CS 4644-DL / 7643-A
ZSOLT KIRA

Generative Models:

Denoising Diffusion Probabilistic Models (DDPMs)

Slides adapted from those by Danfei Xu

- **Assignment 3**
  - In Grace period (ends **July 15th 11:59pm EST)**

- **Projects**
  - Project proposal due **July 26th**

Taxonomy of Generative Models

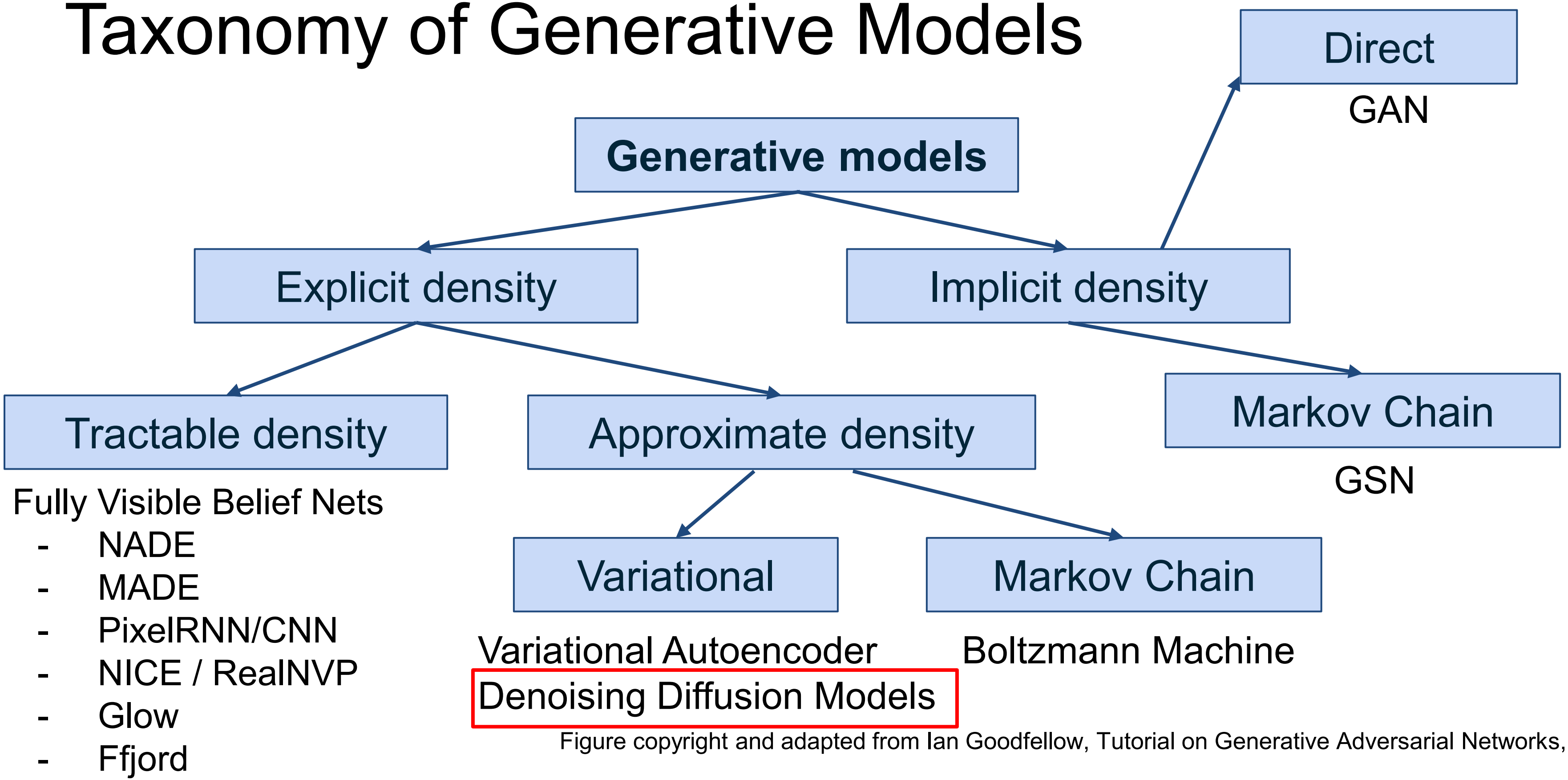


Figure copyright and adapted from Ian Goodfellow, Tutorial on Generative Adversarial Networks, 2017.

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

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

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

$x_0 \longrightarrow x_1 \longrightarrow$

...

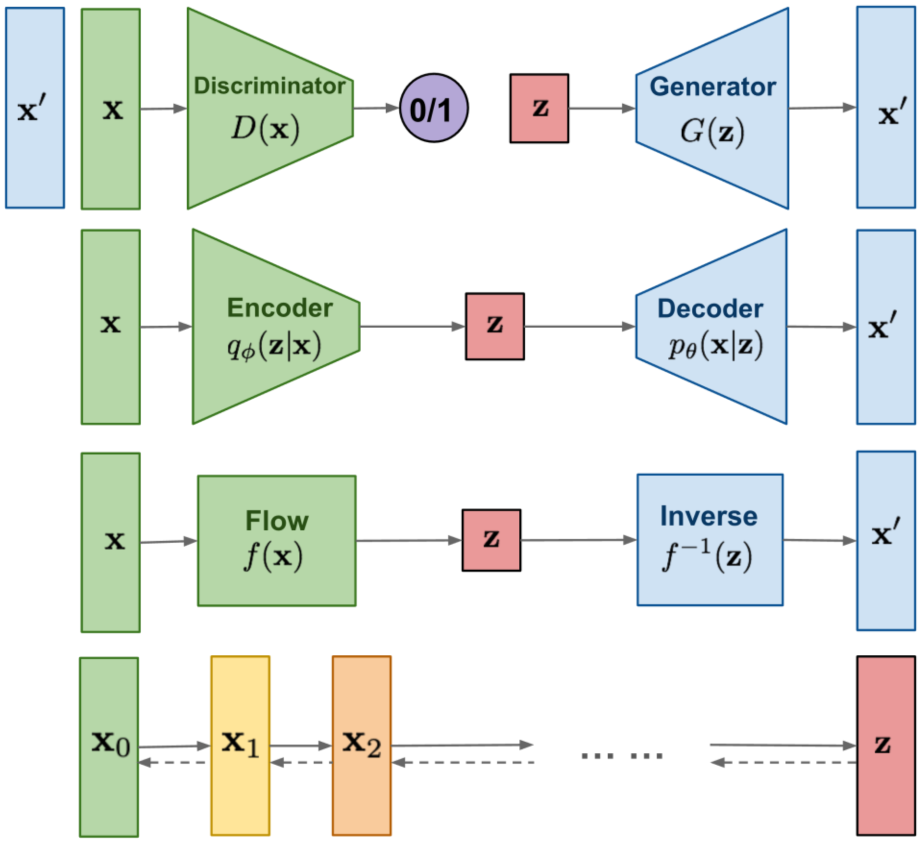
Comparison

GAN: Adversarial training

VAE: maximize variational lower bound

Flow-based models: Invertible transform of distributions

Diffusion models: Gradually add Gaussian noise and then reverse



The Denoising Diffusion Process

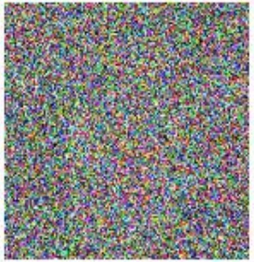
image from dataset

The “forward diffusion” process: add Gaussian noise each step

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

$x_0 \longrightarrow x_1 \longrightarrow \cdots \longrightarrow x_{T-1} \longrightarrow x_T$

...



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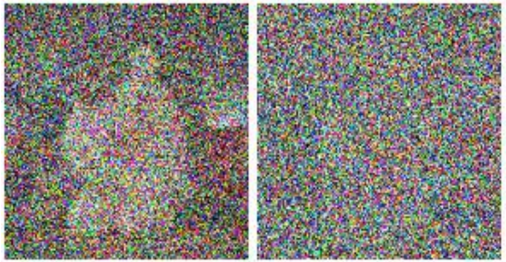
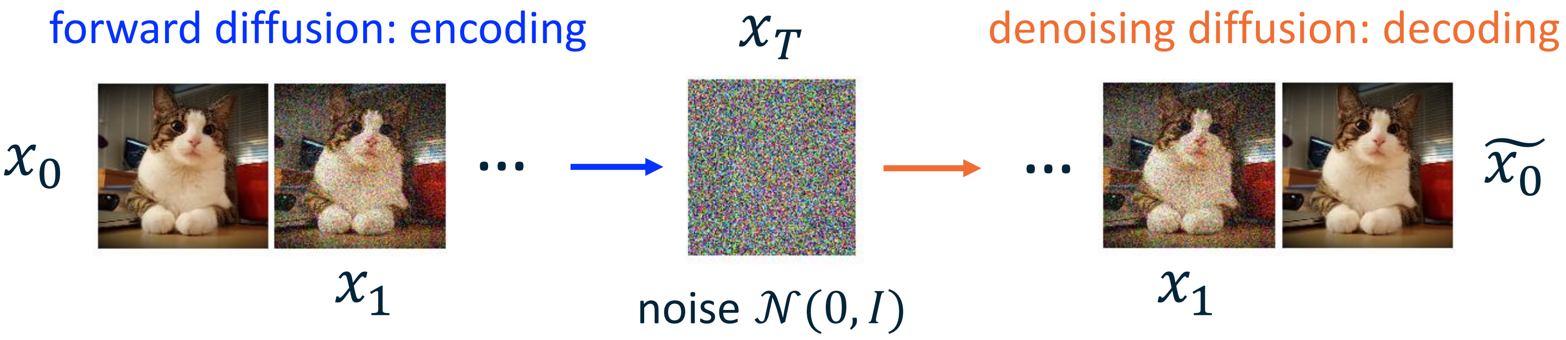


$x_0 \longleftarrow x_1 \longleftarrow \cdots \longleftarrow x_{T-1} \longleftarrow x_T$

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

Ties/inspiration form Annealed Imporantce Sampling in physics

Forward/Reverse Processes



Forward/Reverse Processes

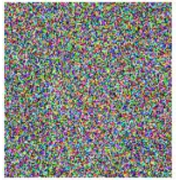
forward diffusion: encoding

x_T

denoising diffusion: decoding

x_0

…



…

$\widetilde{x_0}$

x_1

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

x_1

Known / predefined:

$q(x_{1:T}|x_0)$

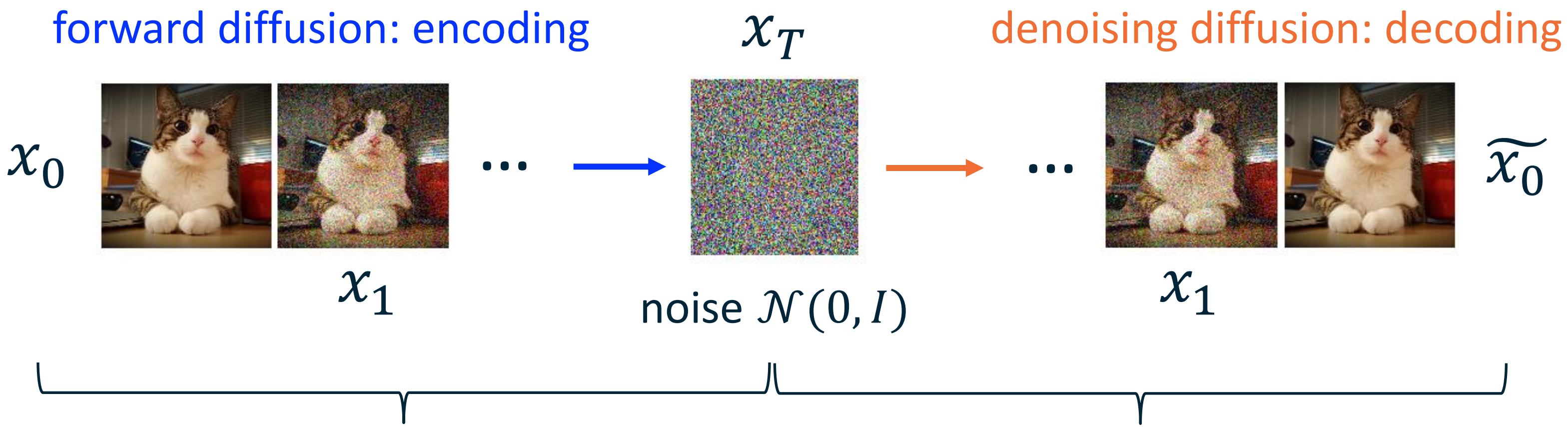
Unknown / learned:

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

Input: x_t

Output: Noise mean to remove, sample & use w/ x_t to get x_{t-1}

Forward/Reverse Processes



Known / predefined:

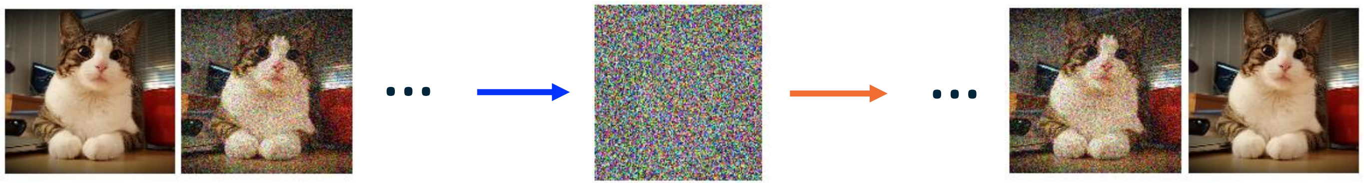
$q(x_{1:T}|x_0)$

Unknown / learned:

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

Use the denoising decoding process to generate new images.

Forward/Reverse Processes



Known / predefined:
$q(x_{1:T}|x_0)$

Unknown / learned:

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

The Diffusion (Encoding) Process

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

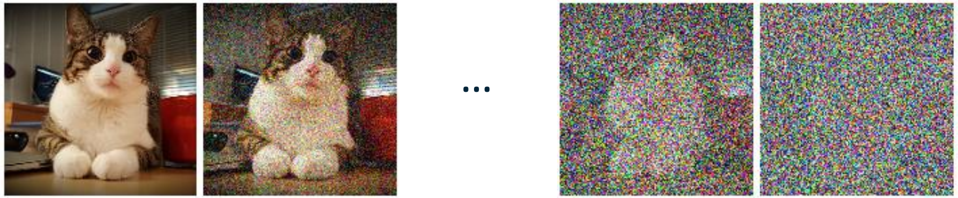
$$q(x_{1:T}|x_0) = \prod_{t=1}^{T} q(x_t|x_{t-1})$$ Probability Chain Rule (Markov Chain)

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

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

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

$x_0 \longrightarrow x_1 \longrightarrow \quad \longrightarrow x_{T-1} \longrightarrow x_T$



The Diffusion (Encoding

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

$$\bar{\alpha}_t = \prod_{s=1} a_s$$

$$\begin{aligned}
\mathrm{q}(x_t|x_{t-1}) &= \mathcal{N}(x_t, \sqrt{1-\beta_t}x_{t-1}, \beta_t I) \\
&= \sqrt{1-\beta_t}x_{t-1} + \sqrt{\beta_t}\epsilon \\
&= \sqrt{\alpha_t}\, x_{t-1} + \sqrt{1-\alpha_t}\,\epsilon \\
&= \sqrt{\alpha_t\alpha_{t-1}}\, x_{t-2} + \sqrt{1-\alpha_t\alpha_{t-1}}\,\epsilon \\
&= \sqrt{\alpha_t\alpha_{t-1}\alpha_{t-2}}\, x_{t-3} + \sqrt{1-\alpha_t\alpha_{t-1}\alpha_{t-2}}\,\epsilon \\
&= \sqrt{\alpha_t\alpha_{t-1}\ldots\alpha_1\alpha_0}\, x_0 + \sqrt{1-\alpha_t\alpha_{t-1}\ldots\alpha_1\alpha_0}\,\epsilon
\end{aligned}$$

$$q(x_t|x_0) = \mathcal{N}(x_t; \sqrt{\bar{\alpha}_t}\, x_0, (1-\bar{\alpha}_t)I) \longleftarrow \boxed{= \sqrt{\bar{\alpha}_t}\, x_0 + \sqrt{1-\bar{\alpha}_t}\,\epsilon}$$

The **known** forward process x_0

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

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

Nice property: samples from an *arbitrary forward step* are also Gaussian-distributed!

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

Gaussian reparameterization trick:

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

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

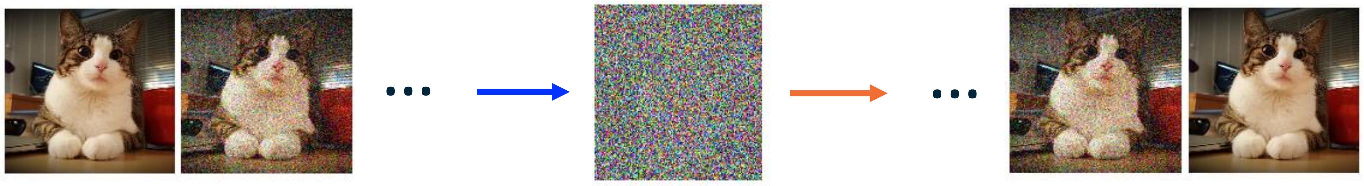
Intuition: We know all distributions in forward process, and can in fact directly compute for any t based on X_0

(square root appears because reparameterization trick has just σ)

The Diffusion and Denoising Process

forward diffusion: encoding $\quad x_T \quad$ denoising diffusion: decoding

x_0



$\widetilde{x_0}$

$x_1 \qquad$ noise $\mathcal{N}(0, I) \qquad x_1$

Known / predefined:

$q(x_{1:T}|x_0)$

Unknown / learned:

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

The Denoising (Decoding) 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

Assume fixed / known variance (simplification)

What is the shape of the mean?

The Denoising (Decoding) Process

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

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Want to learn time-dependent mean

Assume fixed / known variance (simplification)

How do we form a learning objective?

The Denoising (Decoding) Process

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

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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.

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

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

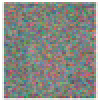
$$\geq \mathrm{E}_q\left[\log \frac{p(x|z)p(z)}{q(z|x)}\right]$$ Evidence Lower Bound (ELBO)

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

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

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

fixed



Easy to optimize / sometimes omitted

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

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

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

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Recall: Gaussian reparameterization trick

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

$$\begin{aligned} q(x_{t-1}|x_t) &= \boldsymbol{q(x_{t-1}|x_t, x_0)} \quad \textbf{(markov assumption)} \\ &= \frac{q(x_t|x_{t-1}, x_0)q(x_{t-1}|x_0)}{q(x_{t|}x_0)} \qquad \text{(Bayes rule)} \\ &= \frac{\mathcal{N}(x_t; \sqrt{a_t}x_{t-1}, \beta_t I)\mathcal{N}(x_{t-1}; \sqrt{\bar{\alpha}_{t-1}}x_{t-1}, (1-\bar{\alpha}_{t-1})I)}{\mathcal{N}(x_t; \sqrt{\bar{\alpha}_t}x_0, (1-\bar{\alpha}_{t-1})I)} \\ &\propto \mathcal{N}\left(x_{t-1}; \frac{\sqrt{a_t}(1-\bar{\alpha}_{t-1})x_t + \sqrt{\bar{\alpha}_{t-1}}(1-a_t)x_0}{1-\sqrt{\bar{\alpha}_t}}, \Sigma_q(t)\right) \qquad \text{(Property of Gaussian)} \end{aligned}$$

The Denoising (Decoding) Process

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

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

$$\mu_q(t) = \frac{1}{\sqrt{\alpha_t}}\left(x_t - \frac{\beta_t}{\sqrt{(1-\bar{\alpha}_t)}}\epsilon\right)$$

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

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

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

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

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

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

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?
See slides at the end! Variational models …

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We know how to learn   Assume fixed / known variance

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

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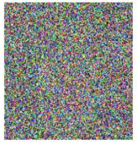
We know how to learn

Assume fixed / known variance

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



$\xrightarrow{p_\theta(x_T|x_{T-1})}$

x_{T-1}

$\xrightarrow{p_\theta(x_{T-1}|x_{T-2})} \cdots \xrightarrow{p_\theta(x_1|x_0)}$

x_0

Generate new images!

