CS 4644-DL / 7643-A ZSOLT KIRA

Generative Models:

Denoising Diffusion Probabilistic Models (DDPMs)

Slides adapted from those by Danfei Xu



- Ffjord

PixelCNN [van der Oord et al. 2016]

Still generate image pixels starting from corner

Dependency on previous pixels now modeled using a CNN over context region (masked convolution)



Figure copyright van der Oord et al., 2016. Reproduced with permission.

$$\begin{split} \log p_{\theta}(x^{(i)}) &= \mathbf{E}_{z \sim q_{\phi}(z|x^{(i)})} \left[\log p_{\theta}(x^{(i)}) \right] & (p_{\theta}(x^{(i)}) \text{ Does not depend on } z) \\ &= \mathbf{E}_{z} \left[\log \frac{p_{\theta}(x^{(i)} \mid z)p_{\theta}(z)}{p_{\theta}(z \mid x^{(i)})} \right] & (\text{Bayes' Rule}) \\ &= \mathbf{E}_{z} \left[\log \frac{p_{\theta}(x^{(i)} \mid z)p_{\theta}(z)}{p_{\theta}(z \mid x^{(i)})} \frac{q_{\phi}(z \mid x^{(i)})}{q_{\phi}(z \mid x^{(i)})} \right] & (\text{Multiply by constant}) \\ &= \mathbf{E}_{z} \left[\log p_{\theta}(x^{(i)} \mid z) \right] - \mathbf{E}_{z} \left[\log \frac{q_{\phi}(z \mid x^{(i)})}{p_{\theta}(z)} \right] + \mathbf{E}_{z} \left[\log \frac{q_{\phi}(z \mid x^{(i)})}{p_{\theta}(z \mid x^{(i)})} \right] & (\text{Logarithms}) \\ &= \mathbf{E}_{z} \left[\log p_{\theta}(x^{(i)} \mid z) \right] - D_{KL}(q_{\phi}(z \mid x^{(i)}) \mid p_{\theta}(z)) + D_{KL}(q_{\phi}(z \mid x^{(i)}) \mid p_{\theta}(z \mid x^{(i)})) \right] \\ & \uparrow \\ \\ \text{Decoder network gives } p_{\theta}(x|z), \text{ can} \\ \text{compute estimate of this term through} \\ \text{sampling. (Sampling differentiable through reparam. trick, see paper.)} \\ \text{This KL term (between Gaussians for encoder and z prior) has nice closed-form solution!} \\ \end{bmatrix}$$

From CS231n, Fei-Fei Li, Justin Johnson, Serena Yeung





Denoising Diffusion Probabilistic Models (DDPMs)

And Conditional Diffusion Models

TEXT DESCRIPTION

An astronaut Teddy bears A bowl of soup

riding a horse lounging in a tropical resort in space playing basketball with cats in space

in a photorealistic style in the style of Andy Warhol as a pencil drawing DALL·E 2

 \rightarrow





https://openai.com/dall-e-2/

TEXT DESCRIPTION

An astronaut Teddy bears A bowl of soup

mixing sparkling chemicals as mad scientists shopping for groceries working on new AI research

as kids' crayon art on the moon in the 1980s underwater with 1990s technology

 \rightarrow







https://openai.com/dall-e-2/



https://openai.com/dall-e-2/

⊙ Watch 321 - 🖓 Fork 5k - 🔶 Starred 33k -

rity 🗠 Insights

pesser Release under	r CreativeML Open RAIL M License	69ae4b3 on Aug 22 🕑 29 commits	n/research/latent-diff
assets	Release under CreativeML Open RAIL	License 2 months ago	
configs	stable diffusion	3 months ago 赵 View license	
data stable diffusion		3 months ago	ago ☆ 33k stars ③ 321 watching ♀ 5k forks
ldm	Idm stable diffusion		
models	add configs for training unconditional/o	ass-conditional ldms 11 months ago	
scripts	Release under CreativeML Open RAIL	License 2 months ago Releases	
LICENSE Release under CreativeML Open RAIL M License		License 2 months ago No releases published	1
B README.md	Release under CreativeML Open RAIL	License 2 months ago	
Stable_Diffusion_v1_I	Model_Card.md Release under CreativeML Open RAIL	License 2 months ago Packages	
environment.yaml	Release under CreativeML Open RAIL	License 2 months ago No packages publishe	d
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Stable Diff	usion	Languages Jupyter Notebool Python 9.8%	k 90.1% Shell 0.1%

