Deep Generative Models

Lecture 12

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AI Masters

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Recap of previous lecture

Neural ODE

$$\boxed{\frac{d\mathbf{x}(t)}{dt} = \mathbf{f}_\theta(\mathbf{x}(t), t);}$$ with initial condition $\mathbf{x}(t_0) = \mathbf{x}_0$

$x(t_0) \sim p_0(x_0)$

Theorem (continuity equation)

If $\mathbf{f}$ is uniformly Lipschitz continuous in $\mathbf{x}$ and continuous in t, then

$$\frac{d \log p_t(\mathbf{x}(t))}{dt} = -\operatorname{tr}\left(\frac{\partial \mathbf{f}(\mathbf{x}(t), t)}{\partial \mathbf{x}(t)}\right)$$

Solution of continuity equation

$$\partial \boxed{\log p_1(\mathbf{x}(1))} = \boxed{\log p_0(\mathbf{x}(0))} - \int_0^1 \operatorname{tr}\left(\frac{\partial \mathbf{f}(\mathbf{x}(t), t)}{\partial \mathbf{x}(t)}\right) dt.$$

$\partial\theta$

- This solution will give us the density along the trajectory (not the total probability path).
- But it is difficult to estimate the last term efficiently.

Chen R. T. Q. et al. Neural Ordinary Differential Equations, 2018

Recap of previous lecture

$$\frac{x_{t+\Delta t} - x_t}{\Delta t} = f$$

SDE basics

Let define stochastic process $\mathbf{x}(t)$ with initial condition $\mathbf{x}(0) \sim p_0(\mathbf{x})$:

$p_t(x)$

$$d\mathbf{x} = \mathbf{f}(\mathbf{x}, t)dt + g(t)d\mathbf{w},$$

Euler

where $\mathbf{w}(t)$ is the standard Wiener process (Brownian motion)

$$\mathbf{w}(t) - \mathbf{w}(s) \sim \mathcal{N}(0, (t-s)\mathbf{I}), \quad d\mathbf{w} = \boldsymbol{\epsilon} \cdot \sqrt{dt}, \text{ where } \boldsymbol{\epsilon} \sim \mathcal{N}(0, \mathbf{I}).$$

Discretization of SDE (Euler method) - SDESolve

$$\mathbf{x}(t + dt) = \mathbf{x}(t) + \mathbf{f}(\mathbf{x}(t), t) \cdot dt + g(t) \cdot \boldsymbol{\epsilon} \cdot \sqrt{dt}$$

- At each moment t we have the density $p_t(\mathbf{x}) = p(\mathbf{x}, t)$.
- $p : \mathbb{R}^m \times [0, 1] \to \mathbb{R}_+$ is a **probability path** between $p_0(\mathbf{x})$ and $p_1(\mathbf{x})$.

Recap of previous lecture

Theorem (Kolmogorov-Fokker-Planck)

Evolution of the distribution $p_t(\mathbf{x})$ is given by the following equation:

$$\boxed{\frac{\partial p_t(\mathbf{x})}{\partial t} = -\text{div}\left(\mathbf{f}(\mathbf{x}, t) p_t(\mathbf{x})\right) + \frac{1}{2} g^2(t) \Delta_{\mathbf{x}} p_t(\mathbf{x})}$$

Langevin SDE (special case)

$$d\mathbf{x} = \frac{1}{2} \frac{\partial}{\partial \mathbf{x}} \log p_t(\mathbf{x}) dt + 1 \cdot d\mathbf{w}$$

The density $p(\mathbf{x}|\boldsymbol{\theta})$ is a **stationary** distribution for the SDE.

Langevin dynamics

Samples from the following dynamics will comes from $p(\mathbf{x}|\boldsymbol{\theta})$ under mild regularity conditions for small enough η.

$$\mathbf{x}_{t+1} = \mathbf{x}_t + \frac{\eta}{2} \nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t|\boldsymbol{\theta}) + \sqrt{\eta} \cdot \boldsymbol{\epsilon}, \quad \boldsymbol{\epsilon} \sim \mathcal{N}(0, \mathbf{I}).$$

Welling M. Bayesian Learning via Stochastic Gradient Langevin Dynamics, 2011

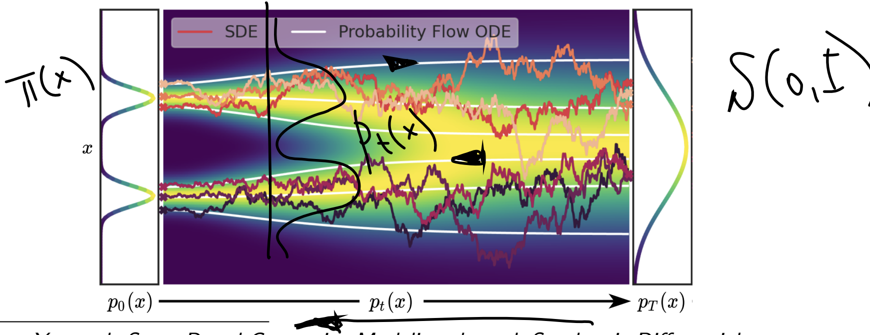
Recap of previous lecture

$d\mathbf{x} = \mathbf{f}(\mathbf{x}, t)dt + g(t)d\mathbf{w}$ – SDE with the probability path $p_t(\mathbf{x})$

