Denoising Diffusion models

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Outline of the course (1/2)

- **Course 1**: Denoising Diffusion Models (introduction & tricks) **(06/02)**
  - Introduction of diffusion models.
  - Connection with ancestral sampling.
  - A variational approach.
- **Course 2**: Denoising Diffusion Models (theory & methodology) **(13/02)**
  - Stochastic processes and time-reversal.
  - Diffusion models as maximum likelihood models.
  - Some extensions of score-based generative models.
  - **Lab session**: implementing a denoising diffusion model.
- Pause **(20/02)**

Outline of the course (2/2)

- **Course 3**: Denoising Diffusion models for inverse problems **(27/02)**
  - Some inverse problems.
  - Denoising Diffusion Restoration Models.
  - Replacement method.
  - Conditioning of the score and guidance.
- **Course 4**: Stable diffusion **(06/03)**
  - Deep dive in stable diffusion.
  - Text conditioning (CLIP).
  - Hierarchical models.
  - **Lab session**: Stable diffusion.
- **Course 5**: Towards Schrödinger bridges **(13/03)**
  - Beyond score-based generative models.
  - The dynamical Schrödinger Bridge problem.
  - Iterative Proportional Fitting.
  - Diffusion Schrödinger Bridge.
  - **Exercise session**: Entropic Optimal Transport and Schrödinger Bridges.

Introduction of denoising diffusion models

- A new **contender**:
  - Denoising **Diffusion Models** also called **Score-Based Generative Models**.
- Having a hard time keeping up with the literature?
  - List of references: https://scorebasedgenerativemodeling.github.io/
- Advantages of the method:
  - **State-of-the-art** results Dhariwal and Nichol (2021); Karras et al. (2022).
  - **High flexibility** Poole et al. (2022); Rombach et al. (2022); Balaji et al. (2022); Saharia et al. (2022).
  - **Theoretical analysis** De Bortoli et al. (2021b); Chen et al. (2022); Pidstrigach (2022); Lee et al. (2022).
- Some drawbacks:
  - **Statistical understanding** is still limited.

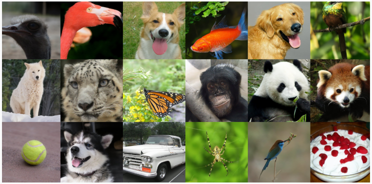
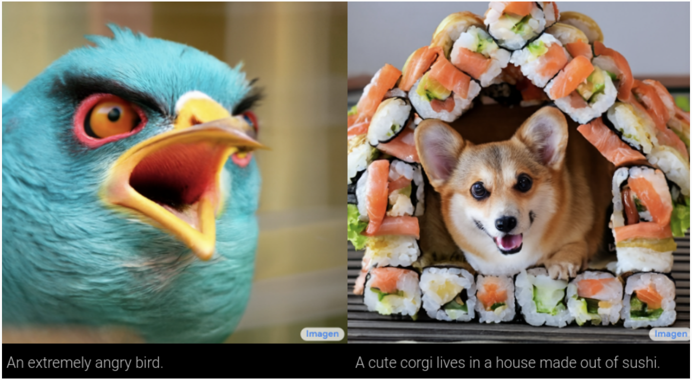


Figure 1: DDM results. Image extracted from Dhariwal and Nichol (2021).

An application: text-to-image

- Text-to-image: Imagen Saharia et al. (2022), DALL-E 2 Ramesh et al. (2022), Stable Diffusion Rombach et al. (2022), Midjourney, EDiff Balaji et al. (2022).



- **CLIP** (Contrastive **L**anguage–**I**mage **P**re-training) Radford et al. (2021).

And beyond images...

Outline

- **Goal of the course**:
  - Introduce DDM in with time-reversal (without relying on stochastic calculus).
  - Present link with other models.

- **Outline of the course**:
  - Introduction of DDM with discrete-time reversal.
  - Introduction of DDM with variational approaches.

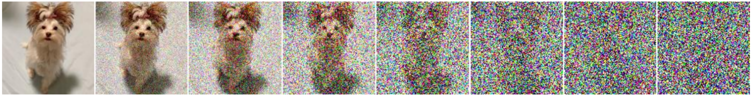


Figure 2: Noising process in DDM. Image extracted from Song et al. (2020b).

Discrete time-reversal and score-based generative modeling

Outline of the section

- In this section we introduce DDM in a **“direct” manner**.
- A bit of “history”:
  - First paper (variational approach) Sohl-Dickstein et al. (2015).
  - First successful application Song and Ermon (2019).
  - Concurrently (variational approach) Ho et al. (2020).
- Our presentation is inspired from Song et al. (2020b).
  - Everything is presented in **discrete-time**.
  - Next lecture we will look at a **continuous-time** version.
  - No **variational** interpretation to start with.
- We present some **techniques** to train DDM.
- In what follows:
  - **Time-reversal in discrete-time**.
  - Links with **annealed Langevin**.
  - **Implementation details and tricks**.

Discrete-time

Principles of DDM

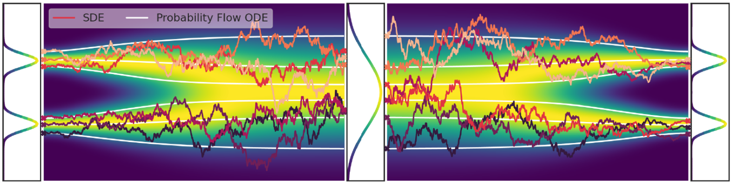


Figure 3: Noising and generative processes in DDM. Image extracted from Song et al. (2020b).