The Denoising Diffusion Algorithm

Algorithm 1 Training

1: **repeat**
2: $\mathbf{x}_0 \sim q(\mathbf{x}_0)$
3: $t \sim \mathrm{Uniform}(\{1, \ldots, T\})$
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

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Algorithm 2 Sampling

1: $\mathbf{x}_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
2: **for** $t = T, \ldots, 1$ **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 Probabilistic Models, Ho *et al.*, 2020

The Denoising Diffusion Algorithm

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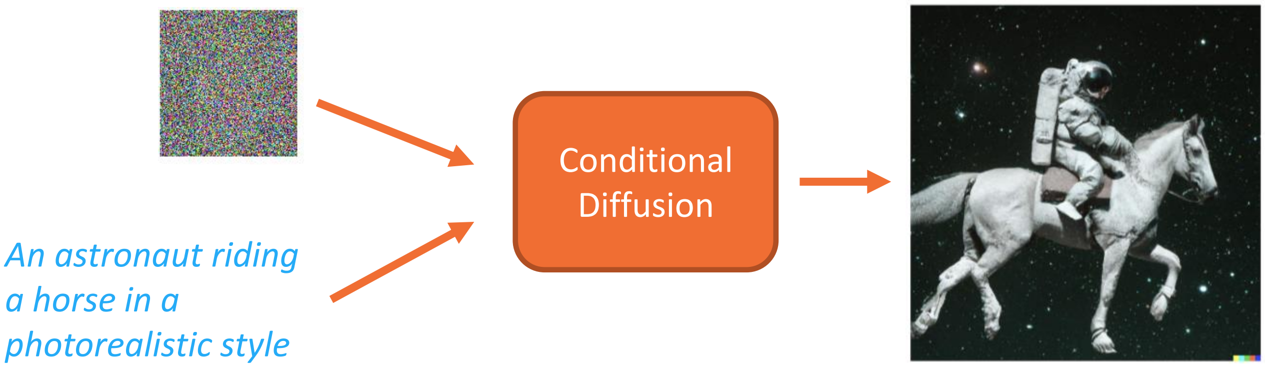
5: **end for**
6: **return** $\mathbf{x}_0$

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

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

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

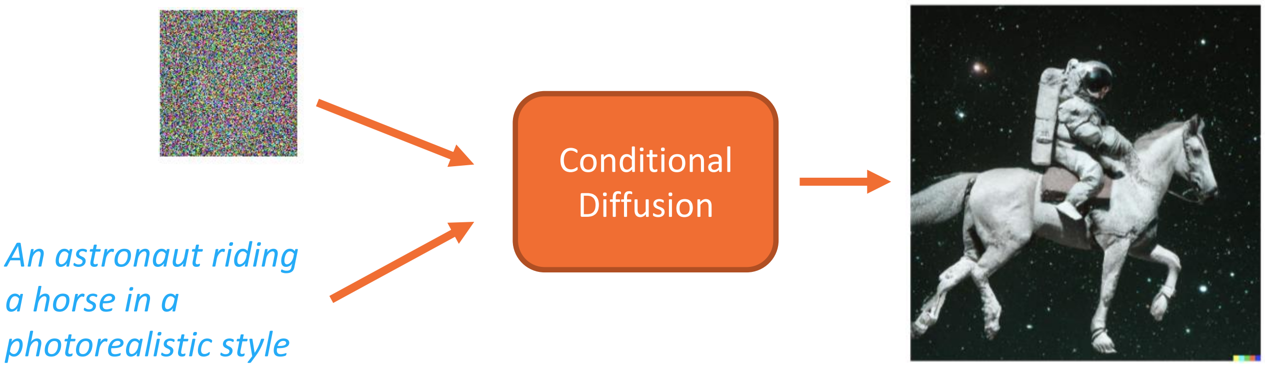
Conditional Diffusion Models



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

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

Conditional Diffusion Models

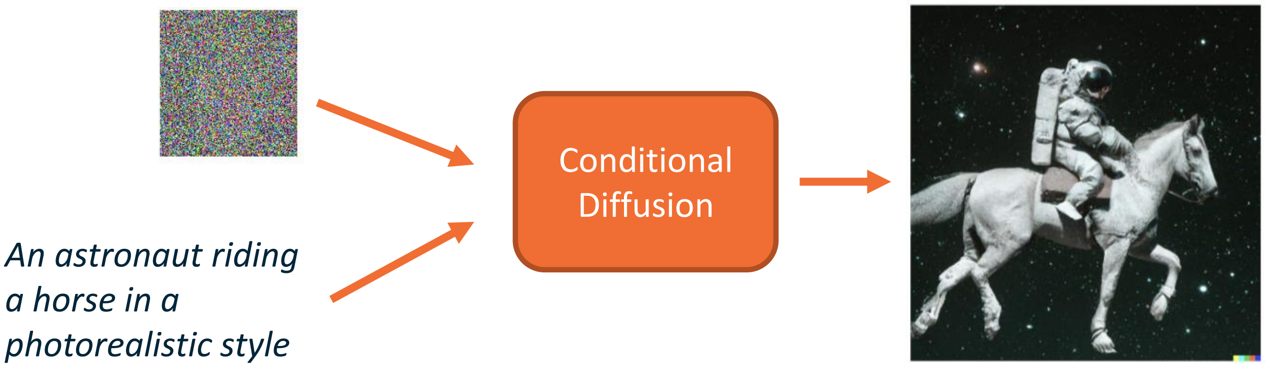


Simple idea: just condition the model on some text labels y!

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

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!

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

Dhariwal & Nichol, 2021

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 Classifier gradient
$x_T \leftarrow$ 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

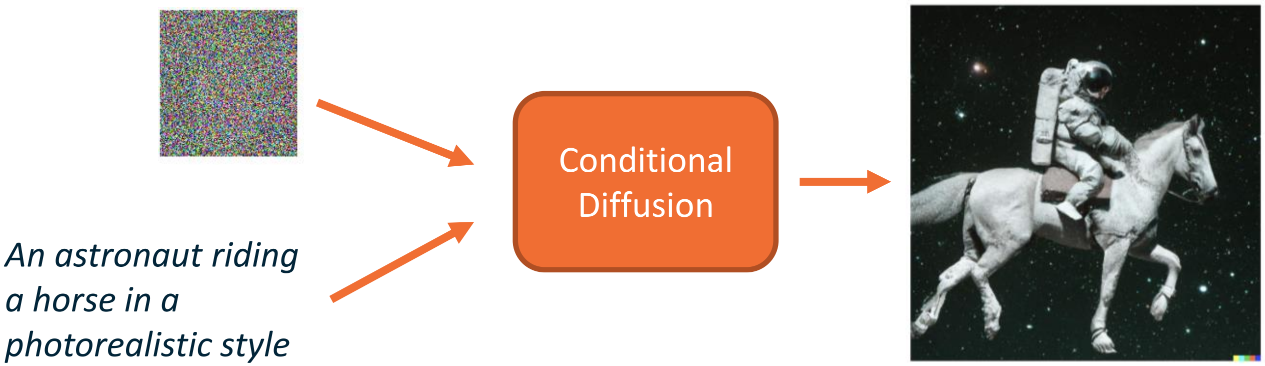
Using the gradient of a trained classifier as guidance

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

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!

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

Ho and Salimans, 2022

Classifier-free guidance

Trade-off for sample quality and sample diversity

Non-guidance

Guidance scale = 1

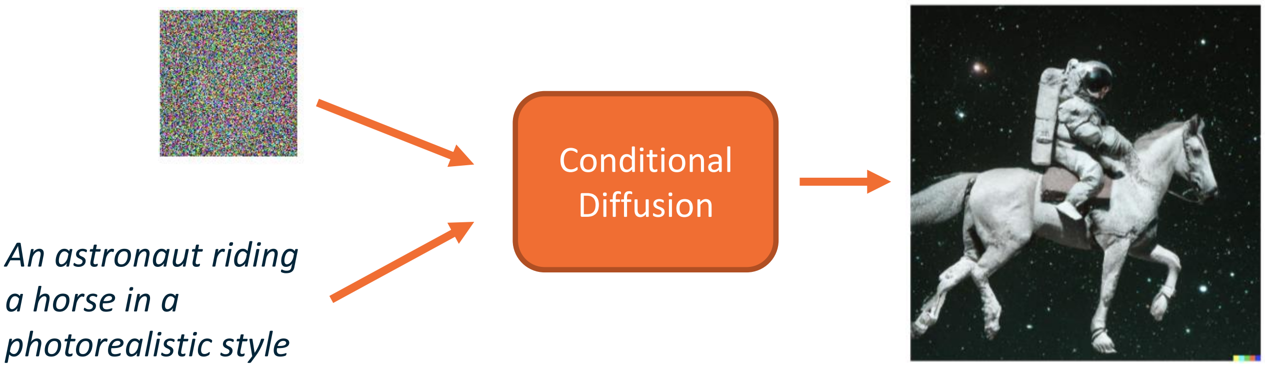
Guidance scale = 3

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

Ho & Salimans, “Classifier-Free Diffusion Guidance”, 2021.

Slide by Soumyadip (Roni) Sengupta

Classifier-free Guided Diffusion



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

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

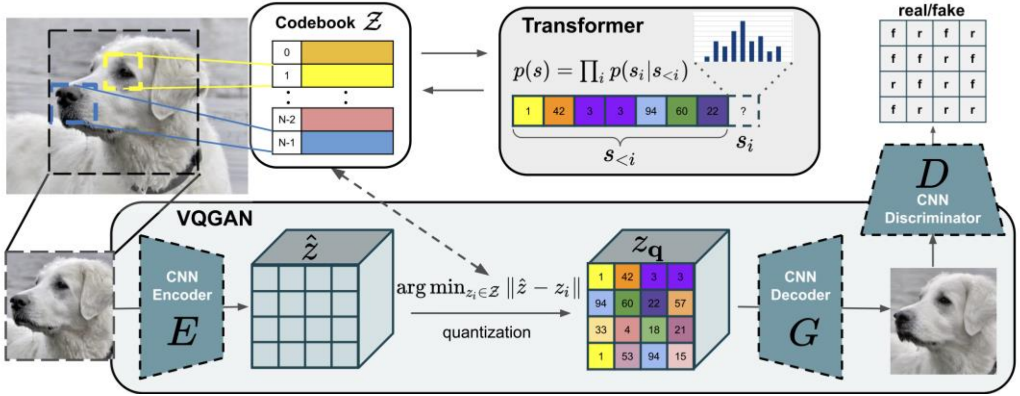
$$\bar{\epsilon}_\theta(x_t,t,y) = (w+1)\epsilon_\theta(x_t,t,y) - w\epsilon_\theta(x_t,t)$$

