CS 4644-DL / 7643-A ZSOLT KIRA

Generative Models:

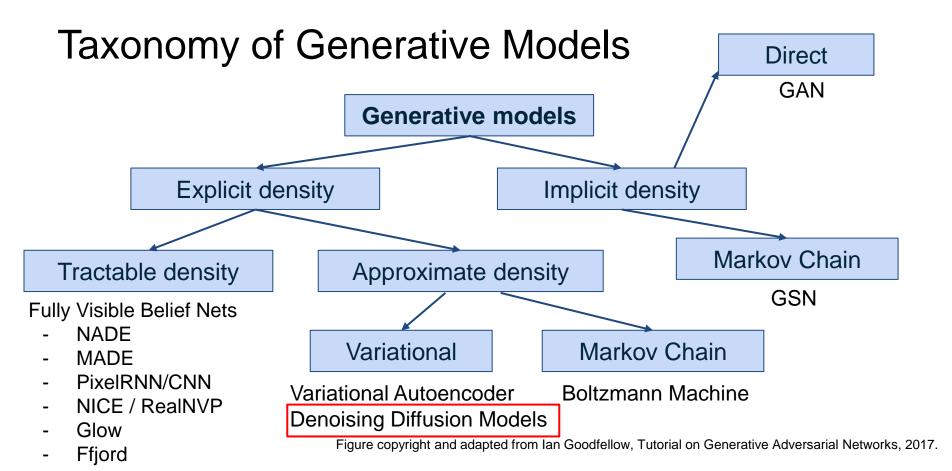
Denoising Diffusion Probabilistic Models (DDPMs)

Slides adapted from those by Danfei Xu

- Assignment 3
 - Due March 9th 11:59pm EST
- Projects
 - Project proposal due March 15th 17th
 - Proposal description out on canvas @256

 Meta office hours today 3pm ET on embeddings

W8: Mar 1	Generative Models (Part I): Generative Adversarial Networks Slides (PDF)
W9: Mar 6	Project Planning Session
W9: Mar 8	Generative Models (Part II): Diffusion Models PS3/HW3 due Mar 9th 11:59pm (grace period Mar 11th), PS4/HW4 out (due Apr 2nd)
W10: Mar 13	Guest Lecture (Mido Assran, Meta) - JePA
W10: Mar 15	Guest Lecture (Michael Auli) - Self-supervised Learning for Audio Project Proposal Due Mar 17th 11:59pm



Denoising Diffusion Probabilistic Models (DDPMs)

And Conditional Diffusion Models

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





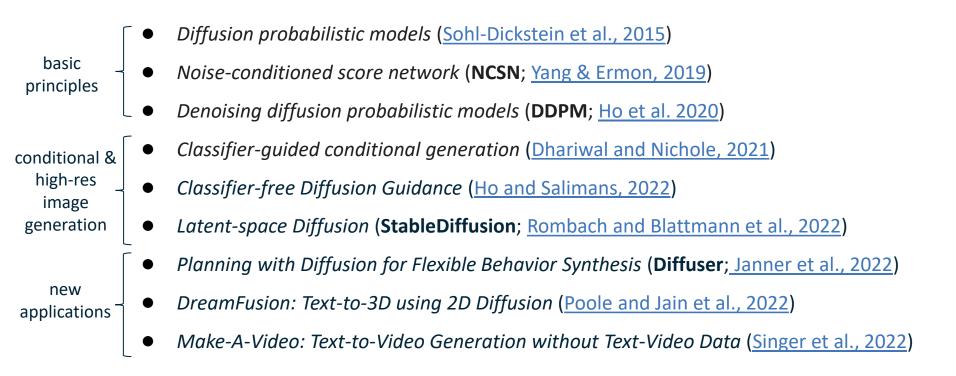








Landscape Highlights of Diffusion Models (Nov 2022)



How to make a new generative model

- Setting: Given unlabeled dataset of data, I want to learn to sample from P(x)
- Define the generative process
- Parameterize it
- Maximum likelihood (often + KL-divergence)
- Approximations
- Optimize parameters!
- Add conditioning, e.g. text

Landscape Highlights of Diffusion Models (Nov 2022)