- **Interpolating** between two distributions:
  - The data distribution is denoted $p_{\text{data}} \in \mathcal{P}(\mathbb{R}^d)$.
  - The easy-to-sample distribution is denoted $p_{\text{ref}} \in \mathcal{P}(\mathbb{R}^d)$.
  - p_{ref} is usually the standard multivariate Gaussian.
- Going from the data to the easy-to-sample distribution: **noising process**.
- Going from the easy-to-sample to the data distribution: **generative process**.
- How to **invert** the forward noising process?

Ancestral sampling

- Let $N \in \mathbb{N}$ with $N > 0$ and consider p a density on $(\mathbb{R}^d)^{N+1}$ such that for any $x_{0:N} = \{x_k\}_{k=0}^N$ we have

$$\boxed{p(x_{0:N}) = p_0(x_0) \prod_{k=0}^{N-1} p_{k+1|k}(x_{k+1}|x_k) \ .}$$

- This the **forward** decomposition of p.
- For any $k \in \{0, \dots, N-1\}$ we define the **marginal** p_{k+1} for any $x_{k+1} \in \mathbb{R}^d$

$$p_{k+1}(x_{k+1}) = \int_{\mathbb{R}^d} p_k(x_k) p_{k+1|k}(x_{k+1}|x_k) \mathrm{d}x_k \ .$$

- Assume that for any $k \in \{0, \dots N\}$, $p_k > 0$ and define $p_{k|k+1}$ for any $x_k, x_{k+1} \in \mathbb{R}^d$

$$\boxed{p_{k|k+1}(x_k|x_{k+1}) = \frac{p_{k+1|k}(x_{k+1}|x_k) p_k(x_k)}{p_{k+1}(x_{k+1})} \ .}$$

- We obtain the **backward** decomposition

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

The noising process (1/2)

- The **ancestral sampling** procedure allows to sample from p **backward**.
  - Access to the **backward transitions** $\{p_{k|k+1}\}_{k=0}^{N-1}$?
  - Tractability of the **forward transitions**?
- In practice we consider:
  - p_{data} admits a density p_0 w.r.t. the Lebesgue measure.
  - The **forward decomposition** is a **noising process**

$$\boxed{p(x_{0:N}) = p_0(x_0) \prod_{k=0}^{N-1} p_{k+1|k}(x_{k+1}|x_k) \ .}$$

- How do we go from the data distribution to the easy-to-sample distribution?
  - **Autoregressive Process**: $X_{k+1} = \alpha X_k + \sqrt{1-\alpha^2} Z_{k+1}$ for $\{Z_k\}_{k \in \mathbb{N}}$ i.i.d. N$(0, \mathrm{Id})$ Gaussian and $alpha < 1$.
  - $\mathrm{Law}(x_k) \to \mathcal{N}(0, \mathrm{Id})$ exponentially fast as $k \to \infty$ (in Wasserstein, TV)

Inverting the noising process (1/3)

- **Ornstein-Ulhenbeck** process: $\mathrm{d}\mathbf{X}_t = -\mathbf{X}_t \mathrm{d}t + \sqrt{2}\mathrm{d}\mathbf{B}_t$.
- **Euler-Maruyama** discretization: $X_{k+1} = (1-\gamma)X_k + \sqrt{2\gamma}Z_{k+1}$.
- **Euler-Maruyama** discretization of the **Ornstein-Ulhenbeck** process converges **exponentially** fast towards $\mathrm{N}(0, \mathrm{Id}/(1-\gamma/2))$.
- Now let us try to **invert** the forward noising process.

$$
\begin{aligned}
&p_{k|k+1}(x_k|x_{k+1}) = p_{k+1|k}(x_{k+1}|x_k)p_k(x_k)/p_{k+1}(x_{k+1}) \\
&= C_0 \exp[-\|x_{k+1} - (1-\gamma)x_k\|^2/(4\gamma)] \exp[\log(p_k(x_k)) - \log(p_{k+1}(x_{k+1}))] \\
&= C_1 \exp[-\|x_{k+1} - (1-\gamma)x_k\|^2/(4\gamma)] \exp[\log(p_k(x_k)) - \log(p_k(x_{k+1}))] \\
&= C_1 \exp[-(\|x_{k+1} - (1-\gamma)x_k\|^2 + 4\gamma\{\log(p_k(x_k)) - \log(p_k(x_{k+1}))\})/(4\gamma)] \; .
\end{aligned}
$$

  - $C_0, C_1 > 0$ constants which depend only on x_{k+1}.
  - $\|x_{k+1} - (1-\gamma)x_k\|^2 =$
    $\|x_k - (1+\gamma)x_{k+1}\|^2 - 2\gamma\|x_{k+1} - x_k\|^2 + \gamma^2\{\|x_k\|^2 - \|x_{k+1}\|^2\}$.
  - $\log(p_k(x_k)) = \log(p_k(x_{k+1})) + \langle \nabla \log p_k(x_{k+1}), x_k - x_{k+1}\rangle +$
    $\int_0^1 \nabla^2 \log p_k((1-t)x_{k+1} + tx_k)(x_k - x_{k+1})^{\otimes 2}\mathrm{d}t$.

