Deep Generative Models: Diffusion Models – SDE perspective

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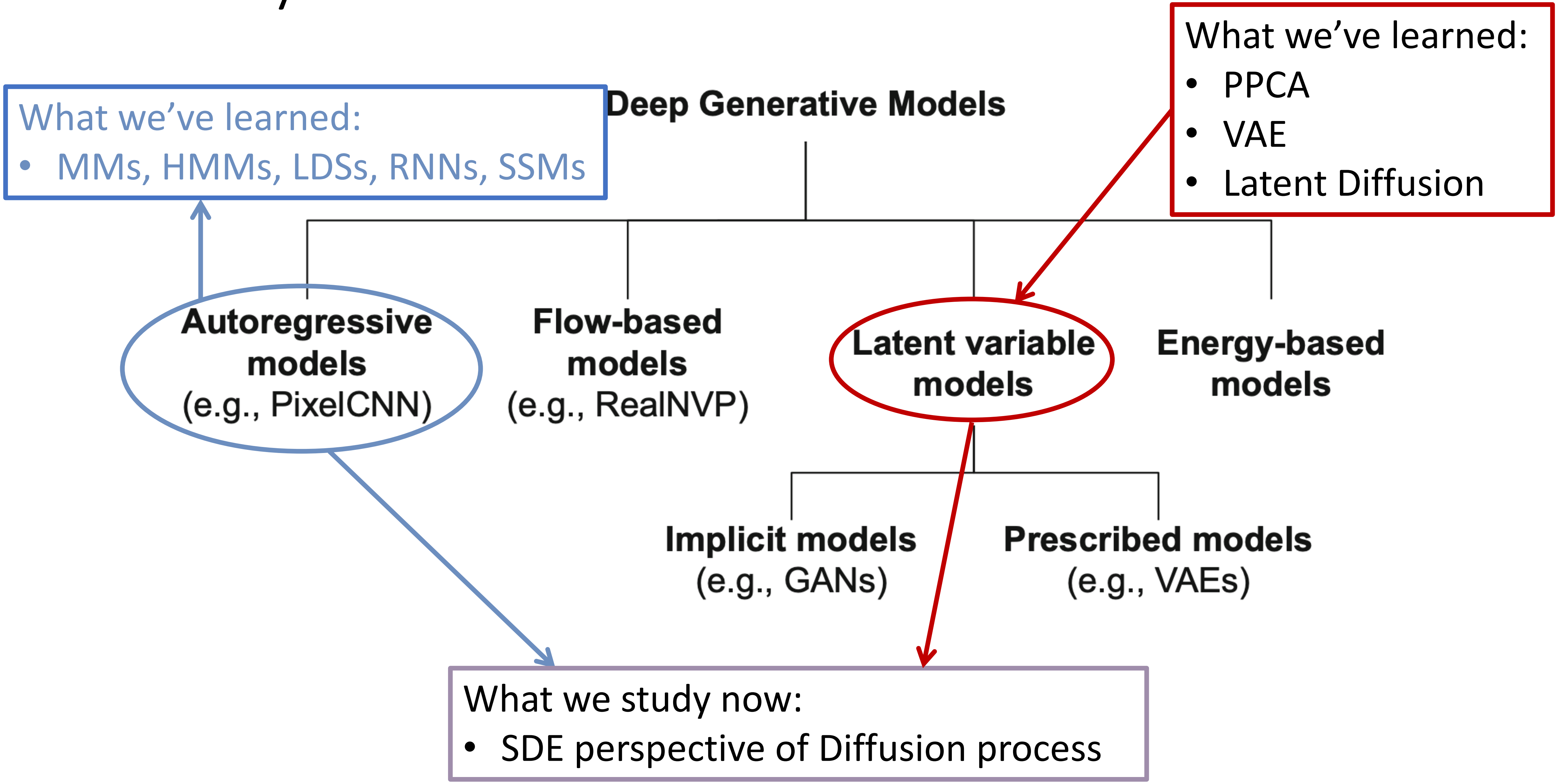
Taxonomy of Generative Models



Stochastic Differential Equation

- SDE is a differential equation in which one or more terms is a stochastic process.

$$dx_t = \mu(x_t, t)dt + \sigma(x_t, t)\mathrm{d}w_t$$

- $\mu(x_t, t)$ is called as the drift coefficient,
- $\sigma(x_t, t)$ is called the diffusion coefficient,
- w_t is called the Weiner process and has the following properties:
    1. <u>Initial zero condition</u>: $w_0 = 0$ a.s. (acronym for “almost surely” – any event that satisfies with probability 1)
    2. <u>Independent increments</u>: For every $t, u \geq 0$, the increments $\mathrm{w}_{t+u} - w_t$ are independent of $w_{<t}$.
    3. <u>Gaussian increments</u>: For every $t, u \geq 0$, the increments $\mathrm{w}_{t+u} - w_t \sim \mathcal{N}(0, uI)$.
    4. <u>Continuity paths</u>: w_t is continuous in t a.s.
- How to obtain x_t given x_0?