Robin Rombach*, Andreas Blattmann*, Dominik Lorenz, Patrick Esser, Björn Ommer

https://github.com/CompVis/stable-diffusion

CVPR '22 Oral | GitHub | arXiv | Project page

Landscape Highlights of Diffusion Models (Nov 2022)



Landscape Highlights of Diffusion Models (Nov 2022)



The Denoising Diffusion Process

image from dataset

 x_0



The Denoising Diffusion Process

image from dataset

The "forward diffusion" process: add Gaussian noise each step



• • •







The "denoising diffusion" process: generate an image from noise by *denoising* the gaussian noises

The Denoising Diffusion Process

Ties/inspiration form Annealed Imporantce Sampling in physics

Comparison











The **known** forward process



The **known** forward process $x_0 \longrightarrow x_1 \longrightarrow \cdots \longrightarrow x_T$ $q(x_{1:T}|x_0) = \prod_{t=1}^T q(x_t|x_{t-1})$ Probability Chain Rule (Markov Chain)

The **known** forward process $x_0 \longrightarrow x_1 \longrightarrow \cdots \longrightarrow x_T$ $q(x_{1:T}|x_0) = \prod_{t=1}^T q(x_t|x_{t-1})$ Probability Chain Rule (Markov Chain) $q(x_t|x_{t-1}) = \mathcal{N}(x_t; (\sqrt{1-\beta_t} \)x_{t-1}, \beta_t I)$ Conditional Gaussian

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Notation: A Gaussian distribution "for" x_t

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 β_t is the *variance schedule* at the diffusion step t

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https://www.youtube.com/watch?v=HoKDTa5jHvg&t=517s

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 $0 < \beta_1 < \beta_2 < \cdots < \beta_T < 1$, typical value range [0.0001, 0.02], with T = 1000





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Nice property: samples from an *arbitrary forward step* are also Gaussian-distributed! $q(x_t|x_0) = \mathcal{N}(x_t; \sqrt{\overline{\alpha}_t}x_0, (1 - \overline{\alpha}_t)I)$

, where $\alpha_t = (1 - \beta_t)$, $\overline{\alpha}_t = \prod_{s=1}^t \alpha_s$





Nice property: samples from an *arbitrary forward step* are also Gaussian-distributed! $q(x_t|x_0) = \mathcal{N}(x_t; \sqrt{\overline{\alpha}_t}x_0, (1 - \overline{\alpha}_t)I)$

Gaussian reparameterization trick (recall from VAEs!):

$$x_t = \sqrt{\overline{\alpha}_t} x_0 + \sqrt{1 - \overline{\alpha}_t} \epsilon, \qquad \epsilon \sim \mathcal{N}(0, I)$$

(square root appears because reparameterization trick has just σ) $z = \mu + \epsilon * \sigma, \epsilon \sim N(0,1)$

The Diffusion and Denoising Process



The **learned** denoising process $x_0 \leftarrow x_1 \leftarrow \cdots \leftarrow x_T$

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The **learned** denoising process
$$x_0 \leftarrow x_1 \leftarrow \cdots \leftarrow x_T$$

 $p_{\theta}(x_{0:T}) = p(x_T) \prod_{t=1}^{T} p_{\theta}(x_{t-1}|x_t)$ Probability Chain Rule (Markov Chain)
 $p_{\theta}(x_{t-1}|x_t) = \mathcal{N}(x_{t-1}; \mu_{\theta}(x_t, t), \Sigma_q(t))$ Conditional Gaussian
Want to learn time-
dependent mean (simplification)

How do we form a learning objective?

The **learned** denoising process $x_0 \leftarrow x_1 \leftarrow \cdots \leftarrow x_T$ $p_{\theta}(x_{t-1}|x_t) = \mathcal{N}(x_{t-1}; \mu_{\theta}(x_t, t), \Sigma_q(t))$

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High-level intuition: derive a ground truth denoising distribution $q(x_{t-1}|x_t, x_0)$ and train a neural net $p_{\theta}(x_{t-1}|x_t)$ to match the distribution.

