Diffusion Policies

Contents

1 Denoising Diffusion Probabilistic Models

From the paper:

Diffusion models are latent-variable models of the form

$$p_\theta(x_0) := \int p_\theta(x_{0:T})\,\mathrm{d}x_{1:T},$$

where $x_1, \ldots, x_T$ are latents of the same dimensionality as the data $x_0 \sim q(x_0)$. The joint distribution $p_\theta(x_{0:T})$ is called the *reverse process*, and it is defined as a Markov chain with learned Gaussian transitions starting at

$$p(x_T) \;=\; \mathcal{N}\Big(x_T; 0, \mathbf{I}\Big).$$

$$p_\theta(x_{0:T}) := p(x_T) \prod_{t=1}^{T} p_\theta(x_{t-1} \mid x_t), \quad p_\theta(x_{t-1} \mid x_t) := \mathcal{N}\Big(x_{t-1};\, \mu_\theta(x_t, t),\, \Sigma_\theta(x_t, t)\Big). \tag{1}$$

What distinguishes diffusion models from other latent-variable methods is that the approximate posterior $q(x_{1:T} \mid x_0)$, called the *forward process* or *diffusion process*, is fixed to a Markov chain that gradually adds Gaussian noise to the data according to a variance schedule $\beta_1, \ldots, \beta_T$:

$$q(x_{1:T} \mid x_0) := \prod_{t=1}^{T} q(x_t \mid x_{t-1}), \quad q(x_t \mid x_{t-1}) := \mathcal{N}\Big(x_t;\, \sqrt{1-\beta_t}\, x_{t-1},\, \beta_t \mathbf{I}\Big). \tag{2}$$

My notes for understanding:

The needed formulas are:

$$p(x_{t-1} \mid x_t) = \mathcal{N}\Big(x_{t-1};\, \mu_\theta(x_t, t),\, \Sigma_\theta(x_t, t)\Big), \tag{1}$$

$$q(x_{t-1} \mid x_t, x_0) = \mathcal{N}\Big(x_{t-1};\, \tilde{\mu}(x_t, x_0),\, \tilde{\beta}_t\, \mathbf{I}\Big), \tag{2}$$

$$\tilde{\mu}_t = \frac{1}{\sqrt{\alpha_t}}\Big(x_t \;-\; \frac{1-\alpha_t}{\sqrt{1-\alpha_t}}\,\epsilon_t\Big) \tag{3}$$

In my understanding, we have the following:
We first add noise in the forward process:

$$x_t = \sqrt{\alpha_t} x_{t-1} + \sqrt{1-\alpha_t}\epsilon_t$$

Then we express the reverse process as:

$$x_{t-1} = \frac{1}{\sqrt{\alpha_t}}\Big(x_t - \sqrt{1-\alpha_t}\epsilon_t\Big)$$

And here we just need to predict the noise ϵ_t added at time t to get the original image back.

From paper:

A notable property of the forward process is that it admits sampling x_t at an arbitrary timestep t in closed form: using the notation

$$\alpha_t := 1 - \beta_t, \quad \bar{\alpha}_t := \prod_{s=1}^{t} \alpha_s,$$

we have

$$q(x_t \mid x_0) = \mathcal{N}\Big(x_t;\, \sqrt{\bar{\alpha}_t}\, x_0,\, (1 - \bar{\alpha}_t)\, \mathbf{I}\Big). \tag{4}$$

It is not so difficult to arrive at this trough simple calculations.

1.1 Objective

From paper:

We try to minimize the negative log-likelihood:

$$\mathbb{E}_q[-\log p_\theta(\mathbf{x}_0)] \leq \mathbb{E}_q \left[-\log \frac{p_\theta(\mathbf{x}_{0:T})}{q(\mathbf{x}_{1:T}|\mathbf{x}_0)} \right] = \mathbb{E}_q \left[-\log p(\mathbf{x}_T) - \sum_{t \geq 1} \log \frac{p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)}{q(\mathbf{x}_t|\mathbf{x}_{t-1})} \right] =: L$$

Here the inequality follows from Jensen's inequality. We then rewrite the objective as:

$$\mathbb{E}_q \left[D_{KL}(q(\mathbf{x}_T|\mathbf{x}_0) \| p(\mathbf{x}_T)) + \sum_{t>1} D_{KL}(q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) \| p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)) - \log p_\theta(\mathbf{x}_0|\mathbf{x}_1) \right] \tag{4}$$

Which I have yet to understand. We still need to compute some things for the KL divergence:

$$q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) = \mathcal{N}(\mathbf{x}_{t-1}; \tilde{\boldsymbol{\mu}}_t(\mathbf{x}_t, \mathbf{x}_0), \tilde{\beta}_t \mathbf{I}), \quad (6)$$

where:

$$\tilde{\boldsymbol{\mu}}_t(\mathbf{x}_t, \mathbf{x}_0) := \frac{\sqrt{\bar{\alpha}_{t-1}}\beta_t}{1 - \bar{\alpha}_t}\mathbf{x}_0 + \frac{\sqrt{\alpha_t}(1 - \bar{\alpha}_{t-1})}{1 - \bar{\alpha}_t}\mathbf{x}_t \quad \text{and} \quad \tilde{\beta}_t := \frac{1 - \bar{\alpha}_{t-1}}{1 - \bar{\alpha}_t}\beta_t \quad (7)$$

I still need to revisit this part for the derivation.