Lebesgue integral

$$x_t - x_0 = \int_0^t \mu(x_t, t)dt + \int_0^t \sigma(x_t, t)\mathrm{d}w_t$$

μ, and σ must be Lipschitz continuous in (x, t) for the uniqueness and existence of solution.

Itô integral

Fokker-Plank Equations

$dx_t = \mu(x_t, t)dt + \sigma(x_t, t)\mathrm{d}w_t$

- As the time progresses the probability distribution of x_t evolves; this gives us a ordinary differential equation in probability
- The evolution can be characterized in closed form via Fokker-Plank equations:

$$\frac{dp(x_t, t)}{dt} = -\nabla_x \cdot \left(\mu(x_t, t) \cdot p(x_t, t) - \frac{1}{2}\nabla_x(\sigma(x_t, t)^2 \cdot p(x_t, t))\right)$$

  - $\nabla_x \cdot g(x_t, t) = \sum_i \partial_{x_i}\big(g(x_t, t)\big)_i$ is the divergence operation.
- Conservation law: The net change of probability at point (x_t, t) is the same as the flow due to drift and diffusion coefficient.
- In the forward process the time progress from $t: 0 \rightarrow 1$, and initial distribution p_0. The probability ODE can be obtained.
- To obtain reverse process we need to modify the SDE with initial distribution p_1 such that probability ODE matches with forward.

Itô's lemma: Scalar case

$dx_t = \mu(x_t, t)dt + \sigma(x_t, t)\mathrm{d}w_t$

- **Itô** is pronounced as ***ee-toh***.
- Lemma: Suppose $y_t = u(x_t, t)$ is another process defined on x_t, then we have
$$dy_t = \partial_t u(x_t, t)dt + \partial_x u(x_t, t)dx_t + \frac{1}{2}\partial_x^2 u(x_t, t)\sigma(x_t, t)^2 dt.$$
- Intuition: Let us compute the finite difference $u(x_{t+\Delta t}, t + \Delta t) - u(x_t, t)$ using Taylor's series:
$$\begin{aligned} &u(x_{t+\Delta t}, t + \Delta t) - u(x_t, t) \\ &= \partial_t u(x_t, t)\Delta t + \partial_x u(x_t, t)(x_{t+\Delta t} - x_t) + \frac{1}{2}\partial_x^2 u(x_t, t)(x_{t+\Delta t} - x_t)^2 + o(\Delta t^{1.5}). \end{aligned}$$
  - Now as $\Delta\mathrm{t} \to 0$, we have $(x_{t+\Delta t} - x_t)^2 = \sigma(x_t, t)^2\,(w_{t+\Delta t} - w_t)^2 + o(\Delta t^{1.5})$.
  - By Gaussian increment property we have $w_{t+\Delta t} - w_t \sim \mathcal{N}(0, \Delta t)$. Therefore, $w_{t+\Delta t} - w_t$ scales proportionally with Δt, due to which the 3rd term survives.
- The actual proof requires more rigorous arguments refer to [Stochastic Calculus For Finance, Shreve].

Proof for Fokker-Plank Equations

$dx_t = \mu(x_t, t)dt + \sigma(x_t, t)\mathrm{d}w_t$

- From Ito's Lemma we have that for any u we have:

$$\mathrm{d}u(x_t, t) \; = \partial_t u(x_t, t)dt + \partial_x u(x_t, t)dx_t + \frac{1}{2}\partial_x^2 u(x_t, t)\sigma(x_t, t)^2 dt.$$

- Using the forward SDE we have

$$\mathrm{d}u(x_t, t) \; = \left[\partial_t u(x_t, t) + \mu(x_t, t)\partial_x u(x_t, t) + \frac{1}{2}\sigma(x_t, t)^2 \partial_x^2 u(x_t, t)\right] dt + \partial_x u(x_t, t)\, \sigma(x_t, t)\mathrm{d}w_t.$$

