Stochastic differential equations in generative modeling. Diffusion models

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Stochastic differential equations

Stochastic differential equation (SDE) is an integral equation of the form:

$$X_t = X_0 + \int_0^t \mu(X_s, s)ds + \int_0^t \sigma(X_s, s)dw_s \tag{1}$$

where X_t is an unknown stochastic process and

- $\int_0^t \mu(X_s, s)ds$ - Riemann integral
- $\int_0^t \sigma(X_s, s)dw_s$ - Ito integral

There is a short notation for the integral equation above:

$$dX_t = \mu(X_t, t)dt + \sigma(X_t, t)dw_t \tag{2}$$

Stochastic differential equations

If the initial condition X_0 is a random variable with PDF $p(X|t=0)$ and we apply the SDE

$$dX_t = \mu(X_t, t)dt + \sigma(X_t, t)dw_t \tag{3}$$

then the probability density will evolve according to the corresponding Fokker-Planck equation

$$\frac{\partial p(x|t)}{\partial t} = -\frac{\partial}{\partial x}\left(\mu(x,t)p(x|t)\right) + \frac{\partial^2}{\partial x^2}\left(\frac{\sigma(x,t)^2}{2}p(x|t)\right) \tag{4}$$

Stochastic differential equations

Suppose that we have some distribution if initial conditions $X_0 \sim p(x|t=0)$ and we are adding noise to it via the SDE

$$dX_t = \mu(X_t, t)dt + dw_t \tag{5}$$

Which drift $\mu(X_t, t)$ should we choose to stay in the same initial distribution $p_0(x) = p(x|t=0)$?

- Example 1: a night our smartphone camera takes noisy photos, but we want to get sharp and high quality ones.
- Example 2: we want to reduce the noise in the measurement of some physical quantity.

Stochastic differential equations

$$dX_t = \mu(X_t, t)dt + dw_t \tag{6}$$

Which drift $\mu(X_t, t)$ should we choose to stay in the same initial distribution $p_0(x) = p(x|t = 0$?

- It is obvious that we need to somehow predict the noise to stay in the same distribution, but how exactly?
- Let's write Fokker-Planck equation:

$$\frac{\partial p(x|t)}{\partial t} = -\frac{\partial}{\partial x}\left(\mu(x,t)p(x|t)\right) + \frac{\partial^2}{\partial x^2}\left(\frac{\sigma(x,t)^2}{2}p(x|t)\right) \tag{7}$$

We have here $\sigma(x, t) = 1$ and also we want to get stationary density so $\frac{\partial p(x|t)}{\partial t} = 0$. Then

$$0 = -\frac{\partial}{\partial x}\left(\mu(x,t)p(x|t)\right) + \frac{1}{2}\frac{\partial^2}{\partial x^2}\left(p(x|t)\right) \tag{8}$$

Stochastic differential equations

$$dX_t = \mu(X_t, t)dt + dw_t \tag{9}$$

Which drift $\mu(X_t, t)$ should we choose to stay in the same initial distribution $p_0(x) = p(x|t = 0)$?
We have here $\sigma(x, t) = 1$ and also we want to get stationary density so $\frac{\partial p(x|t)}{\partial t} = 0$. Then

$$0 = -\frac{\partial}{\partial x}\left(\mu(x, t)p(x|t) + \frac{1}{2}\frac{\partial}{\partial x}p(x|t)\right) \tag{10}$$

$$C(t) = -\mu(x, t)p(x|t) + \frac{1}{2}\frac{\partial}{\partial x}p(x|t) \tag{11}$$

Since C(t) is arbitrary let's set it to 0 for simplicity. Then

$$\mu(x, t) = \frac{1}{2p(x|t)}\frac{\partial}{\partial x}p(x|t) = \frac{1}{2}\frac{\partial}{\partial x}\log p(x|t) \tag{12}$$

Stochastic differential equations

$$dX_t = \mu(X_t, t)dt + dw_t \tag{13}$$

Which drift $\mu(X_t, t)$ should we choose to stay in the same initial distribution $p_0(x) = p(x|t = 0)$?
Our answer is

$$\mu(x, t) = \frac{1}{2p(x|t)} \frac{\partial}{\partial x} p(x|t) = \frac{1}{2} \frac{\partial}{\partial x} \log p(x|t) \tag{14}$$

Our SDE with the noise compensation is then becomes:

$$dX_t = \frac{1}{2} \frac{\partial}{\partial x} \log p_0(X_t)dt + dw_t \tag{15}$$

Stochastic differential equations

Now we have and SDE which allows us to stay in the same initial distribution $p_0(x)$

$$dX_t = \frac{1}{2}\frac{\partial}{\partial x}\log p_0(X_t)dt + dw_t \tag{16}$$

Intuition: here we perform gradient optimization by minimizing negative log-likelihood to compensate added noise

$$dX_t = -\frac{1}{2}\nabla_x L(X_t)dt + dw_t \tag{17}$$

$L(x) = -\log p_0(x)$ - negative log-likelihood loss.