Ho and Salimans, 2022

Latent-space Diffusion

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

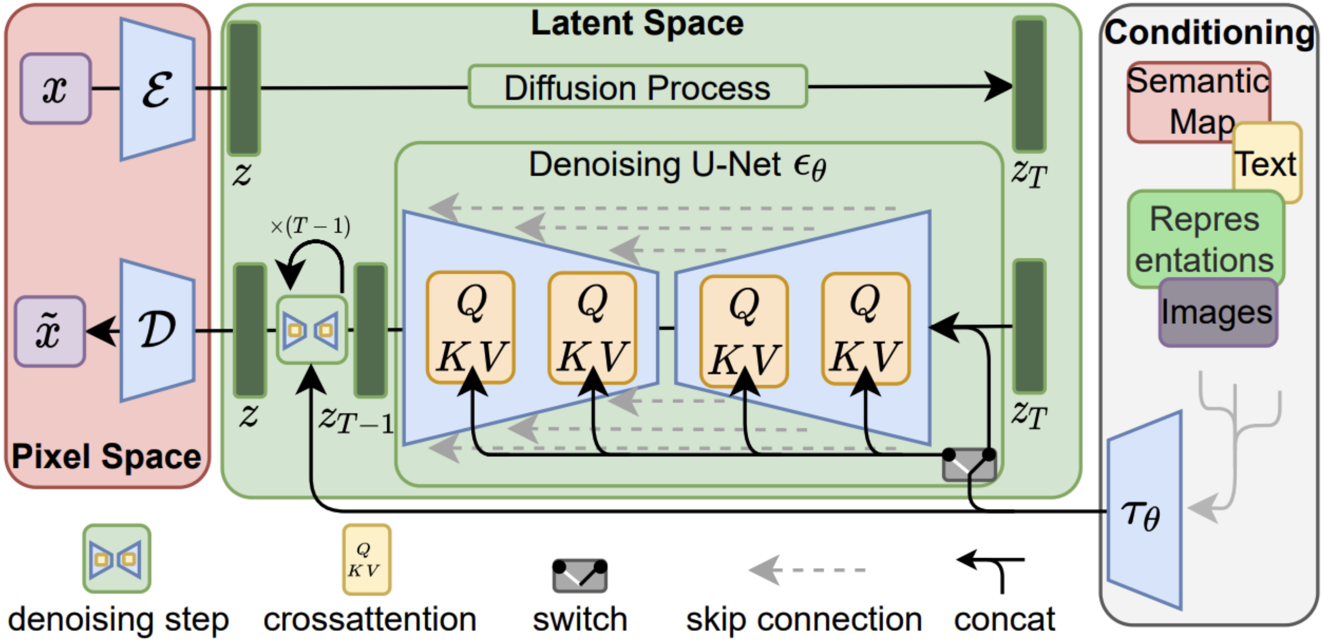
Solution: learn a low-dimensional latent space using a transformer-based autoencoder and *do diffusion on the latent space*!



The latent space autoencoder

Esser and Rombach *et al.*, 2021

“StableDiffusion”



Rombach and Blattmann *et al.*, 2022

“StableDiffusion”

Layout-Conditional Generation

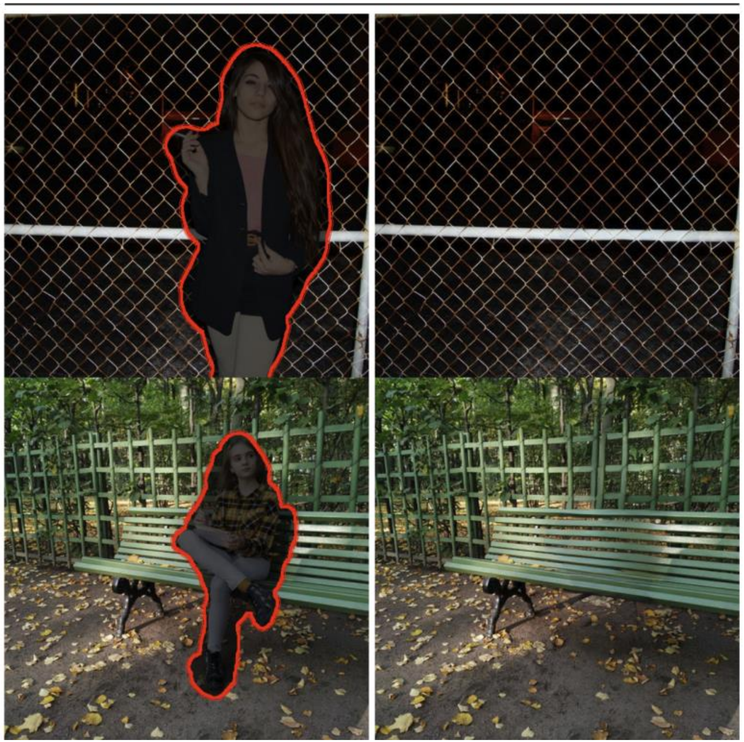
Rombach and Blattmann *et al.*, 2022

"StableDiffusion"

Segmentation-Conditional Generation

Rombach and Blattmann *et al.*, 2022

“StableDiffusion”



Inpainting

Rombach and Blattmann *et al.*, 2022

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

Additional resources / tutorials

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

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!

Reinforcement Learning Introduction

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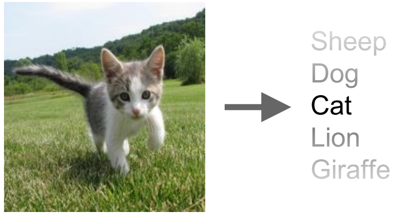
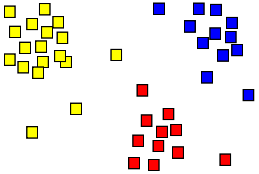
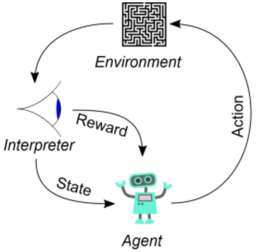
Supervised Learning	Unsupervised Learning	Reinforcement Learning
• Train Input: $\{X, Y\}$ • Learning output: $f : X \rightarrow Y$, $P(y \mid x)$ • e.g. classification	• Input: $\{X\}$ • Learning output: $P(x)$ • Example: Clustering, density estimation, etc.	• Evaluative feedback in the form of **reward** • No supervision on the right action







RL: Sequential decision making in an environment with evaluative feedback.

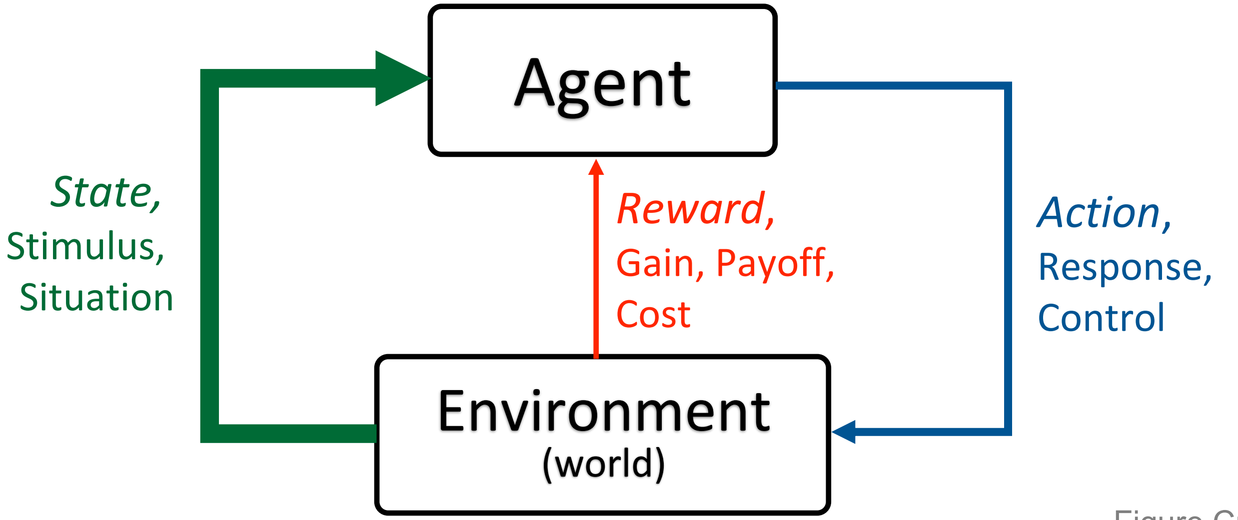


Figure Credit: Rich Sutton

- **Environment** may be unknown, non-linear, stochastic and complex.
- **Agent** learns a **policy** to map states of the environments to actions.
  - Seeking to maximize cumulative reward in the long run.

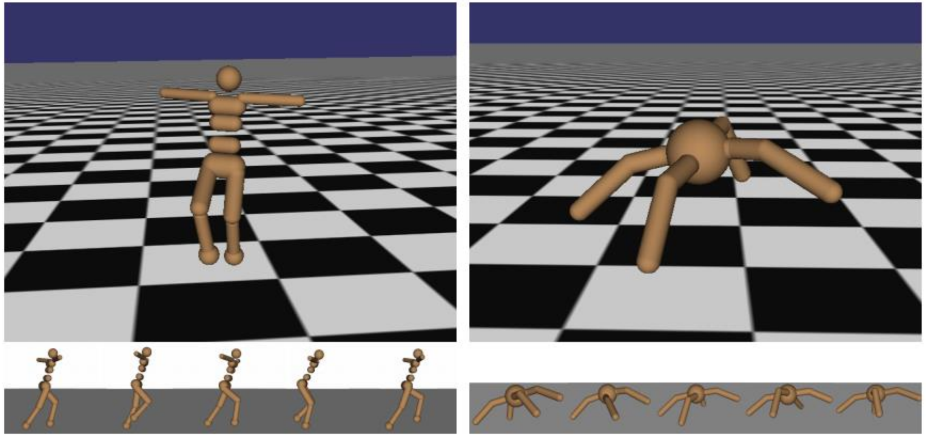
What is Reinforcement Learning?

Signature Challenges in Reinforcement Learning

- Evaluative feedback: Need trial and error to find the right action
- Delayed feedback: Actions may not lead to immediate reward
- Non-stationarity: Data distribution of visited states changes when the policy changes
- Fleeting nature of time and online data

Slide adapted from: Richard Sutton

Robot Locomotion



Figures copyright John Schulman et al., 2016. Reproduced with permission.