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What does it look like? $q(x_{t-1}|x_t, x_0) = \mathcal{N}\left(x_{t-1}; \mu_q(t), \Sigma_q(t)\right)$

$$\mu_{q}(t) = \frac{1}{\sqrt{\alpha_{t}}} \left(x_{t} - \frac{\beta_{t}}{\sqrt{(1 - \overline{\alpha}_{t})}} \epsilon \right), \qquad \epsilon \sim \mathcal{N}(0, I)$$

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The "ground truth" noise that brought x_{t-1} to x_t

The **learned** denoising process $x_0 \leftarrow x_1 \leftarrow \cdots \leftarrow x_T$ $p_{\theta}(x_{t-1}|x_t) = \mathcal{N}(x_{t-1}; \mu_{\theta}(x_t, t), \Sigma_q(t))$

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What does it look like? $q(x_{t-1}|x_t, x_0) = \mathcal{N}\left(x_{t-1}; \mu_q(t), \Sigma_q(t)\right)$

Assuming identical variance $\Sigma_q(t)$, we have:

 $\operatorname{argmin}_{\theta} D_{KL}(q(x_{t-1}|x_t, x_0)| | p_{\theta}(x_{t-1}|x_t)) = \operatorname{argmin}_{\theta} w || \mu_q(t) - \mu_{\theta}(x_t, t)||^2$

Should be variance-dependent, but constant works better in practice

The **learned** denoising process $x_0 \leftarrow x_1 \leftarrow \cdots \leftarrow x_T$ $p_{\theta}(x_{t-1}|x_t) = \mathcal{N}(x_{t-1}; \mu_{\theta}(x_t, t), \Sigma_q(t))$

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Simplified learning objective: $\operatorname{argmin}_{\theta} ||\epsilon - \epsilon_{\theta}(x_t, t)||^2$

Predict the one-step noise that was added (and remove it)!

The **learned** denoising process $x_0 \leftarrow x_1 \leftarrow \cdots \leftarrow x_T$ $p_{\theta}(x_{0:T}) = p(x_T) \prod_{t=1}^{T} p_{\theta}(x_{t-1}|x_t)$ Probability Chain Rule (Markov Chain) $p_{\theta}(x_{t-1}|x_t) = \mathcal{N}(x_{t-1}; \mu_{\theta}(x_t, t), \Sigma_q(t))$ Conditional Gaussian

Assume fixed / known variance

How did we arrive at the learning objective? Let's go back to the basics of variational models ...

(Quick) Derivation!

Connection to VAEs



Connection to VAEs





Variational
Inference $p(x) = \int p(x|z)p(z)dz$ Intractable to estimate! $\log p(x) = E_q \left[\log \frac{p(x|z)p(z)}{q(z|x)} \right] + D_{KL}(q(z|x)) | p(z|x) \right]$ $\geq E_q \left[\log \frac{p(x|z)p(z)}{q(z|x)} \right]$ Evidence Lower Bound (ELBO) - From last lecture on VAEs

Variational
InferenceSimplify to
KL
$$p(x) = \int p(x|z)p(z)dz$$
Intractable to estimate! $\log p(x) = E_q \left[\log \frac{p(x|z)p(z)}{q(z|x)} \right] + D_{KL}(q(z|x)) ||p(z|x))$ $\geq E_q \left[\log \frac{p(x|z)p(z)}{q(z|x)} \right]$ Evidence Lower Bound (ELBO) $\log p(x_0) \geq E_q \left[\log \frac{p(x_0|x_{1:T})p(x_{1:T})}{q(x_{1:T}|x_0)} \right]$ $x = x_0, \ z = x_{1:T}$

Variational
Inference Simplify to

$$kL$$

 $p(x) = \int p(x|z)p(z)dz$ Intractable to estimate!
 $\log p(x) = E_q \left[\log \frac{p(x|z)p(z)}{q(z|x)} \right] + D_{KL}(q(z|x)) |p(z|x))$
 $\geq E_q \left[\log \frac{p(x|z)p(z)}{q(z|x)} \right]$ Evidence Lower Bound (ELBO)

