# Denoising Diffusion Probabilistic Models

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11 / 2025

# Outline


1. What are DDPMs
2. Forward Process
3. Reverse Process
4. Training Algorithm
5. Sampling Algorithm
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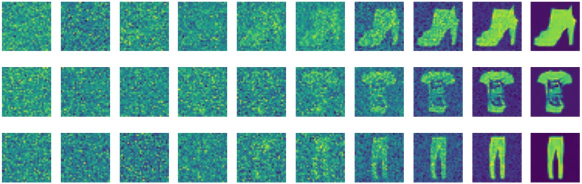
# Overview

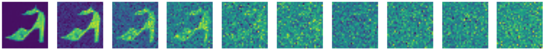
- Denoising Diffusion Probabilistic Models (DDPMs) generate images by iteratively removing noise from a signal until it looks like a real image.



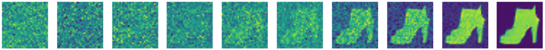
# DDPMs Building Blocks

DDPMs are made of **two iterative processes** defined by different Markov Chains: a **forward** and a **reversion** process.

1. **Forward Process**: gradually adds noise to a image by sampling from a normal distribution according to a Markov Chain



2. **Reverse Process**: removes noise by sampling from a normal distribution according to another Markov Chain



# DDPMs Building Blocks

1. **Forward Process' Distribution**

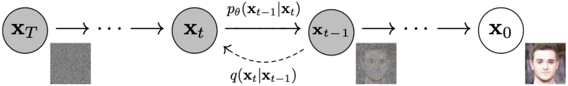
$$q(x_t|x_{t-1}) := \mathcal{N}(x_t; \sqrt{1-\beta_t} \times x_{t-1}; \beta_t I) \tag{1}$$

2. **Reverse Process' Distribution**

$$p(x_T) = \mathcal{N}(x_T; 0; 1) \tag{2}$$

$$p_\theta(x_{0:T}) := p(x_T) \prod_{t=1}^{T} p_\theta(x_{t-1}|x_t) \tag{3}$$

$$p_\theta(x_{t-1}|x_t) := \mathcal{N}(x_{t-1}; \mu_\theta(x_t, t); \Sigma_\theta(x_t, t)) \tag{4}$$



# Forward Process Distribution

- The forward distribution (**q**) is a Normal Distribution with mean as a function of $\mathbf{x_0}$:

$$q(x_t|x_{t-1}) := \mathcal{N}(x_t; \sqrt{1-\beta_t} \times x_{t-1}; \beta_t I) \tag{5}$$

(6)

$\sim \mathcal{N}\left(\sqrt{\bar{\alpha}_\mathbf{t}}\right.$


$\left., (\mathbf{1} - \bar{\alpha}_\mathbf{t})\mathbf{I}\right)$

- $\bar{\alpha}_\mathbf{t}$ is called the cumulative noise and is proportional to the product of the transitions distributions that gradually turns $\mathbf{x_0}$ into $\mathbf{x_t}$.
- The forward distribution let's us produce a noisy signal $\mathbf{x_t}$ from the original $\mathbf{x_0}$ in a single step.

# Forward Process in PyTorch

```python
class DDPMScheduler(nn.Module):
    def __init__(self, num_time_steps: int=1000):

        super().__init__()
        self.beta = torch.linspace(1e-4, 0.02, num_time_steps, requires_grad=False)

        # Alpha is defined as 1 - beta, i.e., 1 - Variance at step t
        alpha = 1 - self.beta

        # The variances are held constant during training, requires_grad = False
        self.alpha = torch.cumprod(alpha, dim=0).requires_grad_(False)

    def forward(self, t):
        return self.beta[t], self.alpha[t]
```

# Forward Process Sampling in PyTorch

Given an input tensor $\mathbf{x_0}$ one can sample from $\mathbf{q}(\mathbf{x_t}|\mathbf{x_0})$ by making the attribution:

```python
# Random sample from dataset
idx = random.randint(0, len(dataset) - 1)
x0, y0 = dataset[idx]

# Sampling 10 signal with increasing noise levels
for t in range(1, 10):
    scheduler = DDPMScheduler(num_time_steps=t + 1)

    # Cumulative noise up until step t
    beta, alpha = scheduler(t)

    e = torch.randn_like(x0, requires_grad=False)
    x_t = (torch.sqrt(alpha)*x0) + (torch.sqrt(1-alpha)*e)
```