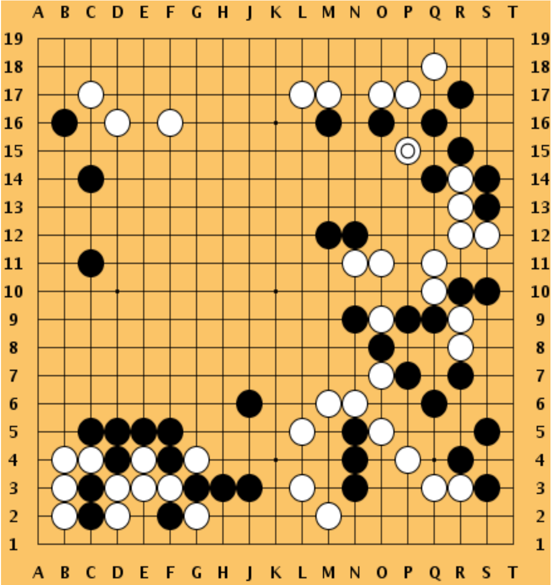
- **Objective**: Make the robot move forward
- **State**: Angle and position of the joints
- **Action**: Torques applied on joints
- **Reward**: +1 at each time step upright and moving forward

Slide Credit: Fei-Fei Li, Justin Johnson, Serena Yeung, CS 231n

Atari Games

- **Objective**: Complete the game with the highest score
- **State**: Raw pixel inputs of the game state
- **Action**: Game controls e.g. Left, Right, Up, Down
- **Reward**: Score increase/decrease at each time step

Go



- **Objective**: Defeat opponent
- **State**: Board pieces
- **Action**: Where to put next piece down
- **Reward**: +1 if win at the end of game, 0 otherwise

Slide Credit: Fei-Fei Li, Justin Johnson, Serena Yeung, CS 231n

- **MDPs**: Theoretical framework underlying RL

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- An MDP is defined as a tuple $(\mathcal{S}, \mathcal{A}, \mathcal{R}, \mathbb{T}, \gamma)$
  - $\mathcal{S}$: Set of possible states
  - $\mathcal{A}$: Set of possible actions
  - $\mathcal{R}(s, a, s')$: Distribution of reward
  - $\mathbb{T}(s, a, s')$: Transition probability distribution, also written as p(s'|s,a)
  - γ : Discount factor

Markov Decision Processes (MDPs)

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Markov Decision Processes (MDPs)

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- **Interaction trajectory**: $\ldots s_t, a_t, r_{t+1}, s_{t+1}, a_{t+1}, r_{t+2}, s_{t+2}, \ldots$
- **Markov property**: Current state completely characterizes state of the environment
- **Assumption**: Most recent observation is a sufficient statistic of history

$$p\left(S_{t+1} = s' | S_t = s_t, A_t = a_t, S_{t-1} = s_{t-1}, \ldots S_0 = s_0\right) = p\left(S_{t+1} = s' | S_t = s_t, A_t = a_t\right)$$

Markov Decision Processes (MDPs)

- In **Reinforcement Learning**, we assume an underlying **MDP** with unknown:
  - Transition probability distribution $\mathbb{T}$
  - Reward distribution $\mathcal{R}$

MDP
$(\mathcal{S}, \mathcal{A}, \mathcal{R}, \mathbb{T}, \gamma)$

MDPs in the context of RL

- In **Reinforcement Learning**, we assume an underlying **MDP** with unknown:
  - Transition probability distribution $\mathbb{T}$
  - Reward distribution $\mathcal{R}$

MDP
$(\mathcal{S}, \mathcal{A}, \mathcal{R}, \mathbb{T}, \gamma)$

- Evaluative feedback comes into play, trial and error necessary
- Deep RL: Use neural network to estimate V/Q, policy, R/T

MDPs in the context of RL

- Solving MDPs by finding the **best/optimal policy**

Solving MDPs: Optimal policy

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- Solving MDPs by finding the **best/optimal policy**

- Formally, a **policy** is a mapping from states to actions

e.g.

State	Action
A →	2
B →	1

Solving MDPs: Optimal policy

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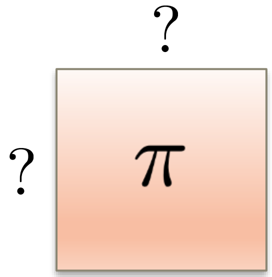
Solving MDPs: Optimal policy

$$n = |\mathcal{S}|$$

$$m = |\mathcal{A}|$$

- Solving MDPs by finding the **best/optimal policy**
- Formally, a **policy** is a mapping from states to actions
  - Deterministic $\pi(s) = a$



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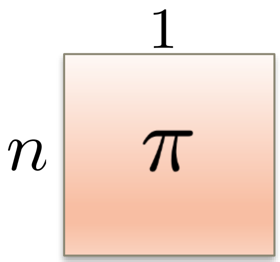

Solving MDPs: Optimal policy

$$n = |\mathcal{S}|$$

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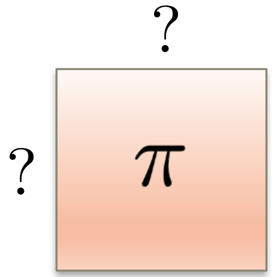

- Solving MDPs by finding the **best/optimal policy**

- Formally, a **policy** is a mapping from states to actions
  - Deterministic $\pi(s) = a$
  - Stochastic $\pi(a|s) = \mathbb{P}(A_t = a | S_t = s)$

Solving MDPs: Optimal policy

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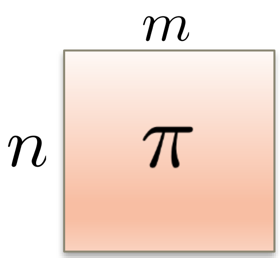

Solving MDPs: Optimal policy

- Solving MDPs by finding the **best/optimal policy**

- Formally, a **policy** is a mapping from states to actions
  - Deterministic $\pi(s) = a$
  - Stochastic $\pi(a|s) = \mathbb{P}(A_t = a|S_t = s)$

- What is a good policy?
  - Maximize **current reward**? Sum of all **future rewards**?
  - **Discounted sum of future rewards**!
    - Discount factor: γ

- Formally, the **optimal policy** is defined as:

$$\pi^* = \arg\max_{\pi} \mathbb{E}\left[\sum_{t\geq 0} \gamma^t r_t | \pi\right]$$

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discounted sum of future rewards

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Solving MDPs: Optimal policy

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discounted sum of future rewards

$$\pi^* = \arg\max_{\pi} \mathbb{E}\left[\sum_{t \geq 0} \gamma^t r_t | \pi\right]$$

?

- Formally, the **optimal policy** is defined as:

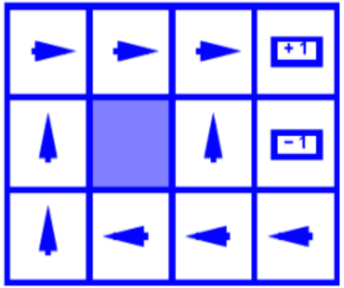
discounted sum of future rewards

$$\pi^* = \arg\max_\pi \mathbb{E}\left[\sum_{t\geq 0} \gamma^t r_t | \pi\right]$$

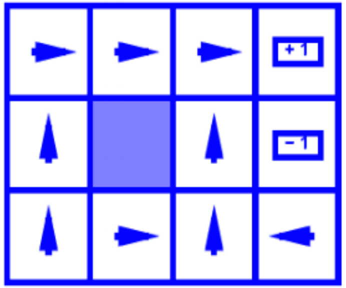
$$\boxed{\boldsymbol{s}_0 \sim p\left(\boldsymbol{s}_0\right), a_t \sim \pi\left(\cdot|\boldsymbol{s}_t\right), \boldsymbol{s}_{t+1} \sim p\left(\cdot|\boldsymbol{s}_t, a_t\right)}$$

Expectation over initial state, actions from policy,
next states from transition distribution

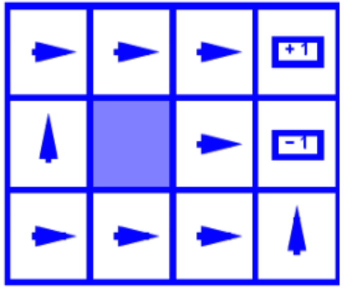
- Some optimal policies for three different grid world MDPs (gamma=0.99)
    - Varying reward for non-absorbing states (states other than +1/-1)



