# Score Matching Langevin Dynamics

References:

- JMLR - Estimation of Non-Normalized Statistical Models ⭐
- Neural Computation - A Connection Between Score Matching and Denoising Autoencoders ⭐
- Tutorial on Diffusion Models for Imaging and Vision ⭐
- Wikipedia - Langevin Dynamics
- Wikipedia - Langevin Equation
- Wikipedia - Fokker-Planck Equation

## Score Matching

Assume we have a continuous random variable $\mathbf{x} \in \mathbb{R}^D$ with some unknown distribution $p(\mathbf{x})$. We want to use a parameterized model $p_{\boldsymbol{\theta}}(\mathbf{x})$ to approximate the true distribution $p(\mathbf{x})$. What we have is a set of i.i.d. samples $\{\mathbf{x}_i\}_{i=1}^N$ from the distribution.

One way to model the distribution is to estimate the **score**, i.e., the gradient of the log-density function with respect to the data. Intuitively, the score is a vector that points in the direction of the steepest increase of the log density.

> This use differs slightly from traditional statistics terminology where score usually refers to the derivative of the log likelihood with respect to parameters, whereas here we are talking about a score with respect to the data. The score we use is called the ***Stein score***.

We denote the real score function as

$$\boldsymbol{\psi}(\mathbf{x}) = \nabla_{\mathbf{x}} \log p(\mathbf{x})$$

and the estimated score function as

$$\mathbf{s}(\mathbf{x}; \boldsymbol{\theta}) = \nabla_{\mathbf{x}} \log p_{\boldsymbol{\theta}}(\mathbf{x}) = \begin{bmatrix} s_1(\mathbf{x}) \\ \vdots \\ s_D(\mathbf{x}) \end{bmatrix}$$

We use $\mathbf{s}(\mathbf{x})$ instead of $\mathbf{s}(\mathbf{x}; \boldsymbol{\theta})$ to denote the estimated score function in the following for simplicity.

We can define the **squared distance** between the estimated and the true score functions as:

$$J(\boldsymbol{\theta}) = \frac{1}{2} \int_{\boldsymbol{\xi} \in \mathbb{R}^D} p(\boldsymbol{\xi}) \|\mathbf{s}(\boldsymbol{\xi}) - \boldsymbol{\psi}(\boldsymbol{\xi})\|^2 d\boldsymbol{\xi}$$

Thus, our **score matching** estimator of $\boldsymbol{\theta}$ is given by

$$\hat{\boldsymbol{\theta}} = \arg\min_{\boldsymbol{\theta}} J(\boldsymbol{\theta})$$

However, we do not know the true score function $\boldsymbol{\psi}(\mathbf{x})$. In practice, we can use non-parametric probability kernel density estimation methods (Parzen window estimation) to get an approximated score function $\hat{\boldsymbol{\psi}}(\mathbf{x})$, and minimize the squared distance between $\mathbf{s}(\mathbf{x})$ and $\hat{\boldsymbol{\psi}}(\mathbf{x})$ instead. This approach is called **Explicit Score Matching (ESM)**.

Instead of explicity matching the true score, Hyvärinen (2005) proposed **Implicit Score Matching**, which avoids the need for a target.

Expanding the formula of squared distance, we have

$$\begin{aligned} J(\boldsymbol{\theta}) &= \frac{1}{2} \int_{\boldsymbol{\xi} \in \mathbb{R}^D} p(\boldsymbol{\xi}) \Big[ \|\mathbf{s}(\boldsymbol{\xi})\|^2 - 2\mathbf{s}(\boldsymbol{\xi})^T \boldsymbol{\psi}(\boldsymbol{\xi}) + \|\boldsymbol{\psi}(\boldsymbol{\xi})\|^2 \Big] d\boldsymbol{\xi} \\ &= \underbrace{\left[ \frac{1}{2} \int_{\boldsymbol{\xi} \in \mathbb{R}^D} p(\boldsymbol{\xi}) \|\mathbf{s}(\boldsymbol{\xi})\|^2 d\boldsymbol{\xi} \right]}_{\text{Term 1}} + \underbrace{\left[ - \int_{\boldsymbol{\xi} \in \mathbb{R}^D} p(\boldsymbol{\xi}) \mathbf{s}(\boldsymbol{\xi})^T \boldsymbol{\psi}(\boldsymbol{\xi}) d\boldsymbol{\xi} \right]}_{\text{Term 2}} + \underbrace{\left[ \frac{1}{2} \int_{\boldsymbol{\xi} \in \mathbb{R}^D} p(\boldsymbol{\xi}) \|\boldsymbol{\psi}(\boldsymbol{\xi})\|^2 d\boldsymbol{\xi} \right]}_{\text{constant}} \end{aligned}$$