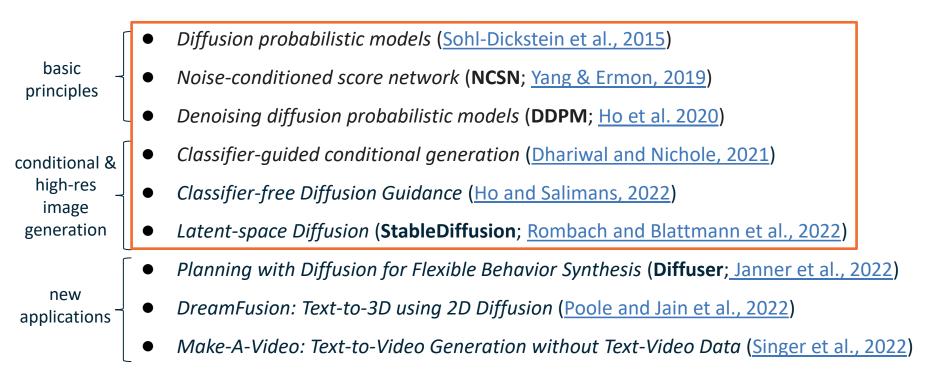


image from dataset

 x_0



image from dataset

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

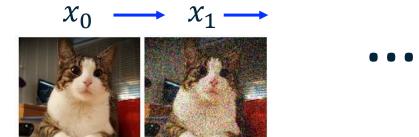
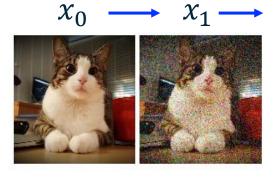


image from dataset

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

noise $\mathcal{N}(0,I)$





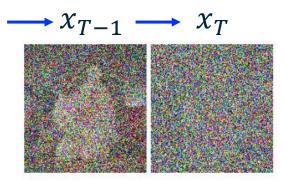
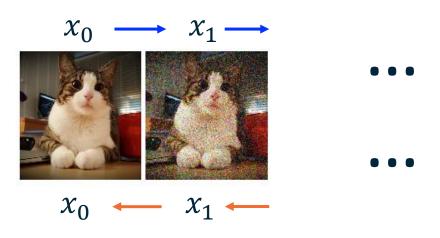


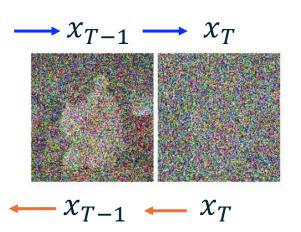
image from dataset

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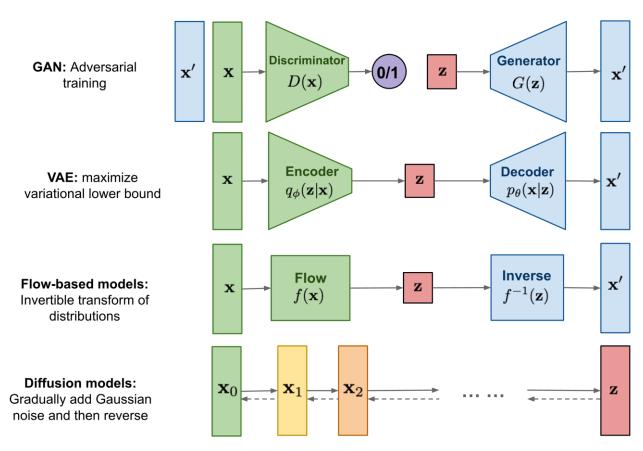


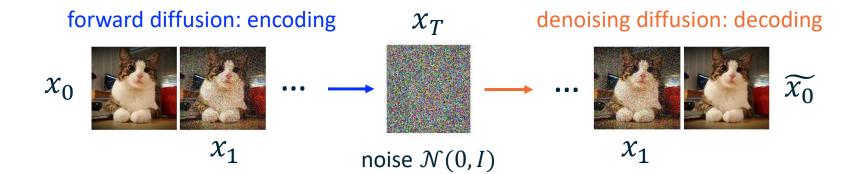
The "denoising diffusion" process: generate an image from noise by denoising the gaussian noises