Inverting the noising process (2/3)

- **Assumption:** $\|x_{k+1} - x_k\|^2 \leq C\gamma$ and $\max(\|x_k\|, \|x_{k+1}\|) \leq C$
  - $\left|\|x_{k+1} - (1-\gamma)x_k\|^2 - \|x_k - (1+\gamma)x_{k+1}\|^2\right| \leq 4C\gamma^2$.
  - $|\log(p_k(x_k)) - \log(p_{k+1}(x_{k+1})) - \langle \nabla \log p_k(x_{k+1}), x_k - x_{k+1}\rangle| \leq D\gamma$.
- Hence, we get that

$$
\begin{aligned}
p_{k|k+1}(x_k|x_{k+1}) &\approx C_2 \exp[-\|x_k - (1+\gamma)x_{k+1}\|^2/(4\gamma)] + \langle \nabla \log p_k(x_{k+1}), x_k - x_{k+1}\rangle] \\
&\approx \mathrm{N}(x_k; x_{k+1} + \gamma\{x_{k+1} + 2\nabla \log p_k(x_{k+1})\}, 2\gamma\, \mathrm{Id})
\end{aligned}
$$

  - The **approximation** is up to a term of order γ in the exponential.
- **Sampling** from the **backward chain**: $X_N \sim p_{\mathrm{ref}}$

$$
\boxed{X_k = X_{k+1} + \gamma\{X_{k+1} + 2\nabla \log p_k(X_{k+1})\} + \sqrt{2\gamma} Z_{k+1}\ .}
$$

- $\nabla \log p_k$ is **untractable**. We are going to approximate this term.

Score-matching (1/4)

- The term $\nabla \log p_k$ is the called the **(Stein) score**.
- Literature on **score matching**: Hyvärinen (2005); Vincent (2011)
- We have the following identity; see e.g. Efron (2011)

$$\begin{aligned}\nabla \log p_k(x_k) &= \nabla p_k(x_k)/p_k(x_k) \\ &= \int_{\mathbb{R}^d} \nabla \log p_{k|0}(x_k|x_0)\ p_{0,k}(x_0, x_k)\mathrm{d}x_0/p_k(x_k) \\ &= \int_{\mathbb{R}^d} \nabla \log p_{k|0}(x_k|x_0)\ p_{0|k}(x_0|x_k)\mathrm{d}x_0\ .\end{aligned}$$

- This can be rewritten

$$\boxed{\nabla \log p_k(x_k) = \mathbb{E}_{p_{0|k}(\cdot|x_k)}[\nabla \log p_{k|0}(x_k|X_0)]\ .}$$

- An **intermediate expression**:
  - $\nabla \log p_{k|0}(x_k|x_0)$ is tractable (forward transition).
  - The **conditional expectation** is not (backward conditional).
- We are going to use the property of the conditional expectation to obtain a **loss function**.

Score matching (2/4)

- We use the following properties of the **conditional expectation**:
  - $Y = \mathbb{E}[X \,|U]$ if $Y = f(U)$, with $f = \arg\min\{\mathbb{E}[\|X - f(U)\|^2] \;:\; f \in \mathrm{L}^2(U)\}$.
- Recall that we have

$$\boxed{\nabla \log p_k(X_k) = \mathbb{E}[\nabla \log p_{k|0}(X_k|X_0)|X_k] \;.}$$

- Using the previous property we have

$$\boxed{\nabla \log p_k = \arg\min\{\mathbb{E}[\|f(X_k) - \nabla \log p_{k|0}(X_k|X_0)\|^2] \;:\; f \in \mathrm{L}^2(p_k)\} \;.}$$

- We obtain a **loss function**:
  - $\nabla \log p_{k|0}(x_k|x_0)$ is tractable (forward transition).
  - The expectation can be approximated with **Monte Carlo** (joint distribution).
- Note that this is valid for $k \in \{0, \ldots, N-1\}$.

Score matching (3/4)

- Recall that the loss function is given by

$$\boxed{\nabla \log p_k = \arg\min\{\mathbb{E}[\|f(X_k) - \nabla \log p_{k|0}(X_k|X_0)\|^2] \;:\; f \in \mathrm{L}^2(p_k)\}\ .}$$

- This **loss function** is called the **D**enoising **S**core **M**atching loss.
  - $\log p_{k|0}(x_k|x_0) = -\|x_k - m_k x_0\|^2/(2\sigma_k^2) + C_k$
  - $m_k = (1-\gamma)^k$, $\sigma_k^2 = \{1-(1-\gamma)^{2k}\}/(1-\gamma/2)$, C_k independent of x_k.
  - $\nabla \log p_{k|0}(x_k|x_0) = -(x_k - m_k x_0)/\sigma_k^2$.
  - $X_k = m_k X_0 + \sqrt{2\gamma}\sum_{j=1}^{k}(1-\gamma)^{k-j} Z_k = m_k X_0 + \sigma_k \hat{Z}_{j+1}$, $\hat{Z}_k \sim \mathrm{N}(0, \mathrm{Id})$.
  - $\nabla \log p_{k|0}(X_k|X_0) = -\hat{Z}_k/\sigma_k^2$.
  - f tries to **predict the residual noise**.

- Another formulation: the loss satisfies

$$\begin{aligned}&\mathbb{E}[\|f(X_k) - \nabla \log p_{k|0}(X_k|X_0)\|^2] \\ &\quad = \mathbb{E}[\|f(X_k)\|^2] - 2\mathbb{E}[\langle f(X_k), \nabla \log p_{k|0}(X_k|X_0)\rangle] + \mathbb{E}[\|\nabla \log p_{k|0}(X_k|X_0)\|^2]\ .\end{aligned}$$

Score matching (4/4)

