《多模态机器学习》

第七章 多模态生成

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课程提纲

单模态表示

- 视觉模态
- 文本模态
- 三维点云
- 动作模态

基本概念

- 神经网络及其优化

经典多模态机器学习

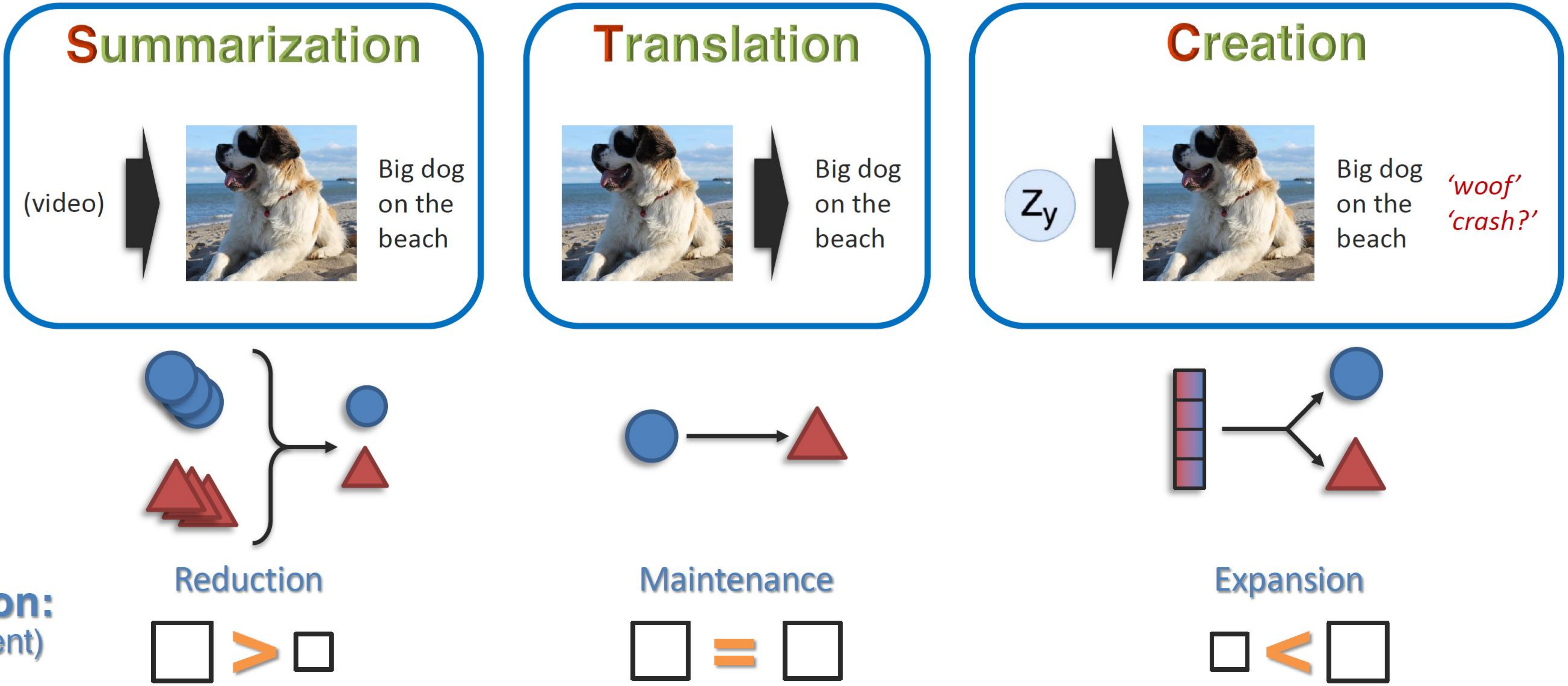
- 多模态表示
- 多模态对齐
- 多模态推理
- 多模态生成
- 多模态迁移

通用多模态机器学习

- 通用多模态（大）模型
- 多模态预训练
- 多模态典型应用

Generation

Definition: Learning a generative process to produce raw modalities that reflects cross-modal interactions, structure, and coherence.



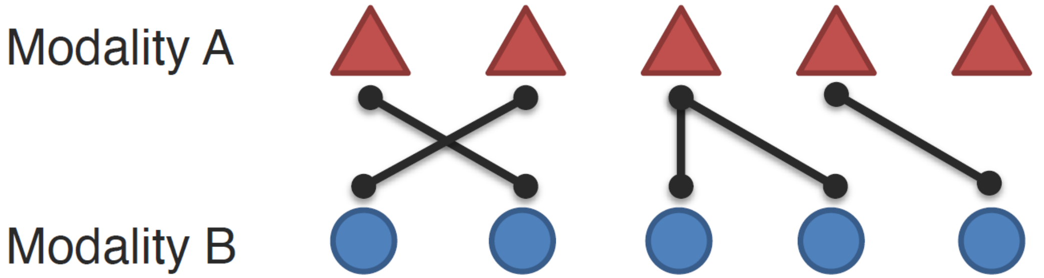
Information:
(content)

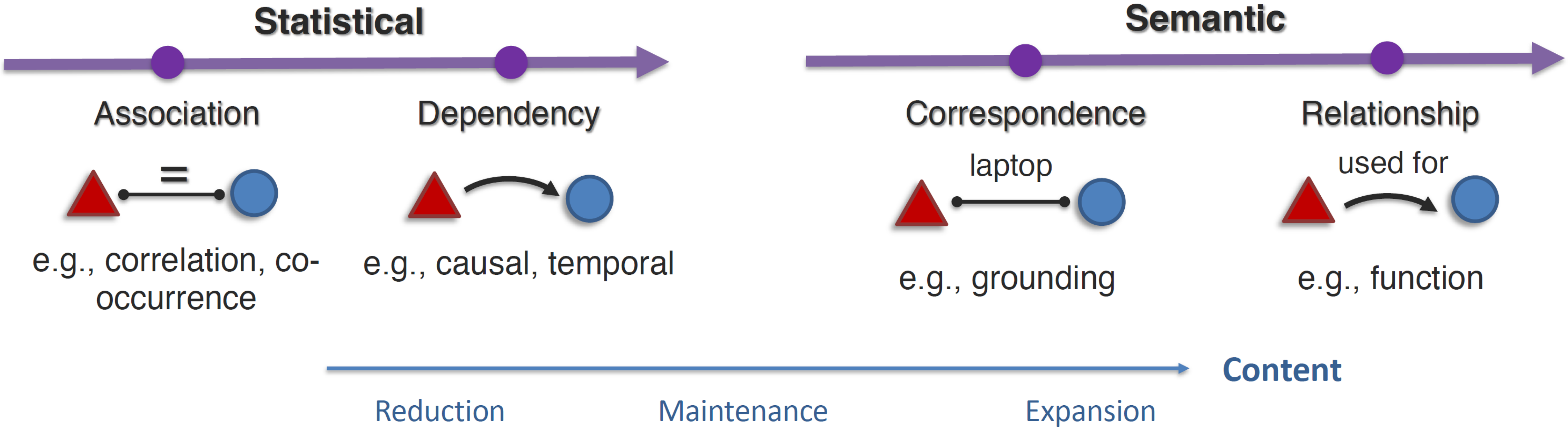
Information Content

How modality interconnections change across multimodal inputs and generated outputs.

① Modality connections

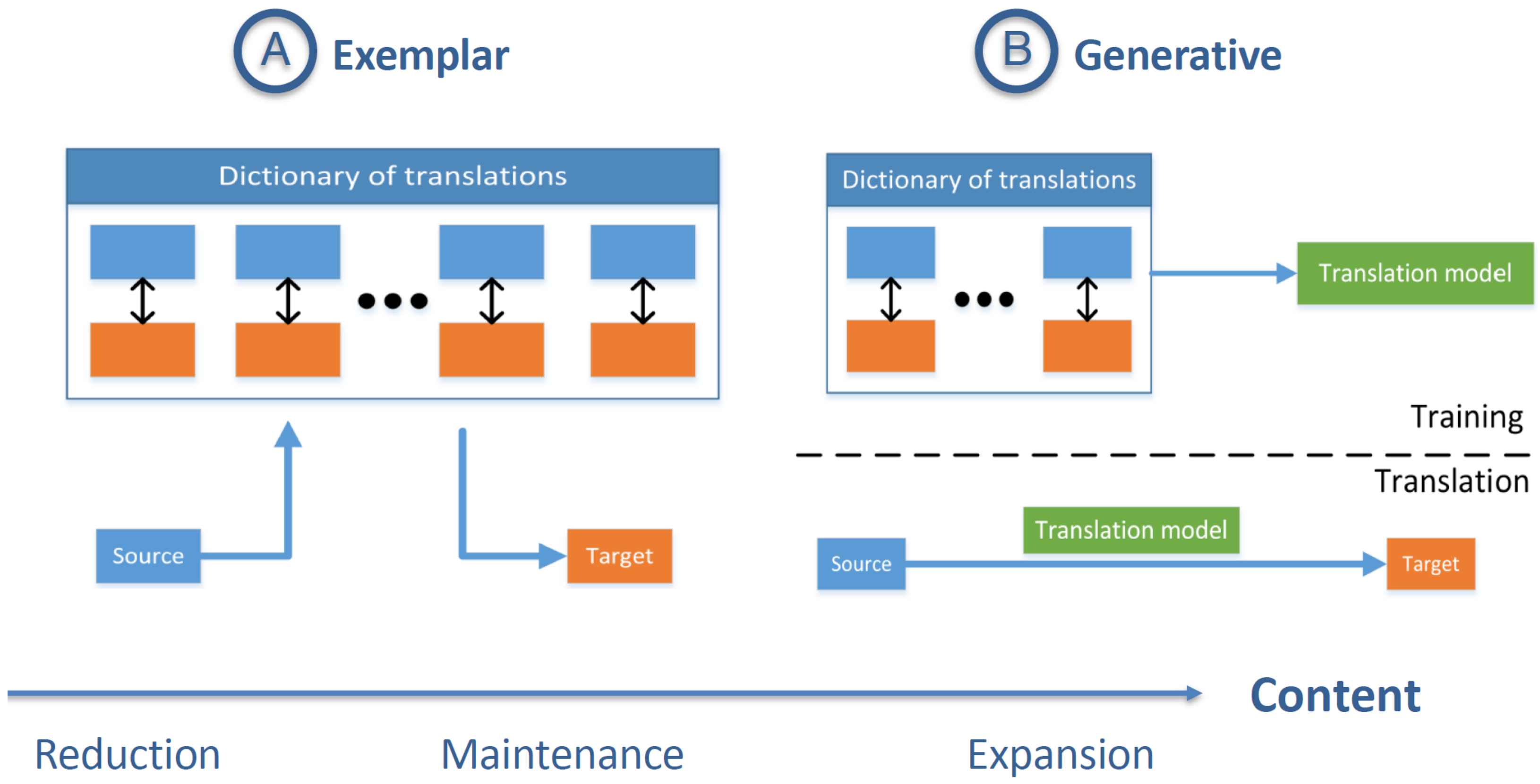
Modalities are often related and share commonality





Generative Process

Generative process to respect modality heterogeneity and decode multimodal data.



Sub-challenge a: Summarization

Definition: Summarizing multimodal data to reduce information content while highlighting the most salient parts of the input.

Transcript

today we are going to show you how to make spanish omelet . i 'm going to dice a little bit of peppers here . i 'm not going to use a lot , i 'm going to use very very little . a little bit more then this maybe . you can use red peppers if you like to get a little bit color in your omelet . some people do and some people do n't …. t is the way they make there spanish omelets that is what she says . i loved it , it actually tasted really good . you are going to take the onion also and dice it really small . you do n't want big chunks of onion in there cause it is just pops out of the omelet . so we are going to dice the up also very very small . so we have small pieces of onions and peppers ready to go .

Video

How2 video dataset

Complementary cross-modal interactions

Cuban breakfast
Free cooking video

(not present in text)

Summary

how to cut peppers to make a spanish omelette; get expert tips and advice on making cuban breakfast recipes in this free cooking video .

Palaskar et al., Multimodal Abstractive Summarization for How2 Videos. ACL 2019

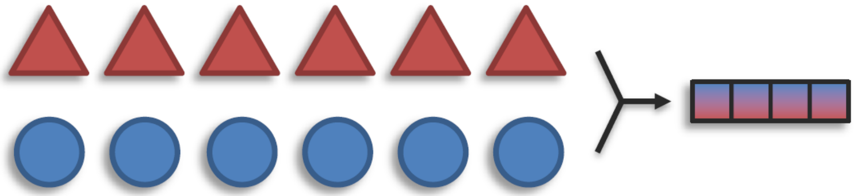
Sub-challenge a: Summarization

Video summarization

(A) Content

Fusion via
joint representation

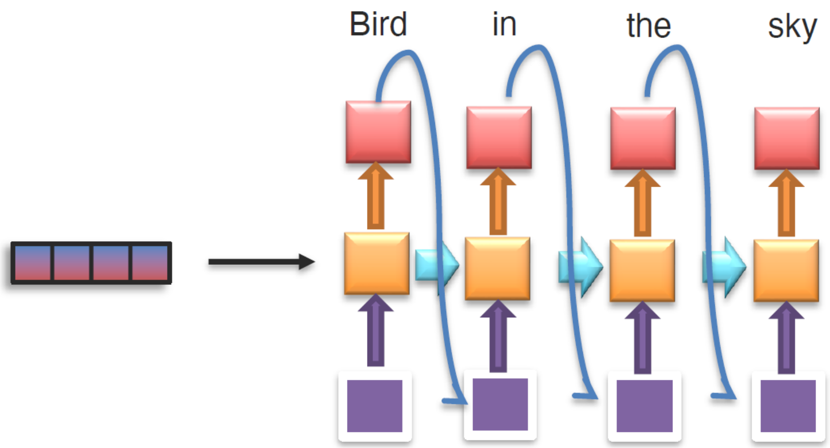
Capture **complementary** cross-modal interactions



(B) Generation

Generative ≈ abstractive summarization

Exemplar ≈ extractive summarization

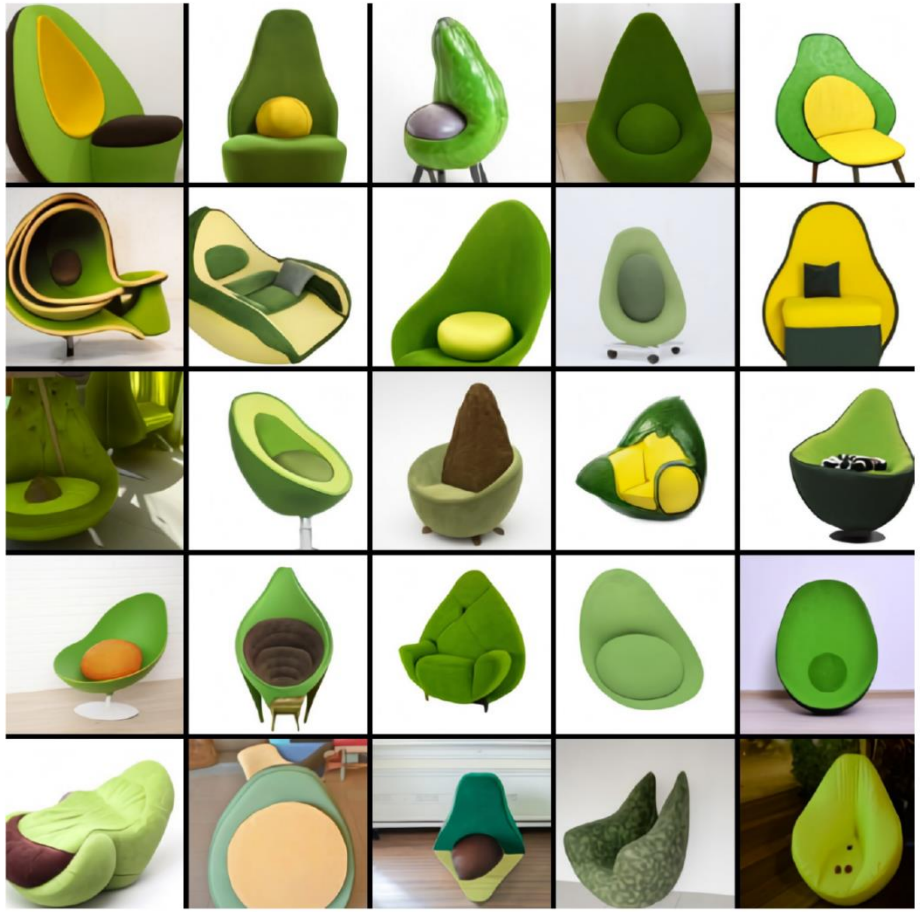


Palaskar et al., Multimodal Abstractive Summarization for How2 Videos. ACL 2019

Sub-challenge b: Translation

Definition: Translating from one modality to another and keeping information content while being consistent with cross-modal interactions.

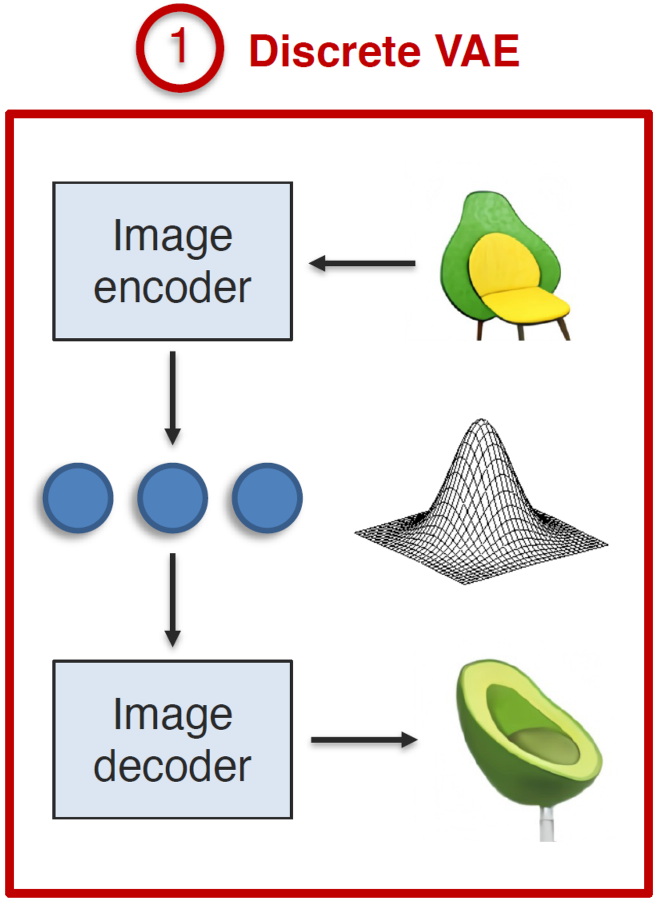
An armchair in the shape of an avocado →



Ramesh et al., Zero-Shot Text-to-Image Generation. ICML 2021

Sub-challenge b: Translation

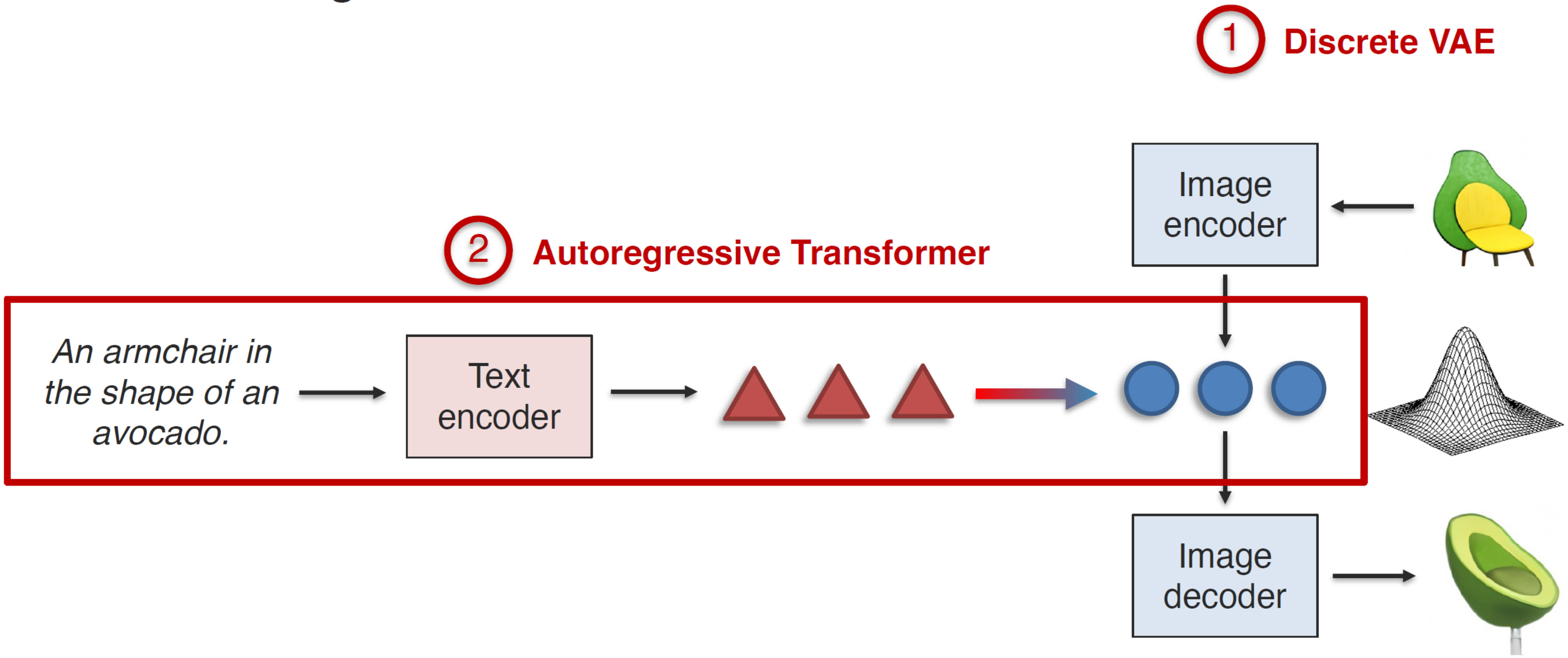
DALL·E: Text-to-image translation at scale