R(s) = -0.03



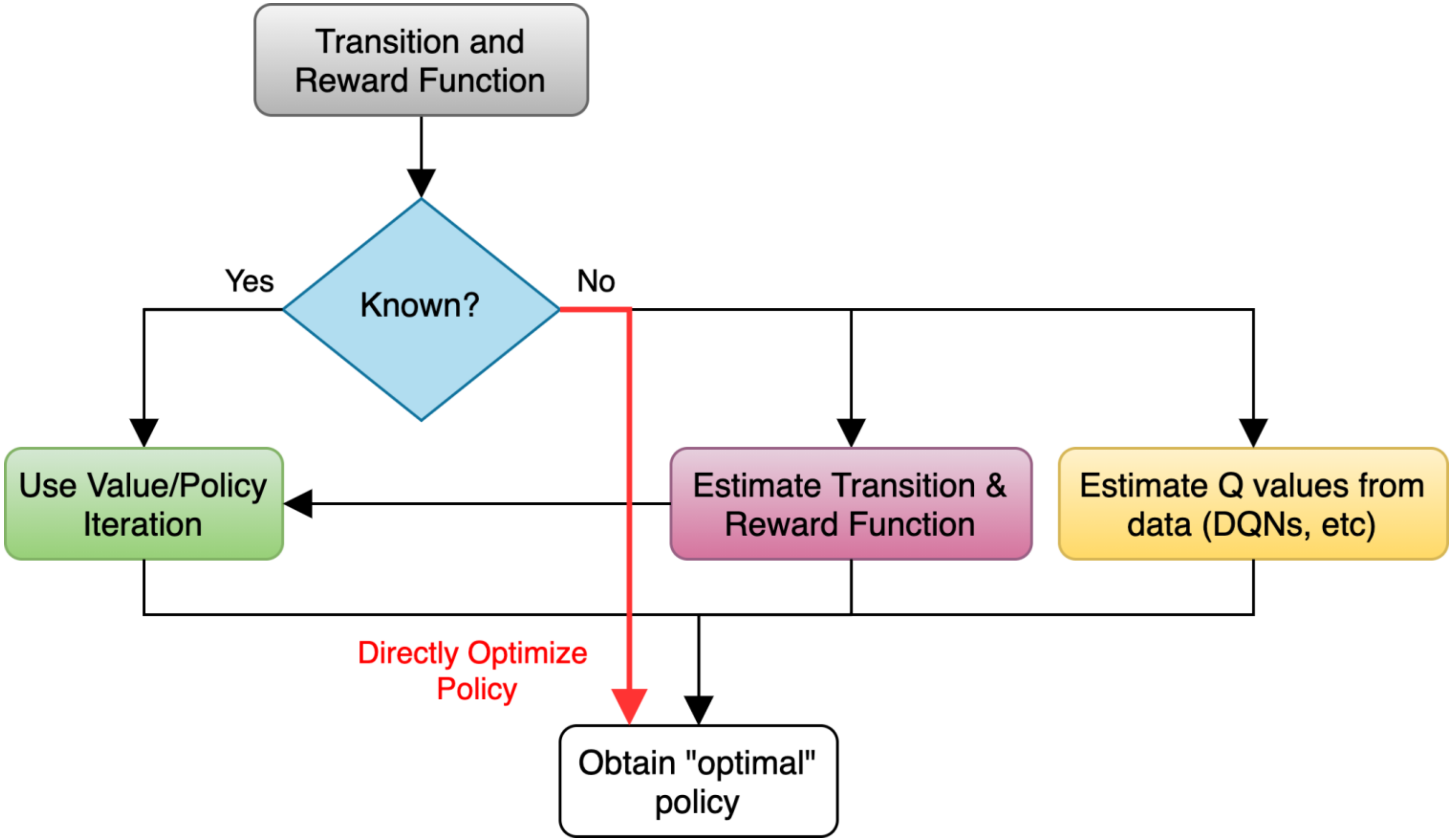
R(s) = -0.4



R(s) = -2.0

Image Credit: Byron Boots, CS 7641

Optimal policy examples



Overview

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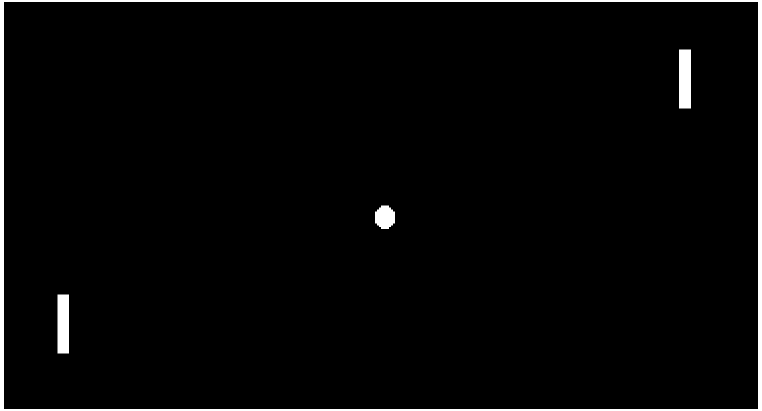

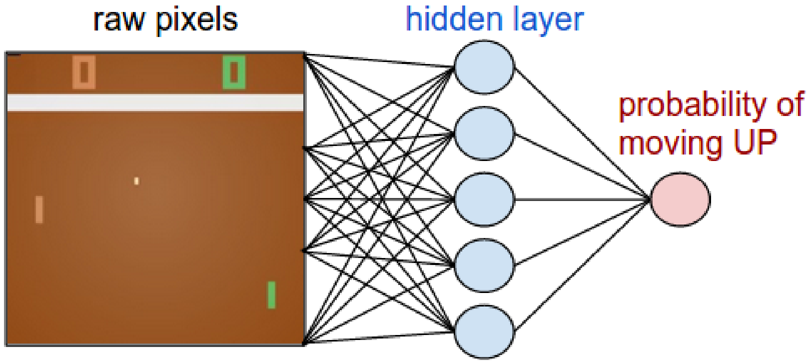

Pong from Pixels

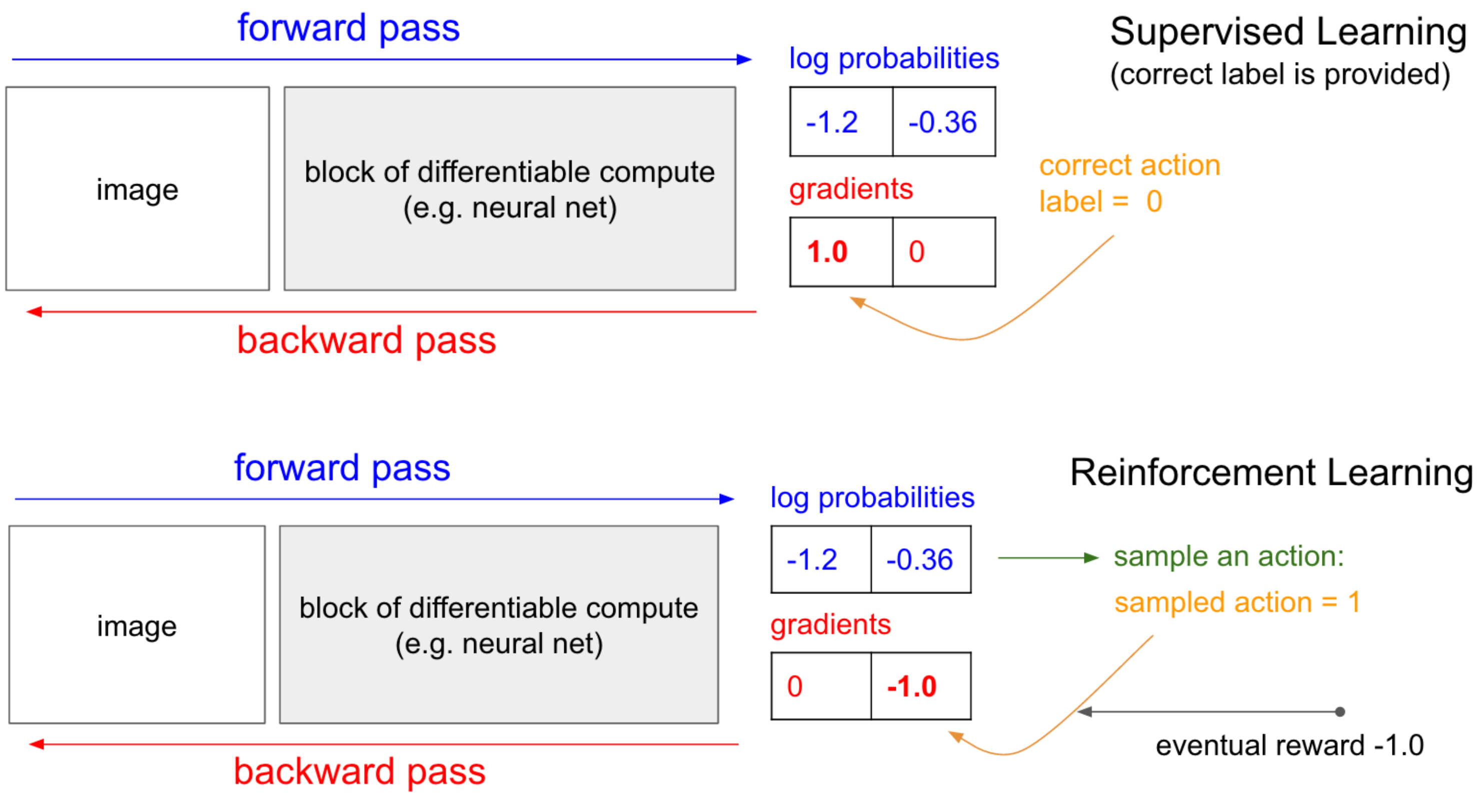

Image Source: http://karpathy.github.io/2016/05/31/rl/

Policy Gradient: Loss Function

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- Slightly re-writing the notation

Let $\tau = (s_0, a_0, \ldots s_T, a_T)$ denote a trajectory

$$\pi_\theta(\tau) = p_\theta(\tau) = p_\theta\left(s_0, a_0, \ldots s_T, a_T\right)$$
$$= p(s_0) \prod_{t=0}^{T} p_\theta\left(a_t \mid s_t\right) \cdot p\left(s_{t+1} \mid s_t, a_t\right)$$

$$\boxed{\arg\max_\theta \mathbb{E}_{\tau \sim p_\theta(\tau)}\left[\mathcal{R}(\tau)\right]}$$

$$J(\theta) = \mathbb{E}_{\tau \sim p_\theta(\tau)} [\mathcal{R}(\tau)]$$

$$= \mathbb{E}_{a_t \sim \pi(\cdot|s_t), s_{t+1} \sim p(\cdot|s_t, a_t)} \left[\sum_{t=0}^{T} \mathcal{R}(s_t, a_t) \right]$$

- How to gather data?
  - We already have a policy: π_θ
  - Sample N trajectories $\{\tau_i\}_{i=1}^{N}$ by acting according to π_θ

$$\approx \frac{1}{N} \sum_{i=1}^{N} \sum_{t=1}^{T} r(s_t^i, a_t^i)$$

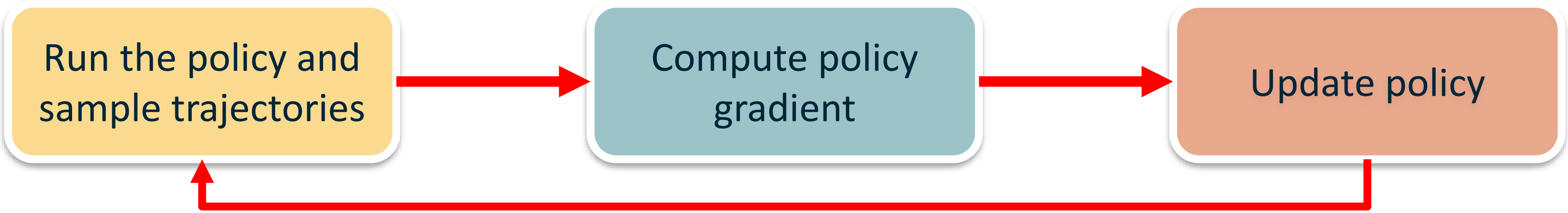
Gathering Data/Experience

- Sample trajectories $\tau_i = \{s_1, a_1, \dots s_T, a_T\}_i$ by acting according to π_θ

- Compute policy gradient as

$$\nabla_\theta J(\theta) \approx \ ?$$

- Update policy parameters: $\theta \leftarrow \theta + \alpha \nabla_\theta J(\theta)$