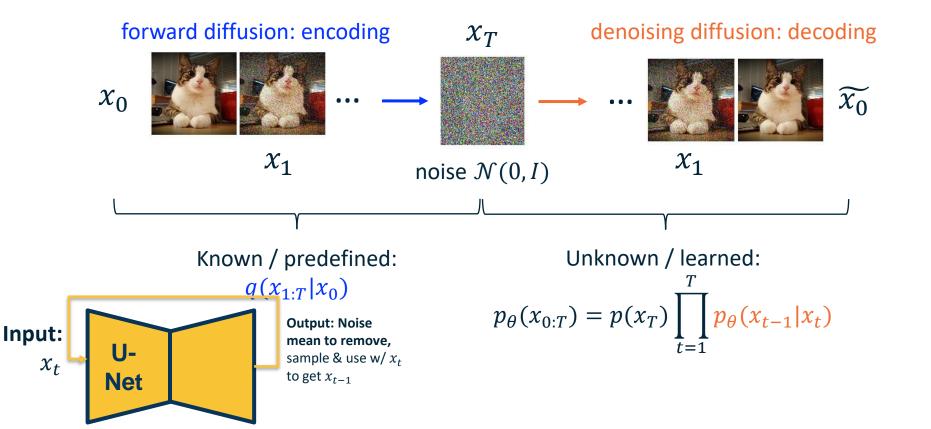


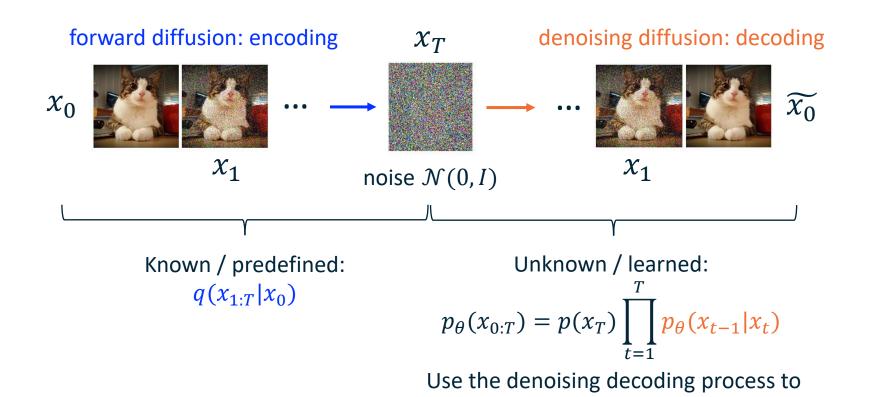
Ties/inspiration form Annealed Imporantce Sampling in physics

Comparison

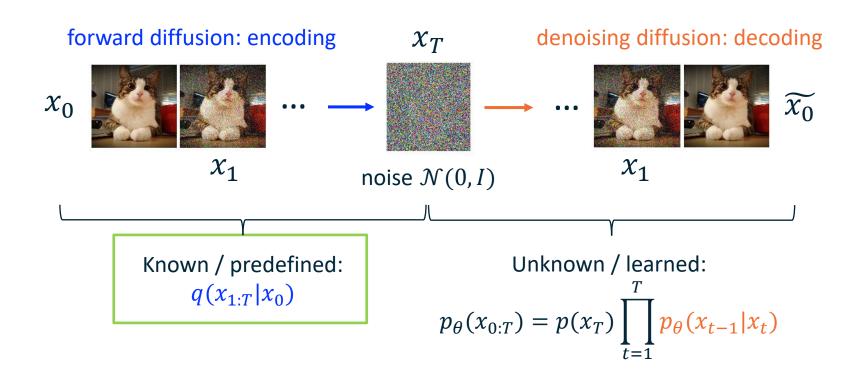








generate new images.



The **known** forward process
$$x_0 \longrightarrow x_1 \longrightarrow \cdots \longrightarrow x_T$$

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Notation: A Gaussian distribution "for" x_t

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

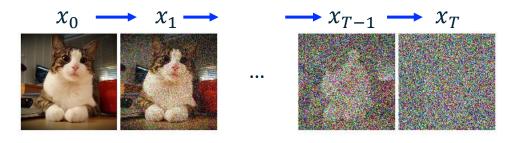
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 Conditional Gaussian