 $\log p(x_0) \ge E_q \left[\log \frac{p(x_0 | x_{1:T}) p(x_{1:T})}{q(x_{1:T} | x_0)} \right] \qquad x = x_0, \ z = x_{1:T}$

... (derivation omitted, see Sohl-Dickstein et al., 2015 Appendix B)

$$= E_q \left[\log \frac{p(x_T) \prod_{t=1}^T p_\theta(x_{t-1}|x_t)}{\prod_{t=1}^T q(x_t|x_{t-1})} \right] \longleftarrow \text{ reverse denoising}$$
 forward diffusion

Variational
Inference Simplify to

$$KL$$

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 $\log p(x) = E_q \left[\log \frac{p(x|z)p(z)}{q(z|x)} \right] + D_{KL}(q(z|x)) ||p(z|x))$
 $\geq E_q \left[\log \frac{p(x|z)p(z)}{q(z|x)} \right]$ Evidence Lower Bound (ELBO)
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Variational
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$$= -E_{q}[D_{KL}(q(x_{T}|x_{0})||p(x_{T}))] - \sum_{t=2}^{T} D_{KL}(q(x_{t-1}|x_{t},x_{0})||p_{\theta}(x_{t-1}|x_{t})) + \log p_{\theta}(x_{0}|x_{1})$$

$$Variational
Inference \rightarrow Simplify to
 KL
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fixed
Easy to optimize / sometimes omitted

Variational
Inference Simplify to
KL

$$p(x) = \int p(x|z)p(z)dz$$
Intractable to estimate!

$$\log p(x) = E_q \left[\log \frac{p(x|z)p(z)}{q(z|x)} \right] + D_{KL}(q(z|x)) ||p(z|x))$$

$$\geq E_q \left[\log \frac{p(x|z)p(z)}{q(z|x)} \right]$$
Evidence Lower Bound (ELBO

$$\log p(x_0) \geq E_q \left[\log \frac{p(x_0|x_{1:T})p(x_{1:T})}{q(x_{1:T}|x_0)} \right]$$

$$x = x_0, \ z = x_{1:T}$$

$$= -\mathbb{E}_{q}\left[D_{KL}\left(q(x_{T}|x_{0})||p(x_{T})\right)\right] - \sum_{t=2}^{T} D_{KL}(q(x_{t-1}|x_{t},x_{0})||p_{\theta}(x_{t-1}|x_{t})) + \log p_{\theta}(x_{0}|x_{1})$$

Maximize the agreement between the predicted reverse diffusion distribution p_{θ} and the "ground truth" reverse diffusion distribution q



$$\begin{array}{c} \text{Variational}\\ \text{Inference} & \longrightarrow & \underset{KL}{\text{Simplify to}} & \longrightarrow & \underset{Reverse Process}{\text{Reverse Process}}\\ => \text{Normal} \\ p(x) = \int p(x|z)p(z)dz & \text{Intractable to estimate!} \\ \log p(x) = & \operatorname{E}_q \left[\log \frac{p(x|z)p(z)}{q(z|x)} \right] + D_{KL}(q(z|x)) | p(z|x)) \\ & \geq & \operatorname{E}_q \left[\log \frac{p(x|z)p(z)}{q(z|x)} \right] & \text{Evidence Lower Bound (ELBO)} \\ \log p(x_0) \geq & \operatorname{E}_q \left[\log \frac{p(x_0|x_{1:T})p(x_{1:T})}{q(x_{1:T}|x_0)} \right] & x = x_0, \ z = x_{1:T} \end{array}$$

$$= -E_{q}[D_{KL}(q(x_{T}|x_{0})||p(x_{T}))] - \sum_{t=2}^{T} D_{KL}(q(x_{t-1}|x_{t},x_{0})||p_{\theta}(x_{t-1}|x_{t})) + \log p_{\theta}(x_{0}|x_{1})$$

