_{t_{k_{i+1}}})/q(x_{t_{k_i}}|x_{t_{k_{i+1}}}, x_0)) q(x_{t_{k_i}}|x_{t_{k_{i+1}}}, x_0) \mathrm{d}x_{t_{k_i}}$.
- $\mathcal{L}_{t_{k_1}, 0} = \int_{\mathbb{R}^d} \log(p_{\theta, 0, t_{k_1}}(x_0|x_{t_{k_1}})) q(x_{t_{k_1}}|x_0) \mathrm{d}x_{t_{k_1}}$.

- To compute $\{\mathcal{L}_{t,s} \ : \ s, t \in \mathcal{T}, \ s < t\}$, we only need $\mathcal{T}$ **forward call** to the network $\mathbf{t}_{\theta^\star}$.

- A **budget** of $K$ steps, which **subsample** $\mathcal{L}_{\mathcal{K}}$ yields the **higher variational bound**?

- If $|\mathcal{K}| \ll |\mathcal{T}|$ then sampling time is **heavily reduced**.

# Dynamic programming

- Create matrices $\mathrm{C} \in \mathbb{R}^{K+1\times N+1}$, $\mathrm{D} \in \mathbb{R}^{K+1\times N+1}$ (recall that $|\mathcal{K}| = K+1$ and $|\mathcal{T}| = N+1$)
- where:
  - $\mathrm{C}(m,n)$ is the **minimal cost** to reach $t_n$ in $m$ steps, i.e.

$$\boxed{\mathrm{C}(m,n) = \min\{\textstyle\sum_{i=1}^{m-1} \mathcal{L}_{t_{k_{i+1}},t_{k_i}} + \mathcal{L}_{t_{k_1},0} \ : \ \mathcal{K} = \{t_{k_0} = 0, \dots, t_{k_m} = t_n\}\} \ .}$$

  - $\mathrm{D}(m,n) = k_{m-1}$ in the decomposition $\mathcal{K} = \{t_{k_0} = 0, t_{k_1}, \dots, t_{k_{m-1}}, t_{k_m} = t_n\}$ which minimizes the **previous cost**.
- We can **fill the lines** recursively using that

$$\mathrm{C}(m,n) = \min\{C(m-1,\ell) + \mathcal{L}_{t_n,t_\ell} \ : \ \ell \in \{0,\dots,N\}, \ t_\ell < t_n\} \ ,$$
$$\mathrm{D}(m,n) = \arg\min\{C(m-1,\ell) + \mathcal{L}_{t_n,t_\ell} \ : \ \ell \in \{0,\dots,N\}, \ t_\ell < t_n\} \ .$$

- Then, the **optimal decomposition** is given by $\mathcal{K} = \{t_{k_0}, \dots, t_{k_K}\}$, where for any $i \in \{0,\dots,K-1\}$, $k_{K-i} = D(K-i, k_{K-i+1})$, with $k_K = N$.
- This is a **dynamic programming** procedure Dijkstra et al. (1959).

# Subsampling results

- Running the **dynamic program** we find the following decomposition

**Figure 8:** Budget of stepsizes. Image extracted from Watson et al. (2021).

- **Consequences**:
  - **More stepsize** near the **data distribution**.
  - **Larger stepsizes** near the **easy-to-sample** distribution.

# Limitations and Extensions

- **Optimizing** the **ELBO** does *not* always correlate with better **FID**.

**Figure 9:** Top and middle are samples (Imagenet) obtained using preset stride strategies. Bottom is the discovering strategy from Watson et al. (2021). Image extracted from Watson et al. (2021).

- Improvement Watson et al. (2022) by differentiating through sample quality (Differentiable Diffusion Sampler Search).
- **Differenciation** through the sampling process. **DDSS** optimize the **Kernel Inception Distance** Bińkowski et al. (2018).

# Conclusion

# Conclusion

- We have introduced **score-based generative models**.
  - Score-based generative models in **continuous time** and results.
  - **Normalizing flows** and **Likelihood computation**.
  - **Acceleration** of SGMs.

- Next time:
  - Introduction of **Schrödinger bridges**.
  - Connection with **Optimal transport**.
  - Introduction of the **Sinkhorn algorithm**.

***See you all on the 14/03!***

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