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

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



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

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



$$x_{T-1}$$
 x_T







The Diffusion (Encoding

The **known** forward process

$$_{-1})$$
 Proba

$$q(x_{1:T}|x_0) = \prod_{t=1}^{n} q(x_t|x_{t-1})$$
 Probab

 $q(x_t|x_0) = \mathcal{N}(x_t; \sqrt{\overline{\alpha}_t}x_0, (1 - \overline{\alpha}_t)I)$

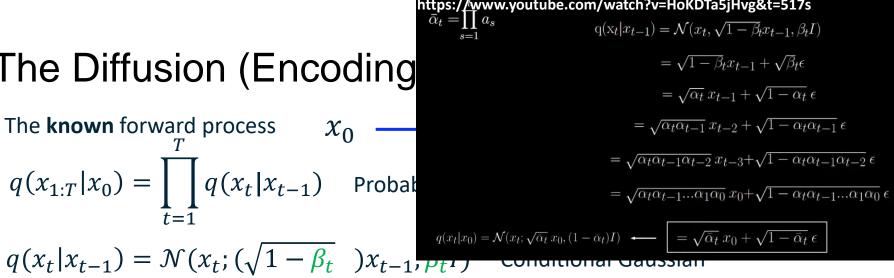
Gaussian reparameterization trick:

Saussian reparameterization trick
$$_{ au}$$
 –

$$z = \mu + \epsilon * \sigma, \epsilon \sim N(0,1)$$

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

(square root appears because reparameterization trick has just σ)



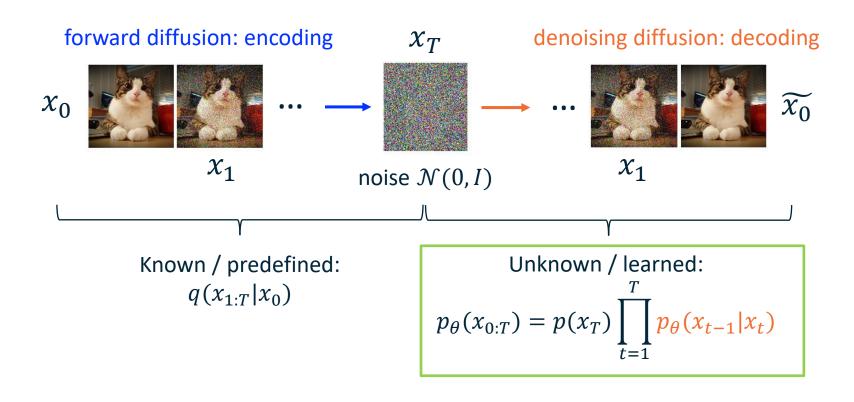
Intuition: We know all

distributions in forward

process, and can in fact directly compute for any t

based on X₀

The Diffusion and Denoising Process



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

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 Want to learn time-dependent mean (simplification)

The **learned** denoising process
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$$\text{Want to learn time-dependent mean} \quad \text{Assume fixed / known variance}$$

$$\text{(simplification)}$$

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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The learning objective: $\operatorname{argmin}_{\theta} D_{KL}(q(x_{t-1}|x_t,x_0)||p_{\theta}(x_{t-1}|x_t))$

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

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

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

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

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

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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 $x_0 \leftarrow x_1 \leftarrow x_T$ $p_{\theta}(x_{t-1}|x_t) = \mathcal{N}(x_{t-1}; \mu_{\theta}(x_t, t), \Sigma_{\sigma}(t))$

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.

The learning objective: $\operatorname{argmin}_{\theta} D_{KL}(q(x_{t-1}|x_t,x_0)||p_{\theta}(x_{t-1}|x_t))$

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

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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
$$x_0 \leftarrow x_1 \leftarrow \cdots \leftarrow x_T$$

$$p_{\theta}(x_{0:T}) = p(x_T) \prod_{t=1}^T p_{\theta}(x_{t-1}|x_t) \quad \text{Probability Chain Rule (Markov Chain)}$$

$$p_{\theta}(x_{t-1}|x_t) = \mathcal{N}(x_{t-1}; \mu_{\theta}(x_t, t), \Sigma_q(t)) \quad \text{Conditional Gaussian}$$
 Assume fixed / known variance

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

(Quick) Derivation!

Reverse Process Variational Simplify to Remove (variance-Bayes + **Predict the** dependent) constant Inference KL => Normal Reparameterization noise!!!