$$\begin{array}{c} \text{Variational}\\ \text{Inference} & \longrightarrow & \underset{KL}{\text{Simplify to}} & \longrightarrow & \underset{Reverse Process}{\text{Reverse Process}}\\ \end{array} \\ p(x) = \int p(x|z)p(z)dz & \text{Intractable to estimate!} \\ \log p(x) = & \operatorname{E}_q \left[\log \frac{p(x|z)p(z)}{q(z|x)} \right] + D_{KL}(q(z|x)) | p(z|x)) \\ & \geq & \operatorname{E}_q \left[\log \frac{p(x|z)p(z)}{q(z|x)} \right] & \text{Evidence Lower Bound (ELBO)} \\ \log p(x_0) \geq & \operatorname{E}_q \left[\log \frac{p(x_0|x_{1:T})p(x_{1:T})}{q(x_{1:T}|x_0)} \right] & x = x_0, \ z = x_{1:T} \end{array}$$

$$= -E_{q}[D_{KL}(q(x_{T}|x_{0})||p(x_{T}))] - \sum_{t=2}^{T} D_{KL}(q(x_{t-1}|x_{t},x_{0})||p_{\theta}(x_{t-1}|x_{t})) + \log p_{\theta}(x_{0}|x_{1})$$

$$q(x_{t-1}|x_{t}) = q(x_{t-1}|x_{t},x_{0}) \quad (\text{markov assumption})$$

$$= \frac{q(x_{t}|x_{t-1},x_{0})q(x_{t-1}|x_{0})}{q(x_{t}|x_{0})} \quad (\text{Bayes rule})$$

$$= \frac{\mathcal{N}(x_{t};\sqrt{a_{t}}x_{t-1},\beta_{t}I)\mathcal{N}(x_{t-1};\sqrt{\overline{a_{t-1}}}x_{t-1},(1-\overline{a_{t-1}})I)}{\mathcal{N}(x_{t};\sqrt{\overline{a_{t}}}x_{0},(1-\overline{a_{t-1}})I)}$$

$$\propto \mathcal{N}\left(x_{t-1}; \frac{\sqrt{a_{t}}(1-\overline{a_{t-1}})x_{t}+\sqrt{\overline{a_{t-1}}}(1-a_{t})x_{0}}{1-\sqrt{\overline{a_{t}}}}, \Sigma_{q}(t)\right) \quad (\text{Property of Gaussian})$$

Variational
InferenceSimplify to
KLReverse Process
=> NormalBayes +
Reparameterization
$$p(x) = \int p(x|z)p(z)dz$$
Intractable to estimate! $\log p(x) = E_q \left[\log \frac{p(x|z)p(z)}{q(z|x)} \right] + D_{KL}(q(z|x)) ||p(z|x)) \right]$ $\geq E_q \left[\log \frac{p(x|z)p(z)}{q(z|x)} \right]$ $\geq E_q \left[\log \frac{p(x|z)p(z)}{q(z|x)} \right]$ Evidence Lower Bound (ELBO) $\log p(x_0) \geq E_q \left[\log \frac{p(x_0|x_{1:T})p(x_{1:T})}{q(x_{1:T}|x_0)} \right]$ $x = x_0, z = x_{1:T}$

$$= -E_{q}[D_{KL}(q(x_{T}|x_{0})||p(x_{T}))] - \sum_{t=2}^{T} D_{KL}(q(x_{t-1}|x_{t},x_{0})||p_{\theta}(x_{t-1}|x_{t})) + \log p_{\theta}(x_{0}|x_{1})$$

$$q(x_{t-1}|x_{t},x_{0}) = \mathcal{N}(x_{t-1};\mu_{q}(t),\Sigma_{q}(t))$$

$$\mu_{q}(t) = \frac{1}{\sqrt{\alpha_{t}}} \left(x_{t} - \frac{\beta_{t}}{\sqrt{(1-\overline{\alpha}_{t})}}\epsilon\right), \quad \epsilon \sim \mathcal{N}(0,I)$$
Proof using by gaussian reperting the second second