Here

$$\text{Term 1} = \frac{1}{2}\int_{\boldsymbol{\xi}\in\mathbb{R}^D} p(\boldsymbol{\xi})\Big[\sum_{i=1}^{D} s_i(\boldsymbol{\xi})^2\Big]d\boldsymbol{\xi}$$

$$\begin{aligned}
\text{Term 2} &= -\int_{\boldsymbol{\xi}\in\mathbb{R}^D} p(\boldsymbol{\xi})\sum_{i=1}^{D} s_i(\boldsymbol{\xi})\psi_i(\boldsymbol{\xi})d\boldsymbol{\xi} \\
&= -\int_{\boldsymbol{\xi}\in\mathbb{R}^D} p(\boldsymbol{\xi})\sum_{i=1}^{D} s_i(\boldsymbol{\xi})\frac{\partial \log p(\boldsymbol{\xi})}{\partial \xi_i}d\boldsymbol{\xi} \\
&= -\int_{\boldsymbol{\xi}\in\mathbb{R}^D} p(\boldsymbol{\xi})\sum_{i=1}^{D} s_i(\boldsymbol{\xi})\frac{1}{p(\boldsymbol{\xi})}\frac{\partial p(\boldsymbol{\xi})}{\partial \xi_i}d\boldsymbol{\xi} \\
&= -\int_{\boldsymbol{\xi}\in\mathbb{R}^D} \sum_{i=1}^{D} s_i(\boldsymbol{\xi})\frac{\partial p(\boldsymbol{\xi})}{\partial \xi_i}d\boldsymbol{\xi} \\
&= -\sum_{i=1}^{D}\int_{\boldsymbol{\xi}\in\mathbb{R}^D} s_i(\boldsymbol{\xi})\frac{\partial p(\boldsymbol{\xi})}{\partial \xi_i}d\boldsymbol{\xi} \\
&= \sum_{i=1}^{D}\int_{\boldsymbol{\xi}\in\mathbb{R}^D} p(\boldsymbol{\xi})\frac{\partial s_i(\boldsymbol{\xi})}{\partial \xi_i}d\boldsymbol{\xi}
\end{aligned}$$

> See Appendix for the proof of the last line.

So we have

$$J(\boldsymbol{\theta}) = \int_{\boldsymbol{\xi}\in\mathbb{R}^D} p(\boldsymbol{\xi})\sum_{i=1}^{D}\Big[\frac{1}{2}s_i(\boldsymbol{\xi})^2 + \frac{\partial s_i(\boldsymbol{\xi})}{\partial \xi_i}\Big]d\boldsymbol{\xi} + \text{constant}$$

We have thus proven the remarkable fact that our objective no longer requires having an explicit score target.

In practice, we have $N$ observations of the random vector $\mathbf{x}$, denoted by $\mathbf{x}_1, \ldots, \mathbf{x}_N$. The sample version of $J$ is obtained as

$$\tilde{J}(\boldsymbol{\theta}) = \frac{1}{N}\sum_{t=1}^{N}\sum_{i=1}^{D}\Big[\frac{1}{2}s_i(\mathbf{x}_t)^2 + \frac{\partial s_i(\mathbf{x}_t)}{\partial (\mathbf{x}_t)_i}\Big] + \text{constant}$$

which is asymptotically equivalent to $J$ due to the law of large numbers. By minimizing $\tilde{J}$, we obtain $\hat{\boldsymbol{\theta}}$ and the corresponding estimator of the score function, $\mathbf{s}(\mathbf{x}; \hat{\boldsymbol{\theta}})$.

