# Your Diffusion Model is Secretly a Zero-Shot Classifier

Alexander C. Li\* Mihir Prabhudesai Shivam Duggal Ellis Brown Deepak Pathak

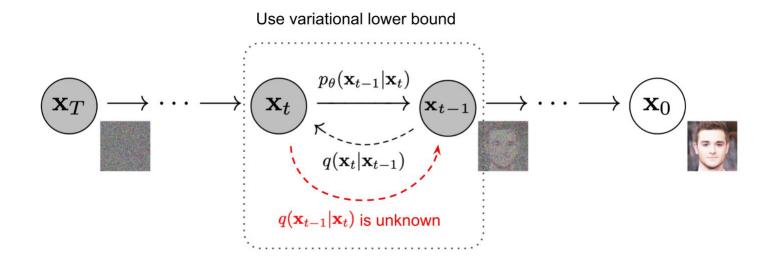
STRUCT Group Seminar Presenter: Zhengbo Xu 2023.04.02

# OUTLINE

- Authorship
- Background
- Method
- Experiments
- Conclusion

### BACKGROUND: Diffusion

#### Overview



$$q(\mathbf{x}_t|\mathbf{x}_{t-1}) = \mathcal{N}(\mathbf{x}_t; \sqrt{1-eta_t}\mathbf{x}_{t-1}, eta_t\mathbf{I}) \quad q(\mathbf{x}_{1:T}|\mathbf{x}_0) = \prod_{t=1}^T q(\mathbf{x}_t|\mathbf{x}_{t-1})$$



$$\mathbf{x}_t = \sqrt{ar{lpha}_t}\mathbf{x}_0 + \sqrt{1-ar{lpha}_t}oldsymbol{\epsilon}$$

Let  $\alpha_t = 1 - \beta_t$  and  $\bar{\alpha}_t = \prod_{i=1}^t \alpha_i$ 

$$q(\mathbf{x}_t|\mathbf{x}_{t-1}) = \mathcal{N}(\mathbf{x}_t; \sqrt{1-eta_t}\mathbf{x}_{t-1}, eta_t\mathbf{I}) \quad q(\mathbf{x}_{1:T}|\mathbf{x}_0) = \prod_{t=1}^T q(\mathbf{x}_t|\mathbf{x}_{t-1})$$

The equation can be written as:

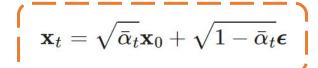
$$\mathbf{x}_{t} = \sqrt{\alpha_{t}} \mathbf{x}_{t-1} + \sqrt{1 - \alpha_{t}} \boldsymbol{\epsilon}_{t-1}$$

$$= \sqrt{\alpha_{t}} \alpha_{t-1} \mathbf{x}_{t-2} + \sqrt{1 - \alpha_{t}} \alpha_{t-1} \bar{\boldsymbol{\epsilon}}_{t-2}$$

$$= \dots$$

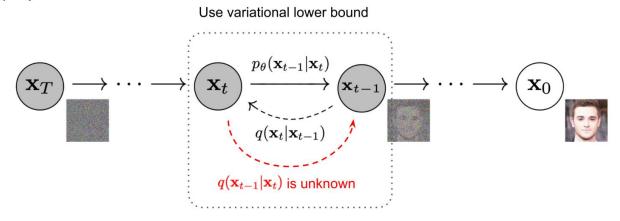
$$= \sqrt{\bar{\alpha}_{t}} \mathbf{x}_{0} + \sqrt{1 - \bar{\alpha}_{t}} \boldsymbol{\epsilon}$$