# Reverse Process' Transitions Distribution

- The reverse distribution is a Normal Distribution with mean and variance as functions of the noisy signal $\mathbf{x_t}$ and the amount of noise that has been added to it $\mathbf{t}$.
-
$$p_\theta(x_{t-1}|x_t) := \mathcal{N}(x_{t-1}; \mu_\theta(x_t, t); \Sigma_\theta(x_t, t)) \tag{7}$$
- What we want is to have a model that is capable of sampling from $\mathbf{p}$ so that $\mathbf{x_{t-1}}$ is indeed a less noisy version of $\mathbf{x_t}$, i.e., a model that can reverse what was done in the forward process.

# Reverse Process' Prior

- Ideally, the Reverse Process would enable us to sample from $\mathbf{x_0}$ directly:

$$p(\mathbf{x}_0) = \int p(\mathbf{x_0}, \mathbf{x_{1:T}})\mathbf{d_{1:T}} \tag{8}$$

$$\tag{9}$$

- Unfortunately, $p(\mathbf{x}_0)$ is very complex due to its multidimensionality. It is **intractable**.
- That is why the training of DDPMs never optmizes $p(\mathbf{x}_0)$ directly. Instead, what is optmized is its lower bound.

# Reverse Process' Transitions Distribution

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$$p(x_T) = \mathcal{N}(x_T; 0; 1) \tag{10}$$

$$p_\theta(x_{0:T}) := p(x_T) \prod_{t=1}^{T} p_\theta(x_{t-1}|x_t) \tag{11}$$

$$p_\theta(x_{t-1}|x_t) := \mathcal{N}(x_{t-1}; \mu_\theta(x_t, t); \Sigma_\theta(x_t, t)) \tag{12}$$

- What we ultimately want is to have a $\mathbf{x}_0$ that is as likely as possible. We can marginalize $\mathbf{x}_0$ using the latent variables $\mathbf{x_{1:T}}$, i.e., by using the noisy images.

# Evidence Lower Bound (ELBO)

- DDPMs are not trained to sample from $p(\mathbf{x}_0)$, but instead to maximize its lower bound ELBO ($L$)
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$$log[p_\theta(\mathbf{x_0})] = log \int_{\mathbf{x_{1:T}}} p(\mathbf{x_0}, \mathbf{x_{1:T}}) d\mathbf{x_{1:T}} \tag{13}$$

$$log[p_\theta(\mathbf{x_0})] = log \int_{\mathbf{x_{1:T}}} p(\mathbf{x_0}, \mathbf{x_{1:T}}) \frac{q(\mathbf{x_{1:T}}|\mathbf{x_0})}{q(\mathbf{x_{1:T}}|\mathbf{x_0})} d\mathbf{x_{1:T}} \tag{14}$$

$$\text{by definition,} \tag{15}$$

$$\mathbb{E}_q[f(\mathbf{x}_{1:T})] = \int q(\mathbf{x}_{1:T}|\mathbf{x}_0)\, f(\mathbf{x}_{1:T})\, d\mathbf{x}_{1:T} \tag{16}$$

$$\implies log[p_\theta(\mathbf{x_0})] = log(\mathbb{E}_q\left[\frac{p(\mathbf{x_{0:T}})}{q(\mathbf{x_{1:T}}|\mathbf{x_0})}\right]) \tag{17}$$

$$\text{the Jensen's inequality tells us} \tag{18}$$

$$f(\mathbb{E}(\mathbf{X})) \geq \mathbb{E}(f(\mathbf{X})) \tag{19}$$

$$\text{for any concave function f. log is concave, hence:} \tag{20}$$

$$log[p_\theta(\mathbf{x_0})] \geq \mathbb{E}_q\left[log \frac{p(\mathbf{x_{0:T}})}{q(\mathbf{x_{1:T}}|\mathbf{x_0})}\right] \tag{21}$$

$$\text{We define the Evidence Lower Bound L as:} \tag{22}$$

$$L := \mathbb{E}_q\left[- log \frac{p(\mathbf{x_{0:T}})}{q(\mathbf{x_{1:T}}|\mathbf{x_0})}\right] \tag{23}$$