- The scalar product satisfies

$$\begin{aligned}\mathbb{E}[\langle f(X_k), \nabla \log p_{k|0}(X_k|X_0)\rangle \,|X_0] &= \int_{\mathbb{R}^d} \langle f(x_k), \nabla \log p_{k|0}(x_k|X_0)\rangle p_{k|0}(x_k|X_0)\mathrm{d}x_k \\ &= \int_{\mathbb{R}^d} \langle f(x_k), \nabla p_{k|0}(x_k|X_0)\rangle \mathrm{d}x_k \\ &= -\int_{\mathbb{R}^d} \mathrm{div}(f(x_k)) p_{k|0}(x_k|X_0)\mathrm{d}x_k \\ &= -\mathbb{E}[\mathrm{div}(f(X_k))\,|X_0]\ .\end{aligned}$$

- Hence the loss satisfies

$$\begin{aligned}&\mathbb{E}[\|f(X_k) - \nabla \log p_{k|0}(X_k|X_0)\|^2] \\ &\quad = \mathbb{E}[\|f(X_k)\|^2 + 2\mathrm{div}(f(X_k))] + \mathbb{E}[\|\nabla \log p_{k|0}(X_k|X_0)\|^2]\ .\end{aligned}$$

- We obtain the **I**mplicit **S**core **M**atching loss function

$$\boxed{\nabla \log p_k = \arg\min\{\mathbb{E}[\tfrac{1}{2}\|f(X_k)\|^2 + \mathrm{div}(f(X_k))] \ : \ f \in \mathrm{L}^2(p_k)\}\ .}$$

- Comparison between ISM/DSM:
  - **DSM**: access to $\nabla \log p_{k|0}$.
  - **ISM**: no need of the **transition density** but computation of a **divergence**.
  - Approximation with the **Hutchinson estimator**.

Training algorithm

- We choose the **DSM** or **ISM** loss for all $k \in \{1, \dots, N\}$
  - $\mathrm{DSM}_k(f) = \mathbb{E}[\|f(X_k) - \nabla \log p_{k|0}(X_k|X_0)\|^2]$.
  - $\mathrm{ISM}_k(f) = \mathbb{E}[\frac{1}{2}\|f(X_k)\|^2 + \mathrm{div}(f(X_k))]$.

- Defining the **integrated** loss:
  - $\ell^{\mathrm{DSM}}(f) = \sum_{k=1}^{N} \lambda_k \mathrm{DSM}_k(f(k, \cdot))$,
  - $\ell^{\mathrm{ISM}}(f) = \sum_{k=1}^{N} \lambda_k \mathrm{ISM}_k(f(k, \cdot))$.
  - We define a **weighting** function $\lambda_k \geq 0$.

- Let $\{\mathbf{s}_\theta\}_{\theta \in \Theta}$ a **a parametric family of functions** such that $\mathbf{s}_\theta : \mathbb{R}_+ \times \mathbb{R}^d \to \mathbb{R}^d$.
  - Usually $\{\mathbf{s}_\theta\}_{\theta \in \Theta}$ is a family of **neural networks**.
  - We optimize $\ell^{\mathrm{DSM}}(\theta) = \ell^{\mathrm{DSM}}(\mathbf{s}_\theta)$ or $\ell^{\mathrm{ISM}}(\theta) = \ell^{\mathrm{ISM}}(\mathbf{s}_\theta)$.

Backward sampling

- Recall the goal:
  - Sample from $p(x_{0:N}) = p_N(x_N) \prod_{k=0}^{N-1} p_{k|k+1}(x_k|x_{k+1})$ (**ancestral sampling**).
  - **Approximate backward**

$$\boxed{p_{k|k+1}(x_k|x_{k+1}) \approx \mathrm{N}(x_k; x_{k+1} + \gamma\{x_{k+1} + 2\nabla \log p_k(x_{k+1})\}, 2\gamma \, \mathrm{Id}).}$$

  - **Approximation of the score** (**DSM** or **ISM** losses).
- Once $\mathbf{s}_{\theta^\star}$ is learned via DSM or ISM losses, i.e. $\mathbf{s}_{\theta^\star}(k, \cdot) \approx \nabla \log p_k$.
- **Sampling scheme**:
  - $X_N \sim \mathrm{N}(0, \mathrm{Id})$ (approximate sampling from p_N).
  - **Approximate ancestral sampling**

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

  - X_1 is approximately distributed according to the **data-distribution**.
- Some remarks:
  - Time-reversal can be obtained in **continuous-time**.
  - Original approach relies on **annealed Langevin** Song and Ermon (2019).
  - Other approaches Ho et al. (2020); Gao et al. (2020).

Links with annealed Langevin

Failure of the score-estimation

- We now present (one) **original approach** by Song and Ermon (2019).
- Goal: **sampling** from the **data distribution** p_0.
  - **Langevin algorithm**: $X_{k+1} = X_k + \gamma \nabla \log p_0(X_k) + \sqrt{2\gamma} Z_{k+1}$.
  - Estimation of the **Stein score** $\nabla \log p_0$ with ISM

$$\boxed{\nabla \log p_0 = \arg\min \{\mathbb{E}[\tfrac{1}{2}\|f(X)\|^2 + \mathrm{div}(f(X))] \ : \ f \in \mathrm{L}^2(p_0)\} \ .}$$

  - $X \sim p_0$.
- **Problems**:
  - **Slow mixing** with Langevin algorithm (non-convexity Eberle (2016)).
  - **Bad score** approximation.

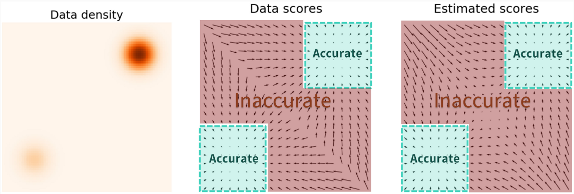


Figure 4: Image extracted from an online tutorial blogpost.