Slide credit: Sergey Levine

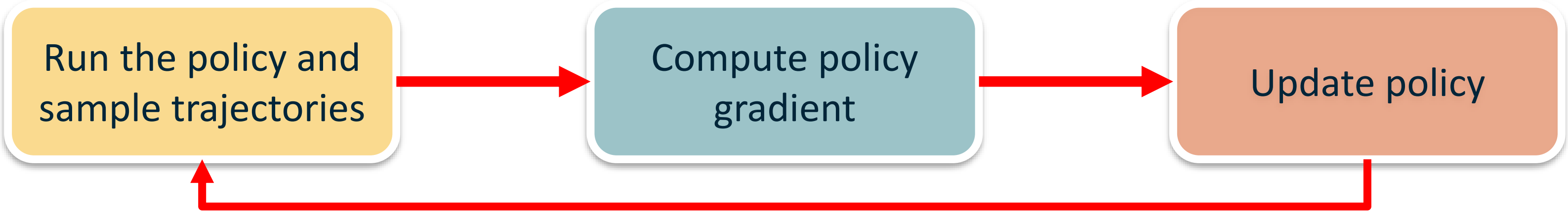
The REINFORCE Algorithm

- Sample trajectories $\tau_i = \{s_1, a_1, \ldots s_T, a_T\}_i$ by acting according to π_θ

- Compute policy gradient as

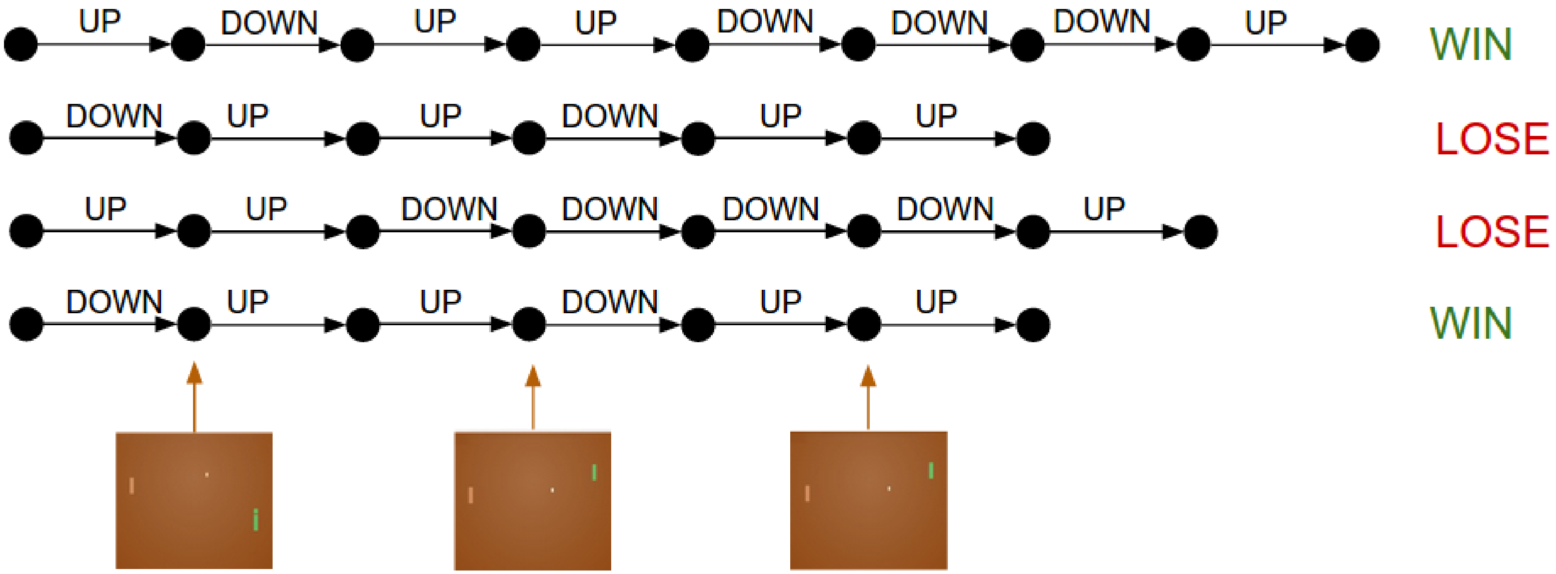
$$\nabla_\theta J(\theta) \approx \frac{1}{N} \sum_i^N \left[\sum_{t=1}^T \nabla_\theta \log \pi_\theta \left(a_t^i \mid s_t^i\right) \cdot \sum_{t=1}^T \mathcal{R}\left(s_t^i \mid a_t^i\right) \right]$$

- Update policy parameters: $\theta \leftarrow \theta + \alpha \nabla_\theta J(\theta)$



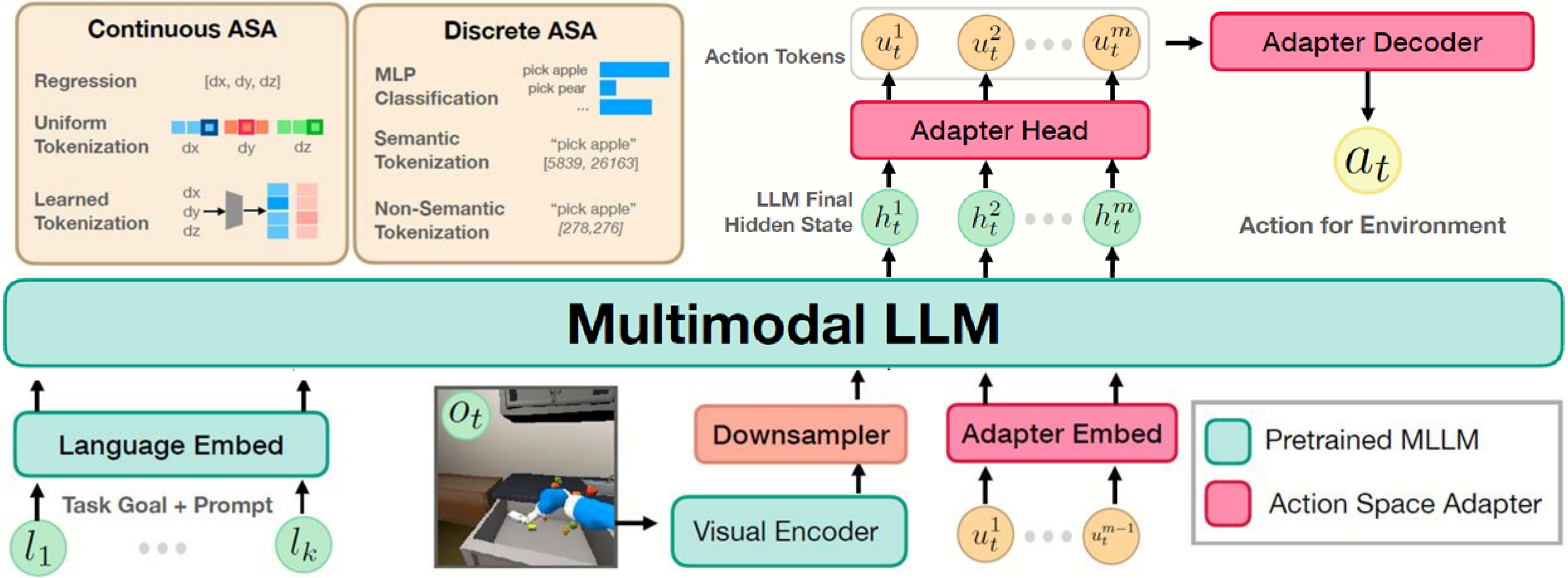
Slide credit: Sergey Levine

The REINFORCE Algorithm



Slide credit: Dhruv Batra

Drawbacks of Policy Gradients



We finetune the Action Space Adaptors (ASAs), downsampler, and MLLM

Szot et al., Grounding Multimodal Large Language Models in Actions, NeurIPS 2024
Szot et al., From Multimodal LLMs to Generalist Embodied Agents: Methods and Lessons, CVPR 2025

(Quick) Derivation!

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

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

Deep Unsupervised Learning using Nonequilibrium Thermodynamics, Sohl-Dickstein *et al.*, 2015

Variational Inference

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

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

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

Deep Unsupervised Learning using Nonequilibrium Thermodynamics, Sohl-Dickstein *et al.*, 2015

Variational Inference → **Simplify to KL**

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

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

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

$$\log p(x_0) \geq \mathrm{E}_q\left[\log \frac{p(x_0|x_{1:T})p(x_{1:T})}{q(x_{1:T}|x_0)}\right]$$ $x = x_0,\ z = x_{1:T}$

Deep Unsupervised Learning using Nonequilibrium Thermodynamics, Sohl-Dickstein *et al.*, 2015

Variational Inference → Simplify to KL

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

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

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

Evidence Lower Bound (ELBO)

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

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

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

$$= \mathrm{E}_q\left[\log \frac{p(x_T)\prod_{t=1}^{T} p_\theta(x_{t-1}|x_t)}{\prod_{t=1}^{T} q(x_t|x_{t-1})}\right]$$

← reverse denoising

← forward diffusion

Deep Unsupervised Learning using Nonequilibrium Thermodynamics, Sohl-Dickstein *et al.*, 2015

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

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

Deep Unsupervised Learning using Nonequilibrium Thermodynamics, Sohl-Dickstein *et al.*, 2015

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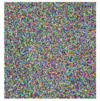
fixed



Easy to optimize / sometimes omitted

Deep Unsupervised Learning using Nonequilibrium Thermodynamics, Sohl-Dickstein *et al.*, 2015

Variational Inference → **Simplify to KL**

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

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

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

$$\log p(x_0) \geq \mathrm{E}_q\left[\log \frac{p(x_0|x_{1:T})p(x_{1:T})}{q(x_{1:T}|x_0)}\right]$$ $x = x_0,\ z = x_{1:T}$

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

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

Maximize the agreement between the predicted reverse diffusion distribution p_θ and the "ground truth" reverse diffusion distribution q

Deep Unsupervised Learning using Nonequilibrium Thermodynamics, Sohl-Dickstein *et al.*, 2015

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

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

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

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

$$\log p(x_0) \geq \mathrm{E}_q\left[\log \frac{p(x_0|x_{1:T})p(x_{1:T})}{q(x_{1:T}|x_0)}\right]$$ $x = x_0,\ z = x_{1:T}$

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

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

Deep Unsupervised Learning using Nonequilibrium Thermodynamics, Sohl-Dickstein *et al.*, 2015