- Now apply expectation on both the sides:

$$\mathrm{d}\mathbb{E}_p[u(x_t, t)] \; = \mathbb{E}_p\left[\partial_t u(x_t, t) + \mu(x_t, t)\partial_x u(x_t, t) + \frac{1}{2}\sigma(x_t, t)^2 \partial_x^2 u(x_t, t)\right] dt.$$

- By exchanging the derivative with the integral, we have:

$$\mathbb{E}_p[\partial_t u(x_t, t)] + \mathbb{E}_{\partial_t p}[u(x_t, t)] = \mathbb{E}_p[\partial_t u(x_t, t)] + \mathbb{E}_p\left[\partial_x u(x_t, t)\mu(x_t, t) + \frac{1}{2}\partial_x^2 u(x_t, t)\sigma(x_t, t)^2\right].$$

- Integration by parts gives us: $\mathbb{E}_{\partial_t p}[u(x_t, t)] = \mathbb{E}_{\partial_x(\mu \cdot p)}[-u(x_t, t)] + \frac{1}{2}\mathbb{E}_{\partial_x(\sigma^2 \cdot p)}[u(x_t, t)].$
- Since these arguments hold true for any u; then the increments must match.

Reversal of the diffusion process

$dx_t = \mu(x_t, t)dt + \sigma(x_t, t)\mathrm{d}w_t$

- Brian Aderson showed this in 1982 which later become a building block in score-matching diffusion models introduced in 2020.
- Theorem: The time-reversal of the SDE $dx_t = \mu(x_t, t)dt + \sigma(x_t, t)\mathrm{d}w_t$ with $x_0 \sim p_0$ is given by $dx'_t = \left(\frac{\nabla_x\left(\sigma(x'_{1-t}, 1-t)^2 \cdot p(x'_{1-t}, 1-t)\right)}{p(x'_t, t)} - \mu(x'_{1-t}, 1-t)\right)dt + \sigma(x'_{1-t}, 1-t)\mathrm{d}\overline{w_t}$ with $x'_0 \sim p_1$, and $(w_t, \overline{w_t})$ are Weiner process.
- Proof: Let us compute the Fokker-Plank equations for reverse SDE.

$$\frac{dp(x'_{1-t}, 1-t)}{dt} = -\nabla_x \cdot \left(\left(-\mu(x'_{1-t}, 1-t) + \frac{\nabla_x\left(\sigma(x'_{1-t}, 1-t)^2 \cdot p(x'_{1-t}, 1-t)\right)}{p(x'_{1-t}, 1-t)}\right) \cdot p(x'_{1-t}, 1-t) - \frac{1}{2}\nabla_x^\top(\sigma(x'_{1-t}, 1-t)^2 \cdot p(x'_{1-t}, 1-t))\right),$$

$$= -(-\nabla_x\left(\mu(x'_{1-t'}, 1-t) \cdot p(x'_{1-t'}, 1-t)\right) + \nabla_x \cdot (\nabla_x \sigma(x'_{1-t}, 1-t)^2 \cdot p(x'_{1-t}, 1-t))) = \frac{dp(x_{1-t}, 1-t)}{d(1-t)}.$$

- The probability ODEs match in both the direction match.
- Due to uniqueness of the solution at each t the solutions to ODE / $p(x_t, t)$ match in both direction.

Special case: SDE $\longrightarrow$ DDPM

- Set $\mu(x,t) = -\frac{1}{2}\sqrt{1 - N\alpha_t} \cdot x_{\mathrm{t}}$, and $\sigma(x,t) = N\sqrt{1-\alpha_t}$.
- We have the forward process: $dx_t = -\frac{1}{2}\sqrt{1-N\alpha_t} \cdot x_t\, dt + N\sqrt{1-\alpha_t} \cdot \mathrm{d}w_t$.
- Now we discretize the time with N scales: $t = \frac{i}{N}$, and $\Delta t = \frac{1}{N}$.
- We can write $dx_t \approx x_{i+1} - x_i$, $-\frac{1}{2}\sqrt{1-N\alpha_t} \cdot x_t\, dt$= $-\frac{1}{2}\sqrt{1-N\alpha_i} \cdot x_{\mathrm{i}}\, \Delta t$, and $\mathrm{N}\sqrt{1-\alpha_t}\mathrm{d}w_t \sim \mathcal{N}\left(\epsilon_i; 0, \sqrt{1-\alpha_t I}\right)$.
- We obtain $x_{i+1} = \left(1 - \frac{1}{2N}\sqrt{1-N\alpha_i}\right)x_i + \sqrt{1-\alpha_t} \cdot \epsilon_i$.
- Let $N \to \infty$, then we have $\left(1 - \frac{1}{2N}\sqrt{1-N\alpha_i}\right) \approx \sqrt{1 - \frac{1}{N} + \alpha_i} \approx \sqrt{\alpha_i}$.
- Finally, we have $x_{i+1} \approx \sqrt{\alpha_i}x_i + \sqrt{1-\alpha_t}\epsilon_i$. This is the same as DDPM.