The power of smoothing

- A solution: **smoothing** the density.
  - **Spreading** the observations lead to **better score estimations**.
  - Smoothing leads to **better landscapes** of the potential and **faster mixing** (removal of spurious minima).
- Problem: we do not target the right density.
  - $p_\sigma = p * \mathrm{N}(0, \sigma^2)$.
  - We have that $\mathrm{Var}(p_\sigma) = \mathrm{Var}(p) + \sigma^2$.
- **Trade-off**:
  - **Small value** of σ: close to p_0, hard to sample.
  - **Large value** of σ: far from p_0, easy to sample.

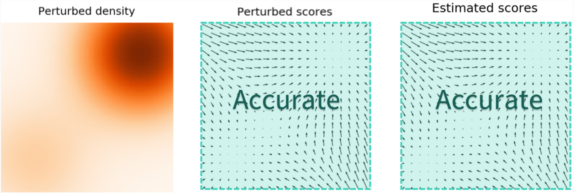


Figure 5: Image extracted from an online tutorial blogpost.

The best of both worlds

- The main of idea of Song and Ermon (2019): **annealed Langevin** dynamics.
  - Starting from a large value of σ_T, sample easily using the **Langevin dynamics**.
  - Reduce the value of $\sigma_T > \sigma_{T-1}$ and **warm-start** the new Langevin dynamics with the previous samples.
  - Repeat the procedure with σ_0 very small (close to the target density).
  - This is an **annealed** procedure.

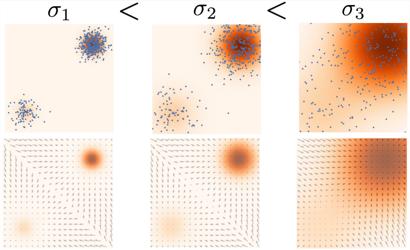


Figure 6: Image extracted from an online tutorial blogpost.

Annealing algorithm

Algorithm 1 Sampling of annealing Langevin dynamics

Input: $\{\sigma_t\}_{t=1}^T$, $\{\gamma\}_{t=1}^T$, K
Initialize $X_T^0 \sim \mathcal{N}(0, \sigma_T \,\mathrm{Id})$.
for $t = T$ to 1 **do**
  for $k = 0$ to $K - 1$ **do**
    Sample $X_t^{k+1} = X_t^k + \gamma_t \mathbf{s}_\theta(\sigma_t, X_t^k) + \sqrt{2\gamma_t} Z_t^{k+1}$
  end for
  $X_{t-1}^0 = X_t^K$
end for
Return X_0^0.

- If $K = 1$ then it is **equivalent to the time-reversal** except that:
  - $\{\gamma_t\}_{t=1}^T$ is *a priori* unrelated to $\{\sigma_t\}_{t=1}^T$ contrary to the time-reversal approach where we would have $\gamma_t = \gamma$ and $\sigma_t^2 = t\gamma$.
  - Main difference is that the **forward** process is the discretization of a **Brownian motion** and not a **Ornstein-Ulhenbeck** process.
  - $X_{k+1} = X_k - \gamma X_k + \sqrt{2\gamma} Z_{k+1}$ in the Ornstein-Ulhenbeck setting and $X_{k+1} = X_k + \sqrt{2\gamma} Z_{k+1}$ in the Brownian case.

Implementation details and tricks

Careful implementation is necessary

- Originally these models were **hard** to train Song and Ermon (2019), see also this blogpost.
- In what follows we describe a **series of tricks** which greatly facilitate the training of these models. These tricks can be found in Song et al. (2020b); Song and Ermon (2020); Nichol and Dhariwal (2021); Ho and Salimans (2021); De Bortoli et al. (2021a); Karras et al. (2022).
- We *do not* discuss the **architecture** here.
- In what follows we discuss the following tricks:
  - Ornstein-Ulhenbeck and discretization
  - Loss function weighting.
  - Exponential Moving Average.
  - Adapted variance and predictor-corrector.
  - Conditional sampling and classifier-free guidance.
  - **(not covered)** Better sampler.
  - **(not covered)** Better architectures.
  - **(not covered)** Self-conditioning.
  - **(not covered)** Latent and hierarchical diffusions.

Ornstein-Ulhenbeck and discretization

- We have introduced **denoising diffusion models** as the discretization of a **Ornstein-Ulhenbeck** process:
  - **Target measure** is $\mathrm{N}(0, \mathrm{Id})$ (approximately), the data should be centered and reduced.
  - **Constant** stepsize discretization is *not* what is done in practice.
- In practice we consider a **schedule** on the stepsize:

$$\boxed{X_k = X_{k+1} + \gamma_k \{X_{k+1} + 2\mathbf{s}_\theta(\textstyle\sum_{j=0}^{k} \gamma_j, X_{k+1})\} + \sqrt{2\gamma_k} Z_{k+1} \ .}$$

  - Linear schedule $\gamma_k = \gamma_{\min} + (\gamma_{\max} - \gamma_{\min})(N-k)/N$ Song et al. (2020b).
  - **Intuition**: we need more stepsizes near the data distribution.
  - Different schedules (cosine, hyperbolic tangent) Song and Ermon (2019); Ho et al. (2020); Nichol and Dhariwal (2021); Karras et al. (2022).

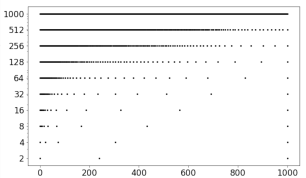


Figure 7: Budget of stepsizes. Image extracted from Watson et al. (2021).