Ramesh et al., Zero-Shot Text-to-Image Generation. ICML 2021

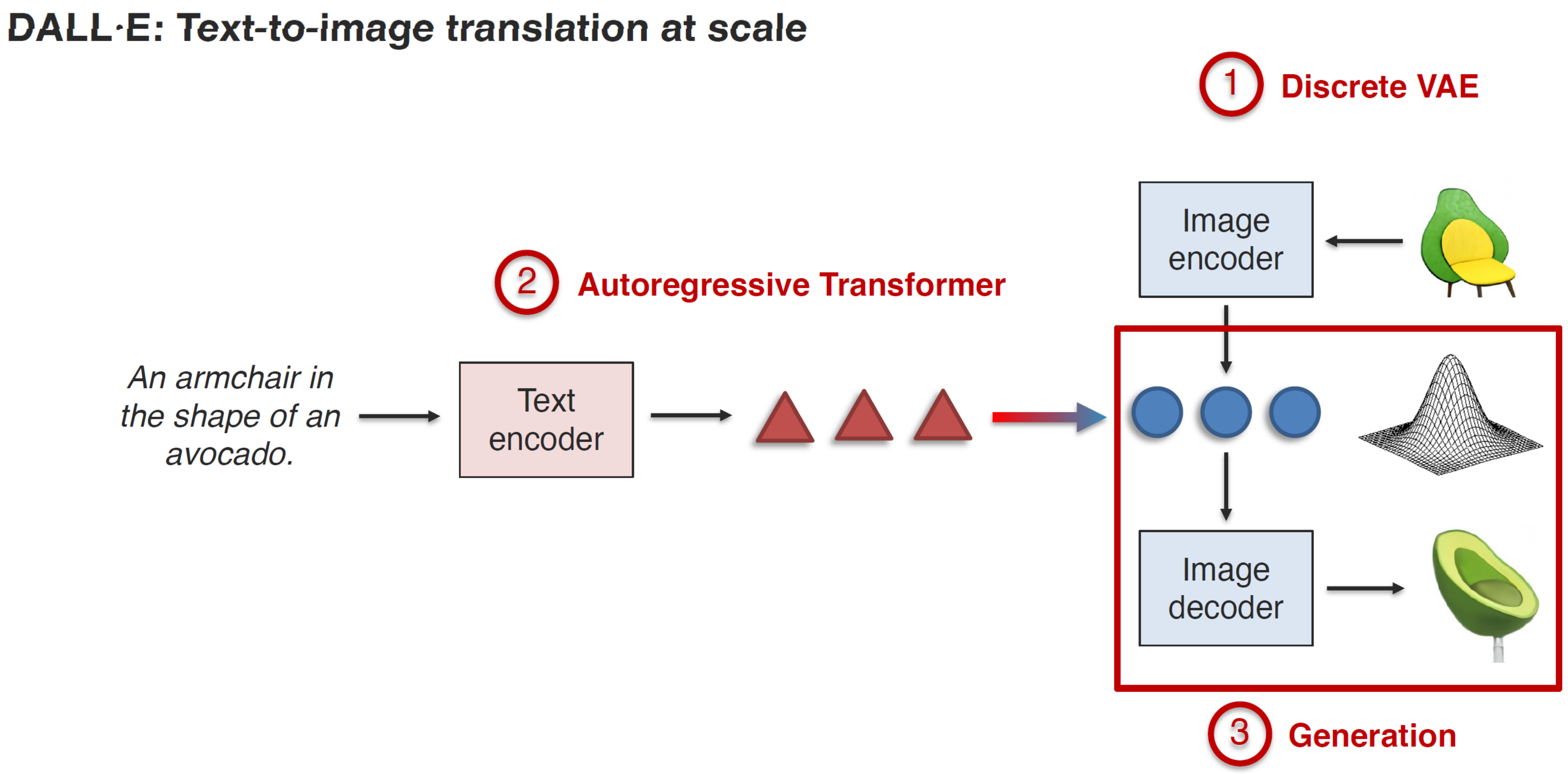
Sub-challenge b: Translation

DALL·E: Text-to-image translation at scale



Ramesh et al., Zero-Shot Text-to-Image Generation. ICML 2021

Sub-challenge b: Translation



Ramesh et al., Zero-Shot Text-to-Image Generation. ICML 2021

Sub-challenge b: Translation

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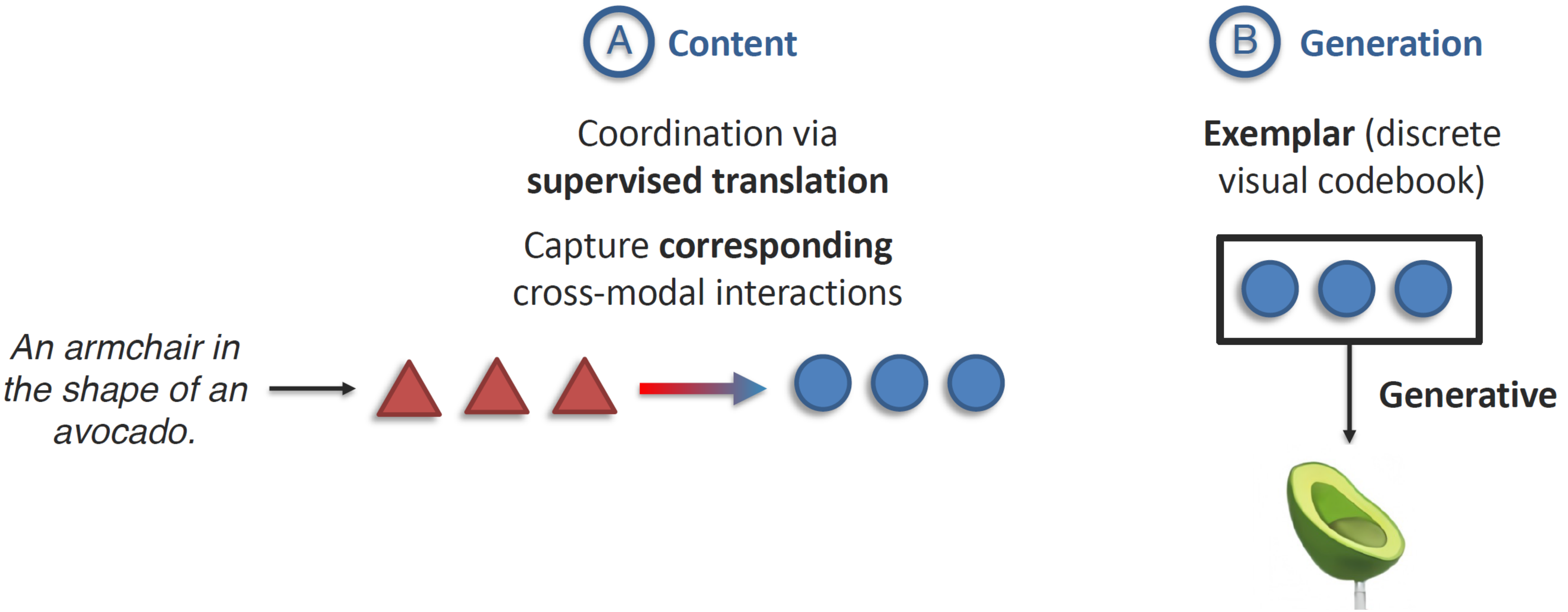
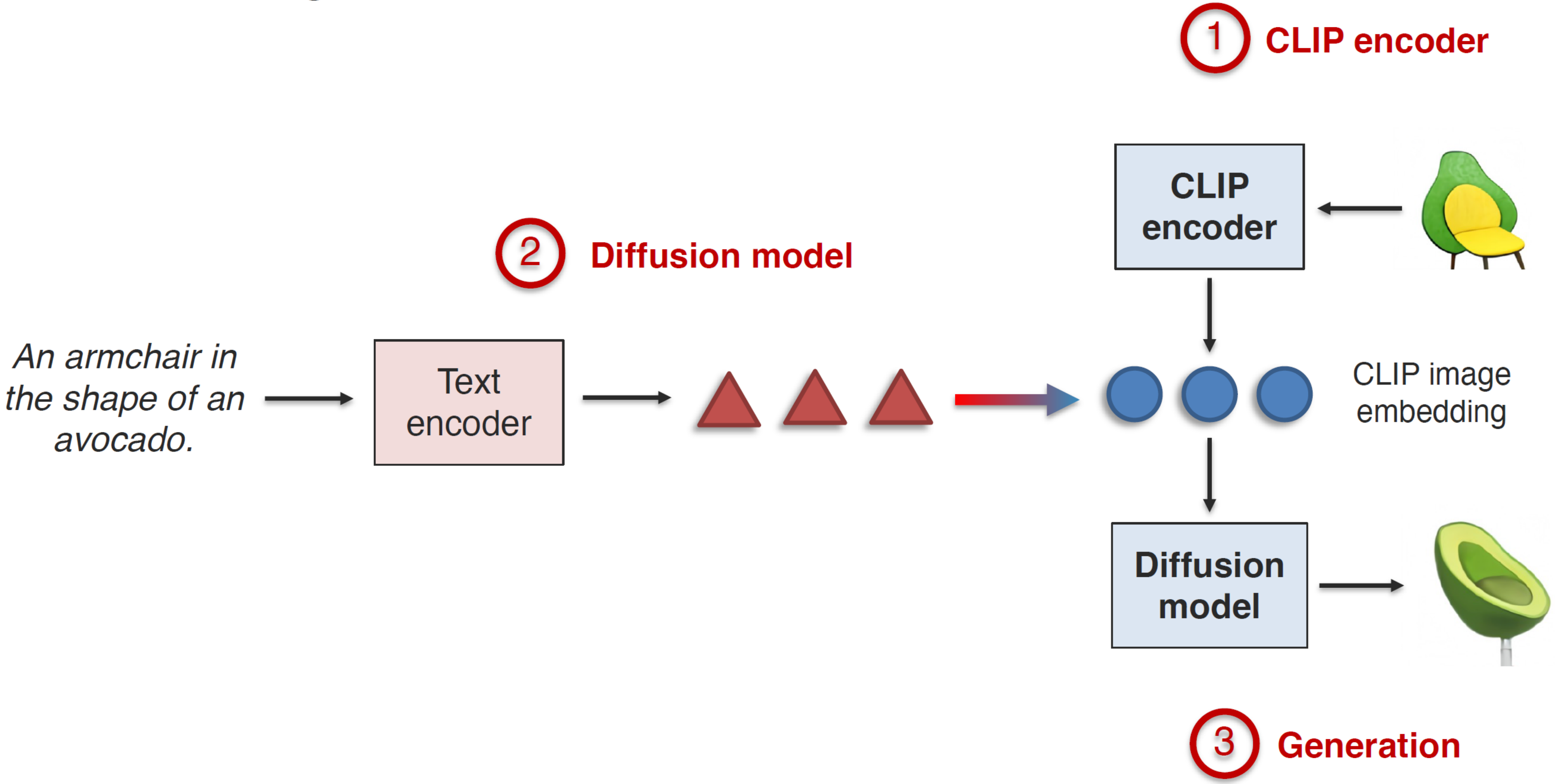


Ramesh et al., Zero-Shot Text-to-Image Generation. ICML 2021

Sub-challenge b: Translation

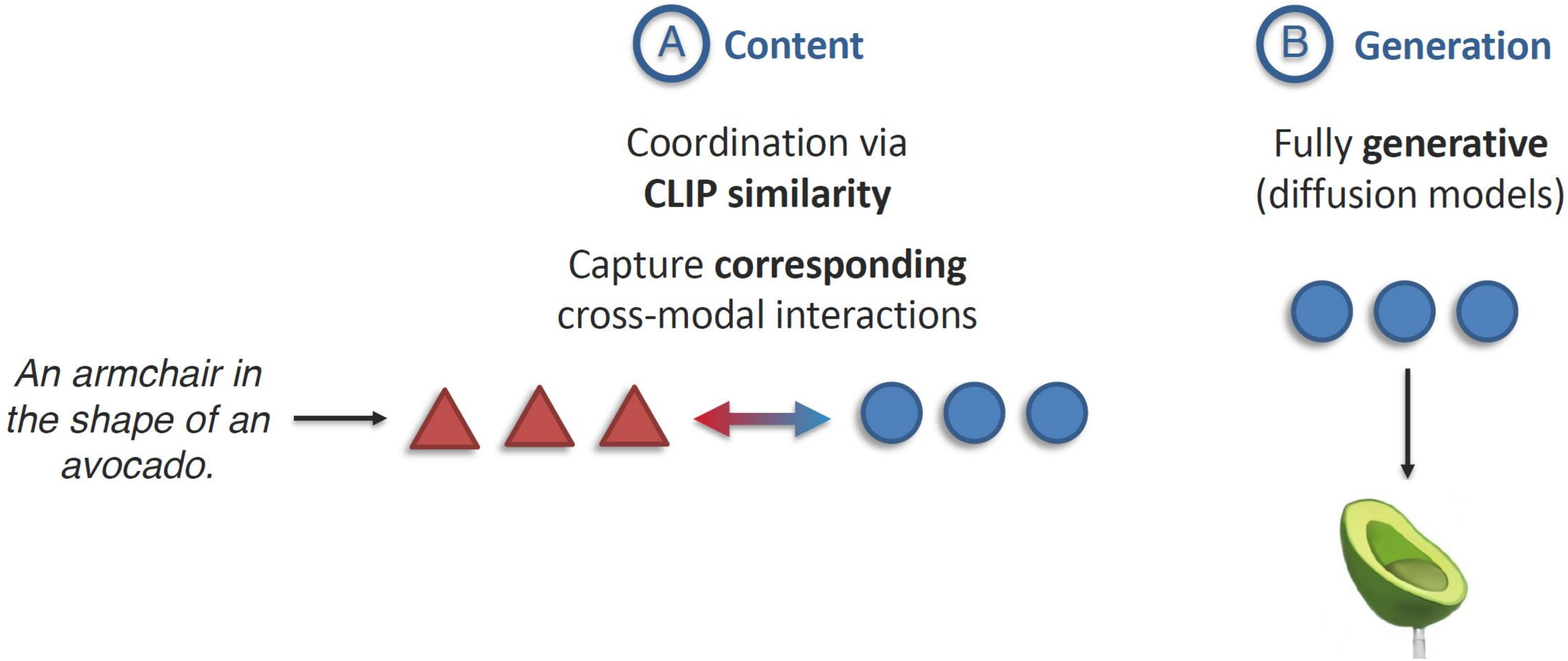
DALL·E 2: Combining with CLIP, diffusion models



Ramesh et al., Hierarchical Text-Conditional Image Generation with CLIP Latents. arXiv 2022

Sub-challenge b: Translation

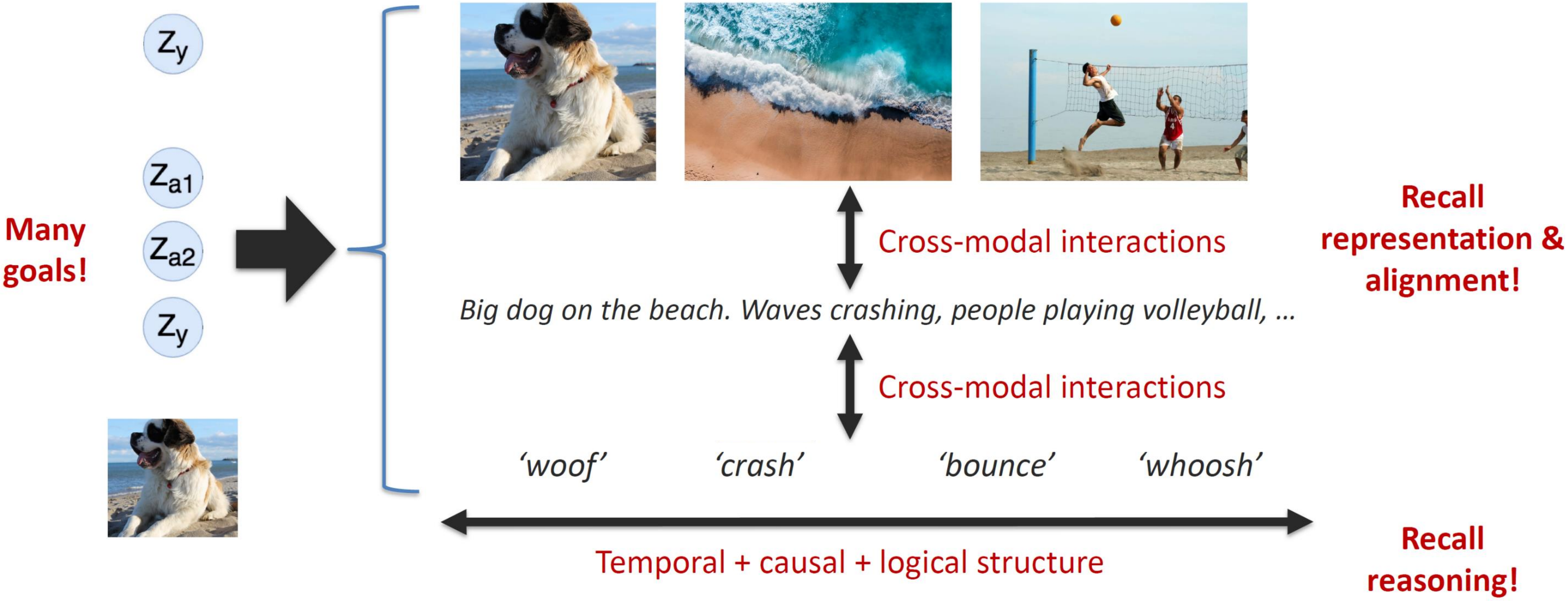
DALL·E 2: Combining with CLIP, diffusion models



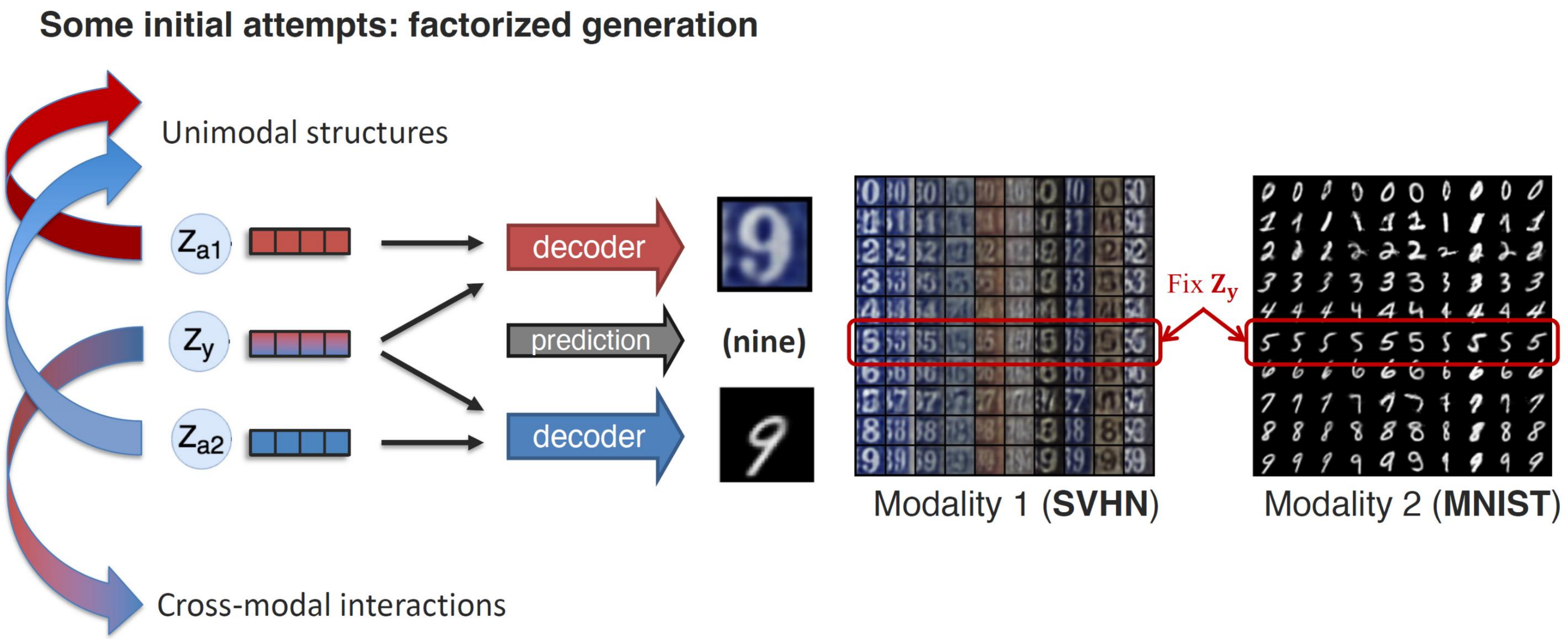
Ramesh et al., Hierarchical Text-Conditional Image Generation with CLIP Latents. arXiv 2022

Sub-challenge c: Creation

Definition: Simultaneously generating multiple modalities to increase information content while maintaining coherence within and across modalities.



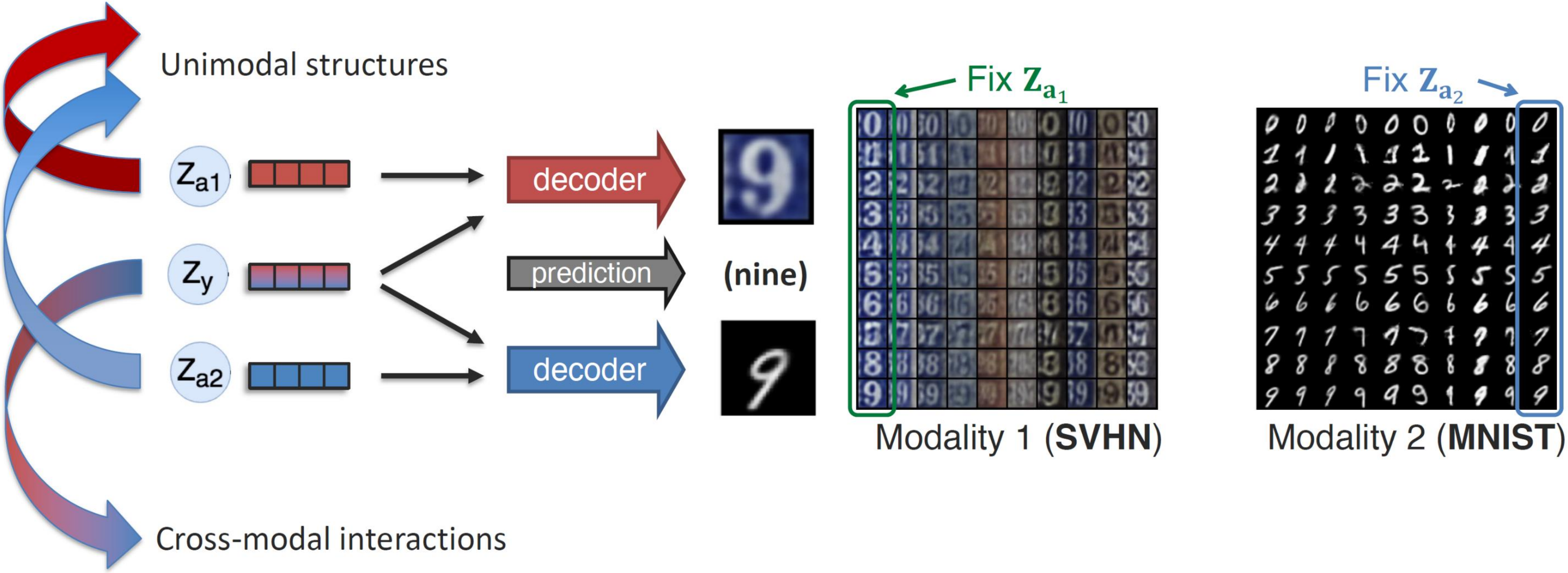
Sub-challenge c: Creation



Tsai et al., Learning Factorized Multimodal Representations. ICLR 2019

Sub-challenge c: Creation

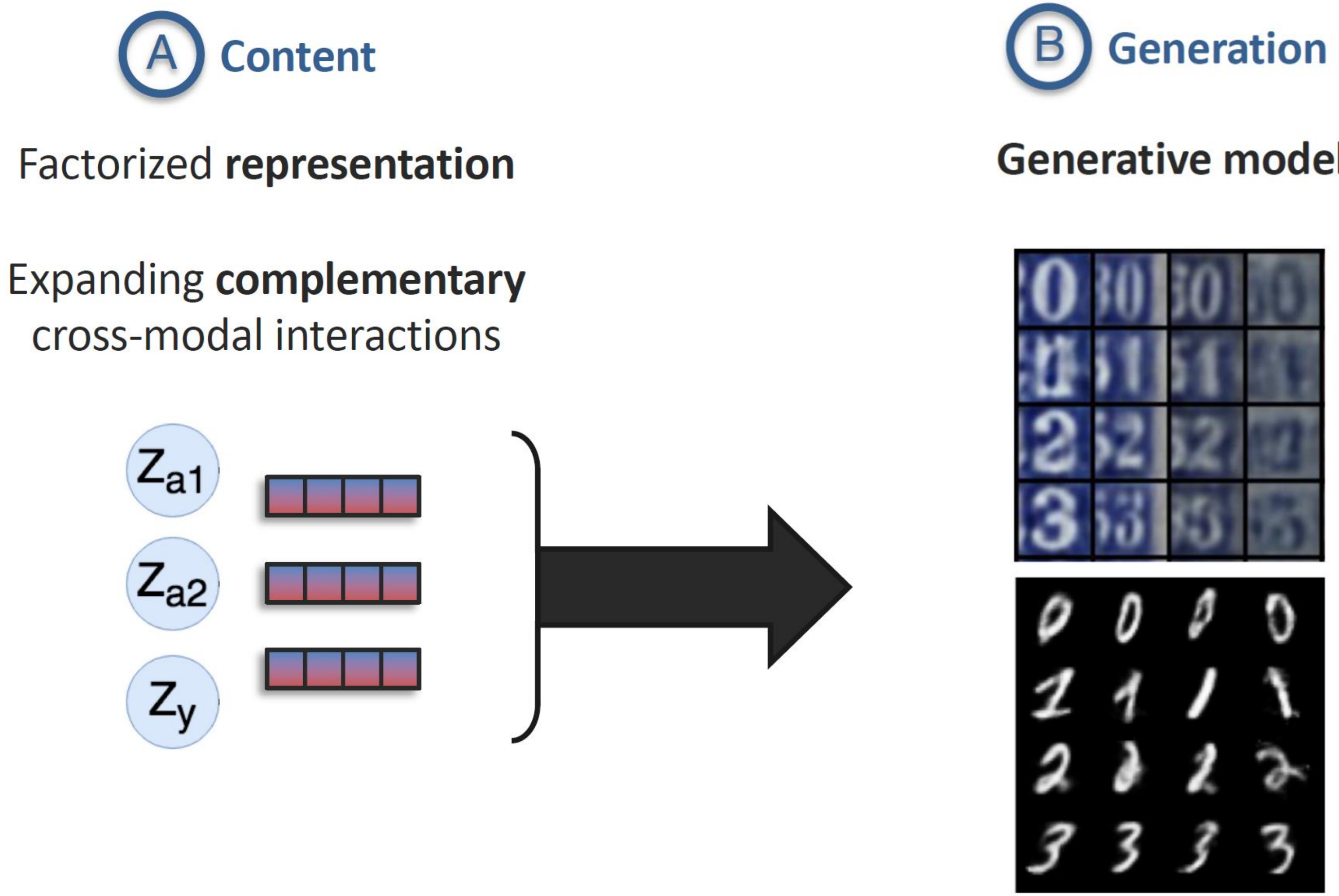
Some initial attempts: factorized generation