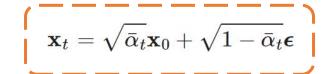


To maximize  $p_{\theta}(\mathbf{x}_0)$ ,

$$egin{aligned} -\log p_{ heta}(\mathbf{x}_0) &\leq -\log p_{ heta}(\mathbf{x}_0) + D_{\mathrm{KL}}(q(\mathbf{x}_{1:T}|\mathbf{x}_0) \| p_{ heta}(\mathbf{x}_{1:T}|\mathbf{x}_0)) \ &= -\log p_{ heta}(\mathbf{x}_0) + \mathbb{E}_{\mathbf{x}_{1:T} \sim q(\mathbf{x}_{1:T}|\mathbf{x}_0)} \Big[ \log rac{q(\mathbf{x}_{1:T}|\mathbf{x}_0)}{p_{ heta}(\mathbf{x}_{0:T})/p_{ heta}(\mathbf{x}_0)} \Big] \ &= -\log p_{ heta}(\mathbf{x}_0) + \mathbb{E}_q \Big[ \log rac{q(\mathbf{x}_{1:T}|\mathbf{x}_0)}{p_{ heta}(\mathbf{x}_{0:T})} + \log p_{ heta}(\mathbf{x}_0) \Big] \ &= \mathbb{E}_q \Big[ \log rac{q(\mathbf{x}_{1:T}|\mathbf{x}_0)}{p_{ heta}(\mathbf{x}_{0:T})} \Big] \end{aligned}$$



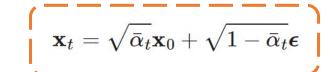




With a long series of derivation...

$$\mathbb{E}_q \Big[ \log \frac{q(\mathbf{x}_{1:T}|\mathbf{x}_0)}{p_{\theta}(\mathbf{x}_{0:T})} \Big] = \mathbb{E}_q [\underbrace{D_{\mathrm{KL}}(q(\mathbf{x}_T|\mathbf{x}_0) \parallel p_{\theta}(\mathbf{x}_T))}_{L_T} + \sum_{t=2}^T \underbrace{D_{\mathrm{KL}}(q(\mathbf{x}_{t-1}|\mathbf{x}_t,\mathbf{x}_0) \parallel p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_t))}_{L_{t-1}} - \log \underbrace{p_{\theta}(\mathbf{x}_0|\mathbf{x}_1)}_{L_0} \Big]$$





With a long series of derivation...

$$\mathbb{E}_q \Big[ \log \frac{q(\mathbf{x}_{1:T}|\mathbf{x}_0)}{p_{\theta}(\mathbf{x}_{0:T})} \Big] = \mathbb{E}_q [\underbrace{D_{\mathrm{KL}}(q(\mathbf{x}_T|\mathbf{x}_0) \parallel p_{\theta}(\mathbf{x}_T))}_{L_T} + \sum_{t=2}^T \underbrace{D_{\mathrm{KL}}(q(\mathbf{x}_{t-1}|\mathbf{x}_t,\mathbf{x}_0) \parallel p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_t))}_{L_{t-1}} - \log p_{\theta}(\mathbf{x}_0|\mathbf{x}_1) \Big]$$

With another long series of derivation...

$$\begin{split} L_t &= \mathbb{E}_{\mathbf{x}_0, \epsilon} \Big[ \frac{1}{2 \|\mathbf{\Sigma}_{\theta}(\mathbf{x}_t, t)\|_2^2} \|\tilde{\boldsymbol{\mu}}_t(\mathbf{x}_t, \mathbf{x}_0) - \boldsymbol{\mu}_{\theta}(\mathbf{x}_t, t)\|^2 \Big] \\ &= \mathbb{E}_{\mathbf{x}_0, \epsilon} \Big[ \frac{1}{2 \|\mathbf{\Sigma}_{\theta}\|_2^2} \|\frac{1}{\sqrt{\alpha_t}} \Big(\mathbf{x}_t - \frac{1 - \alpha_t}{\sqrt{1 - \bar{\alpha}_t}} \boldsymbol{\epsilon}_t \Big) - \frac{1}{\sqrt{\alpha_t}} \Big(\mathbf{x}_t - \frac{1 - \alpha_t}{\sqrt{1 - \bar{\alpha}_t}} \boldsymbol{\epsilon}_{\theta}(\mathbf{x}_t, t) \Big) \|^2 \Big] \\ &= \mathbb{E}_{\mathbf{x}_0, \epsilon} \Big[ \frac{(1 - \alpha_t)^2}{2\alpha_t (1 - \bar{\alpha}_t) \|\mathbf{\Sigma}_{\theta}\|_2^2} \|\boldsymbol{\epsilon}_t - \boldsymbol{\epsilon}_{\theta}(\mathbf{x}_t, t) \|^2 \Big] \\ &= \mathbb{E}_{\mathbf{x}_0, \epsilon} \Big[ \frac{(1 - \alpha_t)^2}{2\alpha_t (1 - \bar{\alpha}_t) \|\mathbf{\Sigma}_{\theta}\|_2^2} \|\boldsymbol{\epsilon}_t - \boldsymbol{\epsilon}_{\theta}(\sqrt{\bar{\alpha}_t} \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \boldsymbol{\epsilon}_t, t) \|^2 \Big] \end{split}$$