> The score matching objective can also be written as
>
> $$\begin{aligned}
> J(\boldsymbol{\theta}) &= \int_{\mathbf{x}\in\mathbb{R}^D} p(\mathbf{x})\Big[\operatorname{tr}\big(\nabla_{\mathbf{x}}\mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x})\big) + \frac{1}{2}\|\mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x})\|_2^2\Big]d\mathbf{x} + \text{constant} \\
> &= \mathbb{E}_{\mathbf{x}\sim p(\mathbf{x})}\Big[\operatorname{tr}\big(\nabla_{\mathbf{x}}\mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x})\big) + \frac{1}{2}\|\mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x})\|_2^2\Big] + \text{constant}
> \end{aligned}$$

# Denoising Score Matching

**Denoising Score Matching (DSM)** is inspired by both the Score Matching principle and the Denoising Autoencoder (DAE) approach.

We denote the clean sample as $\mathbf{x}$, and get the corrupted sample $\tilde{\mathbf{x}}$ by a pre-defined perturbation $q_\sigma(\tilde{\mathbf{x}}|\mathbf{x})$. Denoising score matching defines the following objective:

$$\mathcal{J}_{\text{DSM}}(\boldsymbol{\theta}) = \mathbb{E}_{\mathbf{x}\sim p_{\text{data}}, \tilde{\mathbf{x}}\sim q_\sigma(\tilde{\mathbf{x}}|\mathbf{x})}\Big[\|\mathbf{s}_\theta(\tilde{\mathbf{x}}) - \nabla_{\tilde{\mathbf{x}}}\log q_\sigma(\tilde{\mathbf{x}}|\mathbf{x})\|^2\Big]$$

The underlying intuition is that following the gradient of the log density at some corrupted point, $\tilde{\mathbf{x}}$ should ideally move toward the clean sample $\mathbf{x}$.

Note that if we choose the gaussian kernel $q_\sigma(\tilde{\mathbf{x}}|\mathbf{x}) = \mathcal{N}(\tilde{\mathbf{x}}; \mathbf{x}, \sigma^2\mathbf{I})$, we have

$$\nabla_{\mathbf{x}}\log q_\sigma(\tilde{\mathbf{x}}|\mathbf{x}) = \frac{1}{\sigma^2}(\mathbf{x} - \tilde{\mathbf{x}})$$

The direction $\frac{1}{\sigma^2}(\mathbf{x} - \tilde{\mathbf{x}})$ clearly corresponds to moving from $\tilde{\mathbf{x}}$ back toward clean sample $\mathbf{x}$, and we want $\mathbf{s}_\theta(\tilde{\mathbf{x}})$ to match that as

best it can. Thus, with a **Gaussian kernel**, the DSM objective has a simpler form:

$$\mathcal{J}_{\text{DSM}}(\boldsymbol{\theta}) = \mathbb{E}_{\mathbf{x}\sim p_{\text{data}}}\mathbb{E}_{\tilde{\mathbf{x}}\sim\mathcal{N}(\mathbf{x},\sigma^2\mathbf{I})}\left[\left\|\mathbf{s}_\theta(\tilde{\mathbf{x}}) - \frac{\mathbf{x}-\tilde{\mathbf{x}}}{\sigma^2}\right\|^2\right]$$

Minimizing the objective, we obtain a score estimator $\mathbf{s}_\theta(\tilde{\mathbf{x}})$ which gives the direction that should be followed to move from $\tilde{\mathbf{x}}$ toward $\mathbf{x}$. With some proper sampling algorithm, we can generate samples of $p_{\text{data}}$ starting from any initial point $\mathbf{x}_0$.

# Langevin Dynamics

## Langevin Equation in Physics

**Langevin equation** is a stochastic differential equation (SDE) describing how a system evolves when subjected to a combination of deterministic and fluctuating ("random") forces.