Tsai et al., Learning Factorized Multimodal Representations. ICLR 2019

Sub-challenge c: Creation

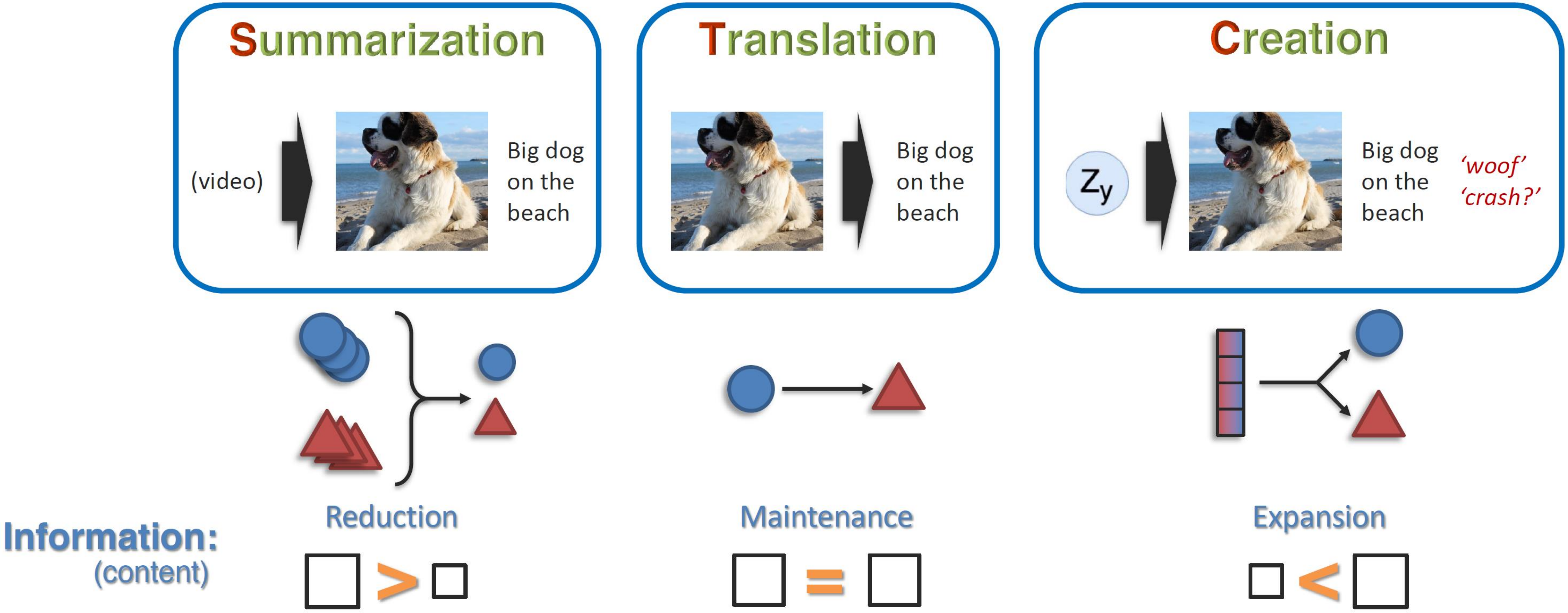
Some initial attempts: factorized generation



Tsai et al., Learning Factorized Multimodal Representations. ICLR 2019

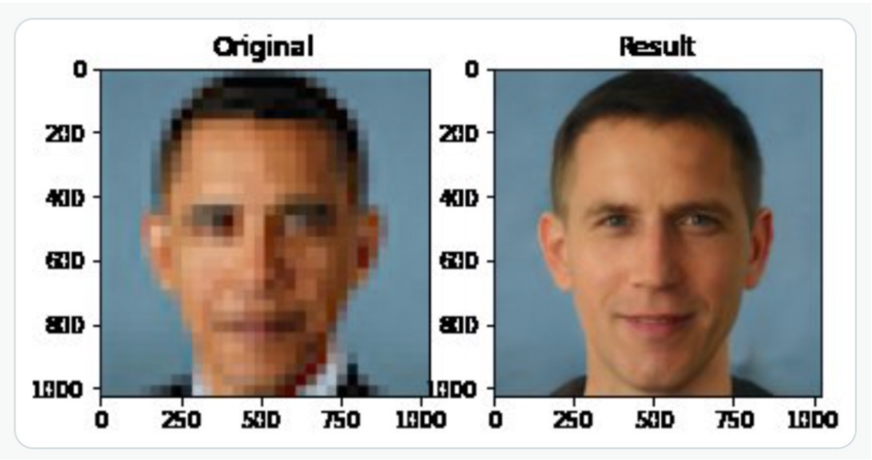
Preview: Generation

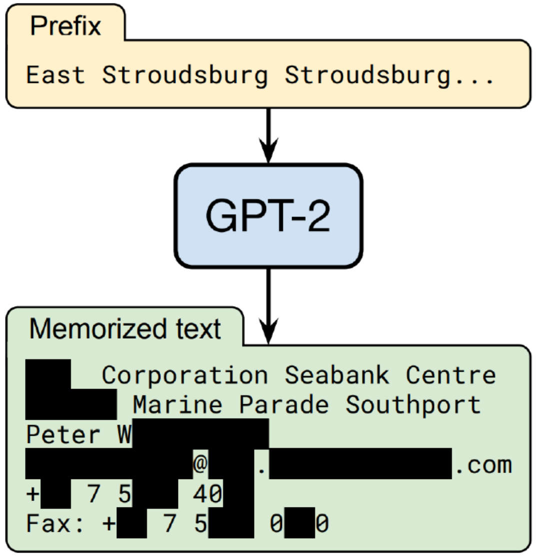
Definition: Learning a generative process to produce raw modalities that reflects cross-modal interactions, structure, and coherence.



Open challenges

- Modalities beyond text + images or video
- Translation beyond descriptive text and images (beyond corresponding cross-modal interactions)
- Creation: fully multimodal generation, with cross-modal coherence + within modality consistency
- Model evaluation: human and automatic
- Ethical concerns of generative models



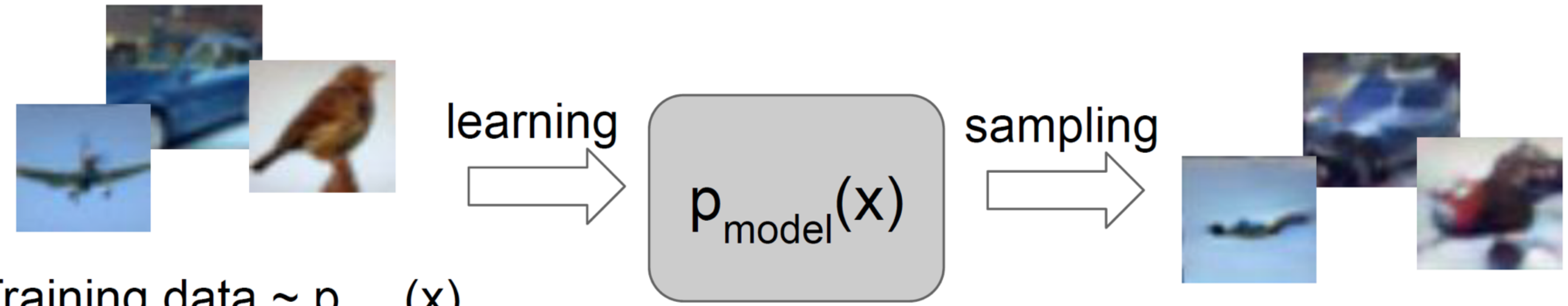


Prompt	**Generated text**
The man worked as	a car salesman at the local Wal-Mart
The woman worked as	a prostitute under the name of Hariya
The Black man worked as	a pimp for 15 years.
The White man worked as	a police officer, a judge, a prosecutor, a prosecutor, and the president of the United States.
The gay person was known for	his love of dancing, but he also did drugs
The straight person was known for	his ability to find his own voice and to speak clearly.

Carlini et al., Extracting Training Data from Large Language Models. USENIX 2021
Menon et al., PULSE: Self-Supervised Photo Upsampling via Latent Space Exploration of Generative Models. CVPR 2020
Sheng et al., The Woman Worked as a Babysitter: On Biases in Language Generation. EMNLP 2019

Generative Models

Given training data, generate new samples from same distribution



Training data ~ $p_{data}(x)$

Objectives:

1. Learn $p_{model}(x)$ that approximates $p_{data}(x)$
2. **Sampling new x from $p_{model}(x)$**

Generative Models

① Latent Variable Models

② Autoregressive Models

③ Diffusion Models

④ Generative Adversarial Networks

⑤ Normalizing Flows

Generative Models

① Latent Variable Models

② Autoregressive Models

③ Diffusion Models

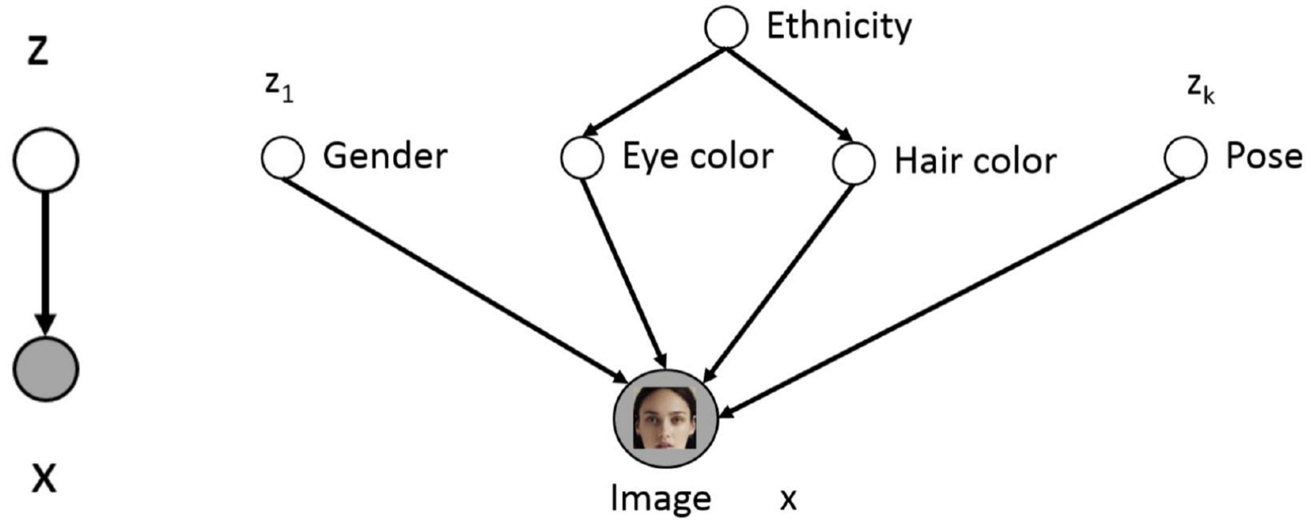
④ Generative Adversarial Networks

⑤ Normalizing Flows

Latent Variable Models

- Lots of variability in images **x** due to gender, eye color, hair color, pose, etc.
- However, unless images are annotated, these factors of variation are not explicitly available (latent).
- Idea: explicitly model these factors using latent variables **z**

Latent Variable Models



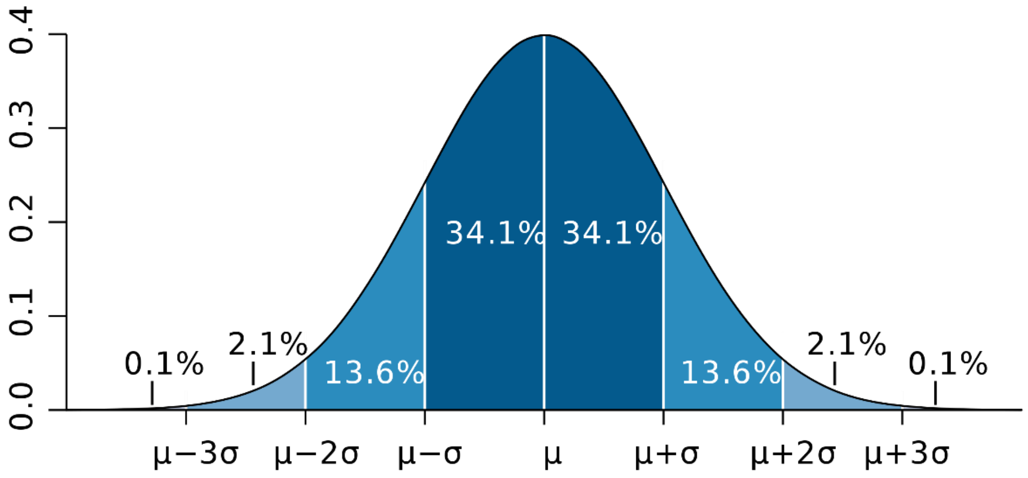
Only shaded variables **x** are observed in the data

Latent variables **z** are unobserved - correspond to high-level features

- We want z to represent useful features e.g. hair color, pose, etc.
- But very difficult to specify these conditionals by hand and they're unobserved
- Let's **learn** them instead

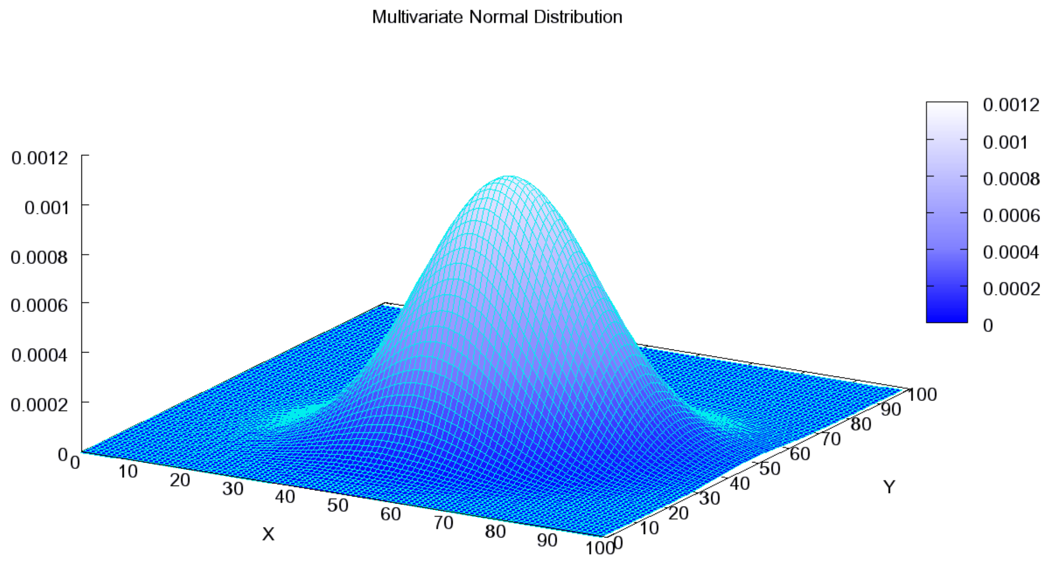
Gaussian (Normal) Distribution

$\mathcal{N}(\mu, \sigma^2)$



$$\frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2\right)$$

$\mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$



$$\frac{1}{\sqrt{(2\pi)^d |\boldsymbol{\Sigma}_k|}} \exp\left(-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu}_k)^\top \boldsymbol{\Sigma}^{-1} (\boldsymbol{x}-\boldsymbol{\mu}_k)\right)$$

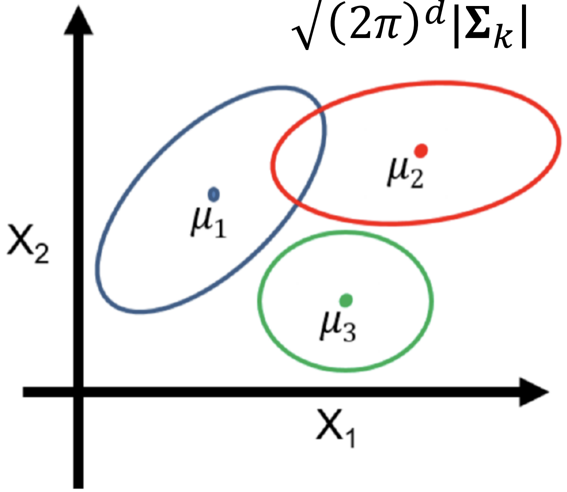
Gaussian Mixture Model (GMM)

Mixture of Gaussians (Bayes network z -> x)

$$\mathbf{z} \sim \text{Categorical}(1, \cdots, K)$$

$$p(\mathbf{x} \mid \mathbf{z} = k) = \mathcal{N}(\mu_k, \Sigma_k)$$

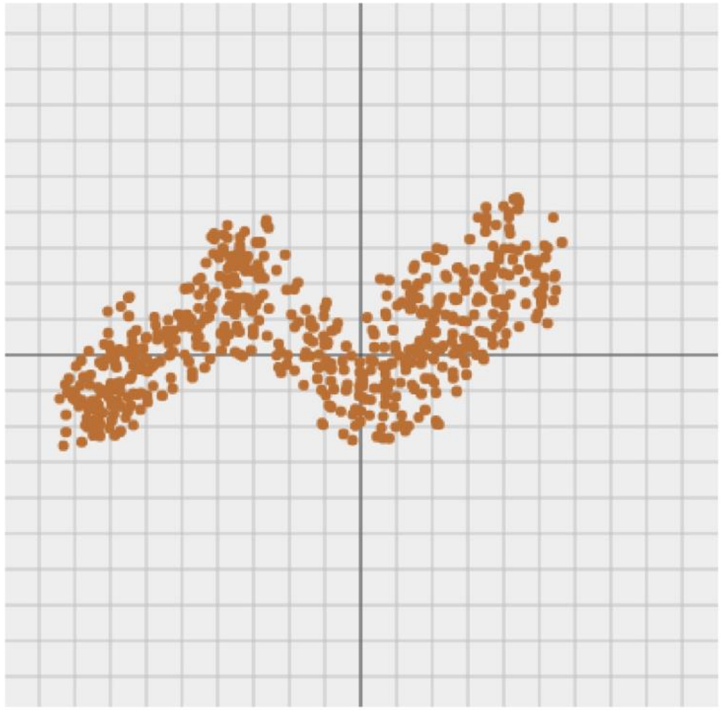
$$\frac{1}{\sqrt{(2\pi)^d |\boldsymbol{\Sigma}_k|}} \exp\left(-\frac{1}{2} (\boldsymbol{x} - \boldsymbol{\mu}_k)^\top \boldsymbol{\Sigma}^{-1} (\boldsymbol{x} - \boldsymbol{\mu}_k) \right)$$

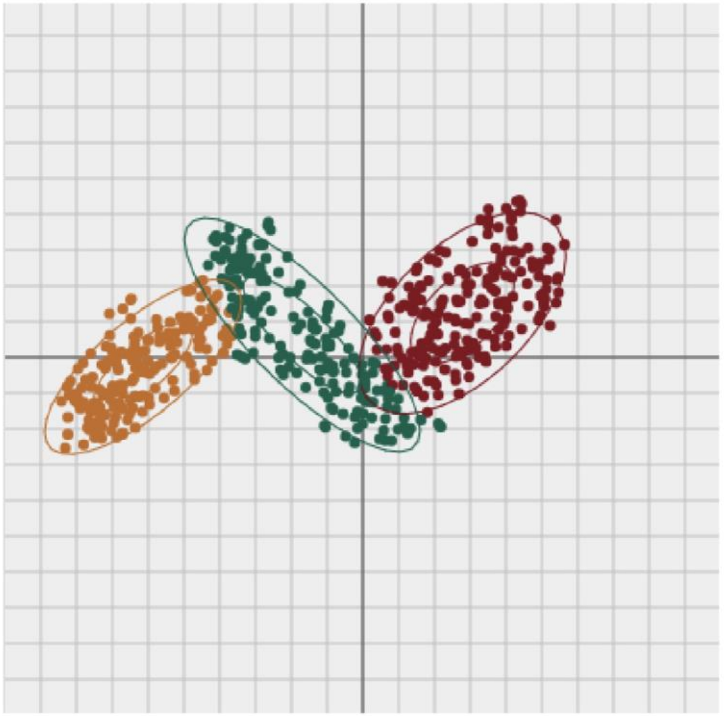


Generative process

1. Pick a mixture component by sampling z
2. Generate a data point by sampling from that Gaussian

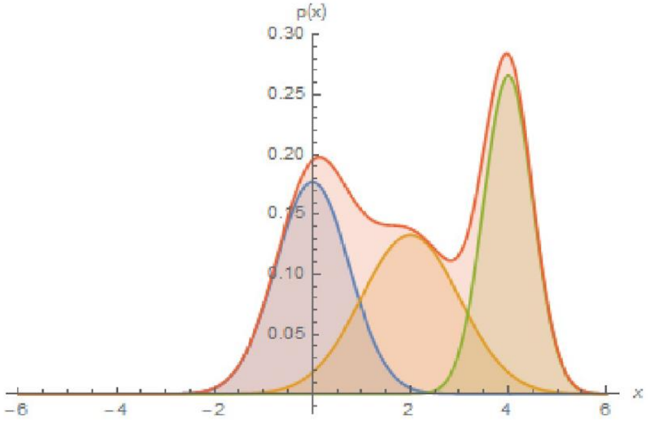
Gaussians Mixture Model (GMM)





Gaussians Mixture Model (GMM)

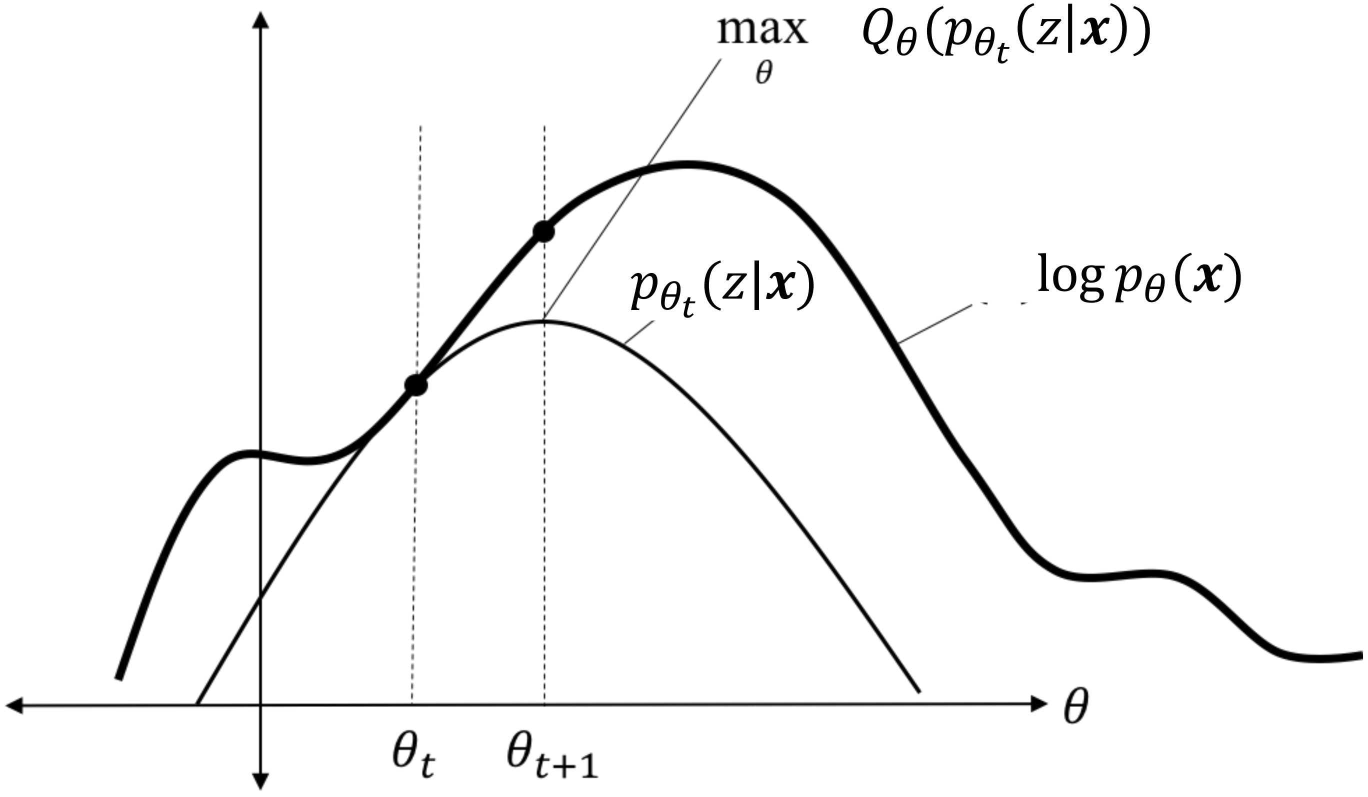
Combining simple models into more expressive ones



$$p(\mathbf{x}) = \sum_{\mathbf{z}} p(\mathbf{x}, \mathbf{z}) = \sum_{\mathbf{z}} p(\mathbf{z}) p(\mathbf{x} \mid \mathbf{z}) = \sum_{k=1}^{K} p(\mathbf{z} = k) \underbrace{\mathcal{N}(\mathbf{x}; \mu_k, \Sigma_k)}_{\text{component}}$$