### BACKGROUND: Diffusion

#### Simply, we have

$$egin{aligned} L_t^{ ext{simple}} &= \mathbb{E}_{t \sim [1,T], \mathbf{x}_0, oldsymbol{\epsilon}_t} \Big[ \|oldsymbol{\epsilon}_t - oldsymbol{\epsilon}_{ heta}(\mathbf{x}_t,t)\|^2 \Big] \ &= \mathbb{E}_{t \sim [1,T], \mathbf{x}_0, oldsymbol{\epsilon}_t} \Big[ \|oldsymbol{\epsilon}_t - oldsymbol{\epsilon}_{ heta}(\sqrt{ar{lpha}_t}\mathbf{x}_0 + \sqrt{1-ar{lpha}_t}oldsymbol{\epsilon}_t,t)\|^2 \Big] \end{aligned}$$

#### Main steps of diffusion:

$$\mathbf{x}_t = \sqrt{\bar{lpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{lpha}_t}\boldsymbol{\epsilon}$$

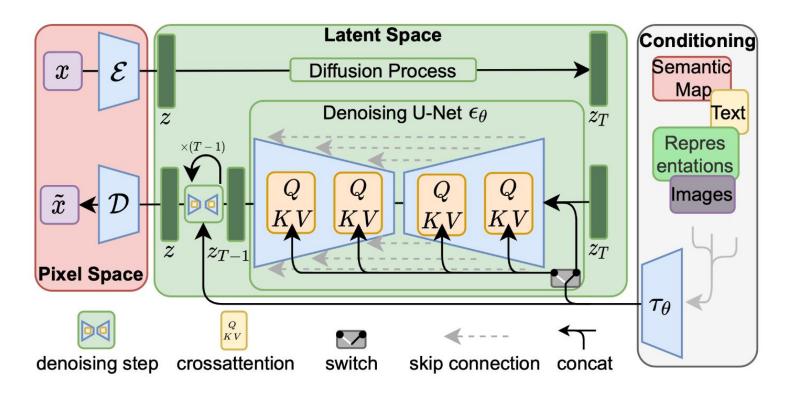
$$\mathbf{x}_t = \sqrt{ar{lpha}_t}\mathbf{x}_0 + \sqrt{1-ar{lpha}_t}oldsymbol{\epsilon} \ \left[ -\log p_{ heta}(\mathbf{x}_0) \leq \mathbb{E}_q \Big[\log rac{q(\mathbf{x}_{1:T}|\mathbf{x}_0)}{p_{ heta}(\mathbf{x}_{0:T})} \Big] 
ight]$$

$$\left\{\mathbb{E}_q\Big[\log\frac{q(\mathbf{x}_{1:T}|\mathbf{x}_0)}{p_{\theta}(\mathbf{x}_{0:T})}\Big]\right. = \mathbb{E}_q[\underbrace{D_{\mathrm{KL}}(q(\mathbf{x}_T|\mathbf{x}_0)\parallel p_{\theta}(\mathbf{x}_T))}_{L_T} + \sum_{t=2}^T\underbrace{D_{\mathrm{KL}}(q(\mathbf{x}_{t-1}|\mathbf{x}_t,\mathbf{x}_0)\parallel p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_t))}_{L_{t-1}} - \log p_{\theta}(\mathbf{x}_0|\mathbf{x}_1)]\right]$$

$$L_t^{ ext{simple}} = \mathbb{E}_{t \sim [1,T], \mathbf{x}_0, oldsymbol{\epsilon}_t} \Big[ \|oldsymbol{\epsilon}_t - oldsymbol{\epsilon}_{ heta}(\mathbf{x}_t,t)\|^2 \Big]$$