Probability flow ODE

There exists ODE with identical the probability path $p_t(\mathbf{x})$ of the form

$$\boxed{d\mathbf{x} = \left(\mathbf{f}(\mathbf{x}, t) - \frac{1}{2}g^2(t)\frac{\partial}{\partial \mathbf{x}}\log p_t(\mathbf{x})\right) dt}$$



Song Y., et al. Score-Based Generative Modeling through Stochastic Differential Equations, 2020

Recap of previous lecture

$$d\mathbf{x} = \mathbf{f}(\mathbf{x}, t)dt, \quad \mathbf{x}(t + dt) = \mathbf{x}(t) + \mathbf{f}(\mathbf{x}, t)dt$$

Reverse ODE

Let $\tau = 1 - t$ ($d\tau = -dt$).

$$d\mathbf{x} = -\mathbf{f}(\mathbf{x}, 1 - \tau)d\tau$$

Reverse SDE

$p_t(x)$

There exists the reverse SDE for the SDE $d\mathbf{x} = \mathbf{f}(\mathbf{x}, t)dt + g(t)d\mathbf{w}$ that has the following form

$$\boxed{d\mathbf{x} = \left(\mathbf{f}(\mathbf{x}, t) \underbrace{- g^2(t)\frac{\partial}{\partial \mathbf{x}} \log p_t(\mathbf{x})}\right) dt + g(t)d\mathbf{w},} \quad dt < 0$$

Sketch of the proof

$$dx = \underbrace{f\, dt} + g(t)\, dw$$

- Convert initial SDE to probability flow ODE.
- Revert probability flow ODE.
- Convert reverse probability flow ODE to reverse SDE.

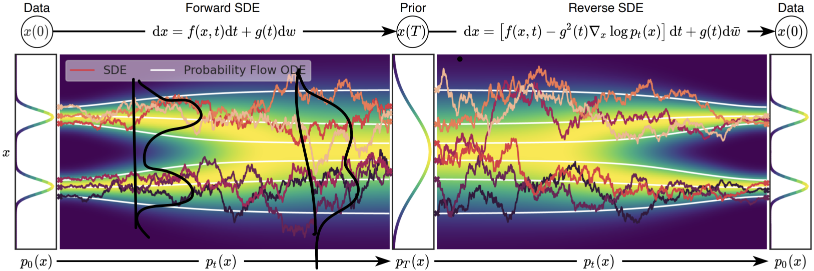
Song Y., et al. Score-Based Generative Modeling through Stochastic Differential Equations, 2020

Recap of previous lecture

$$d\mathbf{x} = \mathbf{f}(\mathbf{x}, t)dt + g(t)d\mathbf{w} - \text{SDE}$$

$$d\mathbf{x} = \left(\mathbf{f}(\mathbf{x}, t) - \frac{1}{2}g^2(t)\frac{\partial}{\partial \mathbf{x}} \log p_t(\mathbf{x})\right) dt - \text{probability flow ODE}$$

$$d\mathbf{x} = \left(\mathbf{f}(\mathbf{x}, t) - g^2(t)\frac{\partial}{\partial \mathbf{x}} \log p_t(\mathbf{x})\right) dt + \boxed{g(t)d\mathbf{w}} - \text{reverse SDE}$$



Song Y., et al. Score-Based Generative Modeling through Stochastic Differential Equations, 2020

Outline

1. Diffusion and Score matching SDEs
2. Score-based generative models through SDEs
3. Flow Matching
4. Conditional Flow Matching

Outline

Score matching SDE

$dx = x(t) - x(t - dt)$

$f(x, t)dt + g(t)d$

Denoising score matching

$$\mathbf{x}_t = \mathbf{x} + \sigma_t \cdot \boldsymbol{\epsilon}_t, \qquad q(\mathbf{x}_t|\mathbf{x}) = \mathcal{N}(\mathbf{x}, \sigma_t^2 \cdot \mathbf{I})$$

$$\mathbf{x}_{t-1} = \mathbf{x} + \sigma_{t-1} \cdot \boldsymbol{\epsilon}_{t-1}, \qquad q(\mathbf{x}_{t-1}|\mathbf{x}) = \mathcal{N}(\mathbf{x}, \sigma_{t-1}^2 \cdot \mathbf{I})$$

$$\boxed{\mathbf{x}_t = \mathbf{x}_{t-1} + \sqrt{\sigma_t^2 - \sigma_{t-1}^2} \cdot \boldsymbol{\epsilon},} \qquad q(\mathbf{x}_t|\mathbf{x}_{t-1}) = \mathcal{N}(\mathbf{x}_{t-1}, (\sigma_t^2 - \sigma_{t-1}^2) \cdot \mathbf{I})$$