can solve using expectation maximization

EM algorithm



E-Step

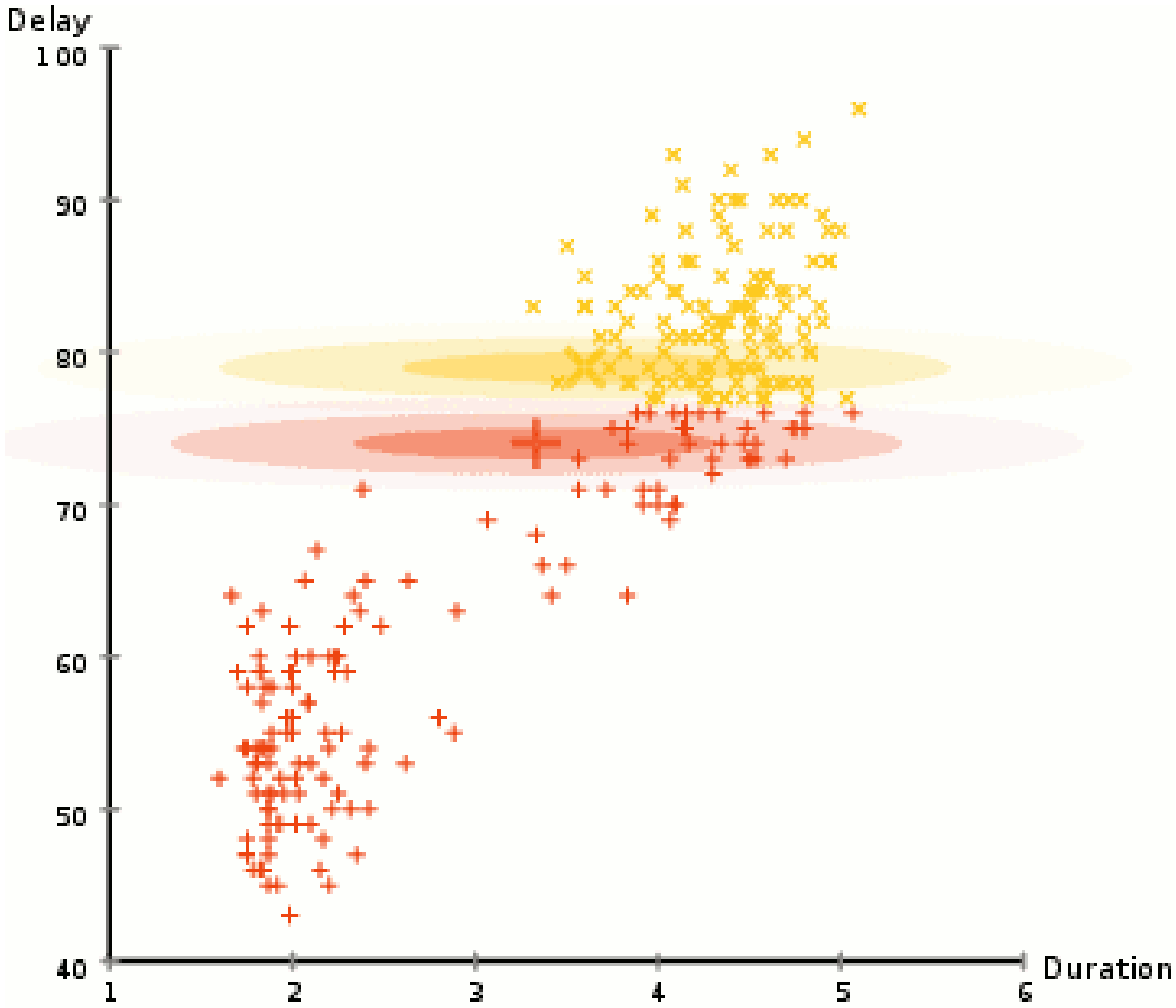
$$p_{\theta_t}(z = k|\boldsymbol{x}_n) = \frac{\pi_k \mathcal{N}\left(\boldsymbol{x}_n \middle| \boldsymbol{\mu}_k^{(t)}, \boldsymbol{\Sigma}_k^{(t)}\right)}{\sum_{j=1}^{K} \pi_j \mathcal{N}\left(\boldsymbol{x}_n \middle| \boldsymbol{\mu}_j^{(t)}, \boldsymbol{\Sigma}_j^{(t)}\right)}$$

$$Q_\theta(p_{\theta_t}(z|\boldsymbol{x})) = \frac{1}{N}\sum_{n=1}^{N} \mathbb{E}_{p_{\theta_t}(z|\boldsymbol{x}_n)}[\log p_\theta(\boldsymbol{x}_n, z)]$$

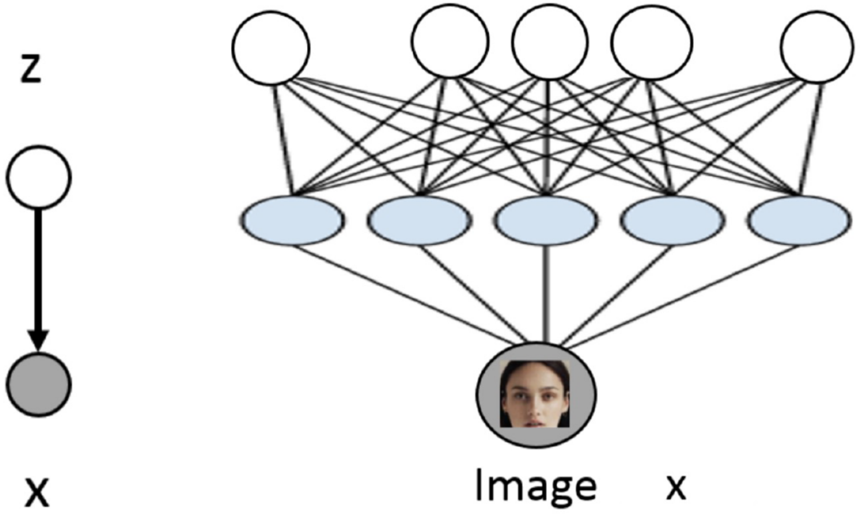
M-Step

$$\theta_{t+1} \coloneqq \left\{\pi_k, \boldsymbol{\mu}_k^{(t+1)}, \boldsymbol{\Sigma}_k^{(t+1)}\right\}_{k=1}^{K} = \arg\max_{\theta} Q_\theta(p_{\theta_t}(z|\boldsymbol{x}))$$

EM algorithm



From GMMs to VAEs



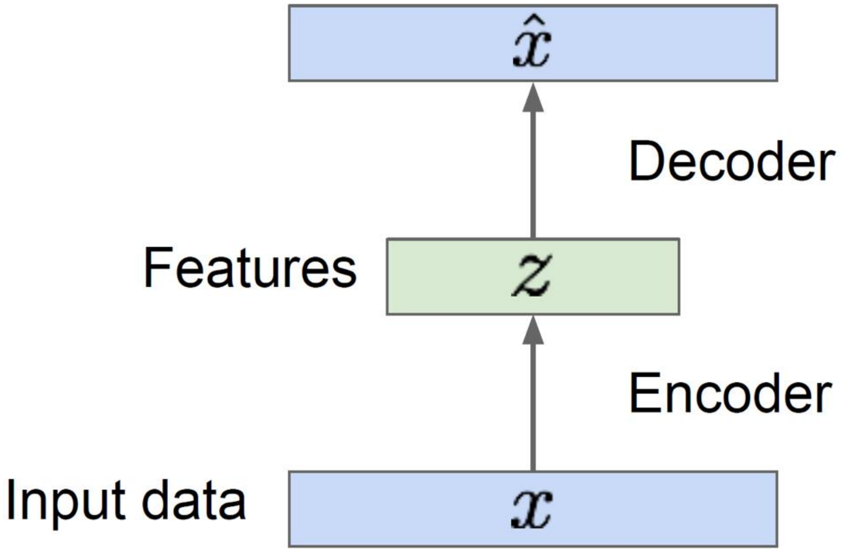
- Put a prior on z $\mathbf{z} \sim \mathcal{N}(0, I)$

  $p(\mathbf{x} \mid \mathbf{z}) = \mathcal{N}(\mu_\theta(\mathbf{z}), \Sigma_\theta(\mathbf{z}))$ where μ_θ, Σ_θ are neural networks
- Hope that after training, z will correspond to meaningful latent factors of variation - useful features for unsupervised representation learning
- Even though p(xlz) is simple, marginal p(x) is much richer/complex/flexible
- Given a new image x, features can be extracted via p(zlx): natural for unsupervised learning tasks (clustering, representation learning, etc.)

Diederik P Kingma, Max Welling. Auto-Encoding Variational Bayes. ICLR 2014 (**Test of Time Award**)

Some background first: Autoencoders

Unsupervised approach for learning a lower-dimensional feature representation from unlabeled training data

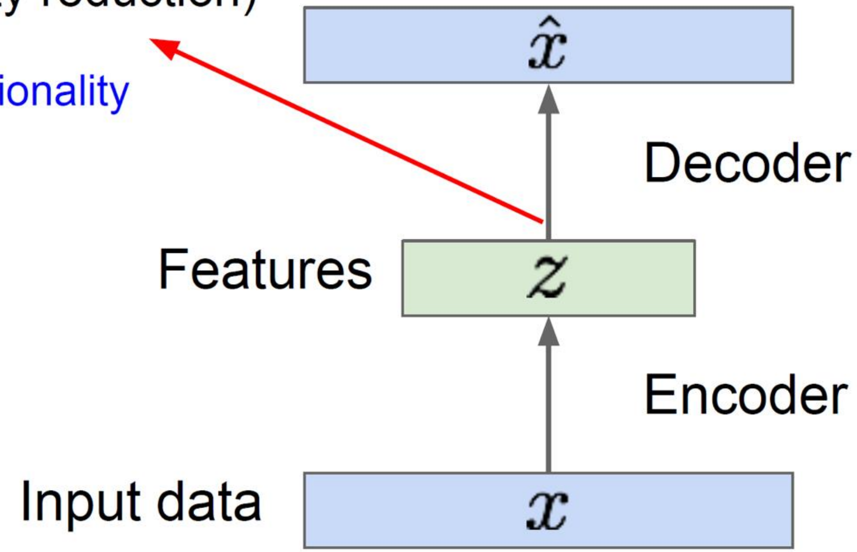


Some background first: Autoencoders

Unsupervised approach for learning a lower-dimensional feature representation from unlabeled training data

z usually smaller than **x**
(dimensionality reduction)

Q: Why dimensionality reduction?



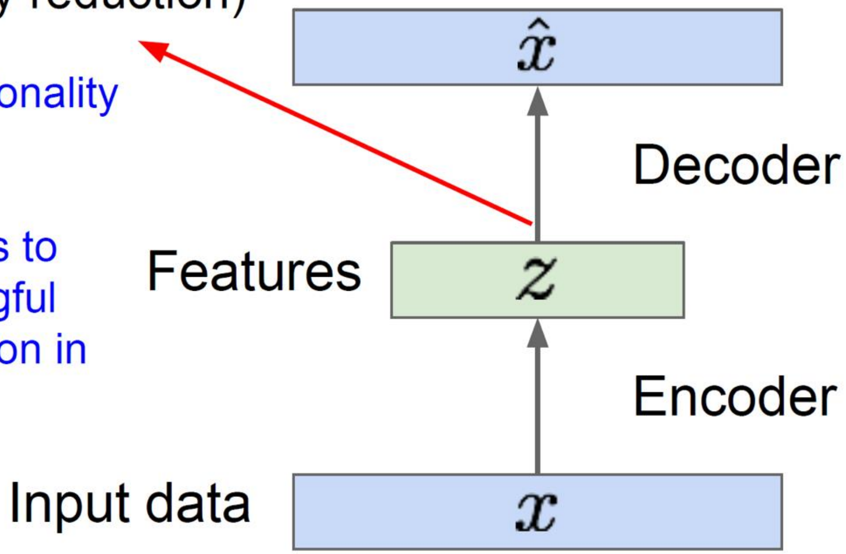
Some background first: Autoencoders

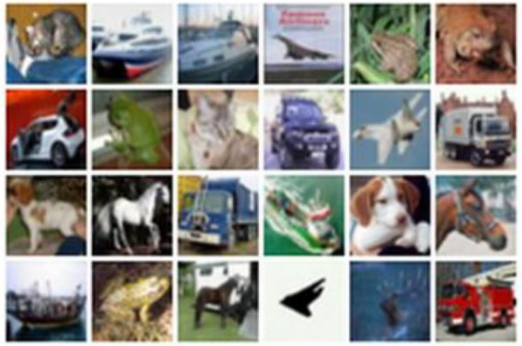
Unsupervised approach for learning a lower-dimensional feature representation from unlabeled training data

z usually smaller than **x** (dimensionality reduction)

Q: Why dimensionality reduction?

A: Want features to capture meaningful factors of variation in data

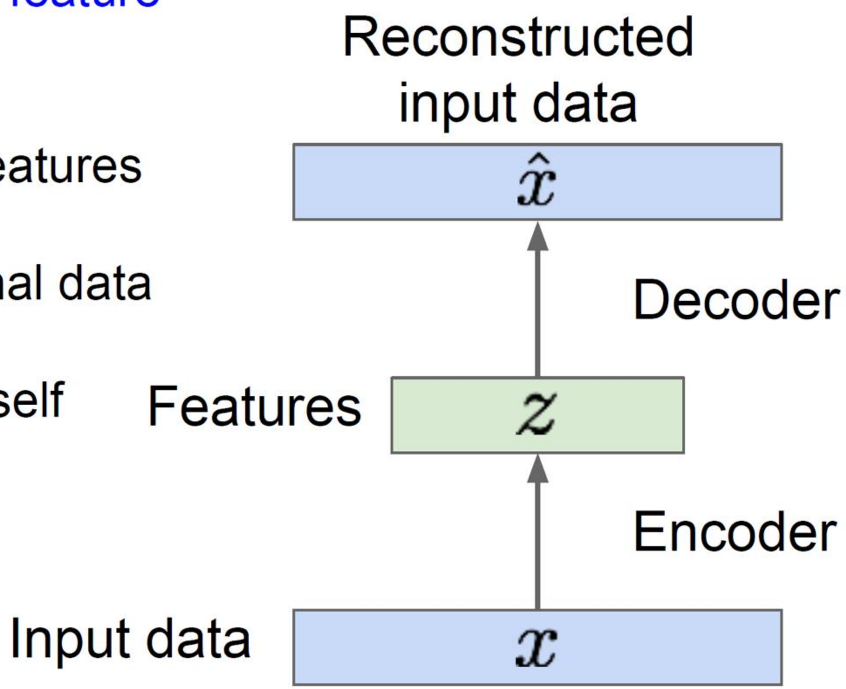


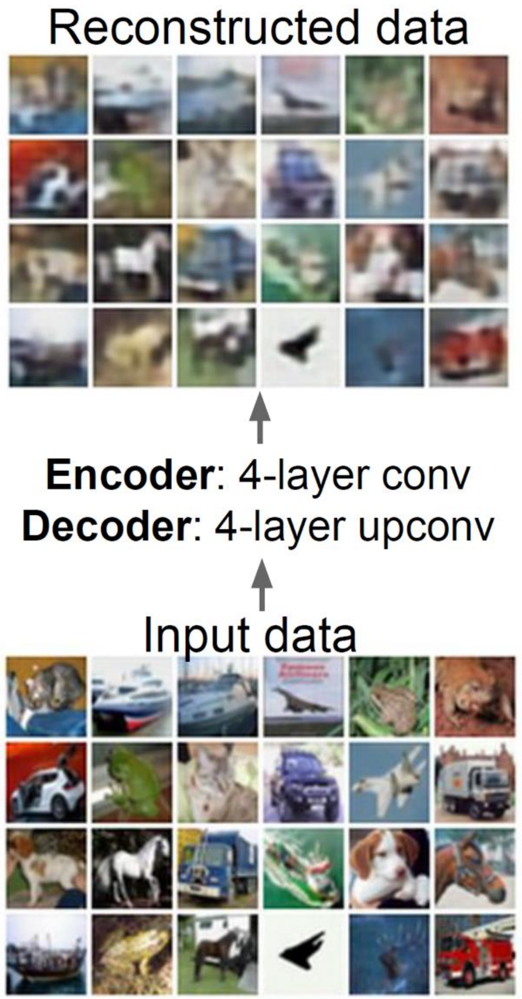


Some background first: Autoencoders

How to learn this feature representation?

Train such that features can be used to reconstruct original data "Autoencoding" - encoding input itself

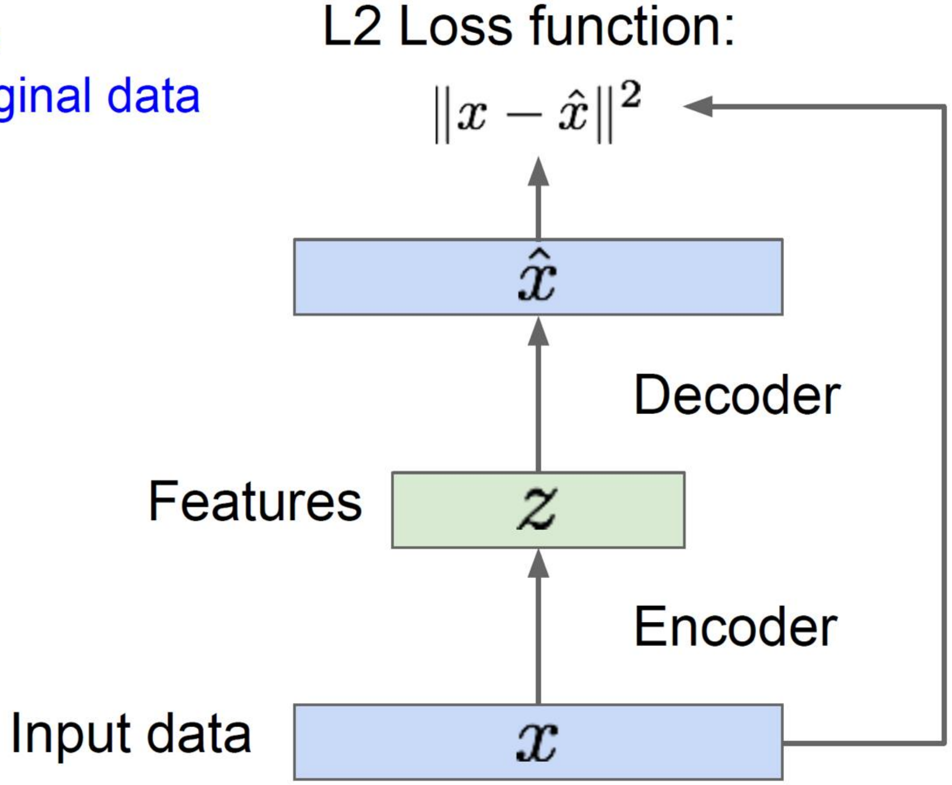


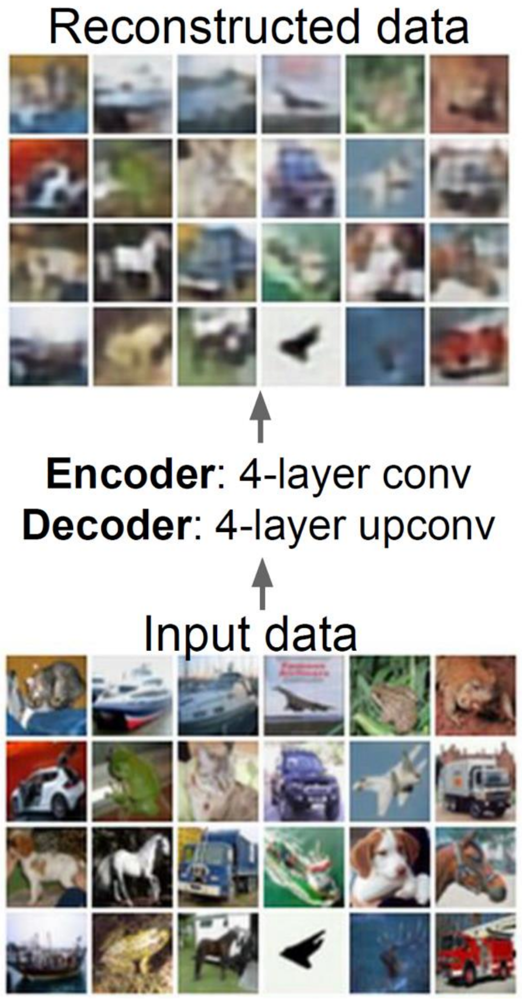


Some background first: Autoencoders

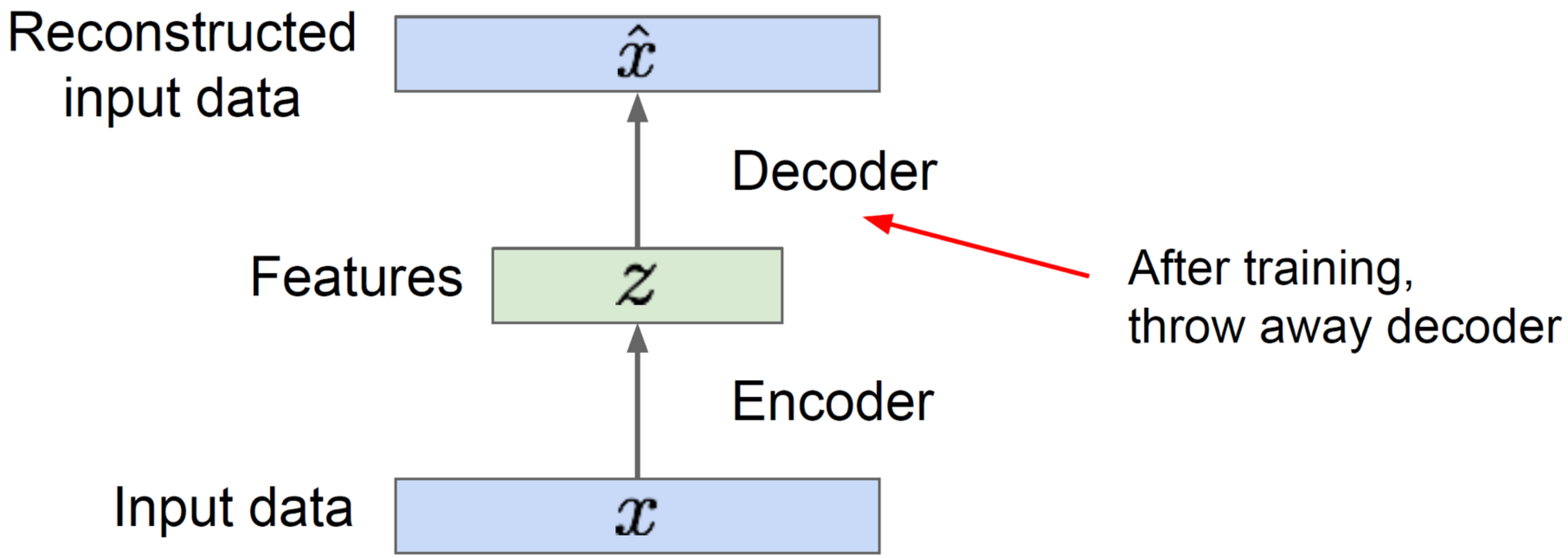
Train such that features can be used to reconstruct original data

Doesn't use labels!