### BACKGROUND: Stable Diffusion

#### Latent diffusion model

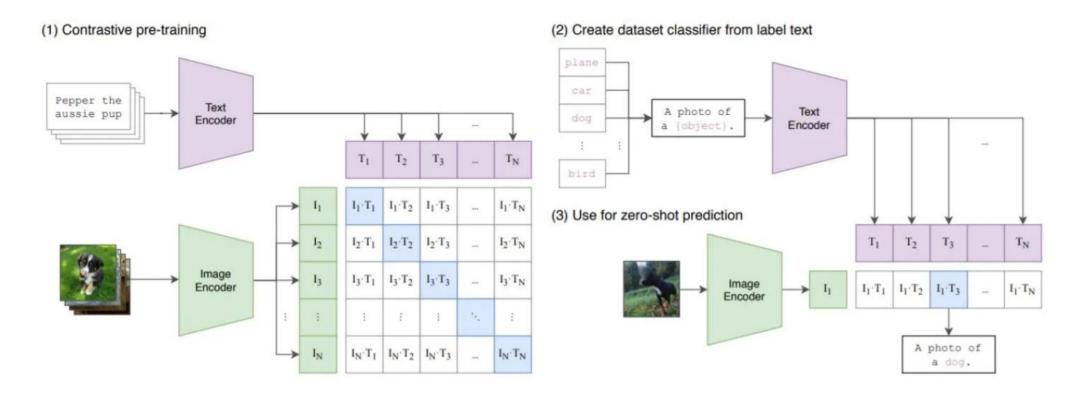


$$egin{aligned} \operatorname{Attention}(\mathbf{Q},\mathbf{K},\mathbf{V}) &= \operatorname{softmax}\Big(rac{\mathbf{Q}\mathbf{K}^{ op}}{\sqrt{d}}\Big) \cdot \mathbf{V} \ \end{aligned}$$
 where  $\mathbf{Q} &= \mathbf{W}_Q^{(i)} \cdot arphi_i(\mathbf{z}_i),$   $\mathbf{K} &= \mathbf{W}_K^{(i)} \cdot au_{ heta}(y),$   $\mathbf{V} &= \mathbf{W}_V^{(i)} \cdot au_{ heta}(y)$   $\end{aligned}$   $\mathbf{Attention}$ 

$$L_{LDM} := \mathbb{E}_{\mathcal{E}(x), \epsilon \sim \mathcal{N}(0,1), t} \left[ \left\lVert \epsilon - \epsilon_{ heta} \left( z_t, t 
ight) 
ight
Vert_2^2 
ight]$$

### BACKGROUND: CLIP

#### CLIP and OpenCLIP



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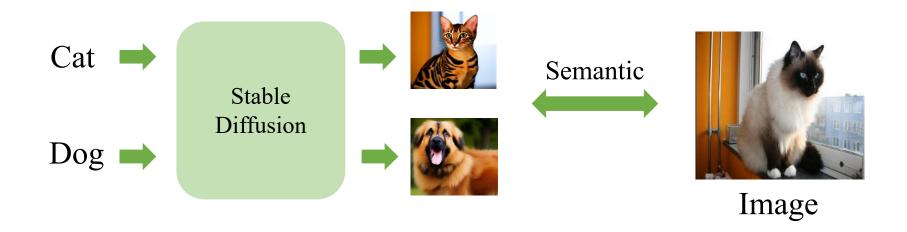
How to do classification task using diffusion model? Generally,

Stable Diffusion



Image

How to do classification task using diffusion model? Generally,



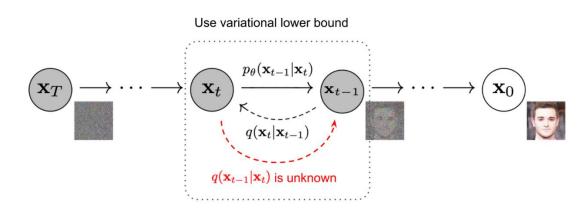
#### Quick Review: main steps of diffusion

$$\mathbf{x}_t = \sqrt{\bar{lpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{lpha}_t}\boldsymbol{\epsilon}$$

$$\mathbf{x}_t = \sqrt{ar{lpha}_t}\mathbf{x}_0 + \sqrt{1-ar{lpha}_t}oldsymbol{\epsilon} \quad egin{bmatrix} -\log p_{ heta}(\mathbf{x}_0) \leq \mathbb{E}_q igg[\log rac{q(\mathbf{x}_{1:T}|\mathbf{x}_0)}{p_{ heta}(\mathbf{x}_{0:T})}igg] \end{pmatrix}$$