Let turn this Markov chain to the continuous stochastic process $\mathbf{x}(t)$ taking $T \to \infty$:

$$\begin{aligned} \boxed{\mathbf{x}(t) = \mathbf{x}(t - dt)} + \sqrt{\sigma^2(t) - \sigma^2(t - dt)} \cdot \boldsymbol{\epsilon} \\ = \mathbf{x}(t - dt) + \sqrt{\frac{\sigma^2(t) - \sigma^2(t - dt)}{dt} dt} \cdot \boldsymbol{\epsilon} \\ = \mathbf{x}(t - dt) + \sqrt{\frac{d[\sigma^2(t)]}{dt}} \cdot d\mathbf{w} \end{aligned}$$

Song Y., et al. Score-Based Generative Modeling through Stochastic Differential Equations, 2020

Score matching SDE

$\sigma(t)$

$\mathcal{N}(0, \sigma^2 I)$

$$\mathbf{x}(t) = \mathbf{x}(t - dt) + \sqrt{\frac{d[\sigma^2(t)]}{dt}} \cdot d\mathbf{w}$$

Denois.
sc. match

$\boxed{\text{Variance Exploding}}$ SDE

$$\boxed{d\mathbf{x} = \sqrt{\frac{d[\sigma^2(t)]}{dt}} \cdot d\mathbf{w}}$$

$\sigma(t)$ is a monotonically increasing function.

$$d\mathbf{x} = \mathbf{f}(\mathbf{x}, t)dt + g(t)d\mathbf{w}, \quad \boxed{\mathbf{f}(\mathbf{x}, t) = 0,} \quad \boxed{g(t) = \sqrt{\frac{d[\sigma^2(t)]}{dt}}}$$

$$d\mathbf{x} = \left(-\frac{1}{2}\frac{d[\sigma^2(t)]}{dt}\frac{\partial}{\partial \mathbf{x}} \log p_t(\mathbf{x})\right) dt \text{ -- probability flow ODE}$$

$$d\mathbf{x} = \left(-\underbrace{\frac{d[\sigma^2(t)]}{dt}}_{g^2(t)}\frac{\partial}{\partial \mathbf{x}} \log p_t(\mathbf{x})\right) dt + \underbrace{\sqrt{\frac{d[\sigma^2(t)]}{dt}}}_{g(t)}d\mathbf{w} \text{ -- reverse SDE}$$

Song Y., et al. Score-Based Generative Modeling through Stochastic Differential Equations, 2020

Diffusion SDE

$dx = \boxed{f\,dt} + \boxed{g\,dw}$

Denoising Diffusion

$$\boxed{\mathbf{x}_t = \sqrt{1-\beta_t}\cdot\mathbf{x}_{t-1} + \sqrt{\beta_t}\cdot\boldsymbol{\epsilon},} \quad q(\mathbf{x}_t|\mathbf{x}_{t-1}) = \mathcal{N}(\sqrt{1-\beta_t}\cdot\mathbf{x}_{t-1}, \beta_t\cdot\mathbf{I})$$

Let turn this Markov chain to the continuous stochastic process taking $T \to \infty$ and taking $\beta_t = \beta(\frac{t}{T}) \cdot \frac{1}{T}$ (with $dt = \frac{1}{T}$)

$$\begin{aligned}
\mathbf{x}(t) &= \sqrt{1-\beta(t)dt}\cdot\mathbf{x}(t-dt) + \sqrt{\beta(t)dt}\cdot\boldsymbol{\epsilon} \approx \\
&\approx (1 - \frac{1}{2}\beta(t)dt)\cdot\mathbf{x}(t-dt) + \sqrt{\beta(t)dt}\cdot\boldsymbol{\epsilon} = \\
&= \mathbf{x}(t-dt) - \frac{1}{2}\beta(t)\mathbf{x}(t-dt)dt + \sqrt{\beta(t)}\cdot d\mathbf{w}
\end{aligned}$$

Variance Preserving SDE

$$d\mathbf{x} = \boxed{-\frac{1}{2}\beta(t)\mathbf{x}(t)}dt + \boxed{\sqrt{\beta(t)}}\cdot d\mathbf{w}$$