Variational Inference → **Simplify to KL** → **Reverse Process => Normal**

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

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

$$\geq \mathrm{E}_q\left[\log\frac{p(X|Z)p(z)}{q(Z|X)}\right]$$ Evidence Lower Bound (ELBO)

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

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

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

$$q(x_{t-1}|x_t) = \boldsymbol{q(x_{t-1}|x_t,x_0)} \quad \textbf{(markov assumption)}$$

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

$$= \frac{\mathcal{N}(x_t;\sqrt{\alpha_t}x_{t-1},\beta_t I)\mathcal{N}(x_{t-1};\sqrt{\bar{\alpha}_{t-1}}x_{t-1},(1-\bar{\alpha}_{t-1})I)}{\mathcal{N}(x_t;\sqrt{\bar{\alpha}_t}x_0,(1-\bar{\alpha}_{t-1})I)}$$

$$\propto \mathcal{N}\left(x_{t-1};\ \frac{\sqrt{\alpha_t}(1-\bar{\alpha}_{t-1})x_t+\sqrt{\bar{\alpha}_{t-1}}(1-a_t)x_0}{1-\sqrt{\bar{\alpha}_t}}, \Sigma_q(t)\right) \qquad \text{(Property of Gaussian)}$$

Deep Unsupervised Learning using Nonequilibrium Thermodynamics, Sohl-Dickstein *et al.*, 2015

Variational Inference → Simplify to KL → Reverse Process => Normal → Bayes + Reparameterization

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

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

$$\log p(x_0) \geq \mathrm{E}_q\left[\log \frac{p(x_0|x_{1:T})p(x_{1:T})}{q(x_{1:T}|x_0)}\right]$$ $x = x_0,\ z = x_{1:T}$

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

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

$$\boxed{\begin{aligned} q(x_{t-1}|x_t, x_0) &= \mathcal{N}\left(x_{t-1}; \mu_q(t), \Sigma_q(t)\right) \\ \mu_q(t) &= \frac{1}{\sqrt{\alpha_t}}\left(x_t - \frac{\beta_t}{\sqrt{(1-\bar{\alpha}_t)}}\epsilon\right), \quad \epsilon \sim \mathcal{N}(0, I) \end{aligned}}$$

Proof using bayes rule and gaussian reparameterization trick

Deep Unsupervised Learning using Nonequilibrium Thermodynamics, Sohl-Dickstein *et al.*, 2015

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Proof using bayes rule and gaussian reparameterization trick

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

Deep Unsupervised Learning using Nonequilibrium Thermodynamics, Sohl-Dickstein *et al.*, 2015

Variational Inference → Simplify to KL → Reverse Process => Normal → Bayes + Reparameterization → Remove (variance-dependent) constant

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

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

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

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

Minimize the difference of distribution means (assuming identical variance)

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

Deep Unsupervised Learning using Nonequilibrium Thermodynamics, Sohl-Dickstein *et al.*, 2015

Learning the Denoising Process

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

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

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

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

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

Learning the Denoising Process

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known during inference

Unknown during inference

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

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

known during inference

Unknown during inference

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

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

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

Learning the Denoising Process

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

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

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

Learning the Denoising Process

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

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

Recall: the simplified t-step forward sample:

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

Learning the Denoising Process

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: $\text{argmin}_\theta ||\epsilon - \epsilon_\theta(\sqrt{\bar{\alpha}_t}x_0 + \sqrt{1-\bar{\alpha}_t}\epsilon, t)||^2$

Recall: the simplified t-step forward sample:

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

Math for Classifier Guidance

Conditional diffusion models

Include condition as input to reverse process

Reverse process: $p_\theta(\mathbf{x}_{0:T}|\mathbf{c}) = p(\mathbf{x}_T)\prod_{t=1}^{T} p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{c}), \quad p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{c}) = \mathcal{N}(\mathbf{x}_{t-1}; \boxed{\boldsymbol{\mu}_\theta(\mathbf{x}_t, t, \mathbf{c}), \boldsymbol{\Sigma}_\theta(\mathbf{x}_t, t, \mathbf{c}))}$

Variational upper bound: $L_\theta(\mathbf{x}_0|\mathbf{c}) = \mathbb{E}_q\left[L_T(\mathbf{x}_0) + \sum_{t>1} D_{\mathrm{KL}}(q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) \parallel \boxed{p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{c})) - \log p_\theta(\mathbf{x}_0|\mathbf{x}_1, \mathbf{c})}\right].$

Incorporate conditions into U-Net

- Scalar conditioning: encode scalar as a vector embedding, simple spatial addition or adaptive group normalization layers.
- Image conditioning: channel-wise concatenation of the conditional image.
- Text conditioning: single vector embedding - spatial addition or adaptive group norm / a seq of vector embeddings - cross-attention.

Classifier guidance

Using the gradient of a trained classifier as guidance

Applying Bayes rule to obtain conditional score function $\nabla_{x_t} log\ q_t(x_t/y)$

$$p(x \mid y) = \frac{p(y \mid x) \cdot p(x)}{p(y)}$$

$$\implies \log p(x \mid y) = \log p(y \mid x) + \log p(x) - \log p(y)$$

$$\implies \nabla_x \log p(x \mid y) = \nabla_x \log p(y \mid x) + \nabla_x \log p(x),$$

$$\nabla_x \log p_\gamma(x \mid y) = \nabla_x \log p(x) + \gamma \nabla_x \log p(y \mid x).$$ ⟵ Classifier

Guidance scale: value >1 amplifies the influence of classifier signal.

$$p_\gamma(x \mid y) \propto p(x) \cdot p(y \mid x)^\gamma.$$

Slide Credits of guidance: https://benanne.github.io/2022/05/26/guidance.html

Classifier guidance

Problems of classifier guidance

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

Classifier

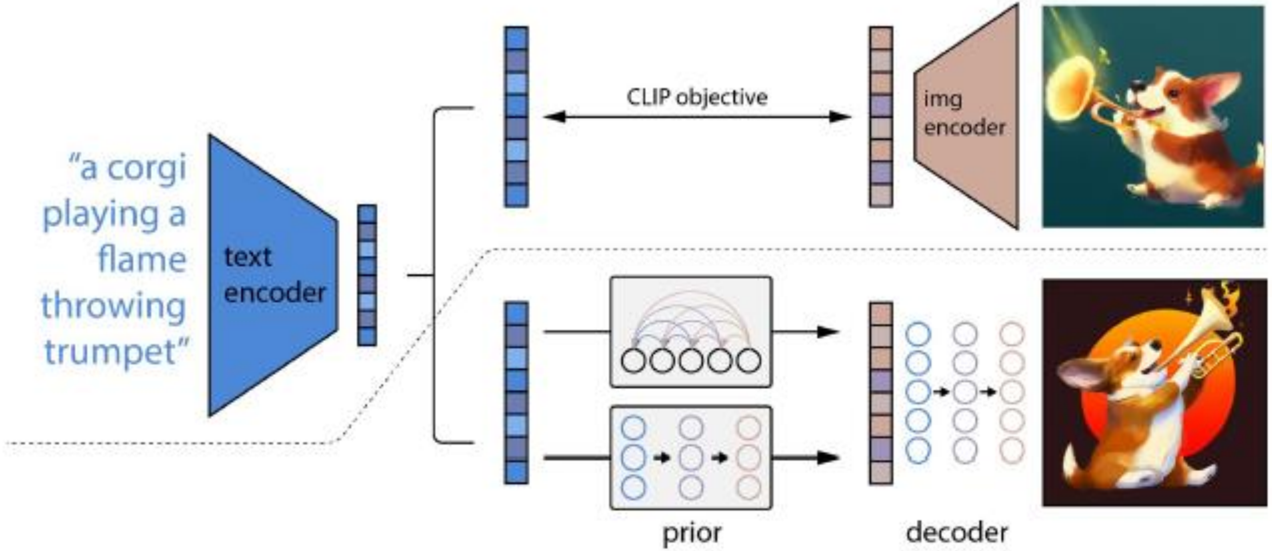
Guidance scale: value >1 amplifies the influence of classifier signal.

- At each step of denoising the input to the classifier is a noisy image x_t . Classifier is never trained on noisy image. So one needs to re-train classifier on noisy images! Can't use existing pre-trained classifiers.
- Most of the information in the input x is not relevant to predicting y, and as a result, taking the gradient of the classifier w.r.t. its input can yield arbitrary (and even adversarial) directions in input space.

Solution 1 (DALL-E 2): Use CLIP Model

DALL·E 2

Model components



Why conditional on CLIP image embeddings?

CLIP image embeddings capture high-level semantic meaning.

Slide by Soumyadip (Roni) Sengupta

Classifier-free guidance

Get guidance by Bayes' rule on conditional diffusion models

$$p(y \mid x) = \frac{p(x \mid y) \cdot p(y)}{p(x)}$$

$$\implies \log p(y \mid x) = \log p(x \mid y) + \log p(y) - \log p(x)$$

$$\implies \boxed{\nabla_x \log p(y \mid x) = \nabla_x \log p(x \mid y) - \nabla_x \log p(x).}$$

We proved this in classifier guidance.

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

$$\nabla_x \log p_\gamma(x \mid y) = \nabla_x \log p(x) + \gamma \left(\nabla_x \log p(x \mid y) - \nabla_x \log p(x)\right),$$

$$\nabla_x \log p_\gamma(x \mid y) = (1 - \gamma)\nabla_x \log p(x) + \gamma \nabla_x \log p(x \mid y).$$

Score function for unconditional diffusion model

Score function for conditional diffusion model

Slide by Soumyadip (Roni) Sengupta

Classifier-free guidance

Get guidance by Bayes' rule on conditional diffusion models

$$\hat{\epsilon} = (1+\omega)\epsilon_\theta(x_t, y) - \omega\epsilon_\theta(x_t)$$

$$\nabla_x \log p_\gamma(x \mid y) = (1-\gamma)\nabla_x \log p(x) + \gamma\nabla_x \log p(x \mid y).$$

Score function for unconditional diffusion model

Score function for conditional diffusio model

In practice:

- Train a conditional diffusion model p(x|y), with *conditioning dropout*: some percentage of the time, the conditioning information y is removed (10-20% tends to work well).
- The conditioning is often replaced with a special input value representing the absence of conditioning information.
- The resulting model is now able to function both as a conditional model p(x|y), and as an unconditional model p(x), depending on whether the conditioning signal is provided.
- During inference / sampling simply mix the score function of conditional and unconditional diffusion model based on guidance scale.