$$\left[\mathbb{E}_q \left[\log \frac{q(\mathbf{x}_{1:T}|\mathbf{x}_0)}{p_{\theta}(\mathbf{x}_{0:T})}\right] \right. = \mathbb{E}_q \left[\underbrace{D_{\mathrm{KL}}(q(\mathbf{x}_T|\mathbf{x}_0) \parallel p_{\theta}(\mathbf{x}_T))}_{L_T} + \sum_{t=2}^T \underbrace{D_{\mathrm{KL}}(q(\mathbf{x}_{t-1}|\mathbf{x}_t,\mathbf{x}_0) \parallel p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_t))}_{L_{t-1}} - \log p_{\theta}(\mathbf{x}_0|\mathbf{x}_1)\right]$$

$$L_t^{ ext{simple}} = \mathbb{E}_{t \sim [1,T], \mathbf{x}_0, oldsymbol{\epsilon}_t} \Big[ \|oldsymbol{\epsilon}_t - oldsymbol{\epsilon}_{ heta}(\mathbf{x}_t,t)\|^2 \Big]$$



How to do classification task using diffusion model? Theoretically,

$$p_{\theta}(\mathbf{x}_0 \mid \mathbf{c}) = \int_{\mathbf{x}_{1:T}} p(\mathbf{x}_T) \prod_{t=1}^{T} p_{\theta}(\mathbf{x}_{t-1} \mid \mathbf{x}_t, \mathbf{c}) \, d\mathbf{x}_{1:T}$$

How to do classification task using diffusion model?

Theoretically,

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Bayes' rule:

$$p_{\theta}(\mathbf{c}_i \mid \mathbf{x}) = \frac{p(\mathbf{c}_i) \ p_{\theta}(\mathbf{x} \mid \mathbf{c}_i)}{\sum_j p(\mathbf{c}_j) \ p_{\theta}(\mathbf{x} \mid \mathbf{c}_j)}$$

How to do classification task using diffusion model?

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Suppose  $p(\mathbf{c}_i) = \frac{1}{N}$ ,

We can use  $p_{\theta}(\mathbf{x} \mid \mathbf{c}_i)$  to predict class.

How to predict  $p_{\theta}(\mathbf{x} \mid \mathbf{c}_i)$ ?

Using definition is too slow:

$$p_{\theta}(\mathbf{x}_0 \mid \mathbf{c}) = \int_{\mathbf{x}_{1:T}} p(\mathbf{x}_T) \prod_{t=1}^T p_{\theta}(\mathbf{x}_{t-1} \mid \mathbf{x}_t, \mathbf{c}) \, d\mathbf{x}_{1:T}$$

The variational lower bound:

$$\log p_{\theta}(\mathbf{x}_0 \mid \mathbf{c}) \ge \mathbb{E}_q \left[ \log \frac{p_{\theta}(\mathbf{x}_{0:T}, \mathbf{c})}{q(\mathbf{x}_{1:T} \mid \mathbf{x}_0)} \right]$$

$$-\log p_{ heta}(\mathbf{x}_0) \leq \ \mathbb{E}_q \Big[\log rac{q(\mathbf{x}_{1:T}|\mathbf{x}_0)}{p_{ heta}(\mathbf{x}_{0:T})} \Big]$$

#### Using

$$\left[\mathbb{E}_q \Big[\log \frac{q(\mathbf{x}_{1:T}|\mathbf{x}_0)}{p_{\theta}(\mathbf{x}_{0:T})}\Big] \right] = \mathbb{E}_q [\underbrace{D_{\mathrm{KL}}(q(\mathbf{x}_T|\mathbf{x}_0) \parallel p_{\theta}(\mathbf{x}_T))}_{L_T} + \sum_{t=2}^T \underbrace{D_{\mathrm{KL}}(q(\mathbf{x}_{t-1}|\mathbf{x}_t,\mathbf{x}_0) \parallel p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_t))}_{L_{t-1}} - \log p_{\theta}(\mathbf{x}_0|\mathbf{x}_1)]\right]$$

$$L_t^{ ext{simple}} = \mathbb{E}_{t \sim [1,T], \mathbf{x}_0, oldsymbol{\epsilon}_t} \Big[ \|oldsymbol{\epsilon}_t - oldsymbol{\epsilon}_ heta(\mathbf{x}_t,t)\|^2 \Big] \, \Big]$$

#### We have

$$\log p_{\theta}(\mathbf{x}_0 \mid \mathbf{c}) \ge \mathbb{E}_q \left[ \log \frac{p_{\theta}(\mathbf{x}_{0:T}, \mathbf{c})}{q(\mathbf{x}_{1:T} \mid \mathbf{x}_0)} \right] = -\mathbb{E}_{t,\epsilon} \left[ \|\epsilon - \epsilon_{\theta}(\mathbf{x}_t, \mathbf{c})\|^2 \right] + C$$