Proof using bayes rule and gaussian reparameterization trick

$$\begin{array}{c} \text{Variational}\\ \text{Inference} & \longrightarrow & \underset{KL}{\text{Simplify to}}\\ \text{KL} & \longrightarrow & \underset{Reverse Process}{\text{Process}} & \longrightarrow & \underset{Reparameterization}{\text{Bayes +}}\\ p(x) = \int p(x|z)p(z)dz & \text{Intractable to estimate!} \\ \log p(x) = & \operatorname{E}_q \left[\log \frac{p(x|z)p(z)}{q(z|x)} \right] + D_{KL}(q(z|x)) | p(z|x)) \\ & \geq & \operatorname{E}_q \left[\log \frac{p(x|z)p(z)}{q(z|x)} \right] & \text{Evidence Lower Bound (ELBO)} \\ \log p(x_0) \geq & \operatorname{E}_q \left[\log \frac{p(x_0|x_{1:T})p(x_{1:T})}{q(x_{1:T}|x_0)} \right] & x = x_0, \ z = x_{1:T} \end{array}$$

$$= -E_{q}[D_{KL}(q(x_{T}|x_{0})||p(x_{T}))] - \sum_{t=2}^{T} D_{KL}(q(x_{t-1}|x_{t},x_{0})||p_{\theta}(x_{t-1}|x_{t})) + \log p_{\theta}(x_{0}|x_{1})$$

$$q(x_{t-1}|x_{t},x_{0}) = \mathcal{N}\left(x_{t-1};\mu_{q}(t),\Sigma_{q}(t)\right)$$

$$\mu_{q}(t) = \frac{1}{\sqrt{\alpha_{t}}}\left(x_{t} - \frac{\beta_{t}}{\sqrt{(1-\overline{\alpha_{t}})}}\epsilon\right), \quad \epsilon \sim \mathcal{N}(0,I)$$
Proof using bayes rule and gaussian reparameterization

The "ground truth" noise that brought x_{t-1} to x_t

trick

$$\begin{array}{c} \begin{array}{c} \mbox{Variational}\\ \mbox{Inference} \end{array} \rightarrow \begin{array}{c} \mbox{Simplify to}\\ \mbox{KL} \end{array} \rightarrow \begin{array}{c} \mbox{Reverse Process}\\ \mbox{=> Normal} \end{array} \rightarrow \begin{array}{c} \mbox{Bayes +}\\ \mbox{Reparameterization} \end{array} \rightarrow \begin{array}{c} \mbox{Remove (variance-dependent) constant} \end{array} \end{array} \\ p(x) = \int p(x|z)p(z)dz \qquad \mbox{Intractable to estimate!} \end{array} \\ \mbox{log } p(x) = E_q \left[\log \frac{p(x|z)p(z)}{q(z|x)} \right] + D_{KL}(q(z|x)) | p(z|x) \right) \\ \mbox{$\geq E_q} \left[\log \frac{p(x|z)p(z)}{q(z|x)} \right] \qquad \mbox{Evidence Lower Bound (ELBO)} \end{aligned} \\ \mbox{Intractable } p(x_0) \geq E_q \left[\log \frac{p(x_0|x_{1:T})p(x_{1:T})}{q(x_{1:T}|x_0)} \right] \qquad x = x_0, \ z = x_{1:T} \end{array}$$

$$= -E_q [D_{KL}(q(x_T|x_0)||p(x_T))] - \sum_{t=2}^T D_{KL}(q(x_{t-1}|x_t, x_0)||p_{\theta}(x_{t-1}|x_t)) + \log p_{\theta}(x_0|x_1)$$

Minimize the difference of distribution means (assuming identical variance)

$$\operatorname{argmin}_{\theta} w || \mu_q(t) - \mu_{\theta}(x_t, t) ||^2$$

Reverse Process

=> Normal

Simplify to

KL

Variational

Inference

The **learned** denoising process
$$x_0 \leftarrow x_1 \leftarrow \cdots \leftarrow x_T$$

 $p_{\theta}(x_{0:T}) = p(x_T) \prod_{t=1}^{T} p_{\theta}(x_{t-1}|x_t)$
 $p_{\theta}(x_{t-1}|x_t) = \mathcal{N}(x_{t-1}; \mu_{\theta}(x_t, t), \Sigma(t))$ Conditional Gaussian

Bayes +

Reparameterization

Remove (variance-

dependent) constant

Predict the

noise!!!