Song Y., et al. Score-Based Generative Modeling through Stochastic Differential Equations, 2020

Diffusion SDE

Variance Preserving SDE

$$d\mathbf{x} = -\frac{1}{2}\beta(t)\mathbf{x}(t)dt + \sqrt{\beta(t)} \cdot d\mathbf{w}$$

$$\mathbf{f}(\mathbf{x}, t) = -\frac{1}{2}\beta(t)\mathbf{x}(t), \quad g(t) = \sqrt{\beta(t)}$$

Variance is preserved if $\mathbf{x}(0)$ has a unit variance.

$$d\mathbf{x} = \left(-\frac{1}{2}\beta(t)\mathbf{x}(t) - \frac{1}{2}\beta(t)\frac{\partial}{\partial \mathbf{x}} \log p_t(\mathbf{x})\right) dt \text{ – probability flow ODE}$$

$$d\mathbf{x} = \underbrace{\left(-\frac{1}{2}\beta(t)\mathbf{x}(t) - \beta(t)\frac{\partial}{\partial \mathbf{x}} \log p_t(\mathbf{x})\right) dt + \sqrt{\beta(t)}d\mathbf{w}} \text{ – reverse SDE}$$

Song Y., et al. Score-Based Generative Modeling through Stochastic Differential Equations, 2020

Diffusion SDE

Euler

$$d\mathbf{x} = \mathbf{f}(\mathbf{x}, t)dt + g(t)d\mathbf{w}$$

Diff.

Score Matching

VAE-ELBO

SDEs

Variance Exploding SDE (NCSN)

$$d\mathbf{x} = \sqrt{\frac{d[\sigma^2(t)]}{dt}} \cdot d\mathbf{w}$$

Variance Preserving SDE (DDPM)

$$d\mathbf{x} = -\frac{1}{2}\beta(t)\mathbf{x}(t)dt + \sqrt{\beta(t)} \cdot d\mathbf{w}$$

Efficient Solvers

DPM++

- Converting SDEs to PF-ODEs gives us the more efficient inference.

Runge Heun

- We can apply any ODESolve procedure to reduce the number of inference steps.

5-10

- In practice it reduces from 100-1000 steps to 20-50 steps.

Lu C. et al. Dpm-solver: A fast ode solver for diffusion probabilistic model sampling in around 10 steps, 2022

Outline

1. Diffusion and Score matching SDEs
2. Score-based generative models through SDEs
3. Flow Matching
4. Conditional Flow Matching

Score-based generative models through SDEs

$\mathcal{N}(\alpha_t x_t, \sqrt{1-\alpha_t}^2)$

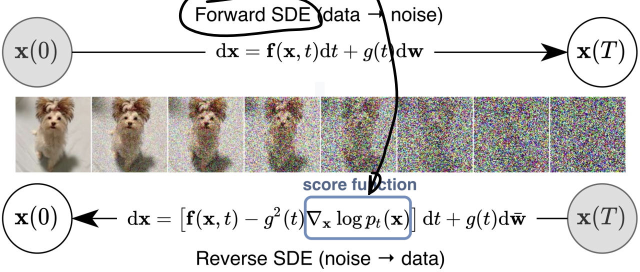
Discrete-in-time objective

$$\mathbb{E}_{\pi(\mathbf{x}_0)}\mathbb{E}_{t\sim U\{1,T\}}\mathbb{E}_{q(\mathbf{x}_t|\mathbf{x}_0)}\left\|\mathbf{s}_{\theta,t}(\mathbf{x}_t) - \nabla_{\mathbf{x}_t}\log q(\mathbf{x}_t|\mathbf{x}_0)\right\|_2^2$$

Is it possible to train score-based diffusion in continuous time?

Continuous-in-time objective

$$\mathbb{E}_{\pi(\mathbf{x}(0))}\mathbb{E}_{t\sim U[0,1]}\mathbb{E}_{q(\mathbf{x}(t)|\mathbf{x}(0))}\left\|\mathbf{s}_{\theta}(\mathbf{x}(t), t) - \nabla_{\mathbf{x}(t)}\log q(\mathbf{x}(t)|\mathbf{x}(0))\right\|_2^2$$



Song Y., et al. Score-Based Generative Modeling through Stochastic Differential Equations, 2020

