

Diffusion Probabilistic Models

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Introduction



Figure: Images generated by DALL.E 2 (Open AI) from text descriptions

Introduction



Inspired by non-equilibrium
thermodynamics

The forward and reverse processes

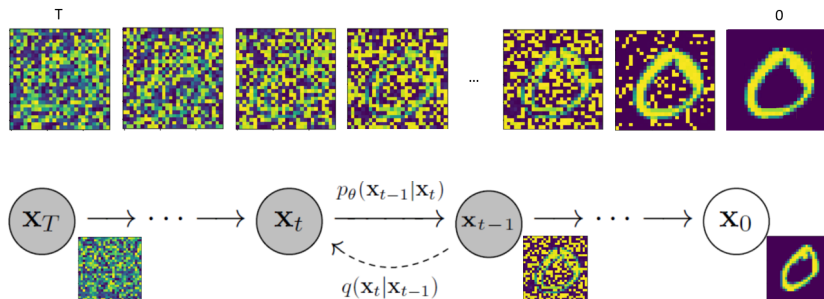


Figure: The Markov chain

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

$$p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t) := \mathcal{N}(\mathbf{x}_{t-1}; \boldsymbol{\mu}_\theta(\mathbf{x}_t, t), \boldsymbol{\Sigma}_\theta(\mathbf{x}_t, t))$$

The forward process

$$q(x_t|x_0) := \mathcal{N}(x_t; \sqrt{\bar{\alpha}_t}x_0, (1 - \bar{\alpha}_t)I)$$
$$x_t = \sqrt{\bar{\alpha}_t}x_0 + \sqrt{1 - \bar{\alpha}_t}\epsilon \text{ where } \epsilon \sim \mathcal{N}(0, I)$$

► The noise schedule : linear, cosine, quadratic, sigmoid

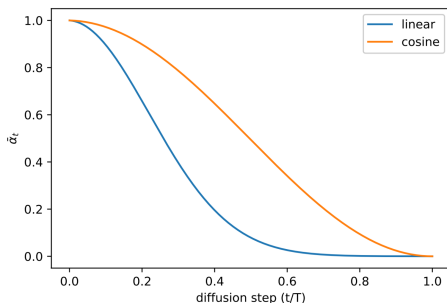


Figure: Comparison of the Linear and Cosine noise schedule (Nichol & Dhariwal, 2021)

The forward process

► The choice of the noise schedule

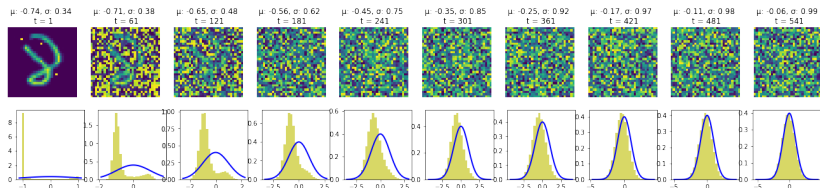


Figure: Linear noise schedule

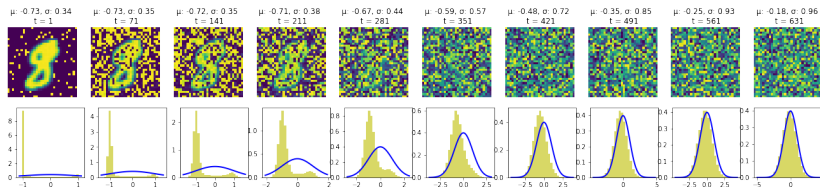


Figure: Cosine noise schedule (optimal according to the papers)

The reverse process

approximated model distribution $p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_t) := \mathcal{N}(\mathbf{x}_{t-1}; \boldsymbol{\mu}_{\theta}(\mathbf{x}_t, t), \boldsymbol{\Sigma}_{\theta}(\mathbf{x}_t, t))$

$$\theta^* = \arg \max_{\theta} \sum_{i=1}^n \log p_{\theta}(x^{(i)})$$

The computed loss function :

$$L_{simple}(\theta) := \mathbb{E}_{t, \mathbf{x}_0, \epsilon} [\|\epsilon - \epsilon_{\theta}(\sqrt{\bar{\alpha}_t} \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \epsilon, t)\|^2]$$