Learning objective: $\operatorname{argmin}_{\theta} ||\mu_q(t) - \mu_{\theta}(x_t, t)||^2$

$$\mu_q(t) = \frac{1}{\sqrt{\alpha_t}} \left(x_t - \frac{\beta_t}{\sqrt{(1 - \overline{\alpha}_t)}} \epsilon \right), \qquad \epsilon \sim \mathcal{N}(0, I)$$

Reverse Process

=> Normal

Simplify to

KL

Variational

Inference

The **learned** denoising process
$$x_0 \leftarrow x_1 \leftarrow \cdots \leftarrow x_T$$

 $p_{\theta}(x_{0:T}) = p(x_T) \prod_{t=1}^{T} p_{\theta}(x_{t-1}|x_t)$
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Do we actually need to learn the entire $\mu_{\theta}(x_t, t)$?

Reverse Process

=> Normal

Simplify to

KL

Variational

Inference

The **learned** denoising process
$$x_0 \leftarrow x_1 \leftarrow \cdots \leftarrow x_T$$

 $p_{\theta}(x_{0:T}) = p(x_T) \prod_{t=1}^{T} p_{\theta}(x_{t-1}|x_t)$
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known during inference
Unknown during inference
Noise that brought x_{t-1} to x_{t}

Reverse Process

=> Normal

The **learned** denoising process
$$x_0 \leftarrow x_1 \leftarrow \cdots \leftarrow x_T$$

 $p_{\theta}(x_{0:T}) = p(x_T) \prod_{t=1}^{T} p_{\theta}(x_{t-1}|x_t)$
 $p_{\theta}(x_{t-1}|x_t) = \mathcal{N}(x_{t-1}; \mu_{\theta}(x_t, t), \Sigma(t))$ Conditional Gaussian

Bayes +

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known during inference
Unknown during inference
Noise that brought x_{t-1} to x_{t}

Idea: just learn ϵ with $\epsilon_{\theta}(x_t, t)$!

Simplify to

KL

Variational

Inference

Reverse Process

=> Normal

Variational

Inference

Simplify to

KL

The **learned** denoising process
$$x_0 \leftarrow x_1 \leftarrow \cdots \leftarrow x_T$$

 $p_{\theta}(x_{0:T}) = p(x_T) \prod_{t=1}^{T} p_{\theta}(x_{t-1}|x_t)$
 $p_{\theta}(x_{t-1}|x_t) = \mathcal{N}(x_{t-1}; \mu_{\theta}(x_t, t), \Sigma(t))$ Conditional Gaussian

Bayes +

Reparameterization

Remove (variance-

dependent) constant

Predict the

noise!!!

Simplified learning objective: $\operatorname{argmin}_{\theta} ||\epsilon - \epsilon_{\theta}(x_t, t)||^2$

Reverse Process

=> Normal

Simplify to

KL

Variational

Inference

The **learned** denoising process
$$x_0 \leftarrow x_1 \leftarrow \cdots \leftarrow x_T$$

 $p_{\theta}(x_{0:T}) = p(x_T) \prod_{t=1}^{T} p_{\theta}(x_{t-1}|x_t)$
 $p_{\theta}(x_{t-1}|x_t) = \mathcal{N}(x_{t-1}; \mu_{\theta}(x_t, t), \Sigma(t))$ Conditional Gaussian

Bayes +

Reparameterization

Remove (variance-

dependent) constant

Predict the

noise!!!

Simplified learning objective: $\operatorname{argmin}_{\theta} ||\epsilon - \epsilon_{\theta}(x_t, t)||^2$

Recall: the simplified *t*-step forward sample: $x_t = \sqrt{\overline{\alpha}_t} x_0 + \sqrt{1 - \overline{\alpha}_t} \epsilon$

Reverse Process

=> Normal

Simplify to

KL

Variational

Inference

The **learned** denoising process
$$x_0 \leftarrow x_1 \leftarrow \cdots \leftarrow x_T$$

 $p_{\theta}(x_{0:T}) = p(x_T) \prod_{t=1}^{T} p_{\theta}(x_{t-1}|x_t)$
 $p_{\theta}(x_{t-1}|x_t) = \mathcal{N}(x_{t-1}; \mu_{\theta}(x_t, t), \Sigma(t))$ Conditional Gaussian

Simplified learning objective: $\operatorname{argmin}_{\theta} ||\epsilon - \epsilon_{\theta} (\sqrt{\overline{\alpha}_t} x_0 + \sqrt{1 - \overline{\alpha}_t} \epsilon, t)||^2$