Score-based generative models through SDEs

$dx = f\,dt + g\,dw$

Continuous-in-time objective

$$\mathbb{E}_{\pi(\mathbf{x}(0))}\mathbb{E}_{t\sim U[0,1]}\mathbb{E}_{q(\mathbf{x}(t)|\mathbf{x}(0))}\left\|\mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x}(t),t) - \nabla_{\mathbf{x}(t)}\log q(\mathbf{x}(t)|\mathbf{x}(0))\right\|_2^2$$

$$q(\mathbf{x}(t)|\mathbf{x}(0)) = \mathcal{N}\left(\underline{\boldsymbol{\mu}(\mathbf{x}(t),\mathbf{x}}(0)), \boldsymbol{\sigma}^2(\mathbf{x}(t),\mathbf{x}(0))\cdot\mathbf{I}\right)$$

$$\nabla_{\mathbf{x}(t)}\log q(\mathbf{x}(t)|\mathbf{x}(0)) = -\frac{1}{\boldsymbol{\sigma}}\odot(\mathbf{x}(t)-\boldsymbol{\mu})$$

$$d\mathbf{x} = \sqrt{\frac{d[\sigma^2(t)]}{dt}}\cdot d\mathbf{w} \text{ — Variance Exploding SDE}$$

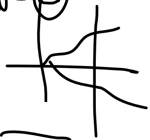
$$d\mathbf{x} = -\frac{1}{2}\beta(t)\mathbf{x}(t)dt + \sqrt{\beta(t)}\cdot d\mathbf{w} \text{ — Variance Preserving SDE}$$

Is it possible to derive the expressions for $\boldsymbol{\mu}(\mathbf{x}(t),\mathbf{x}(0))$ and $\boldsymbol{\Sigma}(\mathbf{x}(t),\mathbf{x}(0))$ for VE-SDE and VP-SDE?

Särkkä S., Solin A. Applied stochastic differential equations, 2019

Score-based generative models through SDEs

$dw = \varepsilon \sqrt{dt}$



$$q(\mathbf{x}(t)|\mathbf{x}(0)) = \mathcal{N}\Big(\boldsymbol{\mu}(\mathbf{x}(t), \mathbf{x}(0)), \boldsymbol{\Sigma}(\mathbf{x}(t), \mathbf{x}(0))\Big)$$

Theorem

Moments of the SDE $d\mathbf{x} = \mathbf{f}(\mathbf{x}, t)dt + g(t)d\mathbf{w}$ satisfies the equations

$$\frac{d\boldsymbol{\mu}(\mathbf{x}(t), \mathbf{x}(0))}{dt} = \mathbb{E}\left[\mathbf{f}(\mathbf{x}(t), t)|\mathbf{x}(0)\right]$$

$$\frac{d\boldsymbol{\Sigma}(\mathbf{x}(t), \mathbf{x}(0))}{dt} = \mathbb{E}\left[\mathbf{f} \cdot (\mathbf{x}(t) - \boldsymbol{\mu})^T + (\mathbf{x}(t) - \boldsymbol{\mu}) \cdot \mathbf{f}^T|\mathbf{x}(0)\right] + g^2(t) \cdot \mathbf{I}$$

Proof

$$\begin{aligned}
\mathbb{E}\left[d\mathbf{x}|\mathbf{x}(0)\right] &= \mathbb{E}\left[\mathbf{f}(\mathbf{x}, t)dt|\mathbf{x}(0)\right] + \mathbb{E}\left[g(t)d\mathbf{w}|\mathbf{x}(0)\right] \\
&= \mathbb{E}\left[\mathbf{f}(\mathbf{x}, t)|\mathbf{x}(0)\right] dt + g(t)\underbrace{\mathbb{E}\left[d\mathbf{w}|\mathbf{x}(0)\right]}_{=0} \\
&= \mathbb{E}\left[\mathbf{f}(\mathbf{x}, t)|\mathbf{x}(0)\right] dt
\end{aligned}$$

Särkkä S., Solin A. Applied stochastic differential equations, 2019

Score-based generative models through SDEs

$$\frac{d\mu}{\mu} = -\frac{1}{2}\beta dt$$

$$\frac{d \ln \mu}{dt} = -\frac{1}{2}\beta$$

Theorem

$$\frac{d\boldsymbol{\mu}(\mathbf{x}(t), \mathbf{x}(0))}{dt} = \mathbb{E}\left[\mathbf{f}(\mathbf{x}(t), t) | \mathbf{x}(0)\right]$$

Proof (continued)

$$\mathbb{E}\left[d\mathbf{x} | \mathbf{x}(0)\right] = \mathbb{E}\left[\mathbf{f}(\mathbf{x}, t) | \mathbf{x}(0)\right] dt$$

$$\frac{d\mathbb{E}\left[\mathbf{x}(t) | \mathbf{x}(0)\right]}{dt} = \frac{d\boldsymbol{\mu}(\mathbf{x}(t), \mathbf{x}(0))}{dt} = \mathbb{E}\left[\mathbf{f}(\mathbf{x}, t) | \mathbf{x}(0)\right]$$