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

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

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

$$\geq \mathbb{E}_q \left[\log \frac{p(x|z)p(z)}{q(z|x)} \right] \qquad \text{Evidence Lower Bound (ELBO)}$$

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

Evidence Lower Bound (ELBO)

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

$$= \mathrm{E}_{q} \left[\log \frac{p(x_{T}) \prod_{t=1}^{T} p_{\theta}(x_{t-1}|x_{t})}{\prod_{t=1}^{T} q(x_{t}|x_{t-1})} \right] \longleftarrow \text{ reverse denoising}$$

$$\longleftarrow \text{ forward diffusion}$$

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

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

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

Easy to optimize / sometimes omitted

fixed

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

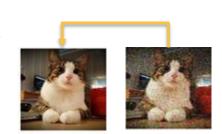
$$\geq \mathbb{E}_q \left[\log \frac{p(x|z)p(z)}{q(z|x)} \right] \qquad \text{Evidence Lower Bound (ELBO)}$$

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



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

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

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Variational Inference Simplify to KL Reverse Process
$$=>$$
 Normal $=>$ Normal $=>$ Normal

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

$$\geq \mathbb{E}_q \left[\log \frac{p(x|z)p(z)}{q(z|x)} \right]$$
 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)

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 $q(x_{t-1}|x_t) = q(x_{t-1}|x_t, x_0)$ (markov assumption) $= \frac{q(x_t|x_{t-1}, x_0)q(x_{t-1}|x_0)}{q(x_{t}|x_0)}$ (Bayes rule)

$$= \frac{1}{q(x_t|x_0)}$$
(Bayes rule)
$$= \frac{\mathcal{N}(x_t; \sqrt{a_t}x_{t-1}, \beta_t I) \mathcal{N}(x_{t-1}; \sqrt{\overline{a}_{t-1}}x_{t-1}, (1-\overline{a}_{t-1})I)}{\mathcal{N}(x_t; \sqrt{\overline{a}_t}x_0, (1-\overline{a}_{t-1})I)}$$

 $\propto \mathcal{N}\left(x_{t-1}; \frac{\sqrt{a_t}(1-\overline{\alpha}_{t-1})x_t+\sqrt{\overline{\alpha}_{t-1}}(1-a_t)x_0}{1-\sqrt{\overline{\alpha}_t}}, \Sigma_q(t)\right)$

(Property of Gaussian)

$$1-\sqrt{u_t}$$

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

$$\geq \mathbb{E}_q \left[\log \frac{p(x|z)p(z)}{q(z|x)} \right]$$
 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)

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

$$q(x_{t-1}|x_t, x_0) = \mathcal{N}\left(x_{t-1}; \mu_q(t), \Sigma_q(t)\right)$$

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

Proof using bayes rule and gaussian reparameterization trick

Variational Inference Simplify to KL Reverse Process
$$\Rightarrow$$
 Normal Reparameterization $p(x) = \int p(x|z)p(z)dz$ Intractable to estimate!

$$D(x|z)p(z)dz$$
 intractable to estimate:

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

$$\geq \mathbb{E}_q \left[\log \frac{p(x|z)p(z)}{q(z|x)} \right]$$
 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)

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

$$q(x_{t-1}|x_t, x_0) = \mathcal{N}\left(x_{t-1}; \mu_q(t), \Sigma_q(t)\right)$$

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

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

Proof using bayes rule and

gaussian reparameterization trick

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

$$\geq \mathbb{E}_q \left[\log \frac{p(x|z)p(z)}{q(z|x)} \right] \qquad \text{Evidence Lower Bound (ELBO)}$$

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

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

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

Minimize the difference of distribution means (assuming identical variance)

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

The **learned** denoising process $x_0 \longleftarrow x_1 \longleftarrow x_T$

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

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

Conditional Gaussian

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

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

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

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

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

Conditional Gaussian

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

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

Do we actually need to learn the entire $\mu_{\theta}(x_t, t)$?