Recall: the simplified *t*-step forward sample:

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

Bayes +

Reparameterization

Remove (variance-

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Predict the

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Reverse Process

Variational

Simplify to

The **learned** denoising process
$$x_0 \leftarrow x_1 \leftarrow \cdots \leftarrow x_T$$

 $p_{\theta}(x_{0:T}) = p(x_T) \prod_{t=1}^{T} p_{\theta}(x_{t-1}|x_t)$
 $p_{\theta}(x_{t-1}|x_t) = \mathcal{N}(x_{t-1}; \mu_{\theta}(x_t, t), \Sigma(t))$ Conditional Gaussian

Bayes +

Remove (variance-

Predict the

noise!!!

Simplified learning objective: $\operatorname{argmin}_{\theta} ||\epsilon - \epsilon_{\theta} (\sqrt{\overline{\alpha}_t} x_0 + \sqrt{1 - \overline{\alpha}_t} \epsilon, t)||^2$

The **learned** denoising process
$$x_0 \leftarrow x_1 \leftarrow \cdots \leftarrow x_T$$

 $p_{\theta}(x_{0:T}) = p(x_T) \prod_{t=1}^{T} p_{\theta}(x_{t-1}|x_t)$ Probability Chain Rule (Markov Chain)
 $p_{\theta}(x_{t-1}|x_t) = \mathcal{N}(x_{t-1}; \mu_{\theta}(x_t, t), \Sigma_q(t))$ Conditional Gaussian

We know how to learn Assume fixed / known variance

Inference time:
$$\mu_{\theta}(x_t, t) = \frac{1}{\sqrt{\alpha_t}} \left(x_t - \frac{\beta_t}{\sqrt{(1 - \overline{\alpha}_t)}} \epsilon_{\theta}(x_t, t) \right)$$

$$x_t$$
 Net x_{t-1}



Generate new images!

The Denoising Diffusion Algorithm

Algorithm 1 Training

1: repeat

2:
$$\mathbf{x}_0 \sim q(\mathbf{x}_0)$$

3:
$$t \sim \text{Uniform}(\{1, \ldots, T\})$$

- 4: $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
- 5: Take gradient descent step on

$$\nabla_{\theta} \left\| \boldsymbol{\epsilon} - \boldsymbol{\epsilon}_{\theta} (\sqrt{\bar{\alpha}_t} \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \boldsymbol{\epsilon}, t) \right\|^2$$

6: until converged

The Denoising Diffusion Probabilistic Models, Ho et al., 2020
The Denoising Diffusion Algorithm

Algorithm 1 Training

1: repeat

2:
$$\mathbf{x}_0 \sim q(\mathbf{x}_0)$$

3:
$$t \sim \text{Uniform}(\{1, \dots, T\})$$

- 4: $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
- 5: Take gradient descent step on

$$\nabla_{\theta} \left\| \boldsymbol{\epsilon} - \boldsymbol{\epsilon}_{\theta} (\sqrt{\bar{\alpha}_t} \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \boldsymbol{\epsilon}, t) \right\|^2$$

6: until converged

Algorithm 2 Sampling

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

The Denoising Diffusion Algorithm

Algorithm 1 Training

1: repeat

2:
$$\mathbf{x}_0 \sim q(\mathbf{x}_0)$$

2: $\mathbf{t}_0 \sim Uniform (1)$

3:
$$t \sim \text{Uniform}(\{1, \dots, T\})$$

- 4: $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
- 5: Take gradient descent step on

$$\nabla_{\theta} \left\| \boldsymbol{\epsilon} - \boldsymbol{\epsilon}_{\theta} (\sqrt{\bar{\alpha}_t} \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \boldsymbol{\epsilon}, t) \right\|^2$$

6: **until** converged

Algorithm 2 Sampling

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

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

The Denoising Diffusion Probabilistic Models, Ho et al., 2020

Visualizing the Diffusion Process on 2D data



Sohl-Dickstein et al., 2015

Conditional Diffusion Models



Conditional Diffusion Models



Simple idea: just condition the model on some text labels y!

 $\epsilon_{\theta}(x_t, y, t)$