Introduction to Diffusion & Flow Models (Dheeraj Nagraj)

Day-1

Generative modeling $x_1, \dots x_n \sim P$ iid generate more samples from $\hat{P} \approx P$

Gen Modeling	MCMC
(i) Sample access $x_1 \dots x_n \sim P$	(i) Probability access $P(x) \propto e^{-F(x)}$
(ii) aim each generated sample is meaningful	(ii) Aim find aggregate stats of P

Random Variables

$F: \Omega \longrightarrow \mathbb{R}^d$ | if $\omega \in \Omega$ $Y = F(\omega)$

↳ random vector.

(*) What do we need to generate "random vectors"?

(1) Source of randomness (i.e. Ω)

(2) A Function "F" to shape it.

Early Ideas

(1) GAN (2) VAE

(*) $z \sim \mathcal{N}(0, I)$ learn $F_\theta(z) \overset{d}{\approx} P$

(ii) SOTA Models Diffusion / Flow based Models.

↳ Easy to train → "Slower to Sample" → Best Quality

Can we generate slowly in many steps?

→ Transform noise to signal

Eg → (1) ODE : $\frac{dx_t}{dt} = \underbrace{v_t(x_t)}_{\text{velocity field}}$ $x_0 \sim \mathcal{N}(0, I)$ $x_1 \sim$ data → Flow Model

(2) SDE → $dX_t = V(t, X_t)dt + \sqrt{2}\, dB_t$ ← Brownian motion
drift ↪ ← Diffusion model

(*) We need to learnn $v_t(x)$ from data $X_1 \dots X_n \sim p$
→ How do we simulate these stochastic DE/ODEs?
→ We will develop theory to answer these questions?
→ We will derive learning algorithms to learn $v_t(x)$.

Intro to ODE

(*) Given a velocity field $v_t(x) : \mathbb{R}^+ \times \mathbb{R}^d \to \mathbb{R}^d$

$$\frac{dx_t}{dt} = v_t(x_t) \qquad \begin{cases} X_0 = x_0 \text{ initial value} \end{cases}$$

→ When can we solve it?
→ When is the solution unique?

Picard Lindelof Theorem → (Comes from Barach's Fixed point theorem)

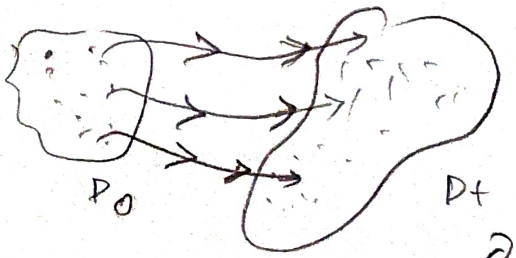
Let $D \subseteq \mathbb{R} \times \mathbb{R}^d$ be a closed box. Let $v(t,x)$ continous in t & lipschitz in x $\Rightarrow \exists\ \epsilon > 0$ s.t. the ODE has a solution for $t \in [t_0 - \epsilon, t_0 + \epsilon]$

(*) This doesn't go till infinite. for e.g. $\frac{dx_t}{dt} = x_t^2 \quad x_0 = 1$

(*) This solution is unique because of Lipschitz property.

(*) Harder question → x_0 is a random vector

$$x_0 \overset{d}{\sim} p_0 \quad | \quad \frac{dx_t}{dt} = v(t, x_t) \qquad x_t \overset{d}{\sim} p_t$$



→ "What is the shape of p_t?"

(*) Continuity Equation $\frac{\partial p_t(x)}{\partial t} + \nabla_x \left(v(t,x)\, p_t(x) \right) = 0$

(*) divergence of $f : \mathbb{R}^d \to \mathbb{R}^d$ $\quad \nabla_x f(x) = \sum_i \frac{\partial f_i(x)}{\partial x_i}$

① $C_c^\infty((0,T)\times\mathbb{R}^d)$ → continous function, ∞ differentiable & compactly supported

If $\phi \in C_c^\infty((0,T)\times\mathbb{R}^d)$ then

(a) $\phi(0,x) = 0$

(b) $\phi(T,x) = 0$

(c) $\phi(t,x) = 0 \quad \forall |x| \geq R_t$

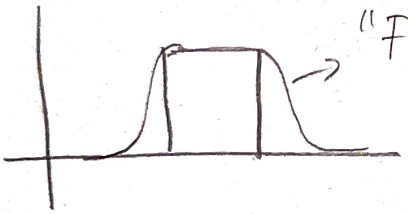
ϕ is called test functions.

Question (i) if we know value of $\int \phi(t,x)\mu(x)dx \quad \forall \phi \in C_c^\infty$ is μ unique?

Let $\mu([a,b]) \quad \forall a,b \in \mathbb{R} \quad b \geq a$



$$\mu([a,b]) = \int \chi_{[a,b]}(x)\, d\mu(x)$$



$$\frac{dx_t}{dt} = v(t,x_t)$$

observation

(1) $\phi(T,x_t) - \phi(0,x_0) = \int_0^T \frac{d}{dt}\phi(t,x_t)dt$

(2) $\phi(T,x_T) - \phi(0,x_0) = 0$

(3) $\frac{d}{dt}\phi(t,x_t) = \frac{\partial}{\partial t}\phi(t,x_t)$

$\forall \phi$

$$0 = \int \left[\frac{\partial}{\partial t}\phi(t,x_t) + \langle v(t,x_t), \nabla\phi(t,x_t)\rangle\right]dt \qquad \nabla_x\phi(t,x_t), v(t,x_t)$$

$$\Rightarrow \int dt \left[\frac{\partial}{\partial t}\phi(t,x_t) + \langle v(t,x_t), \nabla\phi(t,x_t)\rangle\right] = 0$$

→ (Fubini's Theorm) Pushing Forward Interpretation

$$\Rightarrow \int dt \int dP_t(x)\left[\frac{\partial}{\partial t}\phi(t,x_t) + \langle \nabla\phi(t,x), v(t,x_t)\rangle\right] = 0$$

$\forall \phi \in C_c^\infty$

Integration by Parts

$$\int_0^T P_t(x) \frac{\partial}{\partial t} \phi(t,x)\,dt = \underbrace{P_T(x)}_{=0}\phi(T,x) - \underbrace{P_0(x)}_{=0}\phi(0,x) - \int_0^T \left(\frac{\partial}{\partial t} P_t(x)\right)\phi(t,x)\,dt$$

Exercise

$$\int_{\mathbb{R}^d} P_t(x)\,dx \,\langle \nabla\phi(t,x)\, v(t,x)\rangle dx = -\int \phi(t,x)\, \mathrm{div}\,(v(t,x) P_t(x))$$

Now

$$\int \phi(t,x)\left[\frac{\partial}{\partial t} P_t(x) + \nabla_x (V_t(x) P_t(x))\right] = 0 \quad \forall \phi \in C_c^\infty((0,T))$$

$$\Rightarrow \boxed{\frac{\partial}{\partial t} P_t(x) + \mathrm{div}\left(V_t(x) P_t(x)\right) = 0} \rightarrow \text{continuity eqn (CE)}$$