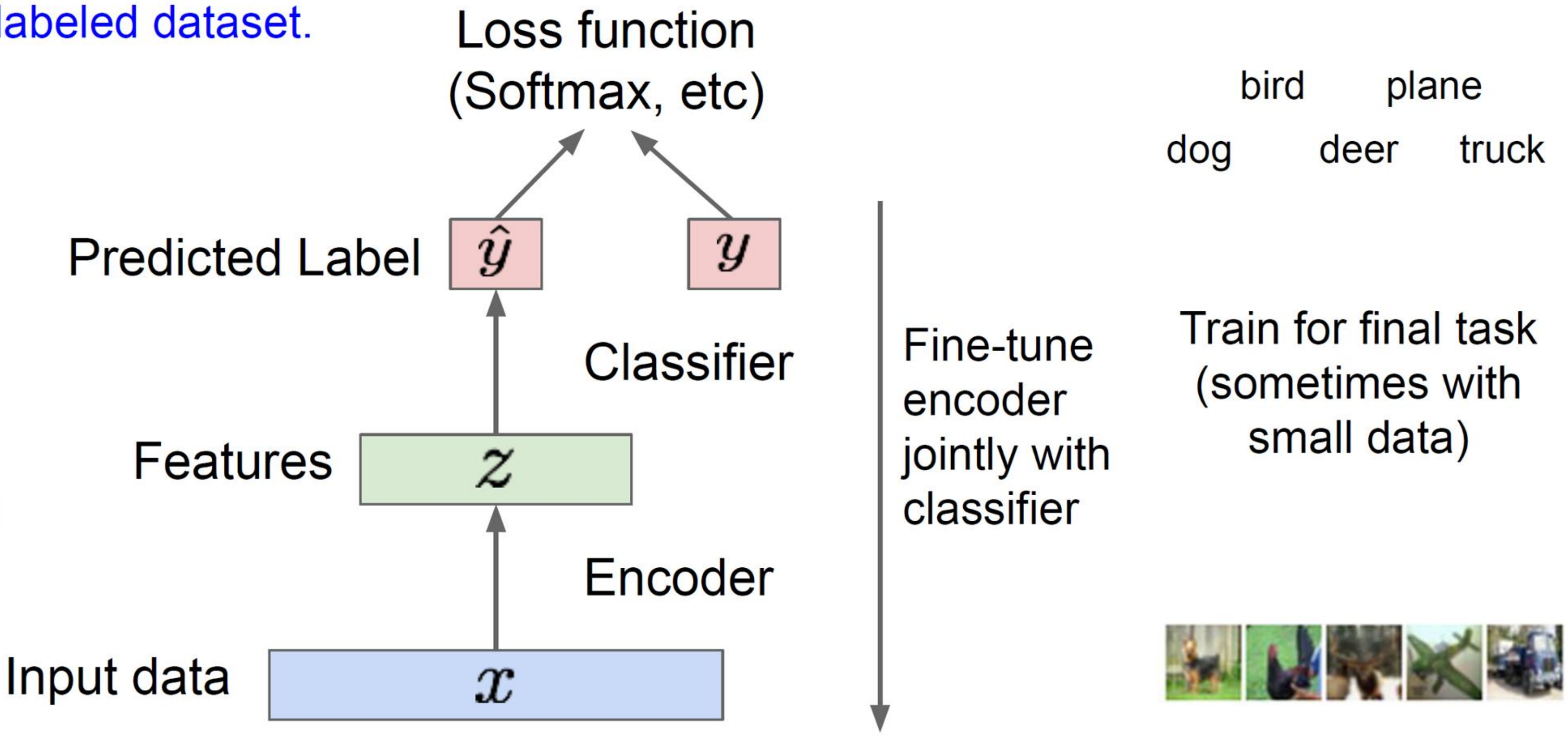
Some background first: Autoencoders



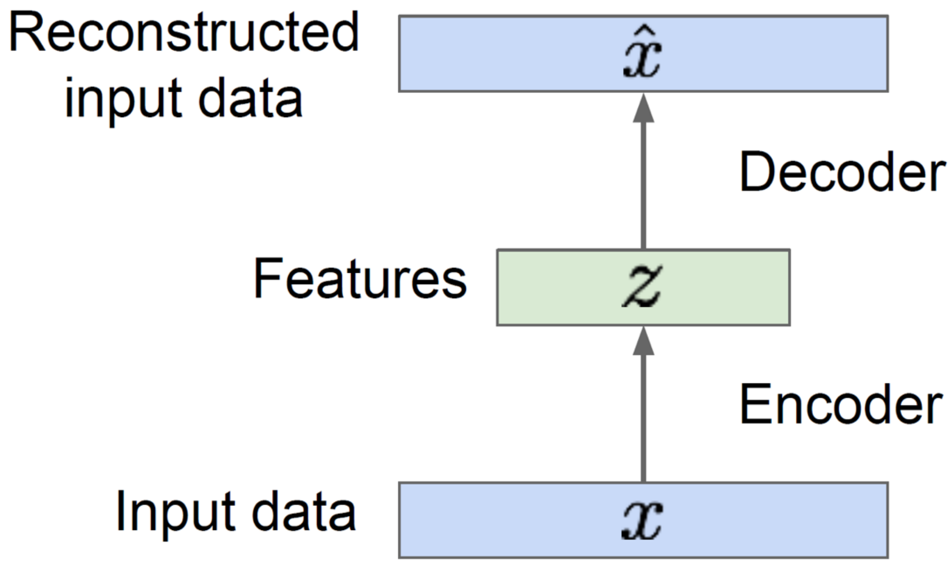
Some background first: Autoencoders

Transfer from large, unlabeled dataset to small, labeled dataset.

Encoder can be used to initialize a **supervised** model



Some background first: Autoencoders



Autoencoders can reconstruct data, and can learn features to initialize a supervised model

Features capture factors of variation in training data.

But we can't generate new images from an autoencoder because we don't know the space of z.

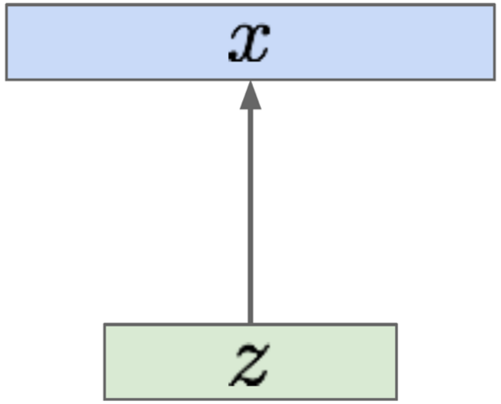
How do we make autoencoder a **generative model**?

Variational Autoencoders

Probabilistic spin on autoencoders - will let us sample from the model to generate data!

Assume training data $\{x^{(i)}\}_{i=1}^{N}$ is generated from the distribution of unobserved (latent) representation **z**

Sample from true conditional $p_{\theta^*}(x \mid z^{(i)})$



Sample from true prior $z^{(i)} \sim p_{\theta^*}(z)$

Kingma and Welling, “Auto-Encoding Variational Bayes”, ICLR 2014

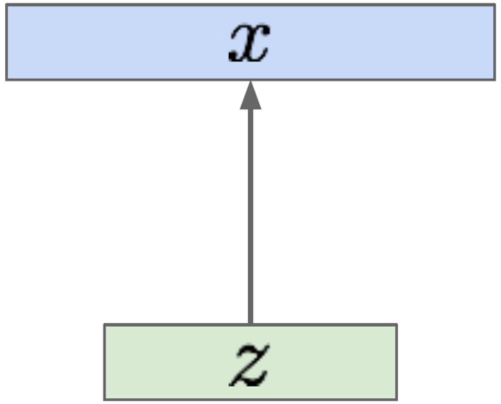
Variational Autoencoders

Probabilistic spin on autoencoders - will let us sample from the model to generate data!

Assume training data $\{x^{(i)}\}_{i=1}^{N}$ is generated from the distribution of unobserved (latent) representation **z**

Intuition (remember from autoencoders!): **x** is an image, **z** is latent factors used to generate **x:** attributes, orientation, etc.

Sample from true conditional
$p_{\theta^*}(x \mid z^{(i)})$



Sample from true prior
$z^{(i)} \sim p_{\theta^*}(z)$

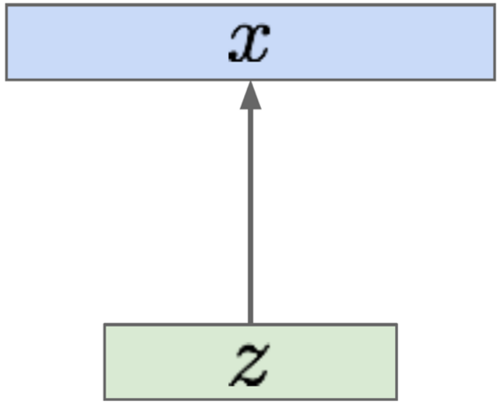
Kingma and Welling, “Auto-Encoding Variational Bayes”, ICLR 2014

Variational Autoencoders

We want to estimate the true parameters θ^* of this generative model given training data x.

Sample from true conditional

$p_{\theta^*}(x \mid z^{(i)})$



Sample from true prior

$z^{(i)} \sim p_{\theta^*}(z)$

Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

Variational Autoencoders

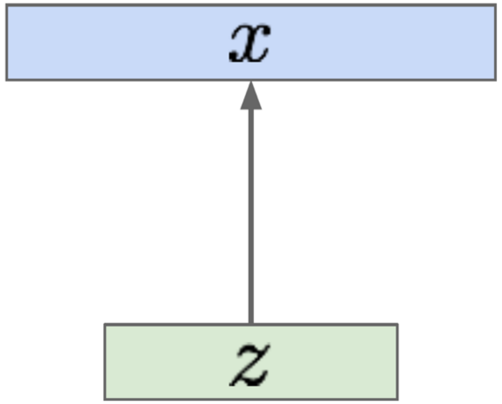
We want to estimate the true parameters θ^* of this generative model given training data x.

Sample from true conditional

$p_{\theta^*}(x \mid z^{(i)})$

Sample from true prior

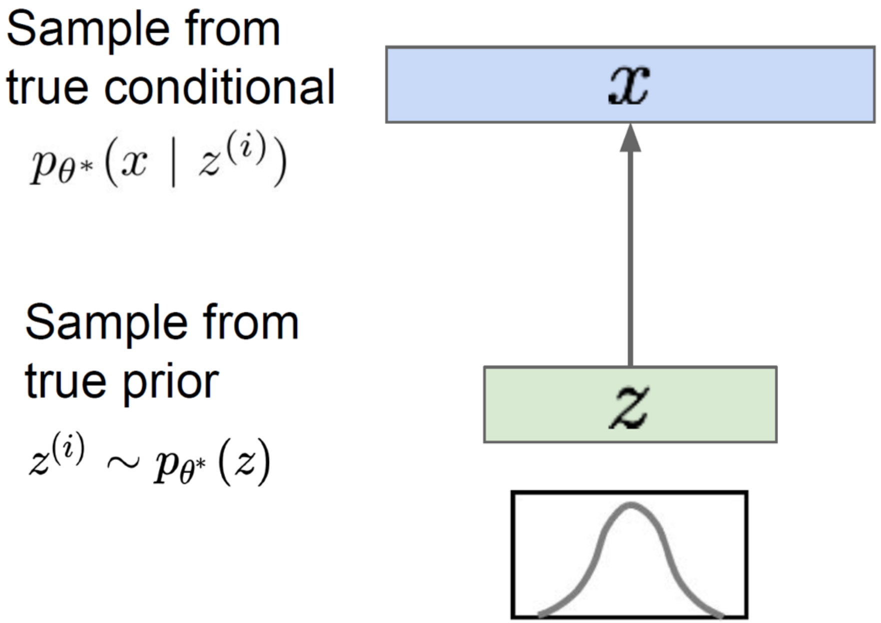
$z^{(i)} \sim p_{\theta^*}(z)$



How should we represent this model?

Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

Variational Autoencoders



We want to estimate the true parameters θ^* of this generative model given training data x.

How should we represent this model?

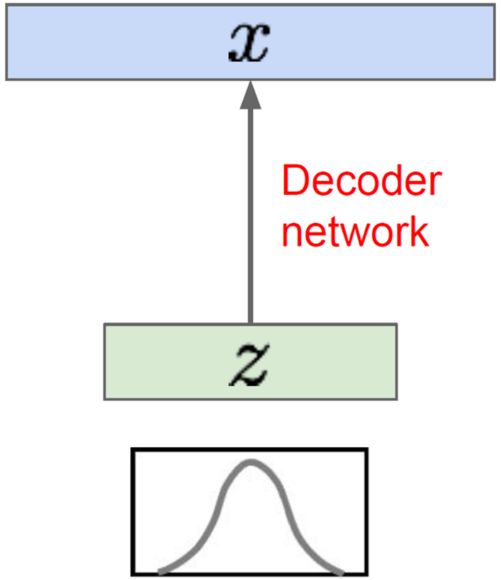
Choose prior p(z) to be simple, e.g. Gaussian. Reasonable for latent attributes, e.g. pose, how much smile.

Kingma and Welling, “Auto-Encoding Variational Bayes”, ICLR 2014

Variational Autoencoders

Sample from
true conditional

$p_{\theta^*}(x \mid z^{(i)})$



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$z^{(i)} \sim p_{\theta^*}(z)$

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How should we represent this model?

Choose prior p(z) to be simple, e.g. Gaussian. Reasonable for latent attributes, e.g. pose, how much smile.

Conditional p(x|z) is complex (generates image) => represent with neural network

Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

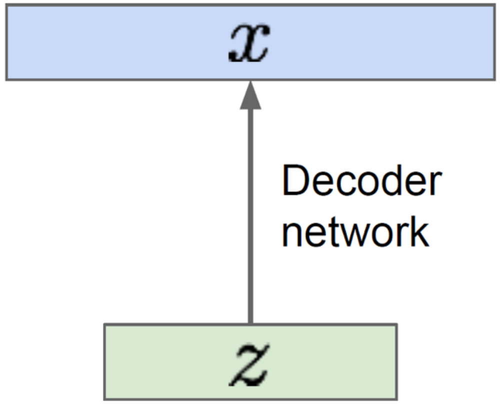
Variational Autoencoders

Sample from true conditional

$p_{\theta^*}(x \mid z^{(i)})$

Sample from true prior

$z^{(i)} \sim p_{\theta^*}(z)$

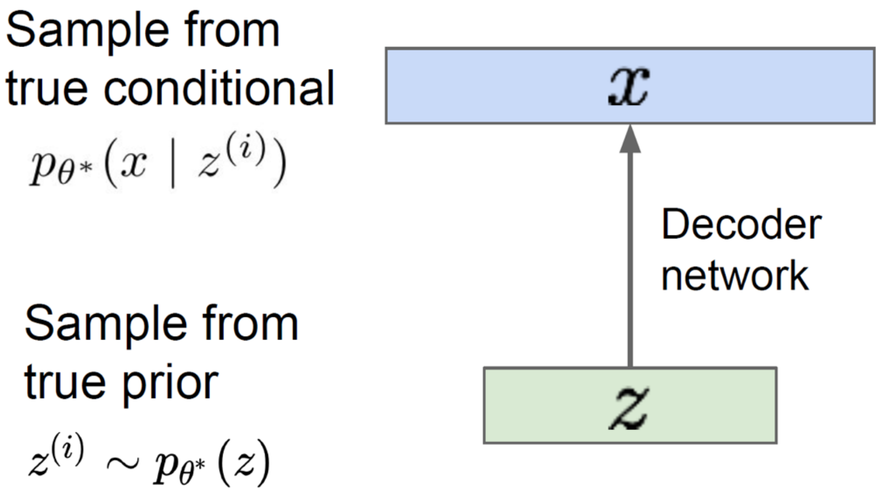


We want to estimate the true parameters θ^* of this generative model given training data x.

How to train the model?

Kingma and Welling, “Auto-Encoding Variational Bayes”, ICLR 2014

Variational Autoencoders



We want to estimate the true parameters θ^* of this generative model given training data x.

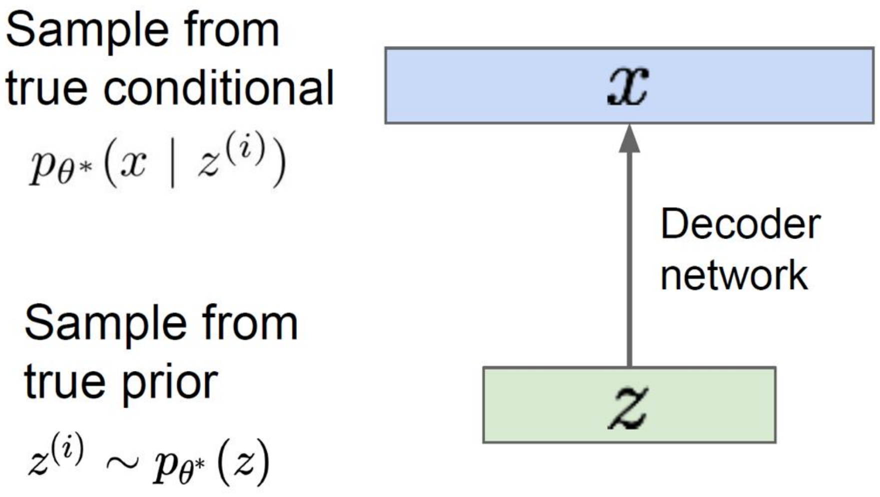
How to train the model?

Learn model parameters to maximize likelihood of training data

$$p_\theta(x) = \int p_\theta(z) p_\theta(x|z) dz$$

Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

Variational Autoencoders



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How to train the model?

Learn model parameters to maximize likelihood of training data

$$p_\theta(x) = \int p_\theta(z) p_\theta(x|z) dz$$

Q: What is the problem with this?

Intractable!

Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

Variational Autoencoders

Data likelihood: $p_\theta(x) = \int p_\theta(z) p_\theta(x|z) dz$

Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

Variational Autoencoders

Data likelihood: $p_\theta(x) = \int p_\theta(z) p_\theta(x|z) dz$

Simple Gaussian prior

Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

Variational Autoencoders

Data likelihood: $p_\theta(x) = \int p_\theta(z) p_\theta(x|z) dz$

Decoder neural network

Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

Variational Autoencoders

Data likelihood: $p_\theta(x) = \int p_\theta(z) p_\theta(x|z) dz$ ✔ ✔

Intractable to compute p(x|z) for every z!

Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

Variational Autoencoders

Data likelihood: $p_\theta(x) = \int p_\theta(z) p_\theta(x|z) dz$ ✔ ✔

Intractable to compute p(x|z) for every z!

$$\log p(x) \approx \log \frac{1}{k} \sum_{i=1}^{k} p(x|z^{(i)}), \text{ where } z^{(i)} \sim p(z)$$

Monte Carlo estimation is too high variance

Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

Variational Autoencoders

Data likelihood: $p_\theta(x) = \int p_\theta(z)p_\theta(x|z)dz$

Posterior density: $p_\theta(z|x) = p_\theta(x|z)p_\theta(z)/p_\theta(x)$

Intractable data likelihood

Kingma and Welling, “Auto-Encoding Variational Bayes”, ICLR 2014

Variational Autoencoders

Data likelihood: $p_\theta(x) = \int p_\theta(z) p_\theta(x|z) dz$

Posterior density also intractable: $p_\theta(z|x) = p_\theta(x|z) p_\theta(z) / p_\theta(x)$

Solution: In addition to modeling $p_\theta(x|z)$, learn $q_\phi(z|x)$ that approximates the true posterior $p_\theta(z|x)$.

Will see that the approximate posterior allows us to derive a lower bound on the data likelihood that is tractable, which we can optimize.

Variational inference is to approximate the unknown posterior distribution from only the observed data x

Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

Variational Autoencoders

$$\log p_\theta(x^{(i)}) = \mathbf{E}_{z \sim q_\phi(z|x^{(i)})} \left[\log p_\theta(x^{(i)}) \right] \quad (p_\theta(x^{(i)}) \text{ Does not depend on } z)$$

Variational Autoencoders

$$\log p_\theta(x^{(i)}) = \mathbf{E}_{z \sim q_\phi(z|x^{(i)})}\left[\log p_\theta(x^{(i)})\right] \quad (p_\theta(x^{(i)}) \text{ Does not depend on } z)$$

Taking expectation wrt. z
(using encoder network) will
come in handy later

Variational Autoencoders

$$\log p_\theta(x^{(i)}) = \mathbf{E}_{z\sim q_\phi(z|x^{(i)})}\left[\log p_\theta(x^{(i)})\right] \quad (p_\theta(x^{(i)}) \text{ Does not depend on } z)$$

$$= \mathbf{E}_z\left[\log \frac{p_\theta(x^{(i)} \mid z)p_\theta(z)}{p_\theta(z \mid x^{(i)})}\right] \quad \text{(Bayes' Rule)}$$

Variational Autoencoders

$$\log p_\theta(x^{(i)}) = \mathbf{E}_{z\sim q_\phi(z|x^{(i)})}\left[\log p_\theta(x^{(i)})\right] \quad (p_\theta(x^{(i)}) \text{ Does not depend on } z)$$

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Variational Autoencoders

$$\log p_\theta(x^{(i)}) = \mathbf{E}_{z\sim q_\phi(z|x^{(i)})}\left[\log p_\theta(x^{(i)})\right] \quad (p_\theta(x^{(i)}) \text{ Does not depend on } z)$$

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$$= \mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right] - \mathbf{E}_z\left[\log \frac{q_\phi(z \mid x^{(i)})}{p_\theta(z)}\right] + \mathbf{E}_z\left[\log \frac{q_\phi(z \mid x^{(i)})}{p_\theta(z \mid x^{(i)})}\right] \quad \text{(Logarithms)}$$

Variational Autoencoders

$$\begin{aligned}
\log p_\theta(x^{(i)}) &= \mathbf{E}_{z\sim q_\phi(z|x^{(i)})}\left[\log p_\theta(x^{(i)})\right] \quad (p_\theta(x^{(i)}) \text{ Does not depend on } z) \\
&= \mathbf{E}_z\left[\log \frac{p_\theta(x^{(i)} \mid z)p_\theta(z)}{p_\theta(z \mid x^{(i)})}\right] \quad (\text{Bayes' Rule}) \\
&= \mathbf{E}_z\left[\log \frac{p_\theta(x^{(i)} \mid z)p_\theta(z)}{p_\theta(z \mid x^{(i)})}\frac{q_\phi(z \mid x^{(i)})}{q_\phi(z \mid x^{(i)})}\right] \quad (\text{Multiply by constant}) \\
&= \mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right] - \mathbf{E}_z\left[\log \frac{q_\phi(z \mid x^{(i)})}{p_\theta(z)}\right] + \mathbf{E}_z\left[\log \frac{q_\phi(z \mid x^{(i)})}{p_\theta(z \mid x^{(i)})}\right] \quad (\text{Logarithms}) \\
&= \mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right] - D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z)) + D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z \mid x^{(i)}))
\end{aligned}$$

The expectation wrt. z (using encoder network) let us write nice KL terms

Variational Autoencoders

$$\log p_\theta(x^{(i)}) = \mathbf{E}_{z\sim q_\phi(z|x^{(i)})}\left[\log p_\theta(x^{(i)})\right] \qquad (p_\theta(x^{(i)}) \text{ Does not depend on } z)$$

$$= \mathbf{E}_z\left[\log \frac{p_\theta(x^{(i)} \mid z)p_\theta(z)}{p_\theta(z \mid x^{(i)})}\right] \qquad \text{(Bayes' Rule)}$$

$$= \mathbf{E}_z\left[\log \frac{p_\theta(x^{(i)} \mid z)p_\theta(z)}{p_\theta(z \mid x^{(i)})} \frac{q_\phi(z \mid x^{(i)})}{q_\phi(z \mid x^{(i)})}\right] \qquad \text{(Multiply by constant)}$$

$$= \mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right] - \mathbf{E}_z\left[\log \frac{q_\phi(z \mid x^{(i)})}{p_\theta(z)}\right] + \mathbf{E}_z\left[\log \frac{q_\phi(z \mid x^{(i)})}{p_\theta(z \mid x^{(i)})}\right] \qquad \text{(Logarithms)}$$

$$= \mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right] - D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z)) + D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z \mid x^{(i)}))$$

Decoder network gives $p_\theta(x|z)$, can compute estimate of this term through sampling (need some trick to differentiate through sampling).

This KL term (between Gaussians for encoder and z prior) has nice closed-form solution!

$p_\theta(z|x)$ intractable (saw earlier), can't compute this KL term :(But we know KL divergence always >= 0.

Variational Autoencoders

$$\log p_\theta(x^{(i)}) = \mathbf{E}_{z\sim q_\phi(z|x^{(i)})}\left[\log p_\theta(x^{(i)})\right] \quad (p_\theta(x^{(i)}) \text{ Does not depend on } z)$$

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$$= \mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right] - D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z)) + D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z \mid x^{(i)}))$$

We want to maximize the data likelihood

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We want to maximize the data likelihood

Tractable lower bound which we can take gradient of and optimize! ($p_\theta(x|z)$ differentiable, KL term differentiable)

Variational Autoencoders

$$\log p_\theta(x^{(i)}) = \mathbf{E}_{z\sim q_\phi(z|x^{(i)})}\left[\log p_\theta(x^{(i)})\right] \quad (p_\theta(x^{(i)}) \text{ Does not depend on } z)$$

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Variational Autoencoders

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Decoder: reconstruct the input data

Encoder: make approximate posterior distribution close to prior

Tractable lower bound which we can take gradient of and optimize! ($p_\theta(x|z)$ differentiable, KL term differentiable)

Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

$$\underbrace{\mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right] - D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z))}_{\mathcal{L}(x^{(i)}, \theta, \phi)}$$

Variational Autoencoders

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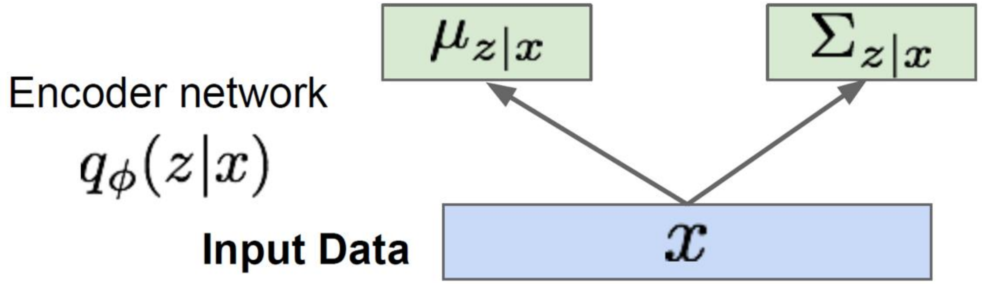
Let's look at computing the KL divergence between the estimated posterior and the prior given some data

Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

$$\underbrace{\mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right] - \boxed{D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z))}}_{\mathcal{L}(x^{(i)}, \theta, \phi)}$$



Variational Autoencoders

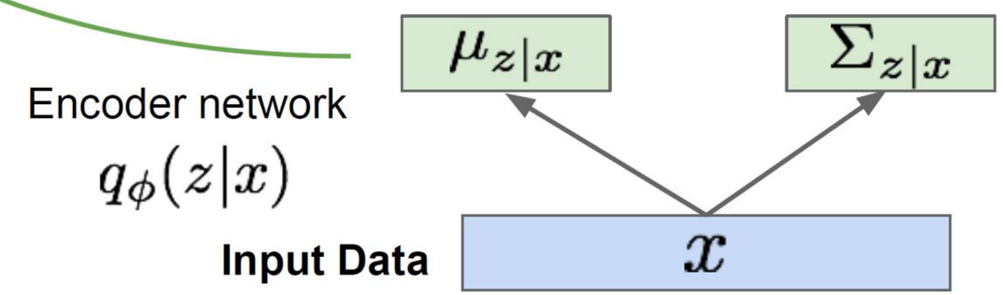
Putting it all together: maximizing the likelihood lower bound

$$\underbrace{\mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right] - \boxed{D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z))}}_{\mathcal{L}(x^{(i)}, \theta, \phi)}$$

$$D_{KL}(\mathcal{N}(\mu_{z|x}, \Sigma_{z|x})||\mathcal{N}(0, I))$$

Have analytical solution

Make approximate posterior distribution close to prior



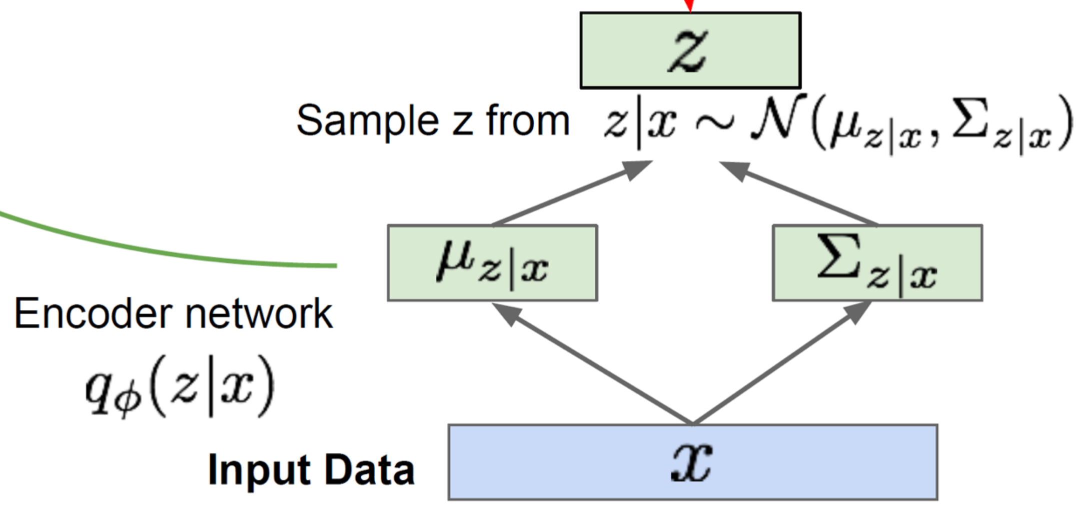
Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

$$\underbrace{\boxed{\mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right]} - D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z))}_{\mathcal{L}(x^{(i)},\theta,\phi)}$$

Make approximate posterior distribution close to prior

Not part of the computation graph!



Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

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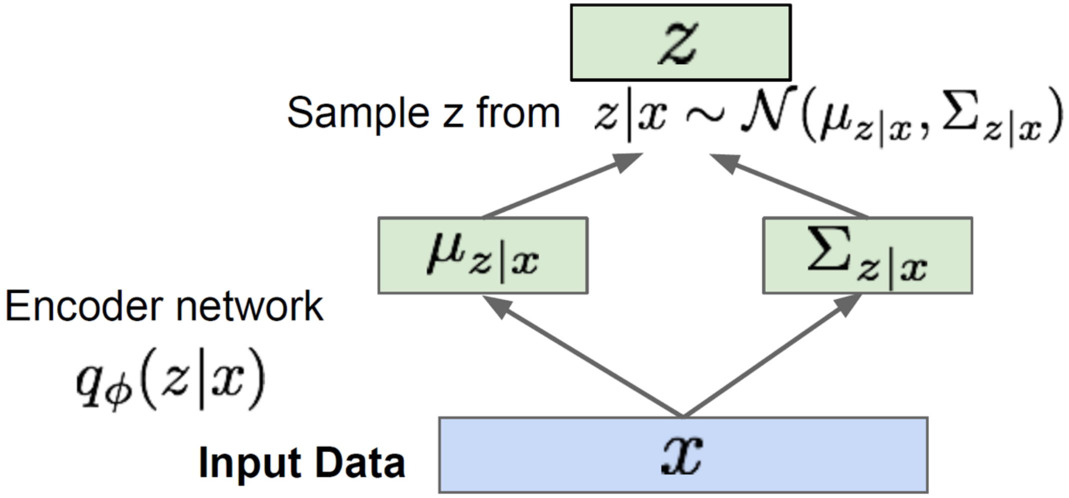
Reparameterization trick to make sampling differentiable:

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

$$z = \mu_{z|x} + \epsilon\sigma_{z|x}$$



Variational Autoencoders

Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

$$\underbrace{\mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right] - D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z))}_{\mathcal{L}(x^{(i)},\theta,\phi)}$$

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

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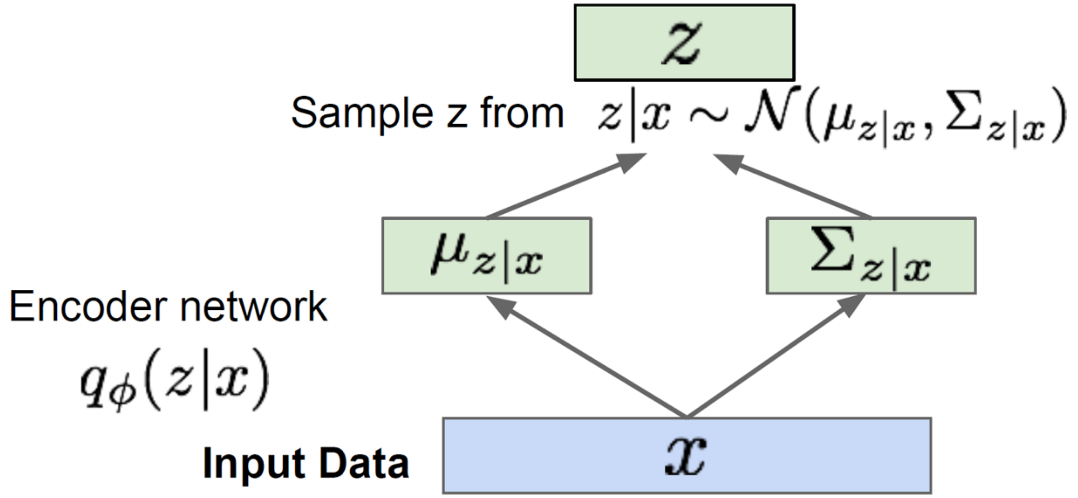
Input to the graph

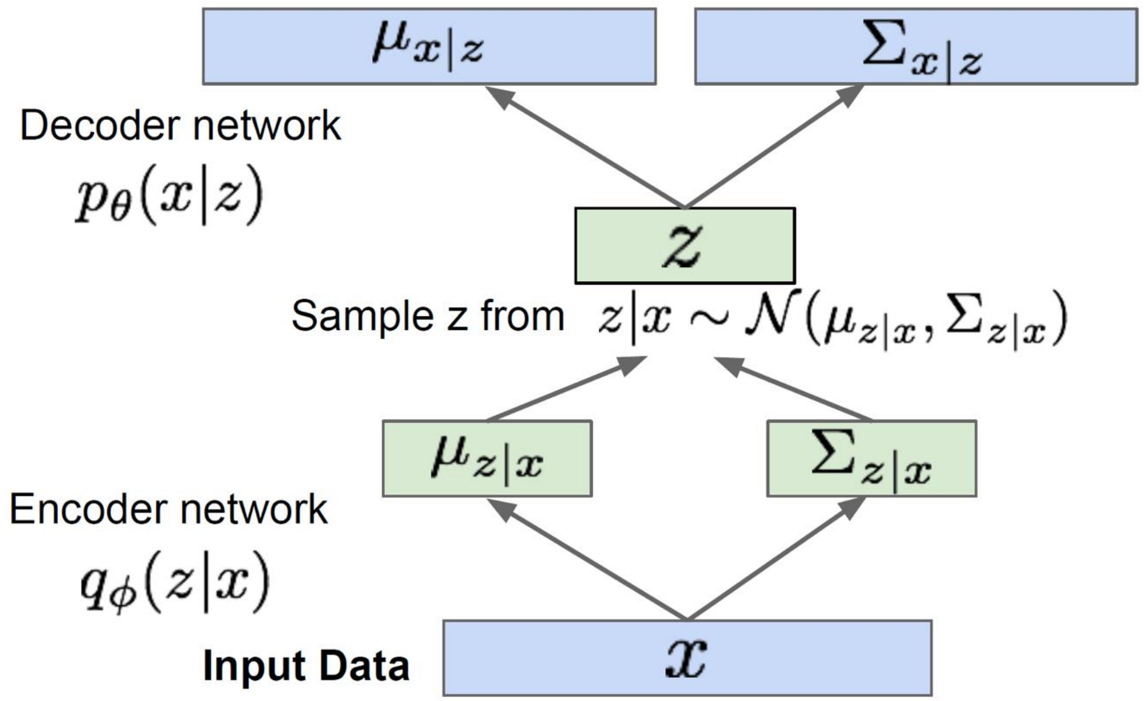
Part of computation graph



Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

$$\underbrace{\mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right] - D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z))}_{\mathcal{L}(x^{(i)},\theta,\phi)}$$



Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

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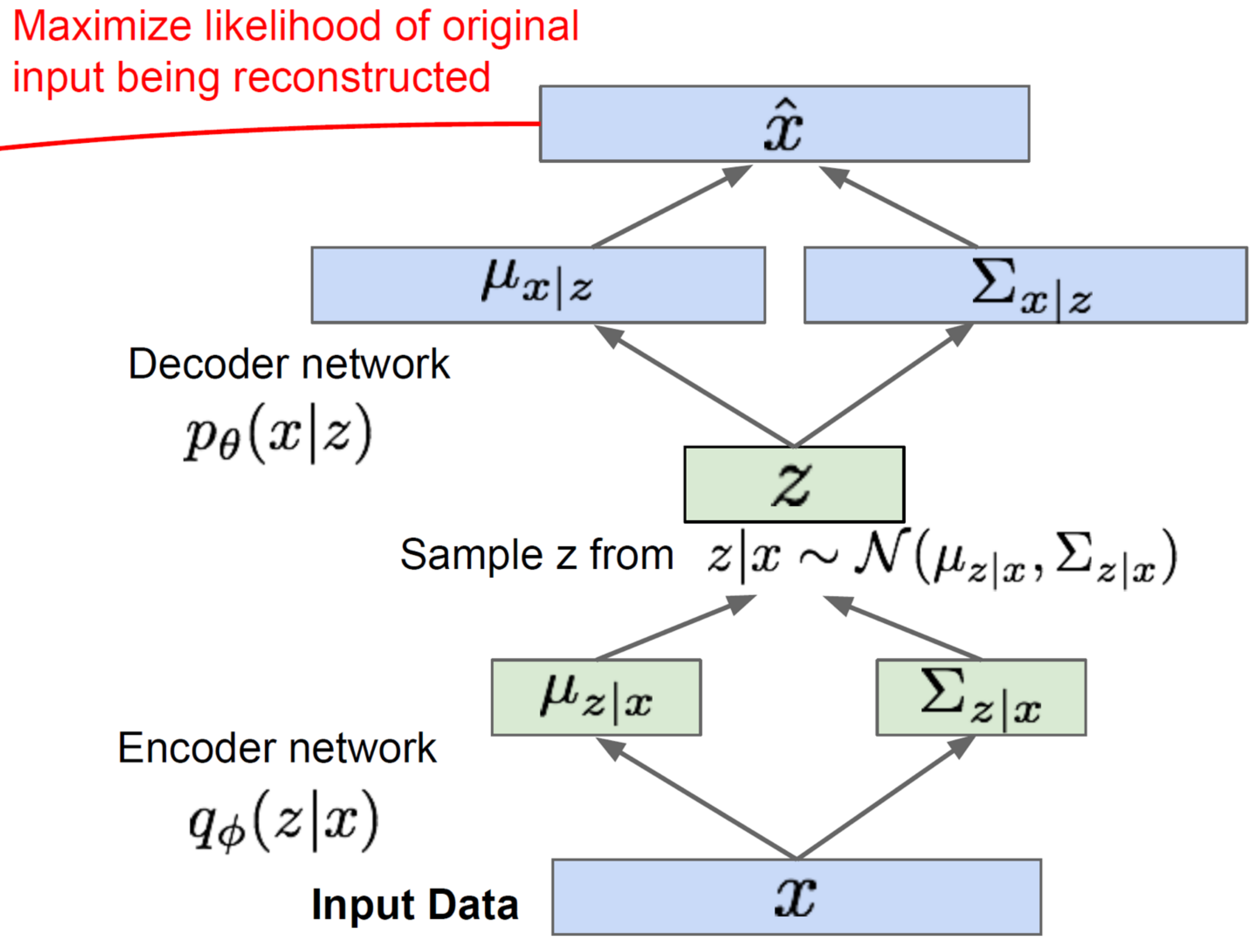
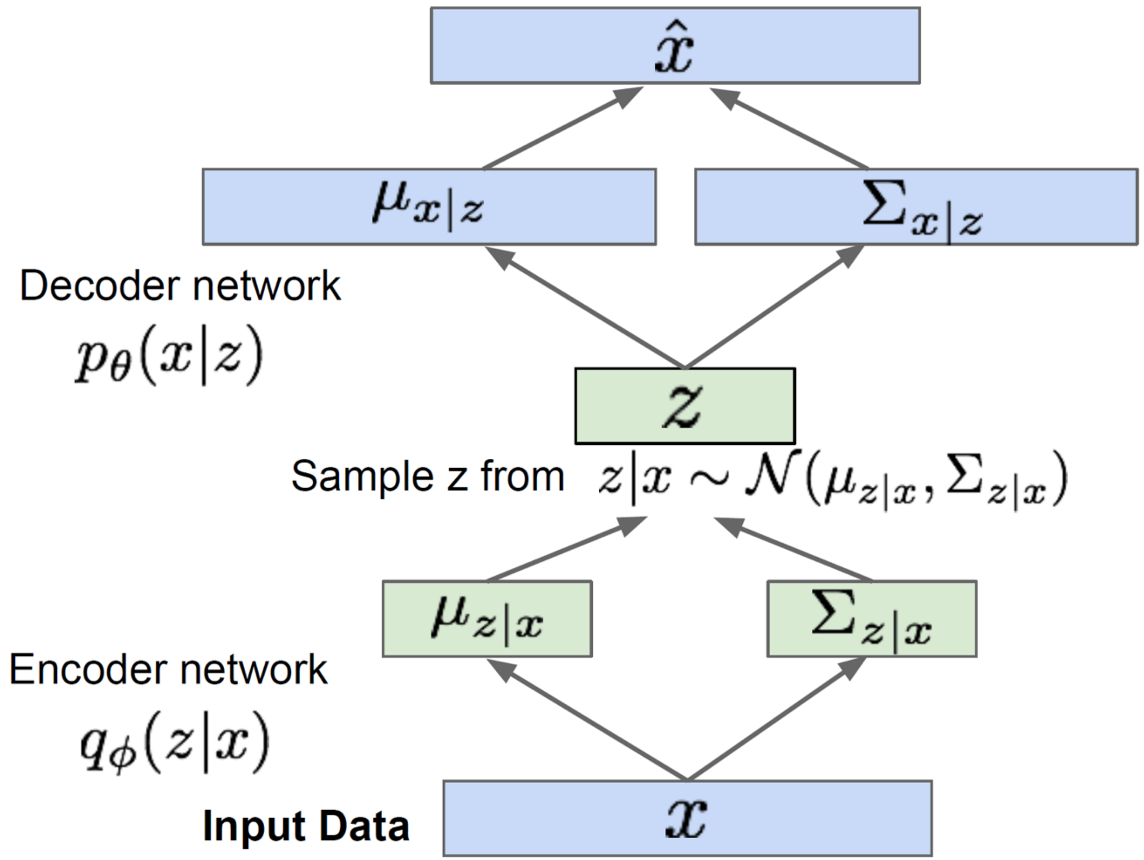


Variational Autoencoders

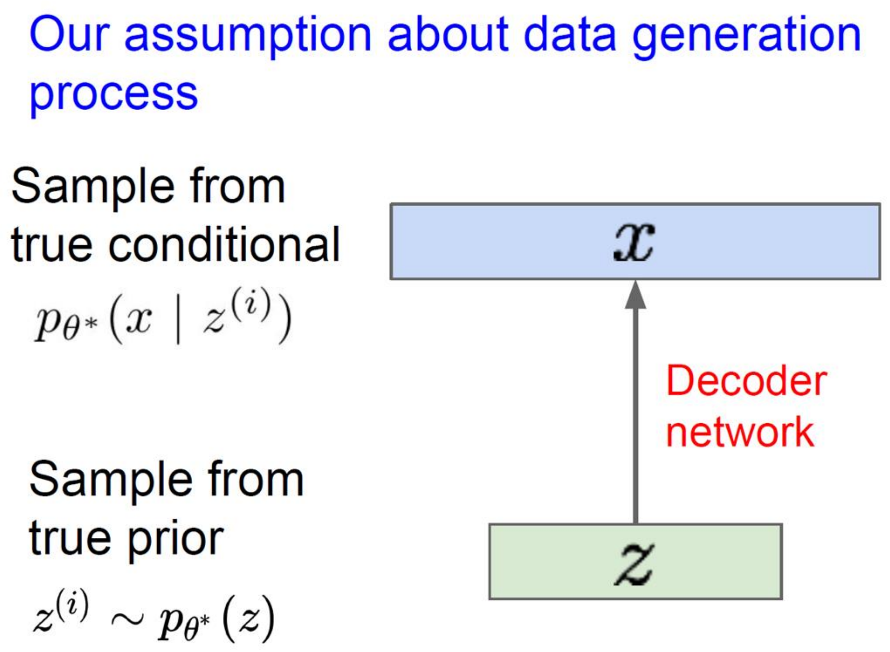
Putting it all together: maximizing the likelihood lower bound

$$\underbrace{\mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right] - D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z))}_{\mathcal{L}(x^{(i)}, \theta, \phi)}$$

For every minibatch of input data: compute this forward pass, and then backprop!



Variational Autoencoders: Generating Data!



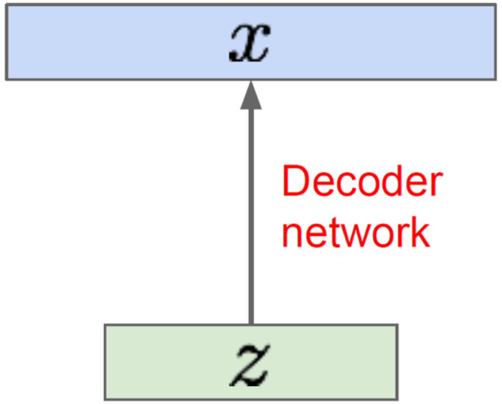
Kingma and Welling, “Auto-Encoding Variational Bayes”, ICLR 2014

Variational Autoencoders: Generating Data!

Our assumption about data generation process

Sample from true conditional

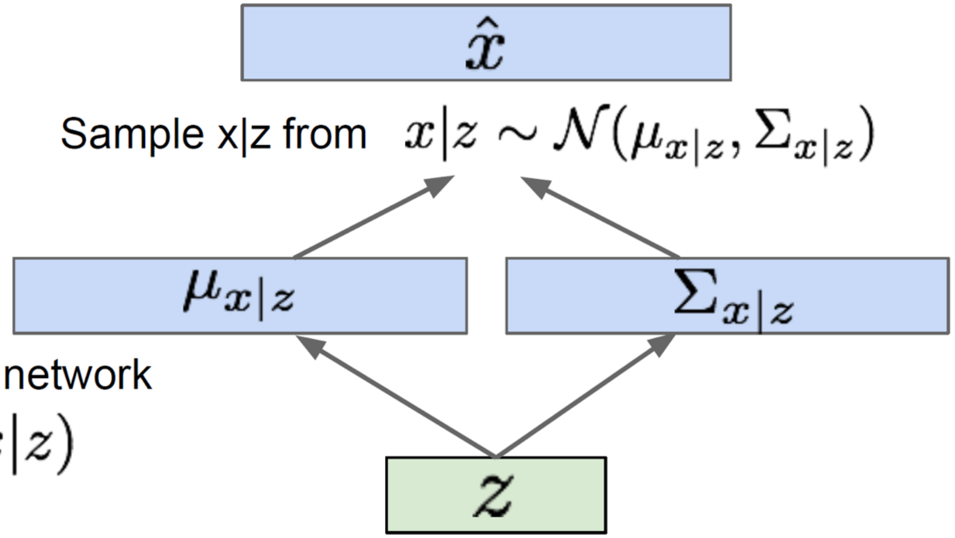
$p_{\theta^*}(x \mid z^{(i)})$



Sample from true prior

$z^{(i)} \sim p_{\theta^*}(z)$

Now given a trained VAE: use decoder network & sample z from prior!



Decoder network

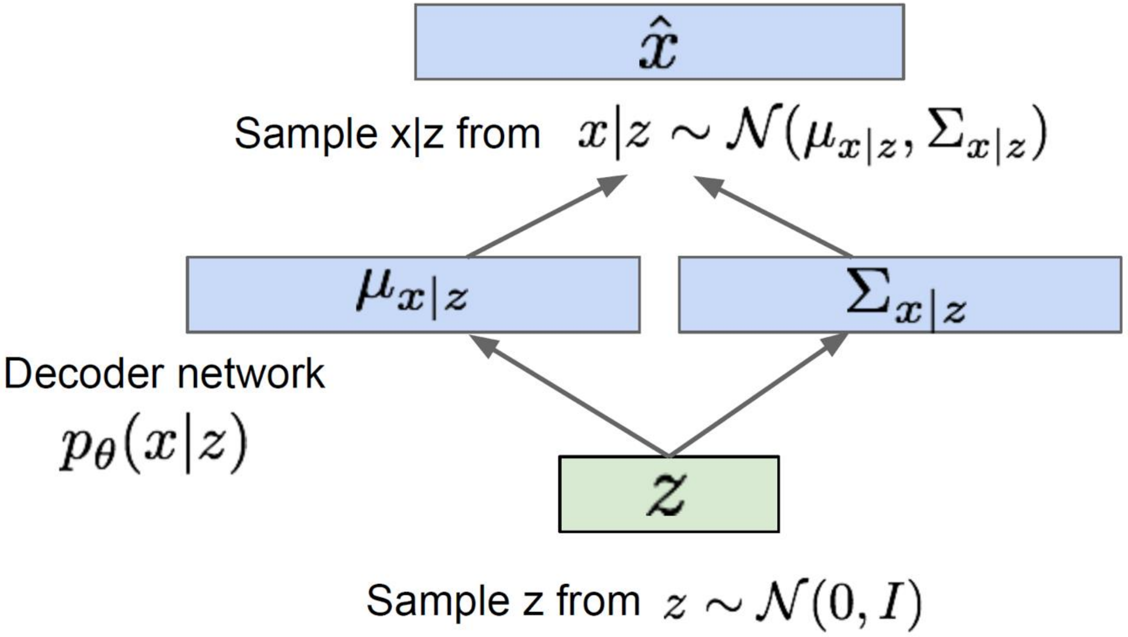
$p_\theta(x|z)$

Sample z from $z \sim \mathcal{N}(0, I)$

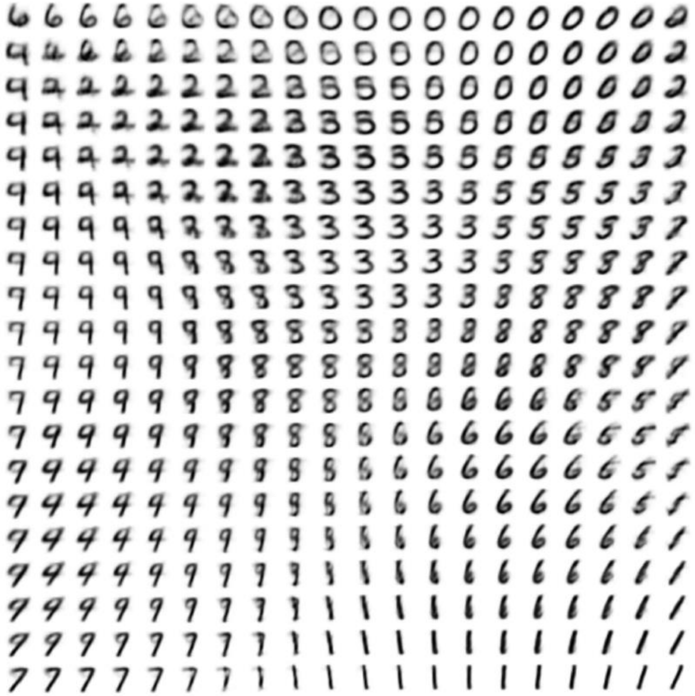
Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

Variational Autoencoders: Generating Data!

Use decoder network. Now sample z from prior!