Combine with Bayes' rule,

$$p_{\theta}(\mathbf{c}_{i} \mid \mathbf{x}) \approx \frac{\exp\{-\mathbb{E}_{t,\epsilon}[\|\epsilon - \epsilon_{\theta}(\mathbf{x}_{t}, \mathbf{c}_{i})\|^{2}] + C\}}{\sum_{j} \exp\{-\mathbb{E}_{t,\epsilon}[\|\epsilon - \epsilon_{\theta}(\mathbf{x}_{t}, \mathbf{c}_{j})\|^{2}] + C\}}$$
$$= \frac{\exp\{-\mathbb{E}_{t,\epsilon}[\|\epsilon - \epsilon_{\theta}(\mathbf{x}_{t}, \mathbf{c}_{i})\|^{2}]\}}{\sum_{j} \exp\{-\mathbb{E}_{t,\epsilon}[\|\epsilon - \epsilon_{\theta}(\mathbf{x}_{t}, \mathbf{c}_{j})\|^{2}]\}}$$

How to predict  $\exp\{-\mathbb{E}_{t,\epsilon}[\|\epsilon - \epsilon_{\theta}(\mathbf{x}_t, \mathbf{c}_j)\|^2]\}$ ?

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How to predict  $\exp\{-\mathbb{E}_{t,\epsilon}[\|\epsilon - \epsilon_{\theta}(\mathbf{x}_t, \mathbf{c}_j)\|^2]\}$ ?

Monte Carlo!

$$\frac{1}{N} \sum_{i=1}^{N} \left\| \epsilon_i - \epsilon_{\theta} (\sqrt{\bar{\alpha}_{t_i}} \mathbf{x} + \sqrt{1 - \bar{\alpha}_{t_i}} \epsilon_i, \mathbf{c}_j) \right\|^2$$

In short,

We just use Bayes' rule and Monte Carlo to classify.

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We just use Bayes' rule and Monte Carlo to classify.

#### Question:

- 1. Why Monte Carlo can predict  $\exp\{-\mathbb{E}_{t,\epsilon}[\|\epsilon \epsilon_{\theta}(\mathbf{x}_t, \mathbf{c}_j)\|^2]\}$ ?
- 2. Why we can use lower bound?

Why Monte Carlo can predict  $\exp\{-\mathbb{E}_{t,\epsilon}[\|\epsilon - \epsilon_{\theta}(\mathbf{x}_t, \mathbf{c}_j)\|^2]\}$ ?

Indeed, it's hard to predict real value.

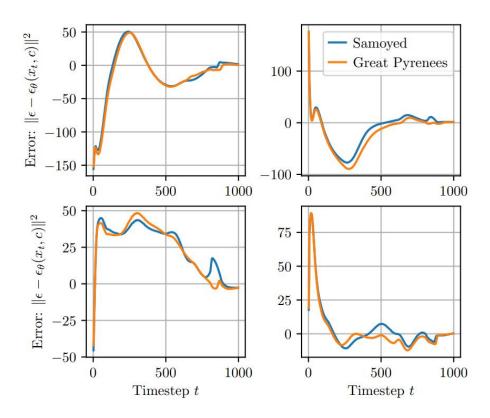
But we only need relative value.

$$p_{\theta}(\mathbf{c}_{i} \mid \mathbf{x}) \approx \frac{\exp\{-\mathbb{E}_{t,\epsilon}[\|\epsilon - \epsilon_{\theta}(\mathbf{x}_{t}, \mathbf{c}_{i})\|^{2}] + C\}}{\sum_{j} \exp\{-\mathbb{E}_{t,\epsilon}[\|\epsilon - \epsilon_{\theta}(\mathbf{x}_{t}, \mathbf{c}_{j})\|^{2}] + C\}}$$