Loss function weighting

- In practice a **weighted** version of the **DSM** loss is used.
  - Recall that the **DSM** loss is given by $\mathrm{DSM}_k(f) = \mathbb{E}[\|f(X_k) - \nabla \log p_{k|0}(X_k|X_0)\|^2]$.
  - $\ell^{\mathrm{DSM}}(f) = \sum_{k=1}^{N} \lambda_k \mathrm{DSM}_k(f(k, \cdot))$.
  - $\nabla \log p_{k|0}(X_k|X_0) = -\hat{Z}_k/\sigma_k^2$
- **Intuition**: λ_k function of σ_k to **stabilize** the loss Song et al. (2020b).
- Additional remarks:
  - In Ho et al. (2020); Nichol and Dhariwal (2021) this loss is given by L_{simple}.
  - Justification with **Girsanov** theory in Song et al. (2021); Huang et al. (2021).
  - Changing the **discretization schedule** is equivalent to do a **time-change** in the original Ornstein-Ulhenbeck process then a **fixed discretization**.

Exponential Moving Average

- The training of the network is **unstable**.
- To regularize this we consider an **E**xponential **M**oving **A**verage of weights.

$$\boxed{\bar{\theta}_{n+1} = (1-m)\bar{\theta}_n + m\theta_n \ .}$$

  - The parameter m corresponds to the **forgetting** of the initial conditions.
  - The parameters $\bar{\theta}_K$ are used at **sampling** times (K is the number of training steps).

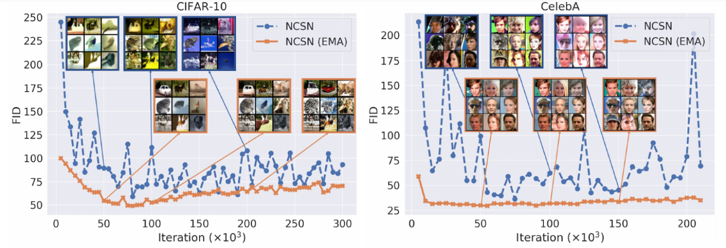


Figure 8: Training instabilities. Image extracted from Song and Ermon (2020).

Adapted variance and predictor-corrector

- Recall that we consider the following **Euler-Maruyama discretization**

$$\boxed{X_k = X_{k+1} + \gamma_k\{X_{k+1} + 2\mathbf{s}_\theta(\textstyle\sum_{j=0}^k \gamma_j, X_{k+1})\} + \sqrt{2\gamma_k} Z_{k+1}\ .}$$

- Instead of a classical Euler-Maruyama discretization we can consider a **Modified Euler-Maruyama** scheme Durham and Gallant (2002).
  - Replace the term $2\gamma_k$ by $2\gamma_k\{\sum_{j=1}^{k-1}\gamma_j / \sum_{j=1}^{k}\gamma_j\}$.
  - This discretization scheme can be found in the literature on **stochastic bridges** De Bortoli et al. (2021a).
  - **Intuition:** smaller variance near the **data distribution**.
- We can also correct the Euler-Maruyama scheme using the **time-reversal** property.
  - We must have $\mathcal{L}(X_k) \approx p_k$.
  - Hence we go from X_{k+1} to $\hat{X}_k$ with the Euler-Maruyama scheme (**predictor**).
  - We refine $\hat{X}_k$ by running a Langevin chain targeting p_k (**corrector**).

$$\boxed{X_k^0 = \hat{X}_k\ , \qquad X_k^{\ell+1} = X_k^\ell + \delta_k \gamma \mathbf{s}_\theta(\textstyle\sum_{j=0}^k \gamma_j, X_k) + \sqrt{2\delta_k} Z_k^{\ell+1}\ .}$$

  - $\{\delta_k\}_{k=0}^N$ is a sequence of stepsizes and we set $X_k = X_k^L$ ($L \in \mathbb{N}$).

Conditional sampling and classifier-free guidance

- If the data distribution contains **classes** (like MNIST, CIFAR-10, LSUN, ImageNet or CelebA when classifying by attributes) then we can exploit this extra **structure**.
- Define a **conditional score** $\mathrm{DSM}_k(f) = \mathbb{E}[\|f(X_k^c, c) - \nabla \log p_{k|0}(X_k^c|X_0^c)\|^2]$.
  - $c \in \{1, \ldots, C\}$ is the class of the image.
  - Then, we can (approximately) sample from the class c by considering $X_N^c \sim \mathrm{N}(0, \mathrm{Id})$

$$\boxed{X_k^c = X_{k+1}^c + \gamma_k\{X_{k+1}^c + 2\mathbf{s}_\theta(\textstyle\sum_{j=0}^k \gamma_j, X_{k+1}^c, c)\} + \sqrt{2\gamma_k} Z_{k+1}\ .}$$

Figure 9: Class conditional generation. Image extracted from Song et al. (2020b).

- Other improvements with **unconditional guidance** Ho and Salimans (2021) or **classifier guidance** Dhariwal and Nichol (2021).

Other approaches

Links with other models

- Until now we have presented two approaches to derive **denoising diffusion models** (DDMs) :
  - A discrete-time **time-reversal** approach.
  - An **annealed Langevin** approach.
- The time-reversal approach is now widely used Song et al. (2020b).

- We now present links with other **generative models**:
  - DDMs as **variational autoencoders** Ho et al. (2020).
- The connection with variational autoencoders allows for:
  - **Extension** to discrete settings
  - **Acceleration** of the sampling dynamics Watson et al. (2021)

- In the next sessions we will see links with **normalizing flows** and **GANs**.