Examples

$$\textbf{NCSN:} \quad \mathbf{f}(\mathbf{x}, t) = 0 \quad \Rightarrow \quad \boldsymbol{\mu} = \mathbf{x}(0)$$

$$\textbf{DDPM:} \quad \boxed{\mathbf{f}(\mathbf{x}, t) = -\frac{1}{2}\beta(t)\mathbf{x}(t)} \quad \Rightarrow \quad \boxed{\frac{d\boldsymbol{\mu}}{dt} = -\frac{1}{2}\beta(t)\boldsymbol{\mu}}$$

$$\alpha_t = \prod \beta_s$$

$$\boldsymbol{\mu} = \mathbf{x}(0) \exp\left(-\frac{1}{2}\int_0^t \beta(s) ds\right)$$

Särkkä S., Solin A. Applied stochastic differential equations, 2019

Score-based generative models through SDEs

$$-\frac{x-\mu}{\sigma}$$

Training

$$\mathbb{E}_{\pi(\mathbf{x}(0))}\mathbb{E}_{t\sim U[0,1]}\mathbb{E}_{q(\mathbf{x}(t)|\mathbf{x}(0))}\left\|\mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x}(t),t)-\nabla_{\mathbf{x}(t)}\log q(\mathbf{x}(t)|\mathbf{x}(0))\right\|_2^2$$

$$q(\mathbf{x}(t)|\mathbf{x}(0))=\mathcal{N}\Big(\boldsymbol{\mu}(\mathbf{x}(t),\mathbf{x}(0)),\boldsymbol{\Sigma}(\mathbf{x}(t),\mathbf{x}(0))\Big)$$

NCSN

$$q(\mathbf{x}(t)|\mathbf{x}(0))=\mathcal{N}\left(\mathbf{x}(0),\left[\sigma^2(t)-\sigma^2(0)\right]\cdot\mathbf{I}\right)$$

DDPM

$$q(\mathbf{x}(t)|\mathbf{x}(0))=\mathcal{N}\left(\mathbf{x}(0)e^{-\frac{1}{2}\int_0^t\beta(s)ds},\left(1-e^{-\int_0^t\beta(s)ds}\right)\cdot\mathbf{I}\right)$$

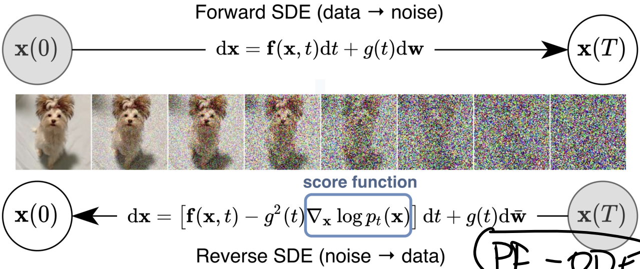
Here we omit the derivations of the variance.

Song Y., et al. Score-Based Generative Modeling through Stochastic Differential Equations, 2020

Score-based generative models through SDEs

Sampling

Solve reverse SDE using numerical solvers (SDESolve).



PF - ODE

- Discretization of the reverse SDE gives us the ancestral sampling.
- Discretization of the probability flow ODE gives us deterministic sampling. DDIM

Song Y., et al. *Score-Based Generative Modeling through Stochastic Differential Equations*, 2020

Outline

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2. Score-based generative models through SDEs
3. Flow Matching
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Continuous-in-time NF

Let return to the ODE dynamic $\mathbf{x}(t)$ in time interval $t \in [0, 1]$

- $\mathbf{x}_0 \sim p_0(\mathbf{x}) = p(\mathbf{x})$, $\mathbf{x}_1 \sim p_1(\mathbf{x}) = \pi(\mathbf{x})$;
- $p(\mathbf{x})$ is a base distribution ($\mathcal{N}(0, \mathbf{I})$) and $\pi(\mathbf{x})$ is a true data distribution.

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}, t), \quad \text{with initial condition } \mathbf{x}(0) = \mathbf{x}_0.$$

KFP theorem (continuity equation)

$$\frac{\partial p_t(\mathbf{x})}{\partial t} = -\text{div}\left(\mathbf{f}(\mathbf{x}, t) p_t(\mathbf{x})\right) \Leftrightarrow \boxed{\frac{d \log p_t(\mathbf{x}(t))}{dt}} = -\text{tr}\left(\frac{\partial \mathbf{f}(\mathbf{x}(t), t)}{\partial \mathbf{x}(t)}\right)$$

- It is hard to solve continuity equation directly because of the trace part.
- There is a method (called adjoint method) that solves this equation directly, but it is unstable and not scalable.