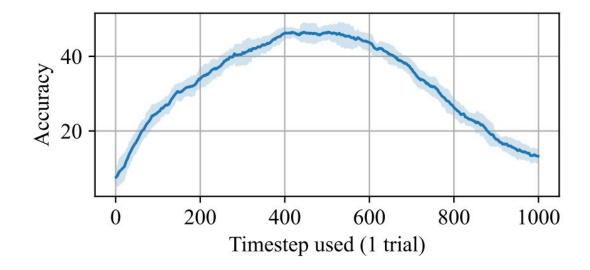
$$= \frac{\exp\{-\mathbb{E}_{t,\epsilon}[\|\epsilon - \epsilon_{\theta}(\mathbf{x}_{t}, \mathbf{c}_{i})\|^{2}]\}}{\sum_{j} \exp\{-\mathbb{E}_{t,\epsilon}[\|\epsilon - \epsilon_{\theta}(\mathbf{x}_{t}, \mathbf{c}_{j})\|^{2}]\}}$$

$$= \frac{1}{\sum_{j} \exp\{\mathbb{E}_{t,\epsilon}[\|\epsilon - \epsilon_{\theta}(\mathbf{x}_{t}, \mathbf{c}_{i})\|^{2} - \|\epsilon - \epsilon_{\theta}(\mathbf{x}_{t}, \mathbf{c}_{j})\|^{2}]\}}$$

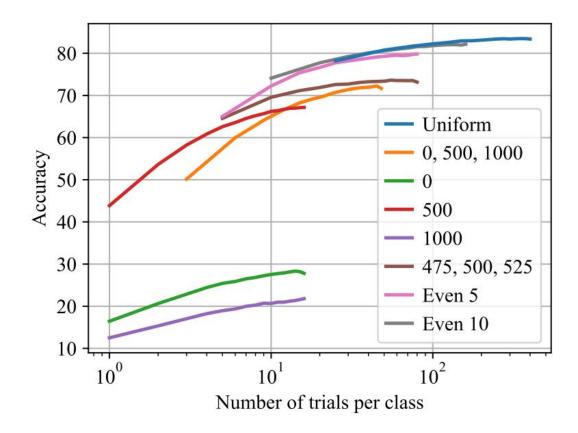
Why we can use lower bound?



How to choose *t* ?



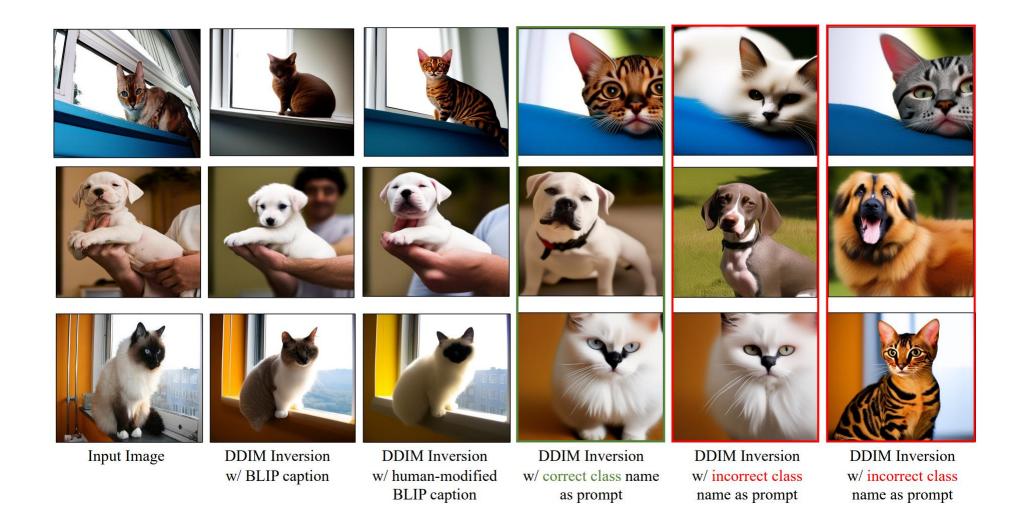
#### How to choose *t* ?



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# EXPERIMENTS: Why does it work?