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

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

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

Conditional Gaussian

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

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

known during inference

Unknown during inference

Recall: this is the "ground truth" noise that brought x_{t-1} to x_t

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

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

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

Conditional Gaussian

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

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

known during inference

Unknown during inference

Recall: this is the "ground truth" noise that brought x_{t-1} to x_t

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

The **learned** denoising process
$$x_0 \longleftarrow x_1 \longleftarrow x_T$$

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

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

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

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

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

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

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

Recall: the simplified t-step forward sample:

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

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

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

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

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

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

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

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

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

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



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
$$x_0 \leftarrow x_1 \leftarrow \cdots \leftarrow x_T$$

$$p_{\theta}(x_{0:T}) = p(x_T) \prod_{t=1}^T p_{\theta}(x_{t-1}|x_t) \quad \text{Probability Chain Rule (Markov Chain)}$$

$$p_{\theta}(x_{t-1}|x_t) = \mathcal{N}(x_{t-1}; \mu_{\theta}(x_t, t), \Sigma_q(t)) \quad \text{Conditional Gaussian}$$

We know how to learn Assume fixed / known variance

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



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

$$p_{\theta}(x_{0:T}) = p(x_T) \prod_{t=1}^T p_{\theta}(x_{t-1}|x_t) \quad \text{Probability Chain Rule (Markov Chain)}$$

$$p_{\theta}(x_{t-1}|x_t) = \mathcal{N}(x_{t-1}; \mu_{\theta}(x_t, t), \Sigma_q(t)) \quad \text{Conditional Gaussian}$$

We know how to learn Assume fixed / known variance

Generate new images!

The Denoising Diffusion Algorithm

Algorithm 1 Training

- 1: repeat
- 2: $\mathbf{x}_0 \sim q(\mathbf{x}_0)$
- 3: $t \sim \text{Uniform}(\{1, \dots, T\})$
- 4: $\epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
- 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 Algorithm

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

$$\nabla_{\theta} \left\| \boldsymbol{\epsilon} - \boldsymbol{\epsilon}_{\theta} (\sqrt{\bar{\alpha}_{t}} \mathbf{x}_{0} + \sqrt{1 - \bar{\alpha}_{t}} \boldsymbol{\epsilon}, t) \right\|^{2}$$

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 x_0

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: $\epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
- 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

$$x_{t} = \sqrt{\bar{\alpha}_{t}}x_{0} + \sqrt{1 - \bar{\alpha}_{t}}\epsilon, \quad \begin{array}{c} \rho_{\theta}(x_{t-1}|x_{t}) \\ \epsilon \sim \mathcal{N}(0, I) \end{array}$$

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 $\mathbf{z} = \mathbf{0}$

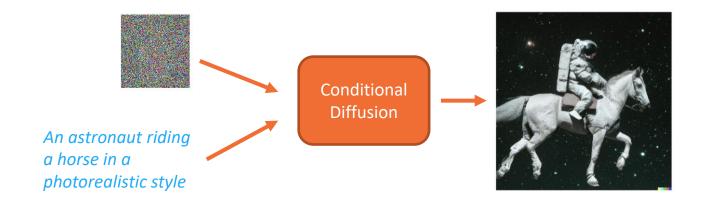
4:
$$\mathbf{x}_{t-1} = \frac{1}{\sqrt{\alpha_t}} \left(\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}} \boldsymbol{\epsilon}_{\theta}(\mathbf{x}_t, t) \right) + \sigma_t \mathbf{z}$$

- 5: end for
- 6: return \mathbf{x}_0

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

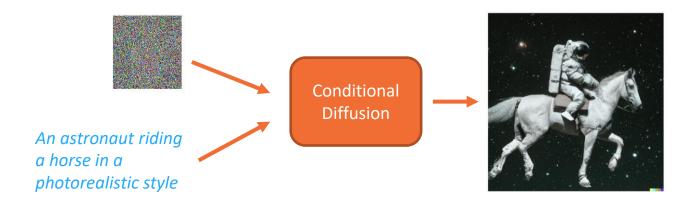
$$\epsilon \sim \mathcal{N}(0, I)$$

Conditional Diffusion Models



Simple idea: just condition the model on some text labels y! $\epsilon_{\theta}(x_t, y, t)$

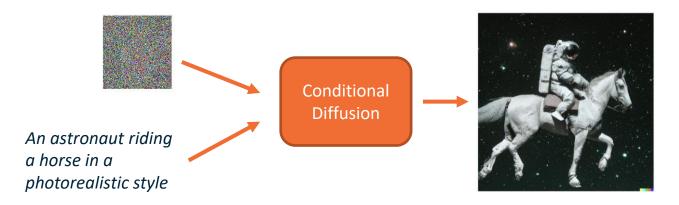
Conditional Diffusion Models



Simple idea: just condition the model on some text labels y! $\epsilon_{\theta}(x_t, y, t)$