The original Langevin equation describes **Brownian motion**. The form is given by

$$m\frac{d\mathbf{v}}{dt} = -\lambda\mathbf{v} + \boldsymbol{\eta}, \quad \boldsymbol{\eta}\sim\mathcal{N}(\mathbf{0}, 2\lambda k_{\text{B}}T\mathbf{I})$$

Here, $\mathbf{v}$ is the velocity of the particle, $\lambda$ is its damping coefficient, $m$ is its mass; $k_{\text{B}}$ is the Boltzmann constant, $T$ is the temperature. The force acting on the particle is written as a sum of

1. a viscous force proportional to the particle's velocity;
2. a random force $\boldsymbol{\eta}(t)$ representing the effect of the collisions with the molecules of the fluid.

The force $\boldsymbol{\eta}(t)$ has a Gaussian probability distribution with correlation function

$$\langle\boldsymbol{\eta}(t), \boldsymbol{\eta}(t')\rangle = 2\lambda k_{\text{B}}T\mathbf{I}\cdot\delta(t-t')$$

This indicates that the random force is time-independent.

## Langevin Dynamics in Generative Models

If we consider other external forces, they can all be represented by a potential force $-\nabla_{\mathbf{x}}U(\mathbf{x})$. The Langevin equation can then be written as

$$m\frac{d\mathbf{v}}{dt} = -\nabla U(\mathbf{x}) - \lambda\mathbf{v} + \boldsymbol{\eta}, \quad \boldsymbol{\eta}\sim\mathcal{N}(\mathbf{0}, 2\lambda k_{\text{B}}T\mathbf{I})$$

Sometimes the inertia (mass) of the particle is negligible in comparison with the damping force. For instance, the pollen in a viscous fluid can be considered as a particle with zero inertia. In this case, the trajectory of the particle is described by the so-called **Overdamped Langevin Equation**:!--https://arxiv.org/pdf/1807.10922--

$$0 = -\nabla U(\mathbf{x}) - \lambda\mathbf{v} + \boldsymbol{\eta}, \quad \boldsymbol{\eta}\sim\mathcal{N}(\mathbf{0}, 2\lambda k_{\text{B}}T\mathbf{I})$$

Or equivalently,

$$\lambda d\mathbf{x} = -\nabla U(\mathbf{x})dt + \sqrt{2\lambda k_{\text{B}}T}\boldsymbol{\epsilon}dt, \quad \boldsymbol{\epsilon}\sim\mathcal{N}(\mathbf{0}, \mathbf{I})$$

In domains other than physics, we often set $\lambda = 1,\ T = 1, k_{\text{B}} = 1$ for simplicity. Then we have

$$d\mathbf{x} = -\nabla U(\mathbf{x})dt + \sqrt{2}\boldsymbol{\epsilon}dt, \quad \boldsymbol{\epsilon}\sim\mathcal{N}(\mathbf{0}, \mathbf{I})$$

If we set the potential as the negative log probability density, i.e., $U(\mathbf{x}) = -\log p(\mathbf{x})$, we get the **overdamped Langevin equation** in **generative modeling**:

$$d\mathbf{x} = \nabla\log p(\mathbf{x})dt + \sqrt{2}\boldsymbol{\epsilon}dt, \quad \boldsymbol{\epsilon}\sim\mathcal{N}(\mathbf{0}, \mathbf{I})$$

The **discrete form** is given as

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

$$\boxed{\mathbf{x}_{t+1} - \mathbf{x}_t = \eta \nabla \log p(\mathbf{x}_t) + \sqrt{2\eta}\mathbf{z}_t, \quad \mathbf{z}_t \sim \mathcal{N}(\mathbf{0}, \mathbf{I})}$$

This is the iteration formula used in generative modeling.

By thermodynamics, the equilibrium distribution of $\mathbf{x}$ is the **Boltzmann distribution**

$$p_{\text{equilibrium}}(\mathbf{x}) = \exp\Big[-\frac{U(\mathbf{x})}{k_{\text{B}}T}\Big]/Z$$

where $Z$ is a normalizing constant. Since we already set $\lambda = 1,\ T = 1, k_{\text{B}} = 1$, which leads to $U(\mathbf{x})/k_{\text{B}}T = -\log p(\mathbf{x})$, we have

$$p_{\text{equilibrium}}(\mathbf{x}) = p(\mathbf{x})$$

So if we choose the negative log probability density as the potential, and iteratively update $\mathbf{x}$ with overdamped Langevin dynamics, $\mathbf{x}$ will eventually converge to a equilibrium distribution $p_{\text{equilibrium}}(\mathbf{x})$, which is exactly the pre-set probability distribution $p(\mathbf{x})$.