### **EXPERIMENTS: Zero-Shot Classification**

8	Zero-shot?	Food101	CIFAR10	<b>FGVC</b>	Oxford Pets	Flowers102	MNIST	STL10	ImageNet	ObjectNet
Synthetic SD Data	<b>√</b>	12.6	35.3	9.4	31.3	22.1	27.9	38.0	18.9	5.2
SD Features	×	73.0	84.0	35.2	75.9	70.0	98.1	87.2	56.6	10.2
Diffusion Classifier (ours)	✓	77.9	76.3	24.3	85.7	56.8	17.4	94.2	58.4	38.56
CLIP ViT-L/14	✓	93.1	94.5	32.7	93.7	79.3	62.6	99.5	73.5	68.5
OpenCLIP ViT-H/14	✓	92.7	97.3	42.3	94.6	79.9	78.2	98.3	76.8	69.2

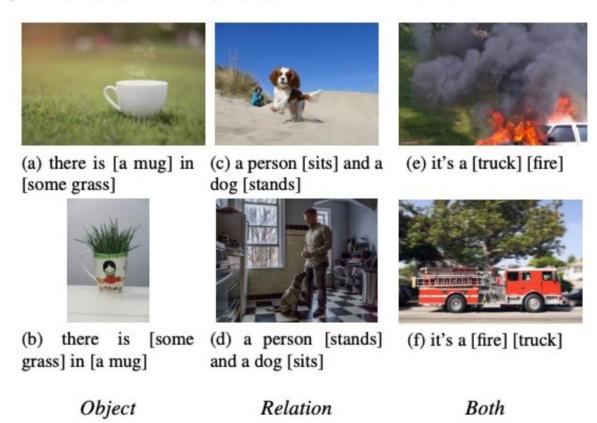
#### Why not as good as CLIP?

- 1. A prompt designed for CLIP
- 2. Training domain without LR, unaesthetic images
- 3. Choice between log-likelihood and high scores

# **EXPERIMENTS:** Relational Reasoning

#### Winoground Benchmark

 $\mathbb{I}[score(C_0, I_0) > score(C_1, I_0) \text{ AND } score(C_1, I_1) > score(C_0, I_1)]$ 



# **EXPERIMENTS:** Relational Reasoning

#### Winoground Benchmark

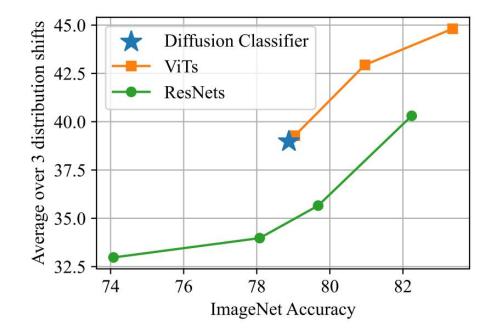
Model	Object	Relation	Both	Average
Random Chance	25.0	25.0	25.0	25.0
CLIP ViT-L/14	27.0	25.8	57.7	28.2
OpenCLIP ViT-H/14	39.0	26.6	57.7	33.0
Diffusion Classifier (ours)	41.8	25.3	69.2	34.0



# **EXPERIMENTS:** Supervised Classification

#### Results with fewer augmentation

Method	ID	OOD				
Without	IN	IN-v2	IN-A	ObjectNet		
ResNet-18	74.1	57.3	15.0	26.6		
ResNet-34	78.1	59.8	10.5	31.6		
ResNet-50	79.7	61.6	9.8	35.6		
ResNet-101	82.2	63.2	19.5	38.2		
ViT-L/32	79.0	61.6	26.3	29.9		
ViT-L/16	81.0	66.6	25.6	36.7		
ViT-B/16	83.4	66.6	30.1	37.8		
Diffusion Classifier	78.9	62.1	22.6	32.3		



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### CONCLUSION

- Diffusion model can be used to zero-shot classification task
- Diffusion model has competitive scores in classification
- Exact choices made during diffusion training affect the classifier

$$\log p_{\theta}(\mathbf{x}_{0} \mid \mathbf{c}) \geq \mathbb{E}_{q} \left[ \log \frac{p_{\theta}(\mathbf{x}_{0:T}, \mathbf{c})}{q(\mathbf{x}_{1:T} \mid \mathbf{x}_{0})} \right] = -\mathbb{E}_{t,\epsilon} \left[ \|\epsilon - \epsilon_{\theta}(\mathbf{x}_{t}, \mathbf{c})\|^{2} \right] + C$$

$$\frac{1}{N} \sum_{i=1}^{N} \left\| \epsilon_{i} - \epsilon_{\theta}(\sqrt{\bar{\alpha}_{t_{i}}} \mathbf{x} + \sqrt{1 - \bar{\alpha}_{t_{i}}} \epsilon_{i}, \mathbf{c}_{j}) \right\|^{2}$$

# Thanks for listening!