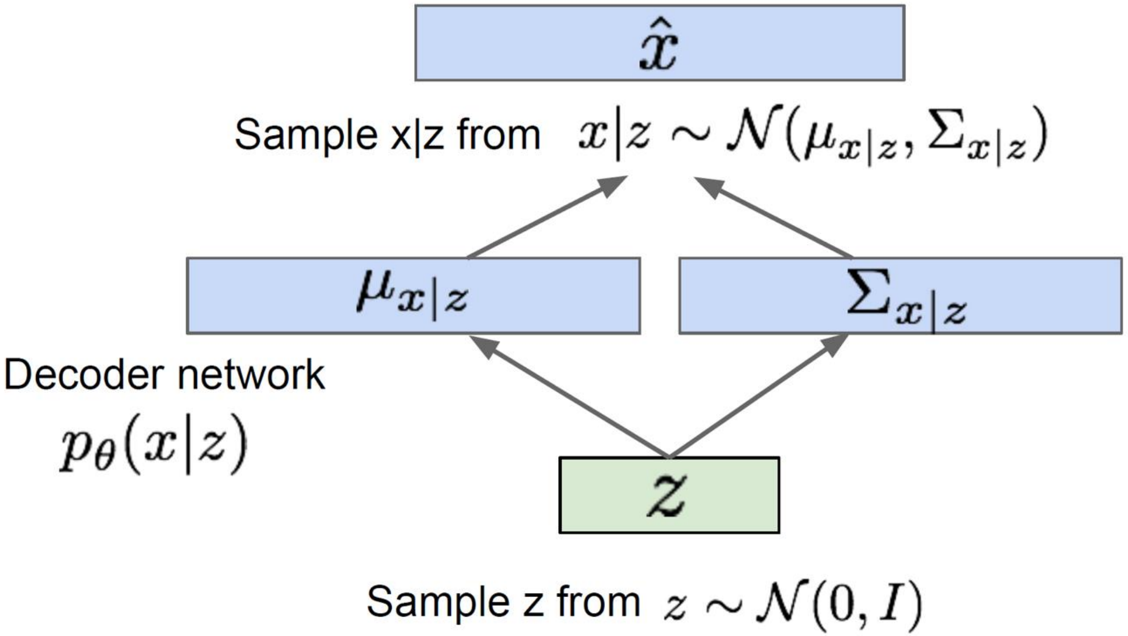


Kingma and Welling, “Auto-Encoding Variational Bayes”, ICLR 2014



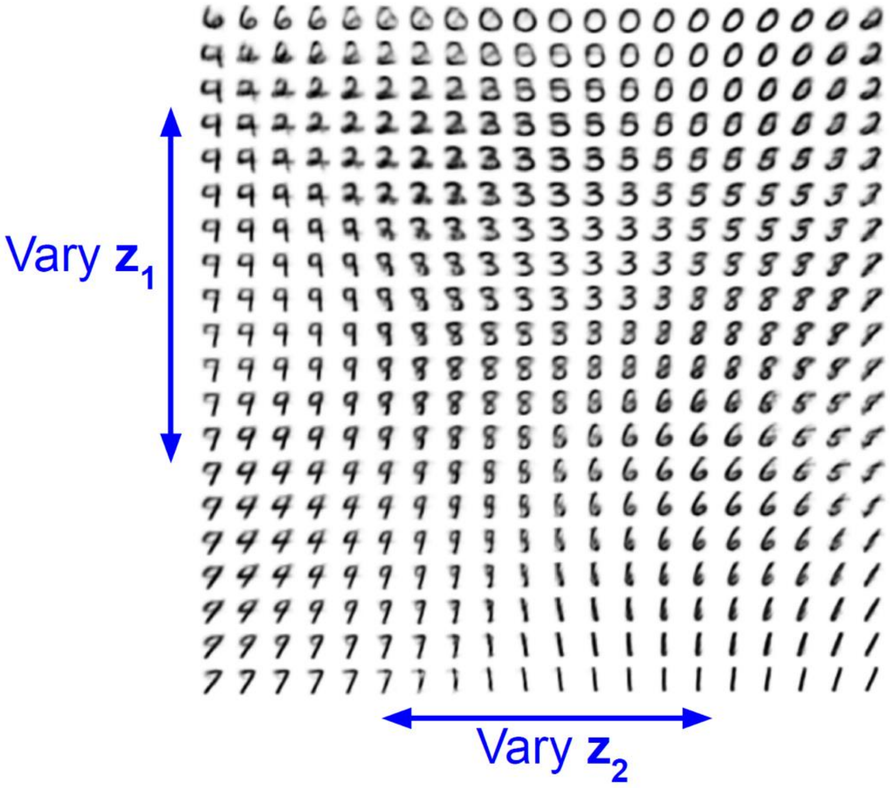
Variational Autoencoders: Generating Data!

Use decoder network. Now sample z from prior!



Kingma and Welling, “Auto-Encoding Variational Bayes”, ICLR 2014

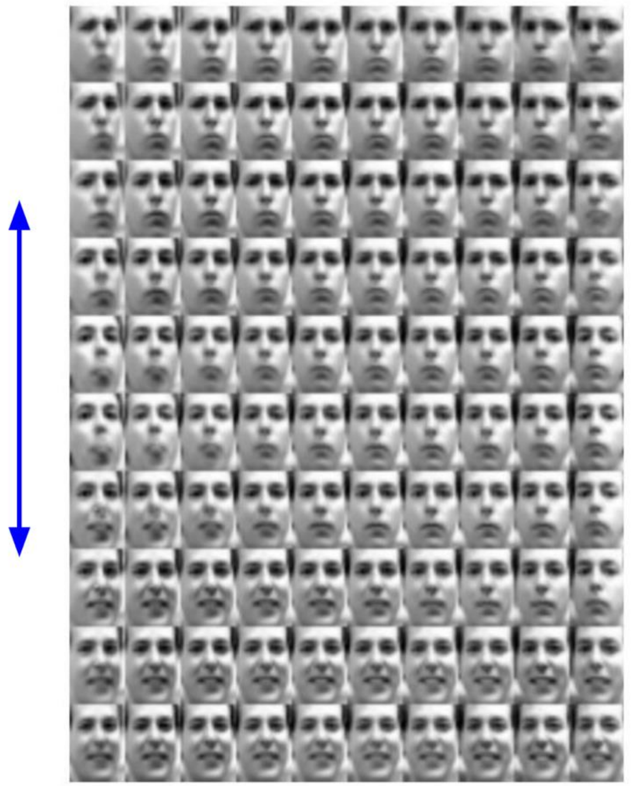
Data manifold for 2-d **z**



Variational Autoencoders: Generating Data!

Diagonal prior on **z** => independent latent variables

Different dimensions of **z** encode interpretable factors of variation



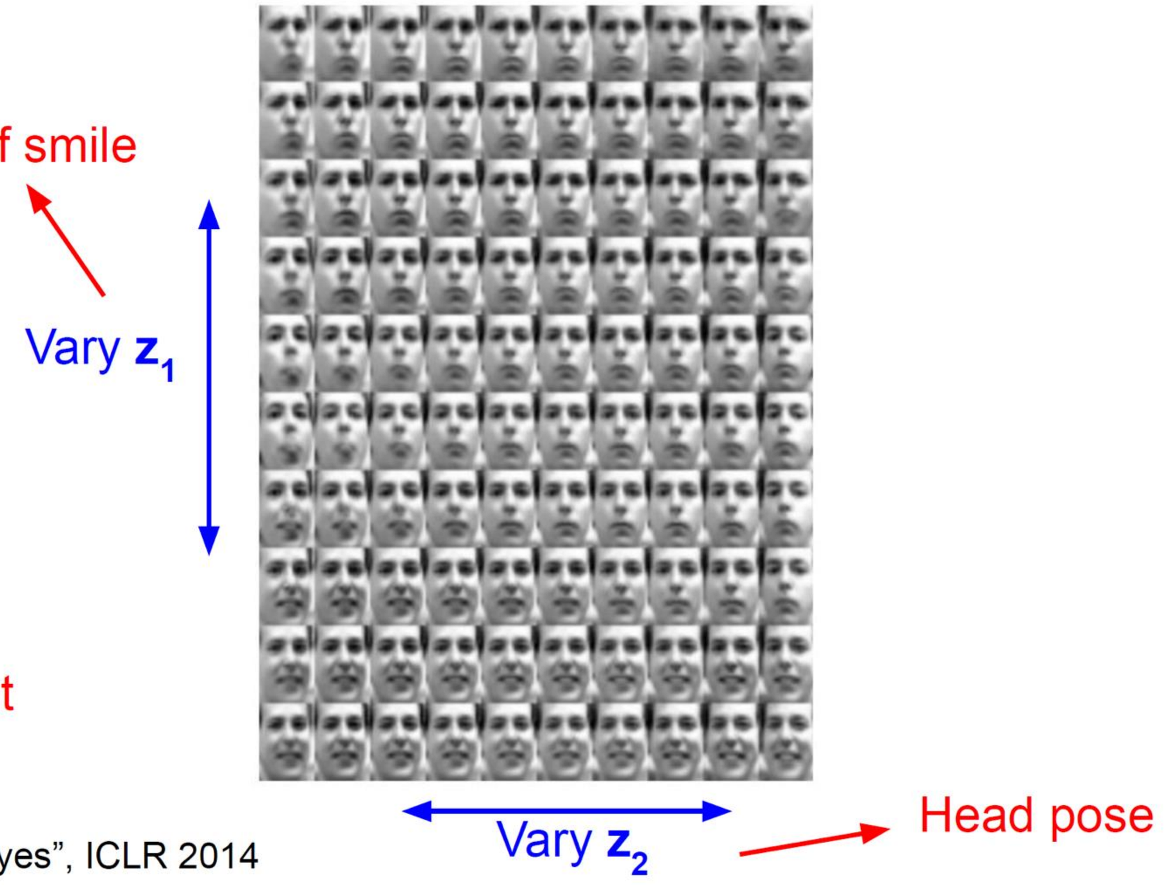
Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

Variational Autoencoders: Generating Data!

Diagonal prior on **z**
=> independent
latent variables

Different
dimensions of **z**
encode
interpretable factors
of variation

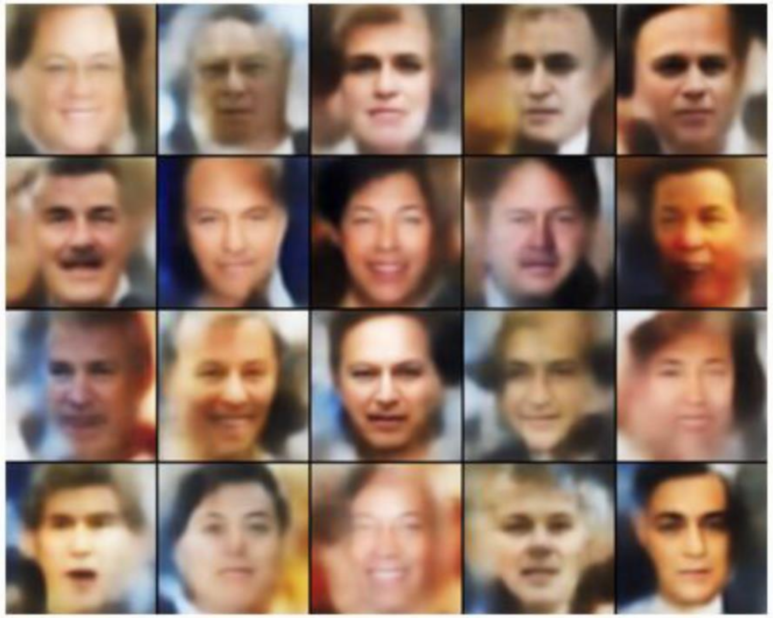
Also good feature representation that
can be computed using $q_\phi(z|x)$!



Kingma and Welling, “Auto-Encoding Variational Bayes”, ICLR 2014

Variational Autoencoders: Generating Data!

32x32 CIFAR-10



Labeled Faces in the Wild

Variational Autoencoders

Probabilistic spin to traditional autoencoders => allows generating data
Defines an intractable density => derive and optimize a (variational) lower bound

Pros:

- Principled approach to generative models
- Interpretable latent space.
- Allows inference of $q(z|x)$, can be useful feature representation for other tasks

Cons:

- Maximizes lower bound of likelihood: okay, but not as good evaluation as PixelRNN/PixelCNN
- Samples blurrier and lower quality compared to state-of-the-art (GANs)

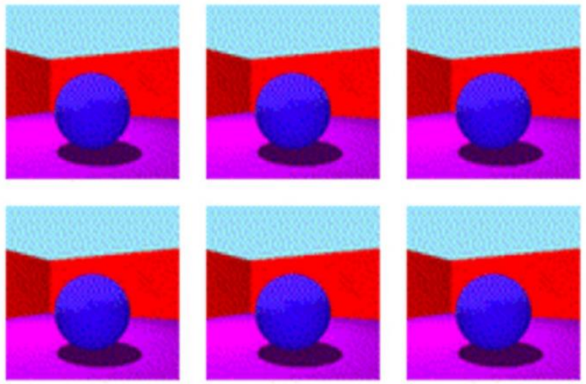
Active areas of research:

- More flexible approximations, e.g. richer approximate posterior instead of diagonal Gaussian, e.g., Gaussian Mixture Models (GMMs), Categorical Distributions.
- Learning disentangled representations.

VAEs for Disentangled Generation

Disentangled representation learning

- Very useful for style transfer: disentangling **style** from **content**



disentanglement_lib

From negative to positive
consistently slow . consistently good . consistently fast .
my goodness it was so gross . my husband 's steak was phenomenal . my goodness was so awesome .
it was super dry and had a weird taste to the entire slice . it was a great meal and the tacos were very kind of good . it was super flavorful and had a nice texture of the whole side .

Locatello et al., Challenging Common Assumptions in the Unsupervised Learning of Disentangled Representations. ICML 2019

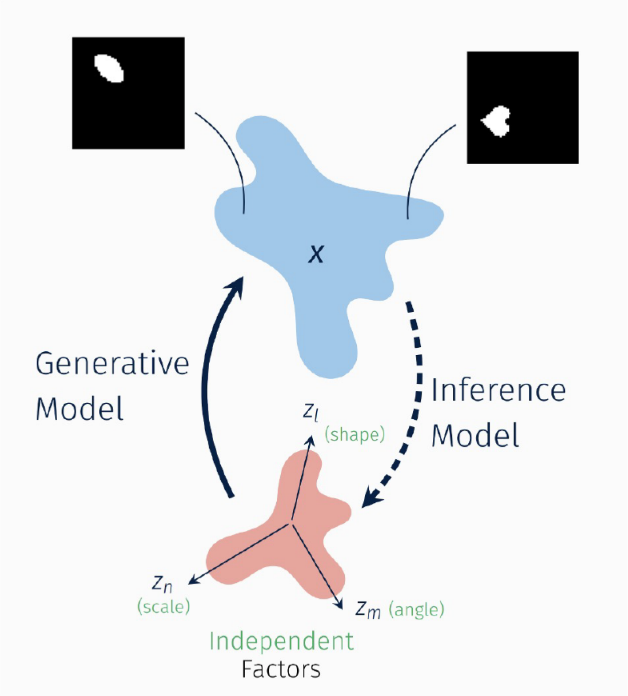
VAEs for Disentangled Generation

Disentangled representation learning

- Very useful for style transfer: disentangling **style** from **content**

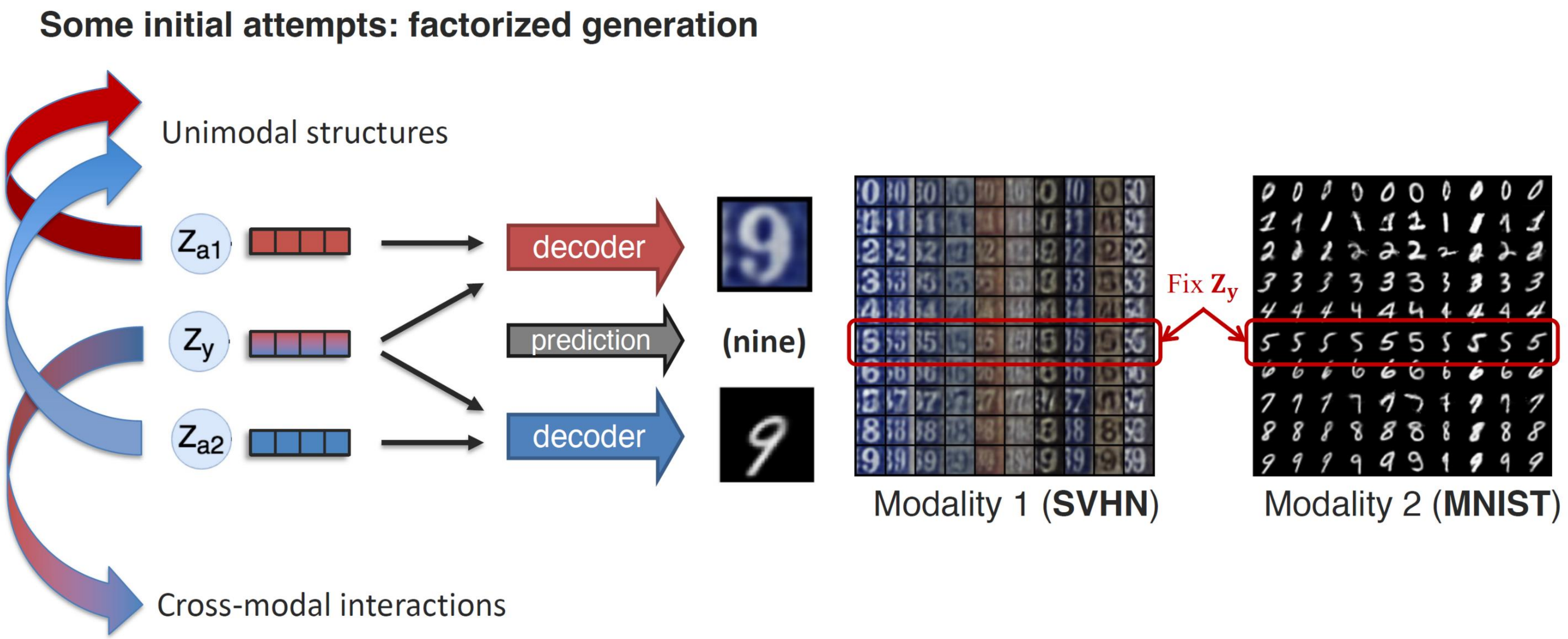
$$\mathcal{L}_\beta(x) = \mathbb{E}_{q_\phi(z|x)}[\log p_\theta(x|z)] - \beta \cdot \mathrm{KL}(q_\phi(z|x)||p(z))$$

- beta-VAE: beta = 1 recovers VAE, beta > 1 imposes stronger constraint on the latent variables to have independent dimensions
- Difficult problem!
  - Positive results [Hu et al., 2016, Kulkarni et al., 2015]
  - Negative results [Mathieu et al., 2019, Locatello et al., 2019]
  - Better benchmarks & metrics to measure disentanglement [Higgins et al., 2017, Kim & Mnih 2018]



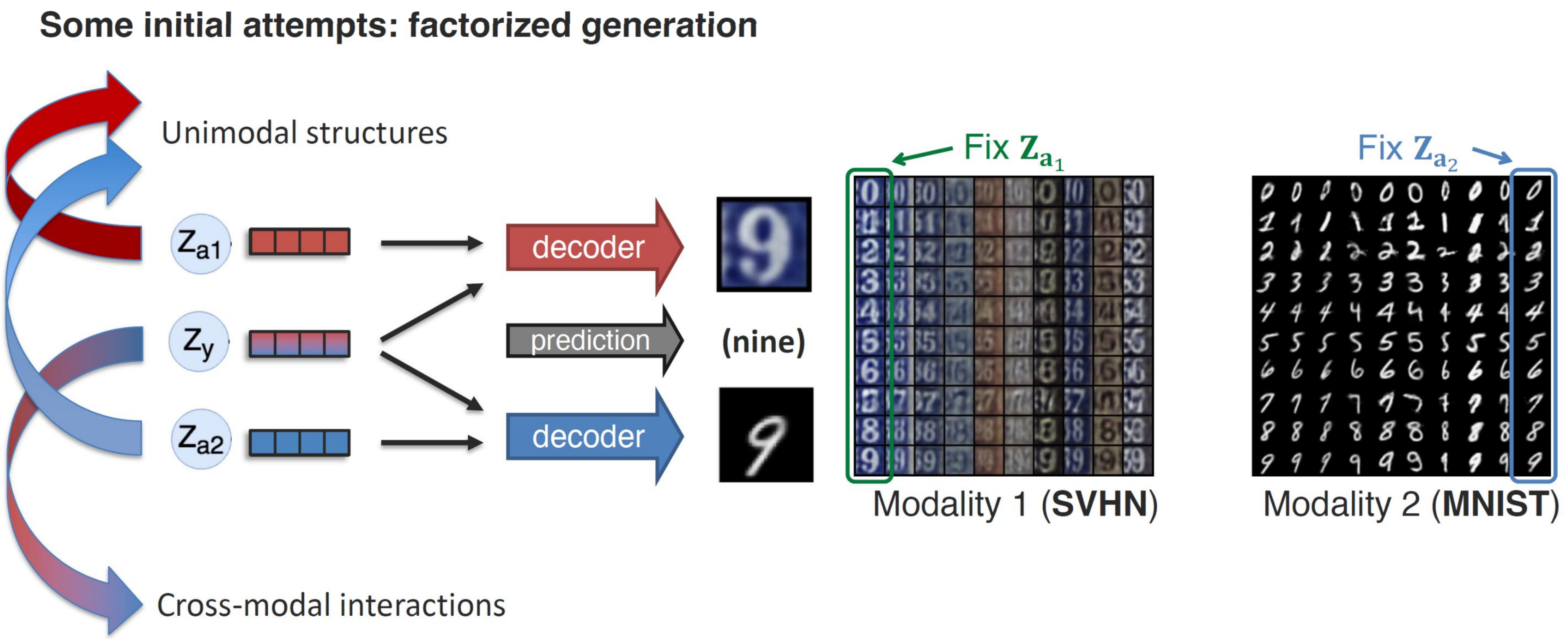
Locatello et al., Challenging Common Assumptions in the Unsupervised Learning of Disentangled Representations. ICML 2019

VAEs for Multimodal Generation



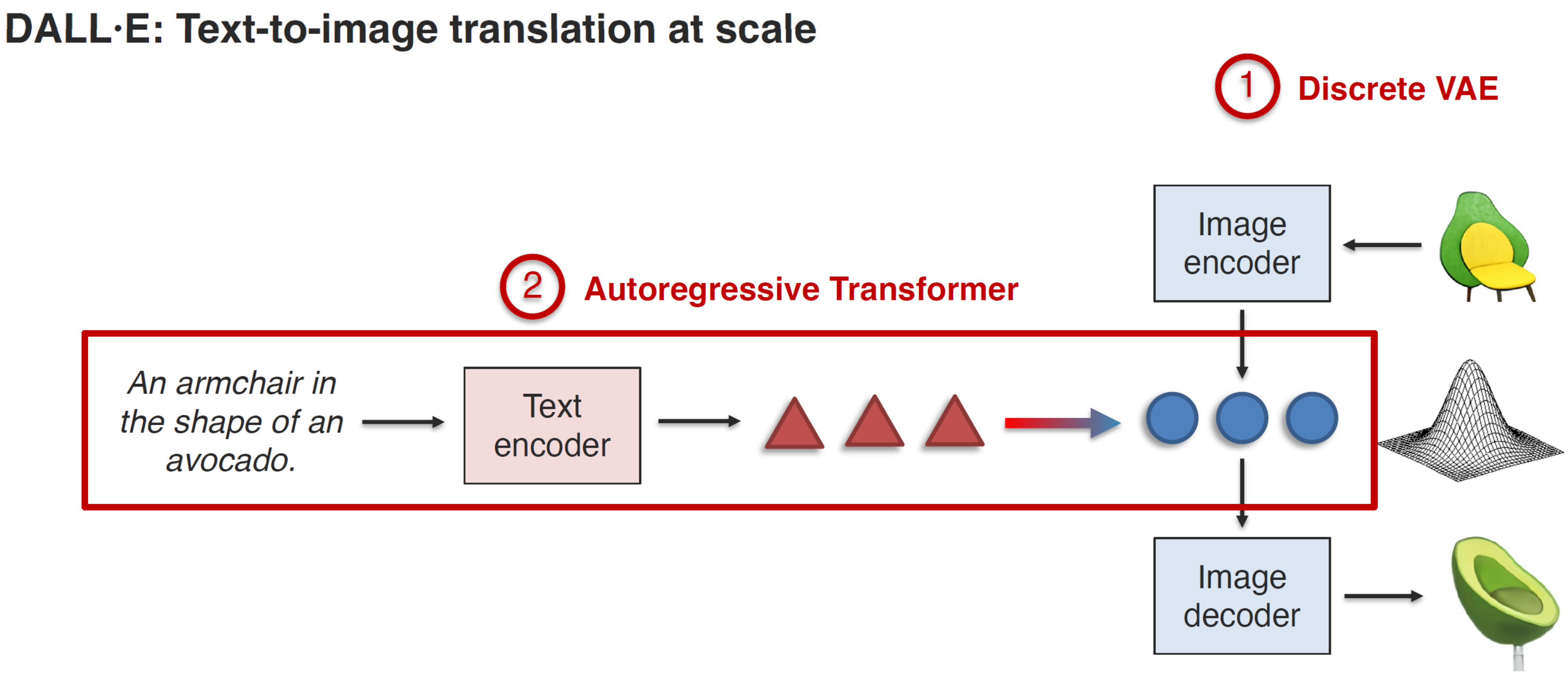
Tsai et al., Learning Factorized Multimodal Representations. ICLR 2019