In other words, for any probability distribution $p(\mathbf{x})$, as long as we know its **score**, i.e., $\nabla p(\mathbf{x})$, we can generate samples from it using overdamped Langevin dynamics.

# Appendix

## Proof of Implicit Score Matching

> Assume $f : \mathbb{R}^D \to \mathbb{R}$ and $g : \mathbb{R}^D \to \mathbb{R}$ are both scalar-valued continuous differentiable functions defined on $\mathbb{R}^D$. Additionally, assume $f(\boldsymbol{\xi})$ and $g(\boldsymbol{\xi})$ both approaches 0 when $\|\boldsymbol{\xi}\|$ approaches infitinty.
>
> By the product rule, we have
>
> $$\frac{\partial[f(\boldsymbol{\xi})g(\boldsymbol{\xi})]}{\partial\xi_1} = f(\boldsymbol{\xi})\frac{\partial g(\boldsymbol{\xi})}{\partial\xi_1} + g(\boldsymbol{\xi})\frac{\partial f(\boldsymbol{\xi})}{\partial\xi_1}$$
>
> Take the integral on the left side, we have
>
> $$\begin{aligned}\int_{\boldsymbol{\xi}\in\mathbb{R}^D}\frac{\partial[f(\boldsymbol{\xi})g(\boldsymbol{\xi})]}{\partial\xi_1}d\boldsymbol{\xi} &= \int_{\xi_2,\xi_3,\ldots,\xi_D}\left[\int_{\xi_1\in\mathbb{R}}\frac{\partial[f(\boldsymbol{\xi})g(\boldsymbol{\xi})]}{\partial\xi_1}d\xi_1\right]d\xi_2 d\xi_3\ldots d\xi_D \\ &= \int_{\xi_2,\xi_3,\ldots,\xi_D}\Big[f(+\infty,\xi_2,\xi_3,\ldots,\xi_D)g(+\infty,\xi_2,\xi_3,\ldots,\xi_D) \\ &\quad -f(-\infty,\xi_2,\xi_3,\ldots,\xi_D)g(-\infty,\xi_2,\xi_3,\ldots,\xi_D)\Big]d\xi_2 d\xi_3\ldots d\xi_D \\ &= \int_{\xi_2,\xi_3,\ldots,\xi_D}\Big[0\cdot 0 - 0\cdot 0\Big]d\xi_2 d\xi_3\ldots d\xi_D \\ &= 0\end{aligned}$$
>
> Take the integral on the right side, we have
>
> $$0 = \int_{\boldsymbol{\xi}\in\mathbb{R}^D} f(\boldsymbol{\xi})\frac{\partial g(\boldsymbol{\xi})}{\partial\xi_1}d\boldsymbol{\xi} + \int_{\boldsymbol{\xi}\in\mathbb{R}^D} g(\boldsymbol{\xi})\frac{\partial f(\boldsymbol{\xi})}{\partial\xi_1}d\boldsymbol{\xi}$$
>
> The same applies for all indices of $\xi_i$.

By definition, $p(\boldsymbol{\xi})$ and $s_i(\boldsymbol{\xi})$ are continuous differentiable functions from $\mathbb{R}^D$ to $\mathbb{R}$. Meanwhile, when $\xi_i$ approached infinity, $p(\boldsymbol{\xi})$ and $s_i(\boldsymbol{\xi})$ is 0. By the above lemma, we have

$$\int_{\boldsymbol{\xi}\in\mathbb{R}^D} s_i(\boldsymbol{\xi})\frac{\partial p(\boldsymbol{\xi})}{\partial\xi_i}d\boldsymbol{\xi} = -\int_{\boldsymbol{\xi}\in\mathbb{R}^D} p(\boldsymbol{\xi})\frac{\partial s_i(\boldsymbol{\xi})}{\partial\xi_i}d\boldsymbol{\xi}$$

## Parzen Density Estimate

The **Parzen density estimate**, also known as **Parzen window method** or **kernel density estimation (KDE)**, is a non-parametric technique for estimating the probability density function (PDF) of a random variable from a finite set of data points.