Problem: Very blurry generation

Classifier-guided Diffusion



Better idea: use the *gradients* from a image captioning model $f_{\varphi}(y|x_t)$ to guide the diffusion process!

$$\bar{\epsilon}_{\theta}(x_t, t) = \epsilon_{\theta}(x_t, t) - \sqrt{1 - \bar{\alpha}_t} \nabla_{x_t} \log f_{\varphi}(y | x_t)$$

Classifier guidance

Using the gradient of a trained classifier as guidance

Algorithm 1 Classifier guided diffusion sampling, given a diffusion model $(\mu_{\theta}(x_t), \Sigma_{\theta}(x_t))$, classifier $p_{\phi}(y|x_t)$, and gradient scale s.

```
Input: class label y, gradient scale s Score model x_T \leftarrow sample from \mathcal{N}(0,\mathbf{I}) for all t from T to 1 do \mu, \Sigma \leftarrow \mu_{\theta}(x_t), \Sigma_{\theta}(x_t) x_{t-1} \leftarrow sample from \mathcal{N}(\mu + s\Sigma \, \nabla_{x_t} \log p_{\phi}(y|x_t), \Sigma) end for return x_0
```

- Train unconditional Diffusion model
- Take your favorite classifier, depending on the conditioning type
- During inference / sampling mix the gradients of the classifier with the predicted score function of the unconditional diffusion model.

Slide by Soumyadip (Roni) Sengupta

Classifier guidance

Using the gradient of a trained classifier as guidance

$$abla_x \log p_\gamma(x \mid y) =
abla_x \log p(x) + \gamma
abla_x \log p(y \mid x).$$

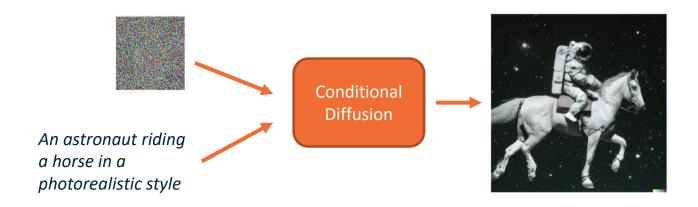




Samples from an unconditional diffusion model with classifier guidance, for guidance scales 1.0 (left) and 10.0 (right), taken from Dhariwal & Nichol (2021).

Slide by Soumyadip (Roni) Sengupta

Classifier-free Guided Diffusion



Classifier-free Guided Diffusion: estimate the gradient of the classifier model with conditional diffusion models!

$$\nabla_{x_t} \log f_{\varphi}(y|x_t) = -\frac{1}{\sqrt{1-\bar{\alpha}_t}} (\epsilon_{\theta}(x_t, t, y) - \epsilon_{\theta}(x_t, t))$$

Classifier-free guidance

Trade-off for sample quality and sample diversity

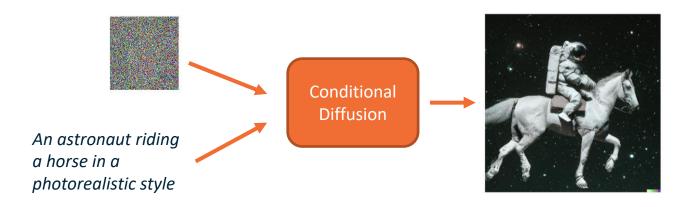


Non-guidance Scale = 1 Guidance scale = 3

Large guidance weight (ω) usually leads to better individual sample quality but less sample diversity.

Ho & Salimans, "Classifier-Free Diffusion Guidance", 2021.