Now we have and SDE which allows us to stay in the same initial distribution $p_0(x)$

$$dX_t = \frac{1}{2}\frac{\partial}{\partial x}\log p_0(X_t)dt + dw_t \tag{18}$$

Example 1: if $p_0(x) = Ce^{-x^2}$ is Gaussian, then our SDE becomes Ornstein–Uhlenbeck process:

$$dX_t = \frac{1}{2}\frac{\partial}{\partial x}\log Ce^{-X_t^2}dt + dw_t =$$

$$= -\frac{1}{2}\frac{\partial}{\partial x}X_t^2 dt + dw_t$$

and then

$$dX_t = -X_t dt + dw_t$$

Stochastic differential equations

Now we have and SDE which allows us to stay in the same initial distribution $p_0(x)$

$$dX_t = \frac{1}{2}\frac{\partial}{\partial x}\log p_0(X_t)dt + dw_t \tag{19}$$

Example 2: if $p_0(x) = Ce^{-U(x)}$ is a particle in a force field $U(x)$.

$$dX_t = \frac{1}{2}\frac{\partial}{\partial x}\log Ce^{-U(X_t)}dt + dw_t =$$

$$= -\frac{1}{2}\frac{\partial}{\partial x}U(X_t)dt + dw_t$$

Note that we don't need to compute the partition function

$$C = \int e^{-U(x)}dx$$

to be able to sample from this distribution.
Note also that potential field equals to the negative log-likelihood loss.

Stochastic differential equations

Now we have and SDE which allows us to stay in the same initial distribution $p_0(x)$

$$dX_t = \frac{1}{2}\frac{\partial}{\partial x}\log p_0(X_t)dt + dw_t \tag{20}$$

The gradient $\frac{1}{2}\frac{\partial}{\partial x}\log p_0(X_t)$ equals to the added noise (not exactly, the denoised sample only must be from the same distribution).

- What if we only have samples from $p_0(x)$ and we don't know the density?

We could train a machine learning algorithm to denoise our samples. This could be done by using the loss function:

$$L(\theta) = \int p_0(X)\int p(\epsilon)||\epsilon_\theta(X+\epsilon) - \epsilon||^2 d\epsilon dX \tag{21}$$

Stochastic differential equations

- What if we only have samples from $p_0(x)$ and we don't know the density?

We could train a machine learning algorithm to denoise our samples. This could be done by using the loss function:

$$L(\theta) = \int p_0(X) \int p(\epsilon) ||\epsilon_\theta(X+\epsilon) - \epsilon||^2 d\epsilon dX \tag{22}$$

Here $\epsilon_\theta(x)$ is a neural network with parameters θ which tries to predict noise from the noisy samples $X + \epsilon$.

$$\epsilon_\theta(x) \approx -\frac{1}{2}\frac{\partial}{\partial x} \log p_0(X_t) \tag{23}$$

And we could sample new data from the same distribution by using our SDE

$$dX_t = \frac{1}{2}\frac{\partial}{\partial x} \log p_0(X_t)dt + dw_t \tag{24}$$

Probability flow ODE

We have considered an SDE

$$dX_t = \mu(X_t, t)dt + dw_t \tag{25}$$

Let's generalize our result to the case if $\sigma(x, t) = \sigma(t)$

$$dX_t = \mu(X_t, t)dt + \sigma(t)dw_t \tag{26}$$

From the Fokker-Planck equation we obtain

$$\mu(x, t) = \frac{1}{p(x|t)} \frac{\sigma(t)^2}{2} \frac{\partial}{\partial x} (p(x|t)) = \frac{\sigma(t)^2}{2} \frac{\partial}{\partial x} \log p(x|t) \tag{27}$$

and the generalized density-conserving SDE becomes

$$dX_t = \frac{\sigma(t)^2}{2} \frac{\partial}{\partial x} \log p(X_t|t)dt + \sigma(t)dw_t \tag{28}$$

Probability flow ODE

Consider an arbitrary SDE of the form

$$dX_t = \mu(X_t, t)dt + \sigma(t)dw_t \tag{29}$$

Density-conserving SDE

$$dX_t = \frac{\sigma(t)^2}{2}\frac{\partial}{\partial x}\log p(X_t|t)dt + \sigma(t)dw_t \tag{30}$$

Now let's consider an ordinary differential equation

$$dX_t = \left[\mu(X_t, t) - \frac{\sigma(t)^2}{2}\frac{\partial}{\partial x}\log p(X_t|t)\right]dt \tag{31}$$

and try to write a Fokker-Planck equation for it

$$\frac{\partial p(x|t)}{\partial t} = -\frac{\partial}{\partial x}\left(\left[\mu(X_t, t) - \frac{\sigma(t)^2}{2}\frac{\partial}{\partial x}\log p(X_t|t)\right]p(x|t)\right) \tag{32}$$