# Evidence Lower Bound (ELBO)

- DDPMs are not trained to sample from $p(\mathbf{x}_0)$, but instead to maximize its lower bound ELBO ($L$)
- With more algebraic manipulation and using the fact that both the forward and reverse processes are Markov Chains, one can derive the following equation:

$$L := \mathbb{E}_q\left[-log\frac{p(\mathbf{x_{0:T}})}{q(\mathbf{x_{1:T}}|\mathbf{x_0})}\right] \tag{25}$$

$$L = \mathbb{E}_q\left[-log\frac{p(\mathbf{x_T})}{q(\mathbf{x_T}|\mathbf{x_0})}\right] - logp_\theta(\mathbf{x_0}|\mathbf{x_1}) - \mathbb{E}_q\left[\sum_{t=2}^{T}\mathbf{D_{KL}}\left[q(\mathbf{x_{t-1}}|\mathbf{x_t},\mathbf{x_0})||p_\theta(\mathbf{x_{t-1}}|\mathbf{x_t}))\right]\right] \tag{26}$$

- **We can conclude that maximizing ELBO (L) is equivalent to minimizing the KL-Divergence between $q(\mathbf{x_{t-1}}|\mathbf{x_t},\mathbf{x_0})$ and $p_\theta(\mathbf{x_{t-1}}|\mathbf{x_t})$, i.e., minimizing the divergence between the forward and reverse processes' distributions.**

# Defining $q(\mathbf{x_{t-1}}|\mathbf{x_t}, \mathbf{x_0})$

$$q(\mathbf{x_{t-1}}|\mathbf{x_t}, \mathbf{x_0}) = \frac{q(\mathbf{x_t}|\mathbf{x_{t-1}}, \mathbf{x_0})q(\mathbf{x_{t-1}}|\mathbf{x_0})}{q(\mathbf{x_t}|\mathbf{x_0})} \tag{27}$$

$$\text{we know the q distribution from Definition, hence} \tag{28}$$

$$q(\mathbf{x_{t-1}}|\mathbf{x_t}, \mathbf{x_0}) \text{ is a product of known Gaussians over another known Gaussian} \tag{29}$$

$$\mu_q(\mathbf{x_t}, \mathbf{x_0}) = \frac{(1-\bar{\alpha}_{t-1})\sqrt{\alpha_t}\mathbf{x_t} + (1-\alpha_t)\sqrt{\bar{\alpha}_{t-1}}\mathbf{x_0}}{(1-\bar{\alpha}_t)} \tag{30}$$

$$\Sigma_q(t) = \frac{(1-\alpha_t)(1-\bar{\alpha}_{t-1})}{1-\bar{\alpha}_t}\mathbf{I} \tag{31}$$

$$\implies q(\mathbf{x_{t-1}}|\mathbf{x_t}, \mathbf{x_0}) = \mathcal{N}(\mathbf{x_{t-1}}; \mu_q(\mathbf{x_t}, \mathbf{x_0}); \Sigma_q(t)) \tag{32}$$

# Defining $p_\theta(\mathbf{x_{t-1}}|\mathbf{x_t})$

$$p_\theta(\mathbf{x_{t-1}}|\mathbf{x_t}) = \mathcal{N}(\mathbf{x_{t-1}}; \mu_\theta(\mathbf{x_t}); \Sigma_\theta(t)) \tag{33}$$

$$\text{from DDPM's paper:} \tag{34}$$

$$\Sigma_\theta(t) = \Sigma_q(t) \tag{35}$$

$$\text{we are only left with the distribution's mean } \mu_\theta \tag{36}$$

$$\implies p_\theta(\mathbf{x_{t-1}}|\mathbf{x_t}) = \mathcal{N}(\mathbf{x_{t-1}}; \mu_\theta(\mathbf{x_t}); \Sigma_q(t)) \tag{37}$$