Chen R. T. Q. et al. Neural Ordinary Differential Equations, 2018

Continuous-in-time NF

KFP theorem (continuity equation)

$$\frac{\partial p_t(\mathbf{x})}{\partial t} = -\text{div}\left(\mathbf{f}(\mathbf{x}, t) p_t(\mathbf{x})\right) \Leftrightarrow \frac{d \log p_t(\mathbf{x}(t))}{dt} = -\text{tr}\left(\frac{\partial \mathbf{f}(\mathbf{x}(t), t)}{\partial \mathbf{x}(t)}\right)$$

- If we know the vector field $\boxed{\mathbf{f}(\mathbf{x}, t)}$ then KFP (or continuity) equation gives us the way to compute the density $p_t(\mathbf{x})$.
- Flow matching gives the alternative way to solve the NeuralODE.

Flow Matching

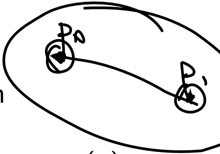
y true

$$\mathbb{E}_{t \sim U[0,1]} \mathbb{E}_{\mathbf{x} \sim p_t(\mathbf{x})} \left\| \mathbf{f}(\mathbf{x}, t) - \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x}, t) \right\|^2 \to \min_{\boldsymbol{\theta}}$$

- Approximate the true vector field $\mathbf{f}(\mathbf{x}, t)$ via $\mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x}, t)$.
- Use $\mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x}, t)$ for deterministic sampling from the ODE.

Lipman Y., et al. Flow Matching for Generative Modeling, 2022

Flow Matching $\rightarrow$ Bridge Match.



$$\mathbb{E}_{t\sim U[0,1]}\mathbb{E}_{\mathbf{x}\sim p_t(\mathbf{x})}\left\|\mathbf{f}(\mathbf{x},t)-\mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x},t)\right\|^2 \rightarrow \min_{\boldsymbol{\theta}}$$

- There exists infinite number of possible $\mathbf{f}(\mathbf{x},t)$ between $\pi(\mathbf{x})$ and $p(\mathbf{x})$.
- The true vector field $\mathbf{f}(\mathbf{x},t)$ is **unknown**.
- We need to select the "best" $\mathbf{f}(\mathbf{x},t)$ and makes the objective tractable.

$KL(p \| W$

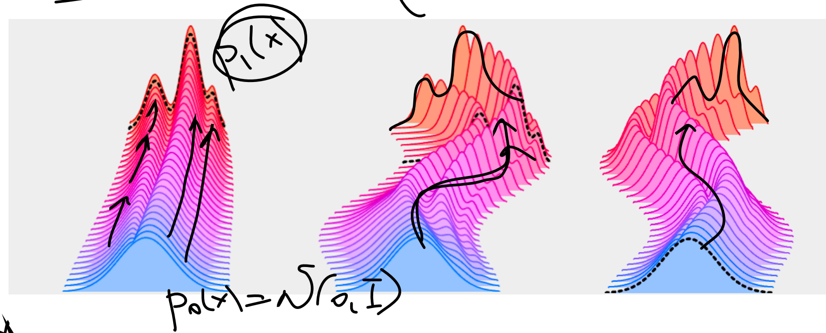


image credit: A Visual Dive into Conditional Flow Matching

Outline

1. Diffusion and Score matching SDEs
2. Score-based generative models through SDEs
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Flow Matching

Latent variable model

Let introduce the latent variable $\mathbf{z}$:

$$p_t(\mathbf{x}) = \int p_t(\mathbf{x}|\mathbf{z})p(\mathbf{z})d\mathbf{z}$$

Here $p_t(\mathbf{x}|\mathbf{z})$ is a **conditional probability path**.
The conditional probability path $p_t(\mathbf{x}|\mathbf{z})$ satisfies KFP theorem

$$\frac{\partial p_t(\mathbf{x}|\mathbf{z})}{\partial t} = -\text{div}\left(\mathbf{f}(\mathbf{x}, \mathbf{z}, t)p_t(\mathbf{x}|\mathbf{z})\right),$$

where $\mathbf{f}(\mathbf{x}, \mathbf{z}, t)$ is a **conditional vector field**.

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}, t) \quad \Rightarrow \quad \frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}, \mathbf{z}, t)$$

What is the relationship between $\mathbf{f}(\mathbf{x}, t)$ and $\mathbf{f}(\mathbf{x}, \mathbf{z}, t)$?