Consider a random variable $X \in \mathbb{R}^d$. We want to estimate its probability density function $f(\mathbf{x})$ using a set of observations $\{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n\}$. Parzen window method gives the estimated density as:

$$\hat{f}(\mathbf{x}) = \frac{1}{n} \sum_{i=1}^{n} \frac{1}{h} K\Big(\frac{\mathbf{x} - \mathbf{x}_i}{h}\Big)$$

where $K$ is the kernel function (normalized to integrate to 1) and $h$ is the **bandwidth** (a hyperparameter).

> It is easy to check that $\hat{f}(\mathbf{x})$ integrals to 1: Denote $\mathbf{u} = (\mathbf{x} - \mathbf{x}_i)/h$, then $d\mathbf{x} = hd\mathbf{u}$, and we have
>
> $$\begin{aligned}
> \int_{\mathbf{x} \in \mathbb{R}^d} \hat{f}(\mathbf{x}) d\mathbf{x} &= \frac{1}{n} \sum_{i=1}^{n} \int_{\mathbf{x} \in \mathbb{R}^d} \frac{1}{h} K\Big(\frac{\mathbf{x} - \mathbf{x}_i}{h}\Big) d\mathbf{x} \\
> &= \frac{1}{n} \sum_{i=1}^{n} \int_{\mathbf{u} \in \mathbb{R}^d} \frac{1}{h} K(\mathbf{u}) h d\mathbf{u} \\
> &= \frac{1}{n} \sum_{i=1}^{n} \underbrace{\int_{\mathbf{u} \in \mathbb{R}^d} K(\mathbf{u}) d\mathbf{u}}_{=1} \\
> &= \frac{1}{n} \cdot n \\
> &= 1
> \end{aligned}$$

Common kernels include:

- **Gaussian**:

$$K(\mathbf{u}) = \frac{1}{(2\pi)^{\frac{d}{2}}} \exp\Big(-\frac{\|\mathbf{u}\|_2^2}{2}\Big)$$

- **Epanechnikov (parabolic)**:

$$K(\mathbf{u}) = \begin{cases} \frac{d+2}{2c_d}(1 - \|\mathbf{u}\|_2^2), & |\mathbf{u}| \le 1 \\ 0, & \text{otherwise} \end{cases}$$

- **Uniform**:

$$K(\mathbf{u}) = \begin{cases} \frac{1}{c_d}, & \|\mathbf{u}\| \le 1 \\ 0, & \text{otherwise} \end{cases}$$

  Here $c_d = \dfrac{\pi^{d/2}}{\Gamma(1 + \frac{d}{2})}$ is the volume of the $d$-dimensional unit ball.

# Denoising Autoencoder

**Denoising autoencoder (DAE)** is a simple modification of classical autoencoder neural networks that are trained not to reconstruct their input but rather to denoise an **artificially corrupted version of their input**.

Let us consider some dataset $\mathbf{X} = \{\mathbf{x}^{(i)}\}_{i=1}^{N}$ consisting of $N$ i.i.d. samples of some continuous or discrete random variable $\mathbf{x} \in \mathbb{R}^d$. Following the logic of autoencoder, the denoising process can be formulated as:

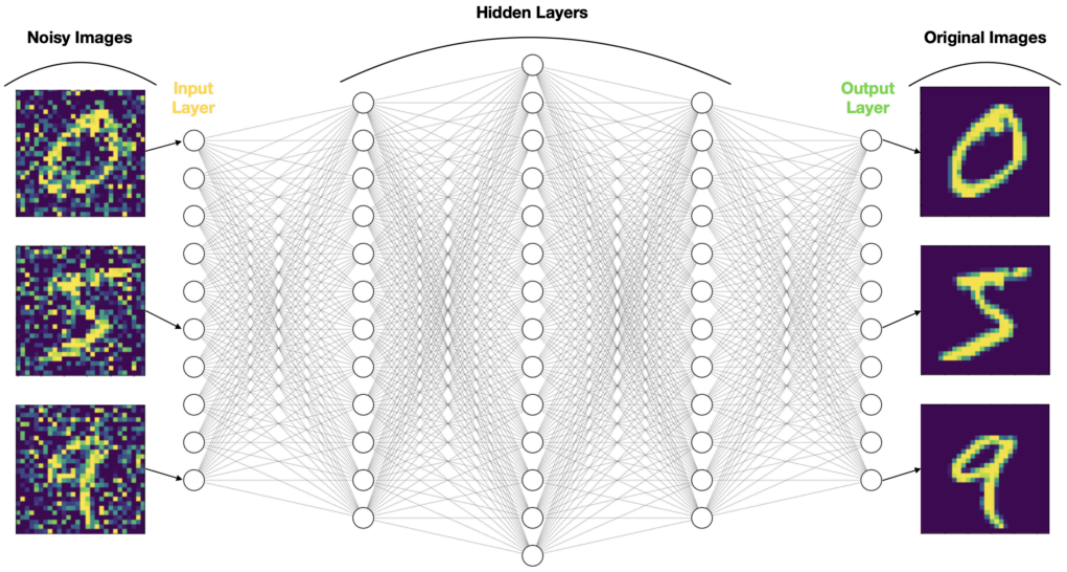
1. Input: denoised sample $\tilde{\mathbf{x}}$;
2. Pass $\tilde{\mathbf{x}}$ through the encoder to obtain the latent variable $\mathbf{z}$;
3. Pass $\mathbf{z}$ through the decoder to obtain the reconstructed data $\mathbf{x}'$.

Usually there is no need to separate the encoder and decoder, as they can be combined into a single network. We denote the network as $f_\theta : \mathbb{R}^d \to \mathbb{R}^d,\ \tilde{\mathbf{x}} \mapsto \mathbf{x}'$.

The training process becomes:

1. Sample an observation $\mathbf{x}$;
2. Corrupt the observation with some noise $\boldsymbol{\epsilon}$ to create $\tilde{\mathbf{x}} = \mathbf{x} + \boldsymbol{\epsilon}$ (usually $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \sigma^2 \mathbf{I})$;

3. Denoise the noisy observation $\tilde{\mathbf{x}}$ to obtain $\mathbf{x}' = f_\theta(\tilde{\mathbf{x}})$;
4. Update the parameters $\theta$ using some loss with $\mathbf{x}$ and $\mathbf{x}'$.




# Fokker-Planck Equation

## Definition

**Fokker–Planck equation** is a partial differential equation that describes the time evolution of the probability density function of a particle under the influence of drag forces and random forces, as in Brownian motion. It is also known as the **Kolmogorov forward equation**.

- **One Dimensional Case**: Consider an **Itô process**:

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

  Here $\mu(X_t, t)$ is the drift, $D(X_t, t) = \sigma^2(X_t, t)/2$ is the diffusion coefficient, and $W_t$ is a standard Wiener process. The **Fokker-Planck equation** for the probability density $p(x, t)$ of the random variable $X_t$ is

  $$\frac{\partial}{\partial t}p(x,t) = -\frac{\partial}{\partial x}\Big[\mu(x,t)p(x,t)\Big] + \frac{\partial^2}{\partial x^2}\Big[D(x,t)p(x,t)\Big]$$

- **Multi-Dimensional Case**: Consider an **Itô process** in $N$ dimensions:

  $$d\mathbf{X}_t = \boldsymbol{\mu}(\mathbf{X}_t, t)dt + \boldsymbol{\sigma}(\mathbf{X}_t, t)d\mathbf{W}_t$$