# Computing the KL Divergence Between $q$ and $p_\theta$

- Now we know we are trying to compute the KL Divergence between two Gaussians with the exact same variance.
- For that, there is the following result that arives from the definition of such divergence

$$d_1(x) = \mathcal{N}(\mu_1, \sigma^2) \tag{38}$$

$$d_2(x) = \mathcal{N}(\mu_2, \sigma^2) \tag{39}$$

$$\text{The KL divergence } D_{KL}(d_1|d_2) \text{ is given by:} \tag{40}$$

$$D_{KL}(d_1|d_2) = \frac{(\mu_1 - \mu_2)^2}{2\sigma^2} \tag{41}$$

$$\text{Hence,} \tag{42}$$

$$\mathbf{D_{KL}}\left[q(\mathbf{x_{t-1}}|\mathbf{x_t}, \mathbf{x_0})||p_\theta(\mathbf{x_{t-1}}|\mathbf{x_t})\right] = \mathbf{D_{KL}}\left(\mathcal{N}(\mathbf{x_{t-1}}; \mu_q(\mathbf{x_t}, \mathbf{x_0}); \Sigma_q(t)), \mathcal{N}(\mathbf{x_{t-1}}; \mu_\theta(\mathbf{x_t}); \Sigma_q(t))\right) \tag{43}$$

$$= \frac{1 - \bar{\alpha}_t}{2(1 - \alpha_t)(1 - \bar{\alpha}_{t-1})}||(\mu_q - \mu_\theta)_2^2|| \tag{44}$$

- **We just need to minimize the difference between the means of the reverse and forward processes' distributions, i.,e., minimize $||(\mu_q - \mu_\theta)_2^2||$.**

# Defining The Model's Prediction

- We can use the prediction of our model as the forward process' mean
- $$\mu_q(\mathbf{x_t}, \mathbf{x_0}) = \frac{(1-\bar{\alpha}_{t-1})\sqrt{\alpha_t}\mathbf{x_t} + (1-\alpha_t)\sqrt{\bar{\alpha}_{t-1}}\mathbf{x_0}}{(1-\bar{\alpha}_t)} \tag{45}$$
$$\text{we can define the prediction} \tag{46}$$
$$\mu_\theta(\mathbf{x_t}) := \hat{\mu}_q(\mathbf{x_t}, \mathbf{x_0}) \tag{47}$$
$$= \frac{(1-\bar{\alpha}_{t-1})\sqrt{\alpha_t}\mathbf{x_t} + (1-\alpha_t)\sqrt{\bar{\alpha}_{t-1}}\mathbf{x}_\theta}{(1-\bar{\alpha}_t)} \tag{48}$$
$$\implies \mathbf{D_{KL}}\left(\mathcal{N}(\mathbf{x_{t-1}}; \mu_\theta(\mathbf{x_t}); \Sigma_q(t)), \mathcal{N}(\mathbf{x_{t-1}}; \mu_q(\mathbf{x_t}, \mathbf{x_0}); \Sigma_q(t))\right) \tag{49}$$
$$= \frac{(1-\bar{\alpha}_t)(\bar{\alpha}_{t-1})}{2(1-\alpha_t)(1-\bar{\alpha}_{t-1})}||(\mathbf{x}_\theta - \mathbf{x_0})_2^2|| \tag{50}$$
- **Theoretically, this equation could be used as the loss function directly, but we can rewrite the images $\mathbf{x}_\theta$ and $\mathbf{x_0}$ in function of the Gaussian noises.**

# Defining The Model's Prediction

- We can rewrite $\mathbf{x_t}$ and $\mathbf{x_0}$ as functions of the added gaussian noises
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$$q(\mathbf{x_t}|\mathbf{x_0}) := \mathcal{N}(x_t; \sqrt{\bar{\alpha}_t} \times x_0; (1-\bar{\alpha}_t)\mathbb{I}) \tag{51}$$

which let's us write (52)

$$\mathbf{x_t} = \sqrt{\bar{\alpha}_t}x_0 + \sqrt{1-\bar{\alpha}_t}\epsilon \tag{53}$$

$$\implies \mathbf{x_0} = \frac{\mathbf{x_t} - \sqrt{1-\bar{\alpha}_t}\epsilon}{\sqrt{\bar{\alpha}_t}} \tag{54}$$

for a Standard Gaussian Noise $\epsilon$. (55)

We can now define our prediction $\hat{\epsilon} = \epsilon_\theta$ (56)

$$\mathbf{x}_\theta = \frac{\mathbf{x_t} - \sqrt{1-\bar{\alpha}_t}\epsilon_\theta}{\sqrt{\bar{\alpha}_t}} \tag{57}$$

$$\implies \frac{(1-\bar{\alpha}_t)(\bar{\alpha}_{t-1})}{2(1-\alpha_t)(1-\bar{\alpha}_{t-1})}||(\mathbf{x}_\theta - \mathbf{x_0})_2^2|| = \frac{(1-\bar{\alpha}_t)(\bar{\alpha}_{t-1})}{2(1-\alpha_t)(1-\bar{\alpha}_{t-1})}\frac{(1-\alpha_t)^2}{(1-\bar{\alpha}_t)\alpha_t}||(\epsilon_\theta - \epsilon)_2^2|| \tag{58}$$