Connections with Variational AutoEncoders

A variational perspective

- We follow the approach of Ho et al. (2020).
- **Variational approach** offers great flexibility:
  - Optimization of the stepsize Watson et al. (2021).
  - Learning of the covariance matrix Nichol and Dhariwal (2021).
  - Non-Markov dynamics Song et al. (2020a).
- Ho et al. (2020) was the first to propose a **discretized Ornstein-Ulhenbeck** Markov chain as a forward process.

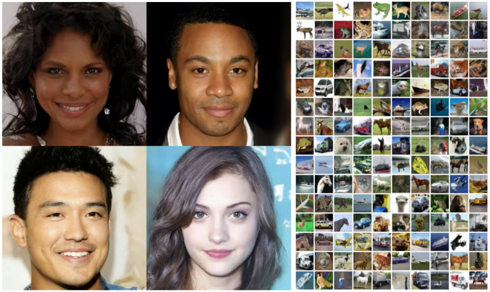


Figure 10: CelebA and CIFAR10 results. Image extracted from Ho et al. (2020).

An Evidence Lower BOund (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**

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

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

$$
\boxed{q_{k+1|k}(x_{k+1}|x_k) = \mathrm{N}(x_{k+1}; (1-\gamma)x_k, 2\gamma \,\mathrm{Id}).}
$$

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

An Evidence Lower BOund (2/2)

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

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

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

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

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

The backward $q_{k|k+1,0}$ (1/2)

- To compute $\mathcal{L}_k$ we need to compute $q_{k|k+1,0}$.
- We know that $q_{k|k+1,0}$ is **Gaussian** with **diagonal covariance** and just need to compute its parameter.
- $q_{k|0} = \mathrm{N}(\alpha_k x_0, \sigma_k \,\mathrm{Id})$ and $q_{k+1|k} = \mathrm{N}(\alpha_{k+1|k}, \sigma_{k+1|k} \,\mathrm{Id})$.
- **Computing the parameters**:
  - $\alpha_{k+1|k} = 1 - \gamma$, $\sigma^2_{k+1|k} = 2\gamma$.
  - $X_{k+1} = (1-\gamma)^k X_0 + \sqrt{2\gamma} \sum_{j=1}^k (1-\gamma)^{k-j} Z_{j+1} = (1-\gamma)^k X_0 + \sigma_{k+1} \hat{Z}_{k+1}$.
  - $\hat{Z}_{k+1} \sim \mathrm{N}(0, \mathrm{Id})$ and $\sigma^2_{k+1} = (1 - (1-\gamma)^{2k})/(1-\gamma/2)$.
  - $\alpha_{k+1} = (1-\gamma)^k$, $\sigma^2_{k+1} = (1 - (1-\gamma)^{2k})/(1-\gamma/2)$.
- We have that

$$\boxed{q_{k|k+1,0}(x_k|x_{k+1}, x_0) = q_{k+1|k}(x_{k+1}|x_k) q_{k|0}(x_k|x_0) / q_{k+1|0}(x_{k+1}|x_0)\ .}$$

  - We can **discard the denominator** (normalizing constant).
  - We can focus on $\log(q_{k+1|k}(x_{k+1}|x_k) q_{k|0}(x_k|x_0))$.

The backward $q_{k|k+1,0}$ (2/2)

- We have that

$$
\begin{aligned}
& -2\log(q_{k+1|k}(X_{k+1}|X_k)q_{k|0}(X_k|X_0)) \\
&= \|X_{k+1}-\alpha_{k+1|k}X_k\|^2/\sigma^2_{k+1|k} + \|X_k-\alpha_k X_0\|^2/\sigma^2_k \\
&= \{\alpha^2_{k+1|k}/\sigma^2_{k+1|k} + (1/\sigma^2_k)\}\|X_k\|^2 - 2\langle \alpha_{k+1|k}/\sigma^2_{k+1|k}X_{k+1} + \alpha_k/\sigma^2_k X_0, X_k\rangle + C \\
&= (1/\sigma^2_{k|k+1})\|X_k\|^2 \\
&\qquad - 2\langle\{\alpha_{k+1|k}/\sigma^2_{k+1|k} + \alpha_k/(\alpha_{k+1}\sigma^2_k)\}X_{k+1} + \alpha_k\sigma_{k+1}/(\alpha_{k+1}\sigma^2_k)\hat{Z}_{k+1}, X_k\rangle + C \\
&= (1/\sigma^2_{k|k+1})\|X_k\|^2 - (2/\sigma^2_{k|k+1})\langle A_{k|k+1}X_{k+1} - B_{k|k+1}\hat{Z}_{k+1}, X_k\rangle + C \\
&= \|X_k - A_{k|k+1}X_{k+1} + B_{k|k+1}\hat{Z}_{k+1}\|^2/(2\sigma^2_{k|k+1}) + D\,.
\end{aligned}
$$

  - C, D constants **independent** from x_k.
  - $\sigma^2_{k|k+1} = (\alpha^2_{k+1|k}/\sigma^2_{k+1|k} + (1/\sigma^2_k))^{-1}$.
  - $A_{k|k+1} = \alpha_{k+1|k}(\sigma_{k|k+1}/\sigma_{k+1|k})^2 + \alpha_k\sigma^2_{k|k+1}/(\alpha_{k+1}\sigma^2_k)$.
  - $B_{k|k+1} = (\alpha_k\sigma_{k+1}\sigma^2_{k+1|k})/(\alpha_{k+1}\sigma^2_k)$.
- Therefore, we **choose the family**

$$
\boxed{\log(p_{\theta,k|k+1}(x_k|x_{k+1})) = \|x_k - A_{k|k+1}x_{k+1} + B_{k|k+1}\hat{z}_{\theta,k+1}(x_{k+1})\|^2/(2\sigma^2_{k|k+1}) + E\,.}
$$

- E is a constant, $\hat{z}_{\theta,k+1}(x_{k+1})$ is a function of x_{k+1} (**estimator of the noise**).