Special case: DDIM $\longrightarrow$ SDE

- Recall the forward process in diffusion models:

$$x_t = \sqrt{\alpha_t} x_{t-1} + \sqrt{1-\alpha_t}\, \epsilon_t,\ \ \epsilon_t \sim \mathcal{N}(\epsilon_t; 0, I)$$

  This is in the discrete time.

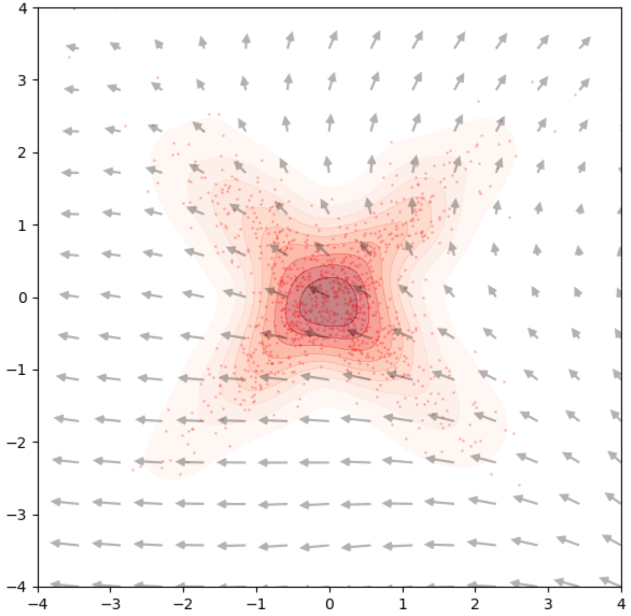
- D$\alpha(t) = N \cdot (1 - \alpha_t), \Delta t = \frac{1}{N}$, where N is the number of noise scales.
- In the limit $N \to \infty$ we have,
  - $x_{t+\Delta t} = \sqrt{1 - \alpha(t)\Delta t} \cdot x_t + \sqrt{\Delta t \cdot \alpha(t)} \cdot \epsilon_t,$
  - $x_{t+\Delta t} \approx \left(1\ - \frac{1}{2}\right) x_t + \sqrt{\alpha(t)} \cdot \sqrt{\Delta t} \cdot \epsilon_t,$
  - $x_{t+\Delta t} - x_t \approx -\frac{\alpha(t)}{2} x_t \cdot \Delta t + \sqrt{\alpha(t)} \cdot \sqrt{\Delta t} \cdot \epsilon_t,$
  - $dx_t \approx -\frac{\alpha(t)}{2} x_t dt + \sqrt{\alpha(t)}\, \sqrt{dt} \cdot \epsilon_t.$
- $\sqrt{dt} \cdot \epsilon_t$ is infinitesimal Normal random variable or Brownian / Weiner process.

Special case: SDE $\longrightarrow$ Score-based models

- Suppose we have zero drift and sample independent noise variance:

Forward: $dx_t = \sigma(t)\mathrm{d}w_t; x_0 \sim p_0,$
Reverse: $dx'_t = \sigma(1-t)^2 \underbrace{\nabla_x ln\big(p(x'_{1-t}, 1-t)\big)}_{\text{Stein's score function}} dt + \sigma(1-t)\mathrm{d}\overline{w}_t; x'_0 \sim p_1.$

- In the reverse process, we are forcing the samples to drift to high- likelihood regions just like in score-based diffusion model.
- After discretizing the reverse process, we obtain: $x'_{t+\Delta t} = x'_t + \sigma(1-t)^2 \Delta \mathrm{t} \nabla_x ln\big(p(x'_{1-t}, 1-t)\big) +$ $\sigma(1-t)\sqrt{\Delta \mathrm{t}} \cdot \epsilon_t$



Vector field of score function