Classifier-free Guided Diffusion



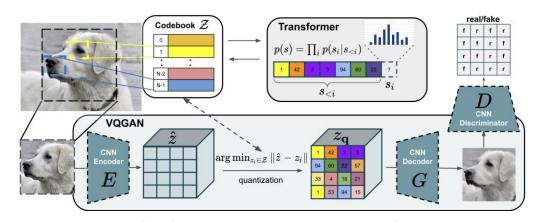
Classifier-free Guided Diffusion: estimate the gradient of the classifier model with conditional diffusion models!

$$\nabla_{x_t} \log f_{\varphi}(y|x_t) = -\frac{1}{\sqrt{1-\bar{\alpha}_t}} (\epsilon_{\theta}(x_t, t, y) - \epsilon_{\theta}(x_t, t))$$
$$\bar{\epsilon}_{\theta}(x_t, t, y) = (w+1)\epsilon_{\theta}(x_t, t, y) - w\epsilon_{\theta}(x_t, t)$$

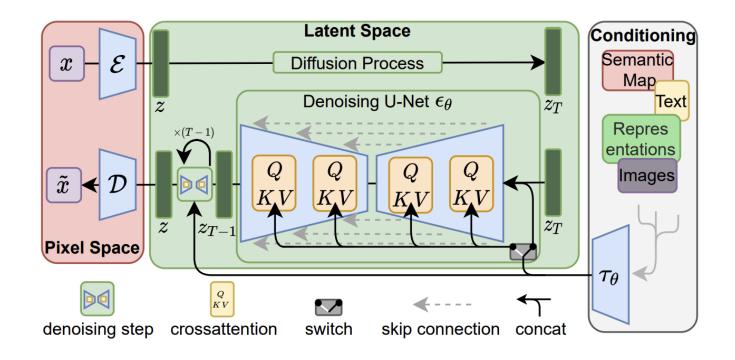
Latent-space Diffusion

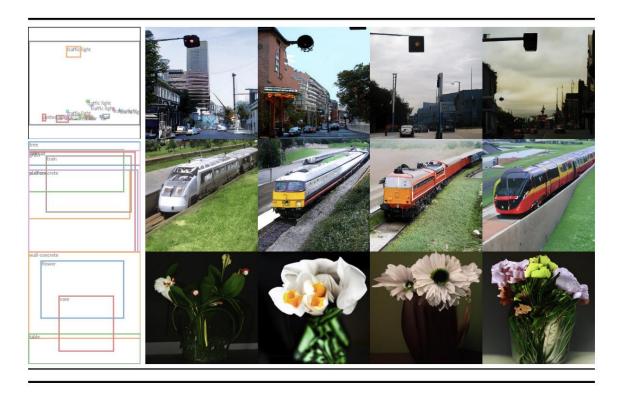
Problem: Hard to learn diffusion process on high-resolution images

Solution: learn a low-dimensional latent space using a transformer-based autoencoder and *do diffusion on the latent space*!



The latent space autoencoder

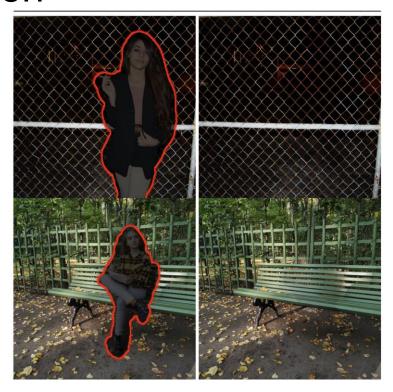




Layout-Conditional Generation



Segmentation-Conditional Generation



Inpainting



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

Additional resources / tutorials

- Overview of the research landscape: What are Diffusion Models?
- More math! <u>Understanding Diffusion Models: A Unified Perspective</u>
- Tutorial with hands-on example: <u>The Annotated Diffusion Model</u>
- Nice introduction videos:
 - o What are Diffusion Models?
 - Diffusion Models | Math Explained
 - Three hours of the math! https://www.youtube.com/watch?v=rLepfNziDPM
- CVPR Tutorial: <u>Denoising Diffusion-based Generative Modeling:</u> Foundations and Applications
- Score functions:
 - In general
 - > For <u>Diffusion models</u>

Summary

- Denoising Diffusion model is a type of generative model that learns the process of "denoising" a known noise source (Gaussian).
- We can construct a learning problem by deriving the evidence lower bound (ELBO) of the denoising process.
- The learning objective is to minimize the KL divergence between the "ground truth" and the learned denoising distribution.
- A simplified learning objective is to estimate the noise of the forward diffusion process.
- The diffusion process can be guided to generate targeted samples.
- Can be applied to many different domains. Same underlying principle.
- Very hot topic!