Sampling from the model

- How to **train** and **sample** the model?
- Recall that we have set

$$\boxed{\log(p_{\theta,k|k+1}(x_k|x_{k+1})) = \|x_k - A_{k|k+1}x_{k+1} + B_{k|k+1}\hat{z}_{\theta,k+1}(x_{k+1})\|^2/(2\sigma^2_{k|k+1}) + E\ .}$$

- Recall that $p_N = \mathrm{N}(0, \mathrm{Id})$. To **sample from the model**:
  - We sample $X_N \sim \mathrm{N}(0, \mathrm{Id})$
  - We consider the **backward update**

$$\boxed{X_k = A_{k|k+1}X_{k+1} - B_{k|k+1}\hat{z}_{\theta,k+1}(X_{k+1}) + \sigma_{k|k+1}Z_{k+1}\ .}$$

- To **train the model** (without the therm $\mathcal{L}_{1|0}$):
  - Minimize $\sum_{k=1}^{N} \mathcal{L}_k(\theta)$, with

$$\boxed{\mathcal{L}_k(\theta) = \mathbb{E}[\|X_k - A_{k|k+1}X_{k+1} + B_{k|k+1}\hat{z}_{\theta,k+1}(X_{k+1})\|^2]/(2\sigma^2_{k|k+1})\ .}$$

Taylor expansion and comparison with DDM (2/2)

- The model is already **similar to DDM**:
  - We sample from $\mathrm{N}(0, \mathrm{Id})$ and use **ancestral sampling**.
  - We train part of the **drift term**.
- The analogy becomes even stronger when considering **Taylor expansion** of $A_{k|k+1}$, $B_{k|k+1}$ and $\sigma_{k|k+1}$:
  - $A_{k|k+1} = 1 + \gamma + o(\gamma)$.
  - $B_{k|k+1} = 2\gamma + o(\gamma)$.
  - $\sigma^2_{k|k+1} = 2\gamma + o(\gamma)$.
- Hence

$$X_k = A_{k|k+1} X_{k+1} - B_{k|k+1} \hat{z}_{\theta,k+1}(X_{k+1}) + \sigma_{k|k+1} Z_{k+1} \ ,$$

- becomes (up to the first order)

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

- We can identify this recursion with the one of DDM if $\hat{z}_{\theta,k+1} \approx -\nabla \log p_{k+1}$, i.e. the neural network approximates the **score**.

Taylor expansion and comparison with DDM (2/2)

- We want to show that $\hat{z}_{\theta,k+1} \approx -\nabla \log p_{k+1}$, i.e. the neural network approximates the **score**.
- Recall that we minimize the sum of the following **loss functions**

$$\mathcal{L}_k(\theta) = \mathbb{E}[\|X_k - A_{k|k+1}X_{k+1} + B_{k|k+1}\hat{z}_{\theta,k+1}(X_{k+1})\|^2]/(2\sigma_{k|k+1}^2) \ .$$

- Up to the first order we get that

$$\boxed{\mathcal{L}_k(\theta) = \mathbb{E}[\|X_k - (1+\gamma)X_{k+1} + 2\gamma\hat{z}_{\theta,k+1}(X_{k+1})\|^2]/(2\gamma) \ .}$$

- But we have $(1+\gamma)X_{k+1} = (1-\gamma^2)X_k + \sqrt{2\gamma}(1+\gamma)Z_{k+1}$.
- Hence, up to the first order we get that

$$\boxed{\mathcal{L}_k(\theta) = \mathbb{E}[\|\sqrt{2\gamma}Z_{k+1} + 2\gamma\hat{z}_{\theta,k+1}(X_{k+1})\|^2]/(2\gamma) \ ,}$$

- This is exactly the **Denoising Score Matching** loss (up to a minus term) times λ_k (the **weighting function** appearing score-based models being fixed to $\lambda_k = 2\gamma$).

The term $\mathcal{L}_0$

- The previous recursion is valid up to $k = 1$.
- p_θ is an **independent decoder** on the pixel of the image.
- We assume that $x_0 \in [-1, 1]^d$

$$\boxed{p_\theta(x_0|x_1) = \prod_{i=1}^{d} \int_{a(x_0^i)}^{b(x_0^i)} \exp[-\left\|x - \mu_\theta(x_1)\right\|^2 / \sigma_1^2] / (2\pi\sigma_1^2)^d \mathrm{d}x \ .}$$

- $a(t) = t + 1/255$ if $t < 1$ and $+\infty$ otherwise.
- $b(t) = t - 1/255$ if $t > -1$ and $-\infty$ otherwise.
- We could also have chosen the classical (non-discrete) **decoding Gaussian of the VAE**.

Figure 11: CelebA results. Image extracted from Ho et al. (2020).

Conclusion

Conclusion

- We have introduced **denoising diffusion models**.
  - Motivation with **state-of-the-art** results.
  - **Ancestral sampling** and time-reversal (discrete-time).
  - **Tricks** and **implementation**.
  - Connection with **EBM** and **VAE**.

- Next time:
  - Denoising diffusion models in **continuous time** and results.
  - **Normalizing flows** and **Likelihood computation**.
  - **Acceleration** of DDMs.
  - A continuous-time **ELBO** with Girsanov and Feynman-Kac theory.

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