  Here $\mathbf{X}_t$ and $\boldsymbol{\mu}(\mathbf{X}_t, t)$ are $N$-dimensional vectors, $\boldsymbol{\sigma}(\mathbf{X}_t, t)$ is an $N \times M$ matrix, and $\mathbf{W}_t$ is an $M$-dimensional standard Wiener process.
  The probability density $p(\mathbf{x}, t)$ for $\mathbf{X}_t$ satisfies the **multi-dimensional Fokker-Planck equation**:

  $$\frac{\partial p(\mathbf{x},t)}{\partial t} = -\sum_{i=1}^{N}\frac{\partial}{\partial x_i}\Big[\mu_i(\mathbf{x},t)p(\mathbf{x},t)\Big] + \sum_{i=1}^{N}\sum_{j=1}^{N}\frac{\partial^2}{\partial x_i \partial x_j}\Big[D_{ij}(\mathbf{x},t)p(\mathbf{x},t)\Big]$$

  Here $\boldsymbol{\mu} = (\mu_1, \ldots, \mu_N)$ is the drift vector, and $\mathbf{D} = \frac{1}{2}\boldsymbol{\sigma}\boldsymbol{\sigma}^T$ is the diffusion tensor.

## Fokker-Planck Equation for Langevin Dynamics

In generative modeling, assume the pre-set probablity distribution is $p_r(\mathbf{x})$, the SDE of **Langevin Dynamics** is given by

$$d\mathbf{X}_t = \nabla \log p_r(\mathbf{x})dt + \sqrt{2}d\mathbf{W}_t$$

Matching Fokker-Planck equation's form, we have

$$\boldsymbol{\mu}(\mathbf{x}, t) = \nabla \log p_r(\mathbf{x})$$

$$\boldsymbol{\sigma}(\mathbf{x}, t) = \sqrt{2}\mathbf{I}$$

$$\mathbf{D}(\mathbf{x}, t) = \frac{1}{2}\boldsymbol{\sigma}\boldsymbol{\sigma}^T = \mathbf{I}$$

$$\mu_i(\mathbf{x}, t) = \frac{\partial}{\partial x_i} \log p_r(\mathbf{x})$$

$$D_{ij}(\mathbf{x}, t) = \delta_{ij}$$

The evolution of the probability density function is given by

$$\begin{aligned}
\frac{\partial p(\mathbf{x}, t)}{\partial t} &= -\sum_{i=1}^{N} \frac{\partial}{\partial x_i} \Big[ \Big( \frac{\partial}{\partial x_i} \log p_r(\mathbf{x}) \Big) p(\mathbf{x}, t) \Big] + \sum_{i=1}^{N} \sum_{j=1}^{N} \frac{\partial^2}{\partial x_i \partial x_j} \Big[ \delta_{ij} p(\mathbf{x}, t) \Big] \\
&= -\sum_{i=1}^{N} \frac{\partial}{\partial x_i} \Big[ \Big( \frac{1}{p_r(\mathbf{x})} \frac{\partial}{\partial x_i} p_r(\mathbf{x}) \Big) p(\mathbf{x}, t) \Big] + \sum_{i=1}^{N} \frac{\partial^2}{\partial x_i^2} \Big[ p(\mathbf{x}, t) \Big] \\
&= -\sum_{i=1}^{N} \frac{\partial}{\partial x_i} \Big[ \frac{p(\mathbf{x}, t)}{p_r(\mathbf{x})} \frac{\partial}{\partial x_i} p_r(\mathbf{x}) \Big] + \sum_{i=1}^{N} \frac{\partial^2}{\partial x_i^2} \Big[ p(\mathbf{x}, t) \Big] \\
&= -\nabla \cdot \Big[ \frac{p(\mathbf{x}, t)}{p_r(\mathbf{x})} \nabla p(\mathbf{x}, t) \Big] + \nabla^2 p(\mathbf{x}, t)
\end{aligned}$$

Assume we have already reached the stationary state $p(\mathbf{x}, t) = p_r(\mathbf{x})$, then $\frac{\partial p(\mathbf{x}, t)}{\partial t} = 0$, which means the probability distribution $p(\mathbf{x}, t)$ converges to the target distribution $p_r(\mathbf{x})$ when $t \to \infty$.