Probability flow ODE

Now let's consider an ordinary differential equation

$$dX_t = \left[\mu(X_t, t) - \frac{\sigma(t)^2}{2} \frac{\partial}{\partial x} \log p(X_t|t) \right] dt \tag{33}$$

and try to write a Fokker-Planck equation for it

$$\frac{\partial p(x|t)}{\partial t} = -\frac{\partial}{\partial x} \left(\left[\mu(X_t, t) - \frac{\sigma(t)^2}{2} \frac{\partial}{\partial x} \log p(X_t|t) \right] p(x|t) \right) =$$

$$= -\frac{\partial}{\partial x} \left[\mu(X_t, t) p(x|t) \right] + \frac{\sigma(t)^2}{2} \frac{\partial}{\partial x} \left[p(x|t) \frac{\partial}{\partial x} \log p(X_t|t) \right],$$

$$p(x|t) \frac{\partial}{\partial x} \log p(X_t|t) = p(x|t) \frac{1}{p(X_t|t)} \frac{\partial}{\partial x} p(X_t|t) = \frac{\partial}{\partial x} p(X_t|t)$$

Probability flow ODE

Now let's consider an ordinary differential equation

$$dX_t = \left[\mu(X_t, t) - \frac{\sigma(t)^2}{2}\frac{\partial}{\partial x}\log p(X_t|t)\right] dt \tag{34}$$

We have obtained the Fokker-Planck equation

$$\frac{\partial p(x|t)}{\partial t} = -\frac{\partial}{\partial x}\left[\mu(X_t, t)p(x|t)\right] + \frac{\sigma(t)^2}{2}\frac{\partial^2}{\partial x^2}p(X_t|t)$$

Note that the same Fokker-Planck equations correspond to the SDE

$$dX_t = \mu(X_t, t)dt + \sigma(t)dw_t$$

Probability flow ODE

This ODE is called the probability flow ODE

$$dX_t = \left[\mu(X_t, t) - \frac{\sigma(t)^2}{2} \frac{\partial}{\partial x} \log p(X_t|t)\right] dt \tag{35}$$

If we start from an initial distribution $p_0(x)$ then the density evolution will be the same as for the SDE

$$dX_t = \mu(X_t, t)dt + \sigma(t)dw_t \tag{36}$$

It means that if we want to numerically solve SDE we instead solve ODE using some advanced high-order solver.

Reverse time SDE

Let's add probability conserving SDE:

$$dX_t = \frac{\sigma(t)^2}{2} \frac{\partial}{\partial x} \log p(X_t|t)dt + \sigma(t)dw_t \tag{37}$$

to the probability flow ODE:

$$dX_t = \left[\mu(X_t, t) - \frac{\sigma(t)^2}{2} \frac{\partial}{\partial x} \log p(X_t|t) \right] dt \tag{38}$$

We will obtain the original forward time SDE:

$$dX_t = \mu(X_t, t)dt + \sigma(t)dw_t \tag{39}$$

Reverse time SDE

Now consider $dt < 0$. In the probability conserving SDE we need to change the sign before dt. So probability-conserving SDE in reverse time becomes

$$dX_t = -\frac{\sigma(t)^2}{2}\frac{\partial}{\partial x}\log p(X_t|t)dt + \sigma(t)dw_t \tag{40}$$

If $dt < 0$ then probability flow ODE stays the same, since ODEs are reversible in time.

Now let's add reverse time ODE and SDE:

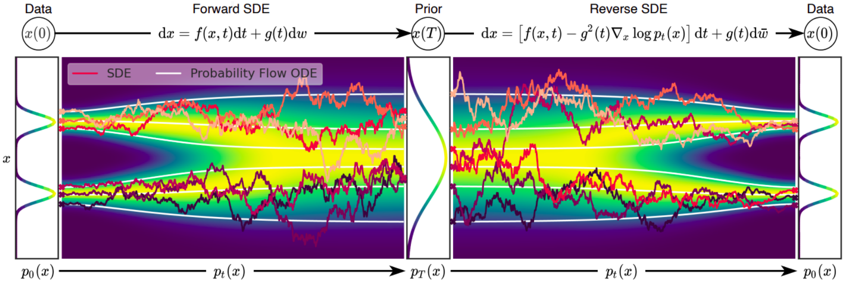
$$dX_t = \left[\mu(X_t, t) - \sigma(t)^2\frac{\partial}{\partial x}\log p(X_t|t)\right]dt + \sigma(t)dw \tag{41}$$

This is the SDE which corresponds the the reverse time probability flow ODE

$$dX_t = \left[\mu(X_t, t) - \frac{\sigma(t)^2}{2}\frac{\partial}{\partial x}\log p(X_t|t)\right]dt, \quad dt < 0 \tag{42}$$

Diffusion models

- Diffusion models leverage reverse time SDE to generate data from a given set of samples.



Good introduction to diffusion models "Understanding Diffusion Models: A Unified Perspective". https://arxiv.org/pdf/2208.11970.pdf