Tong A., et al. Improving and Generalizing Flow-Based Generative Models with Minibatch Optimal Transport, 2023

Flow Matching

$$\frac{\partial p_t(\mathbf{x}|\mathbf{z})}{\partial t} = -\mathrm{div}\left(\mathbf{f}(\mathbf{x}, \mathbf{z}, t) p_t(\mathbf{x}|\mathbf{z})\right),$$

Theorem

The following vector field generates the probability path $p_t(\mathbf{x})$.

$$\mathbf{f}(\mathbf{x}, t) = \mathbb{E}_{p_t(\mathbf{z}|\mathbf{x})} \mathbf{f}(\mathbf{x}, \mathbf{z}, t) = \int \mathbf{f}(\mathbf{x}, \mathbf{z}, t) \frac{p_t(\mathbf{x}|\mathbf{z}) p(\mathbf{z})}{p_t(\mathbf{x})} d\mathbf{z}$$

Proof

$$\frac{\partial p_t(\mathbf{x})}{\partial t} = \frac{\partial}{\partial t} \int p_t(\mathbf{x}|\mathbf{z}) p(\mathbf{z}) d\mathbf{z} = \int \left(\frac{\partial p_t(\mathbf{x}|\mathbf{z})}{\partial t} \right) p(\mathbf{z}) d\mathbf{z} =$$

$$= \int \left(-\mathrm{div}\left(\mathbf{f}(\mathbf{x}, \mathbf{z}, t) p_t(\mathbf{x}|\mathbf{z})\right)\right) p(\mathbf{z}) d\mathbf{z} =$$

$$= -\mathrm{div}\left(\int \mathbf{f}(\mathbf{x}, \mathbf{z}, t) p_t(\mathbf{x}|\mathbf{z}) p(\mathbf{z}) d\mathbf{z} \right) = -\mathrm{div}\left(\mathbf{f}(\mathbf{x}, t) p_t(\mathbf{x})\right)$$

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Flow Matching

$$\frac{dx}{dt} = f(x, t) \longleftrightarrow f(x, z, t)$$

$$S(x, t) = \nabla \log p(x, t)$$

Flow Matching (FM)

$$\mathbb{E}_{t \sim U[0,1]} \mathbb{E}_{\mathbf{x} \sim p_t(\mathbf{x})} \left\| \mathbf{f}(\mathbf{x}, t) - \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x}, t) \right\|^2 \to \min_{\boldsymbol{\theta}}$$

θ^*

Conditional Flow Matching (CFM)

$$\underbrace{\mathbb{E}_{t \sim U[0,1]} \mathbb{E}_{\mathbf{z} \sim p(\mathbf{z})} \mathbb{E}_{\mathbf{x} \sim p_t(\mathbf{x}|\mathbf{z})}}_{\mathbb{E}_{p_t(x)}} \left\| \boxed{\mathbf{f}(\mathbf{x}, \mathbf{z}, t)} - \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x}, t) \right\|^2 \to \min_{\boldsymbol{\theta}}$$

θ^*

$KL(p_\theta \| \pi)$

Theorem

If $\text{supp}(p_t(\mathbf{x})) = \mathbb{R}^m$, then the optimal value of FM objective is equal to the optimal value of CFM objective.

Proof

It is proved similarly with the denoising score matching theorem.

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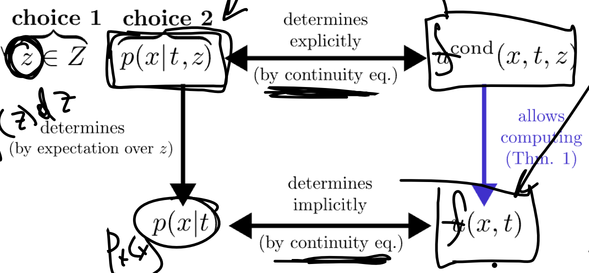
Conditional Flow Matching

$\|f - f_\theta\|^2$

$\int p(z)dz$



$\int p_t(z|x)$

$p_t(x)$

$\|f - f_\theta\|^2$

- We do not want to model $p_t(\mathbf{x})$ because it is complex.
- We showed that it is possible to solve CFM task instead of FM task.
- Let choose the convenient conditioning latent variable $\mathbf{z}$.
- Let parametrize $\int p_t(\mathbf{x}|\mathbf{z}) p(z)dz$ instead of $p_t(\mathbf{x})$. It must satisfy the following constraints

$$p(\mathbf{x}) = \mathcal{N}(0, \mathbf{I}) = \mathbb{E}_{p(\mathbf{z})} p_0(\mathbf{x}|\mathbf{z}); \quad \pi(\mathbf{x}) = \mathbb{E}_{p(\mathbf{z})} p_1(\mathbf{x}|\mathbf{z}).$$

image credit: A Visual Dive into Conditional Flow Matching

Summary

- Score matching (NCSN) and diffusion models (DDPM) are the discretizations of the SDEs (variance exploding and variance preserving).
- It is possible to train the continuous-in-time score-based generative models through forward and reverse SDEs.
- Discretization of the reverse SDE gives the ancestral sampling of the DDPM.
- Flow matching suggests to fit the vector field directly.
- Conditional flow matching introduces the latent variable $\mathbf{z}$ to reformulate the initial task in terms of conditional dynamics.