Algorithm 1 Training

```
1: repeat  
2:  $\mathbf{x}_0 \sim q(\mathbf{x}_0)$   
3:  $t \sim \text{Uniform}(\{1, \dots, T\})$   
4:  $\epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$   
5: Take gradient descent step on  
    $\nabla_{\theta} \|\epsilon - \epsilon_{\theta}(\sqrt{\bar{\alpha}_t} \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \epsilon, t)\|^2$   
6: until converged
```

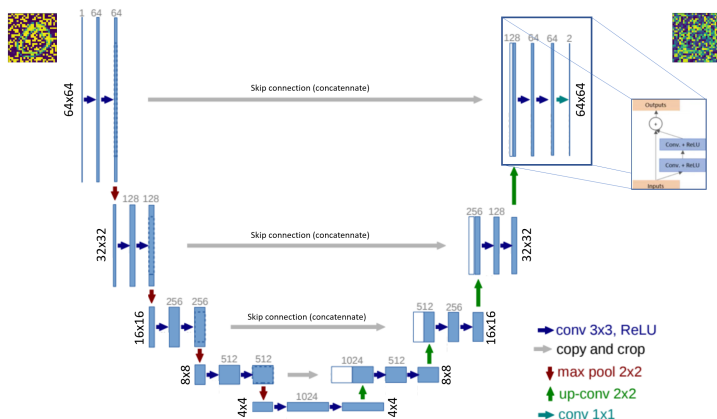
Algorithm 2 Sampling

```
1:  $\mathbf{x}_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$   
2: for  $t = T, \dots, 1$  do  
3:  $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$  if  $t > 1$ , else  $\mathbf{z} = \mathbf{0}$   
4:  $\mathbf{x}_{t-1} = \frac{1}{\sqrt{\alpha_t}} \left( \mathbf{x}_t - \frac{1 - \alpha_t}{\sqrt{1 - \bar{\alpha}_t}} \epsilon_{\theta}(\mathbf{x}_t, t) \right) + \sigma_t \mathbf{z}$   
5: end for  
6: return  $\mathbf{x}_0$ 
```

Figure: Pseudo Code

The reverse process

► The Neural Network architecture : the U-net



Results

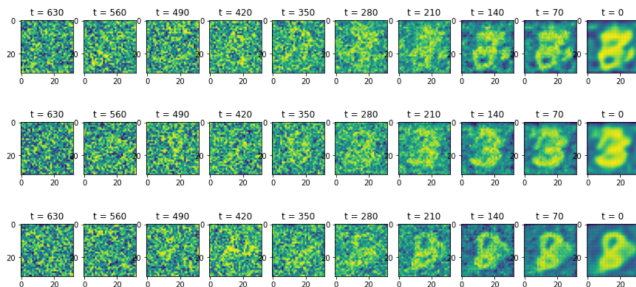


Figure: Preliminary results

► Parameters :

Epochs = 10

Image size =
32x32

Variance schedule :
sigmoid

$T = 700$

NN : Simple Unet

Embedding :
Sinusoidal Position

Areas for improvement

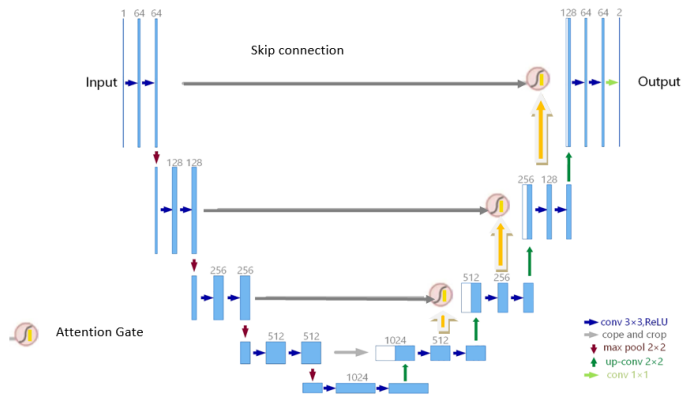


Figure: Attention U-Net Structure

References

[1] Denoising Diffusion Probabilistic Models [Jonathan Ho, Ajay Jain , Pieter Abbeel]

[2] <file:///C:/Users/bendr/OneDrive/Bureau/M2%20IASD/Data%20Science%20Pro%20Denoising%20diffusion%20implicit%20models.pdf>

[3] <https://www.youtube.com/watch?v=GAYJ81M58y8>

[4] <https://lilianweng.github.io/posts/2021-07-11-diffusion-models/>

[5] <https://www.youtube.com/watch?v=a4Yfz2FxxiYt=13s>