- **The DDPM paper authors mention that optimizing $||(\epsilon_\theta - \epsilon)_2^2||$ without the scaling factor with the cumulative noise $\alpha_t$ is enough.**

# Noise Predictor Training

1: **repeat**
2: $\mathbf{x_0} \sim \mathbf{q}(\mathbf{x_0})$ ▷ Sample image from training set
3: $\mathbf{t} \sim \mathbf{Uniform}(\{\mathbf{1}, \ldots, \mathbf{T}\})$ ▷ Sample the step of the Forward Process Markov Chain
4: $\epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ ▷ Sample standard gaussian noise to be added to the input
5: $\mathbf{x_t} = \sqrt{\bar{\alpha}_\mathbf{t}}\mathbf{x_0} + \sqrt{\mathbf{1} - \bar{\alpha}_\mathbf{t}}\epsilon$ ▷ Forward Process/ Generating Noisy Image
6: Take Gradient Descent Step on $\nabla_\theta(||\epsilon - \epsilon_\theta(\mathbf{x_t}, \mathbf{t})||)$
7: **until** converged

# Sampling Algorithm Derivation

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$$p_\theta(\mathbf{x_{t-1}}|\mathbf{x_t}) = \mathcal{N}(\mathbf{x_{t-1}}; \mu_\theta(\mathbf{x_t}); \Sigma_q(t)) \tag{59}$$

$$\mu_\theta(\mathbf{x_t}) = \frac{(1-\bar{\alpha}_{t-1})\sqrt{\alpha_t}\mathbf{x_t} + (1-\alpha_t)\sqrt{\bar{\alpha}_{t-1}}\mathbf{x}_\theta}{(1-\bar{\alpha}_t)} \tag{60}$$

$$\mathbf{x}_\theta = \frac{\mathbf{x_t} - \sqrt{1-\bar{\alpha}_t}\epsilon_\theta}{\sqrt{\bar{\alpha}_t}} \tag{61}$$

$$\implies \mu_\theta(\mathbf{x_t}) = \frac{\mathbf{x_t}}{\sqrt{\alpha_t}} - \frac{(1-\alpha_t)(\sqrt{1-\bar{\alpha}_t})}{(1-\bar{\alpha}_t)(\sqrt{\alpha_t})}\epsilon_\theta = \frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x_t} - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\epsilon_\theta\right) \tag{62}$$

$$\Sigma_\theta(t) = \Sigma_q(t) = \frac{(1-\alpha_t)(1-\bar{\alpha}_{t-1})}{1-\bar{\alpha}_t}\mathbf{I} \tag{63}$$

We now have defined $\mathbf{x_{t-1}}$'s mean and variance given $\mathbf{x_t}$ which let's us write it as (64)

$$\mathbf{x_{t-1}} = \mu_\theta(\mathbf{x_t}) + \sqrt{\Sigma_\theta(t)}\mathbf{z} \tag{65}$$

$$\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I}) \tag{66}$$

# Sampling Algorithm

**repeat**
$\mathbf{x_T} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ ▷ Sample random noisy image
$\mathbf{T} \sim \mathbf{Uniform}(\{\mathbf{1}, \ldots, \mathbf{1000}\})$ ▷ Sample random length of the Denoising Chain
**for** $\mathbf{t} = \mathbf{T}, \ldots, \mathbf{1}$ **do**
$\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ if $t > 1$ else $\mathbf{z} = \mathbf{0}$
$\mathbf{x_{t-1}} = \frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x_t} - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\epsilon_\theta(\mathbf{x_t}, \mathbf{t})\right) + \sqrt{\Sigma_\theta(t)}\mathbf{z}$ ▷ Sampling $\mathbf{x_{t-1}}$ from $p_\theta(\mathbf{x_{t-1}}|\mathbf{x_t})$
**end for**
**return** $\mathbf{x_0}$

# References I


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# References II

[6] Yang, X. (2017). *Understanding the Variational Lower Bound*. https://xyang35.github.io/2017/04/14/variational-lower-bound/

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# Hora da Implementação :)