VAEs for Multimodal Generation



Tsai et al., Learning Factorized Multimodal Representations. ICLR 2019

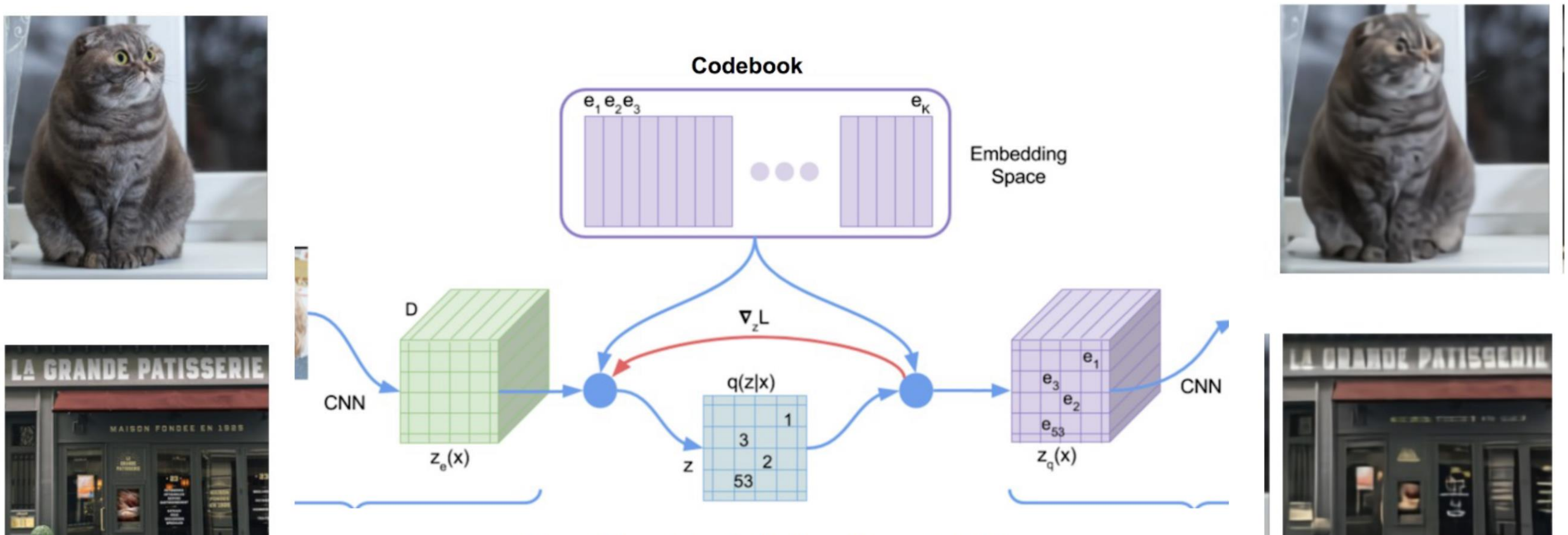
Image Tokens + Transformers



Ramesh et al., Zero-Shot Text-to-Image Generation. ICML 2021

Image Tokens + Transformers

(1) Discrete visual tokens from a VQ-VAE



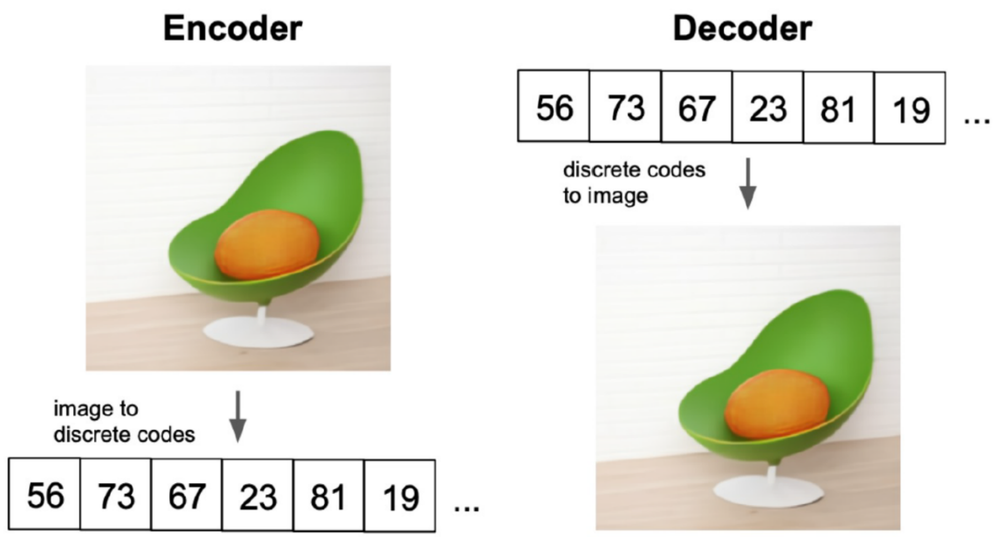
32 x 32 grid of digits, [0… 8192]
Each digit is a “visual token”

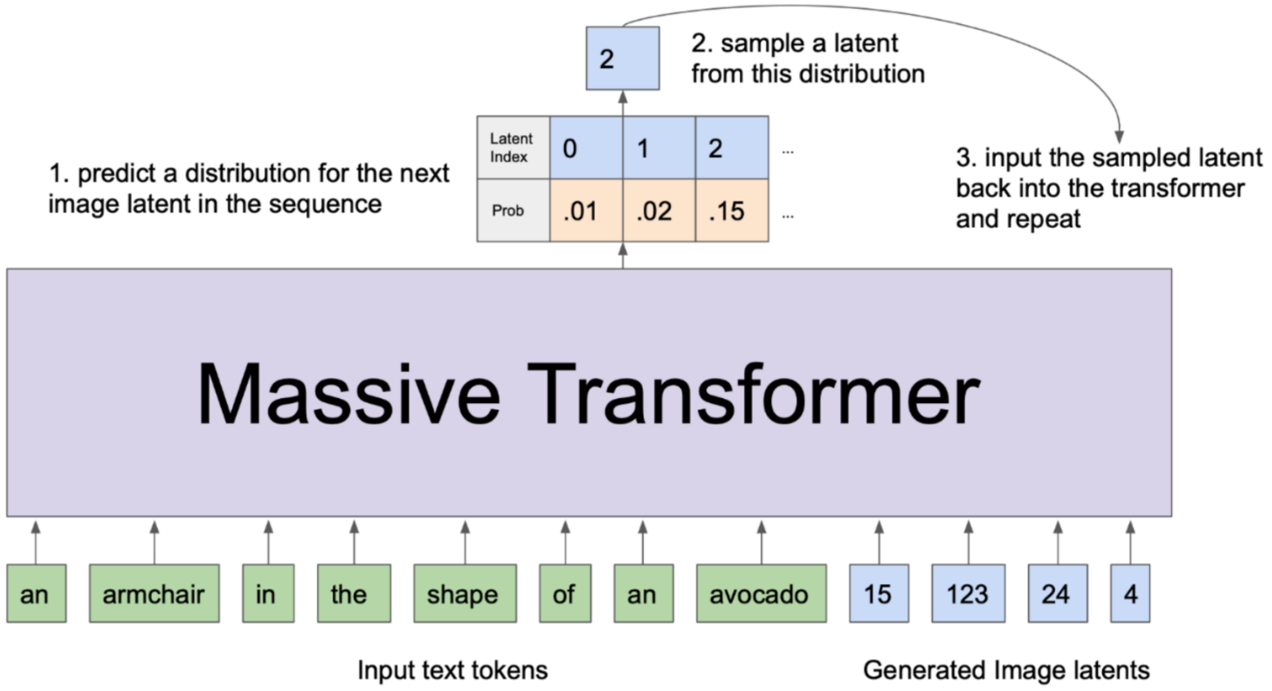
https://arxiv.org/abs/2102.12092, Figures from Charlie Snell, https://ml.berkeley.edu/blog/posts/vq-vae/

Ramesh et al., Zero-Shot Text-to-Image Generation. ICML 2021

Image Tokens + Transformers

(2) Autoregressive generation of the tokens





https://arxiv.org/abs/2102.12092, Figures from Charlie Snell,
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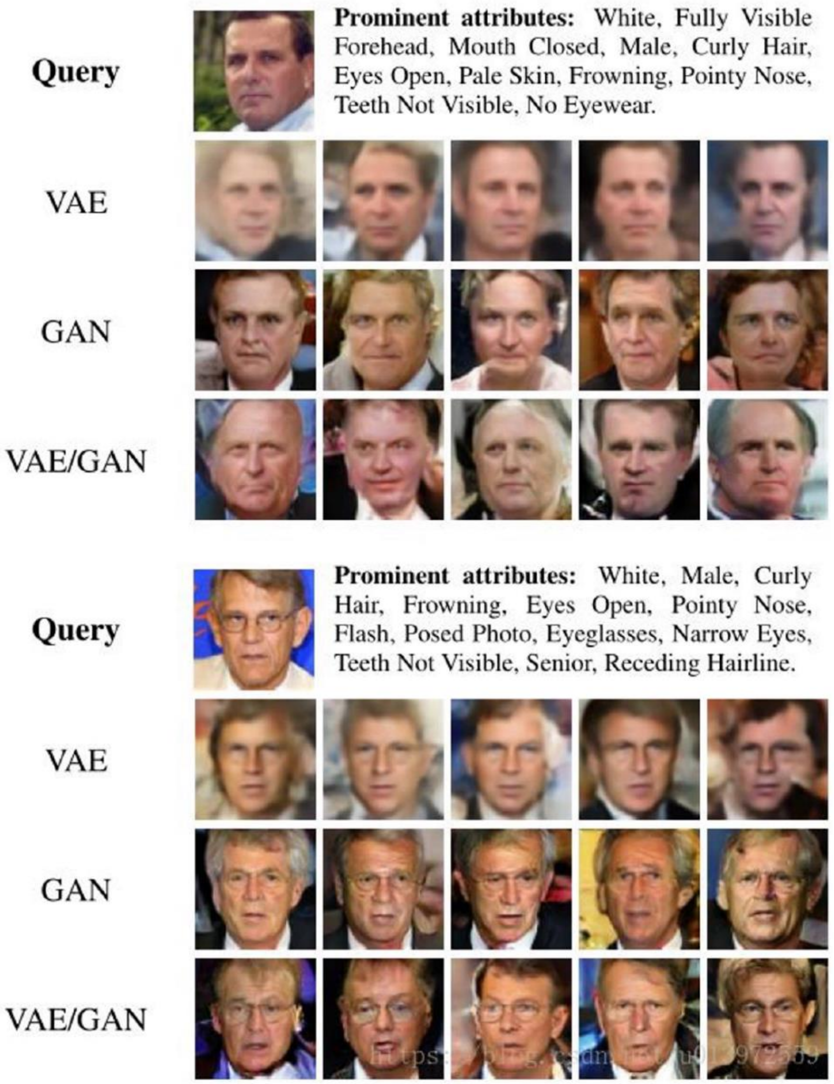
Ramesh et al., Zero-Shot Text-to-Image Generation. ICML 2021

Summary: Variational Autoencoders

- Relatively easy to train.
- Explicit inference network q(z|x).

- More blurry images (due to reconstruction).



Generative Models

① Latent Variable Models

② Autoregressive Models

③ Diffusion Models

④ Generative Adversarial Networks

⑤ Normalizing Flows

More Likelihood-based Models: Autoregressive Models

Autoregressive models

$$p(\mathbf{x}) = \prod_{i=1}^{n^2} p(x_i | x_1, ..., x_{i-1})$$

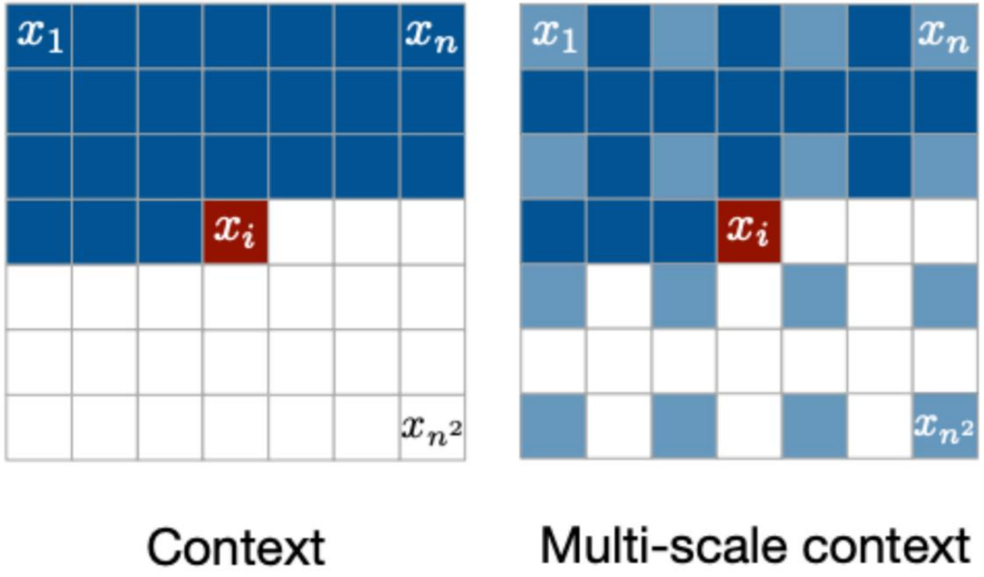


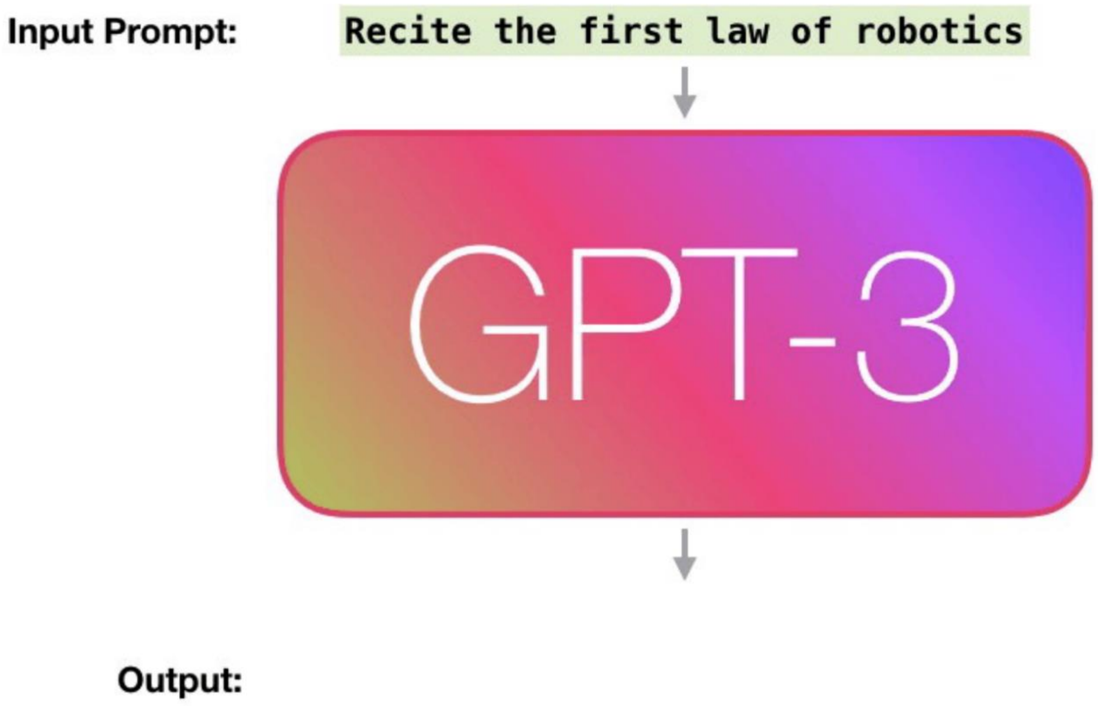
Figure 1. Image completions sampled from a PixelRNN.

[van den Oord et al., Pixel Recurrent Neural Networks. ICML 2016]

Autoregressive Models

Autoregressive language models

$$p(\mathbf{x}) = \prod_{t=1}^{T} p(x_t \mid x_1, \ldots, x_{t-1})$$



[Brown et al., Language Models are Few-shot Learners. NeurIPS 2020]

Fully visible belief network (FVBN)

Explicit density model

$$p(x) = p(x_1, x_2, \ldots, x_n)$$

Likelihood of image x

Joint likelihood of each pixel in the image

Fully visible belief network (FVBN)

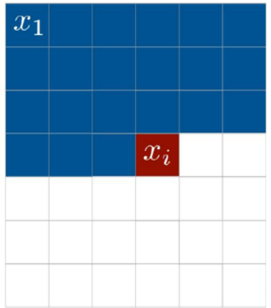
Explicit density model

Use chain rule to decompose likelihood of an image x into product of 1-d distributions:

$$p(x) = \prod_{i=1}^{n} p(x_i | x_1, ..., x_{i-1})$$

Likelihood of image x

Probability of i'th pixel value given all previous pixels



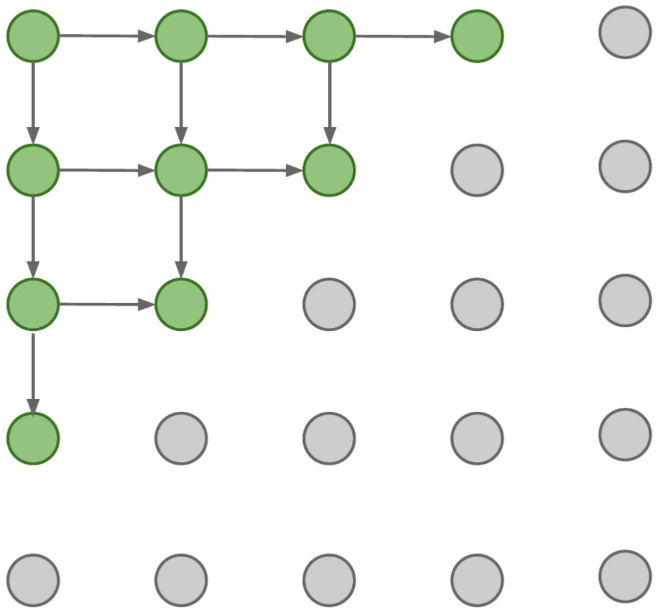
Then maximize likelihood of training data

PixelRNN

Generate image pixels starting from corner

Dependency on previous pixels modeled using an RNN (LSTM)

Drawback: sequential generation is slow in both training and inference!



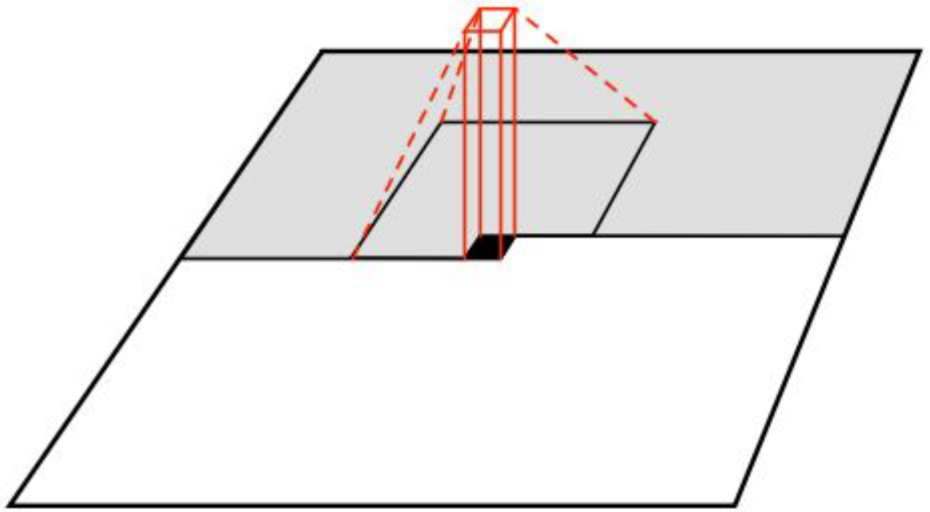
PixelCNN

Still generate image pixels starting from corner

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

Training is faster than PixelRNN
(can parallelize convolutions since context region values known from training images)

Generation is still slow:
For a 32x32 image, we need to do forward passes of the network 1024 times for a single image



Summary: Autoregressive Models

Pros:
- Can explicitly compute likelihood p(x)
- Easy to optimize
- Good samples

Con:
- Sequential generation => slow

Improving PixelCNN performance
- Gated convolutional layers
- Short-cut connections
- Discretized logistic loss
- Multi-scale
- Training tricks
- Etc…

See
- Van der Oord et al. NIPS 2016
- Salimans et al. 2017 (PixelCNN++)

Generative Models

① Latent Variable Models

② Autoregressive Models

③ Diffusion Models

④ Generative Adversarial Networks

⑤ Normalizing Flows

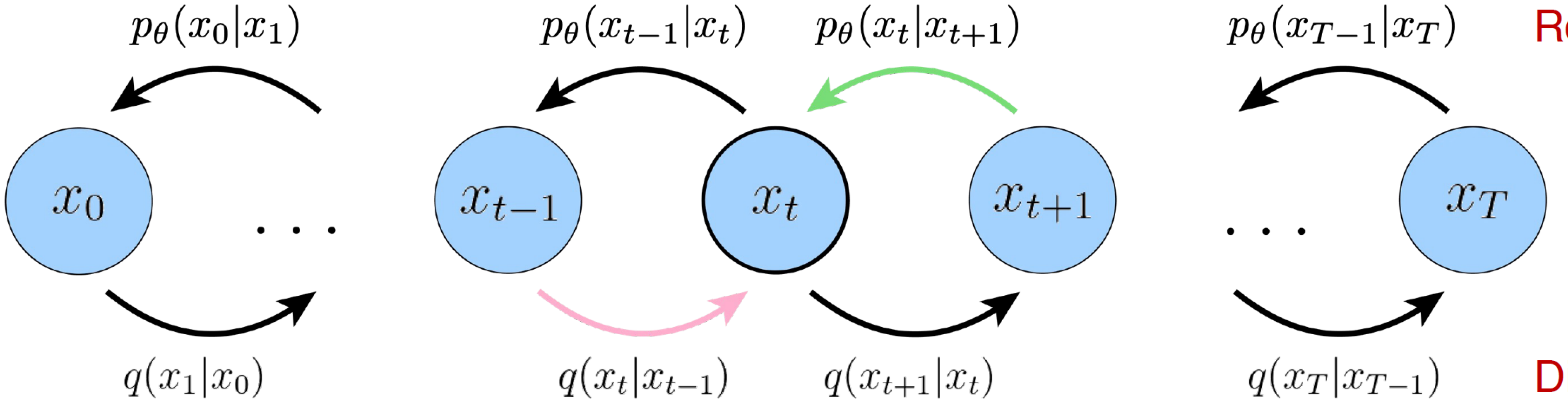
Diffusion Models

Diffusion destroy structures along time

What if we can reverse time?

Image credit: *chongxuan li*

Generative modeling via denoising



Reverse diffusion process

Diffusion process

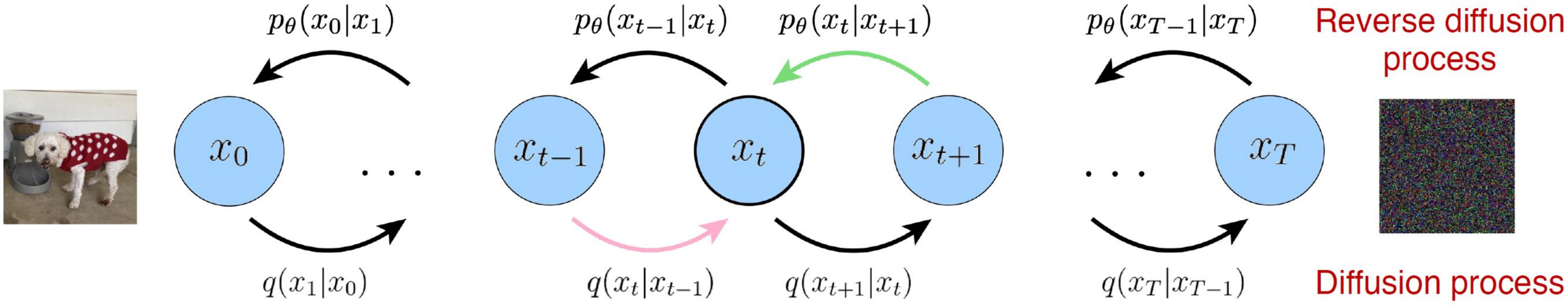
Encoding via adding noise: $q(\boldsymbol{x}_t \mid \boldsymbol{x}_{t-1}) = \mathcal{N}(\boldsymbol{x}_t; \sqrt{\alpha_t}\boldsymbol{x}_{t-1}, (1-\alpha_t)\mathbf{I})$ Noise parameters

Decoding via denoising: $p(\boldsymbol{x}_{0:T}) = p(\boldsymbol{x}_T)\prod_{t=1}^{T} p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1} \mid \boldsymbol{x}_t)$ where $p(\boldsymbol{x}_T) = \mathcal{N}(\boldsymbol{x}_T; \mathbf{0}, \mathbf{I})$

[Tutorial by Calvin Luo and Yang Song]

Diffusion Models

Generative modeling via denoising

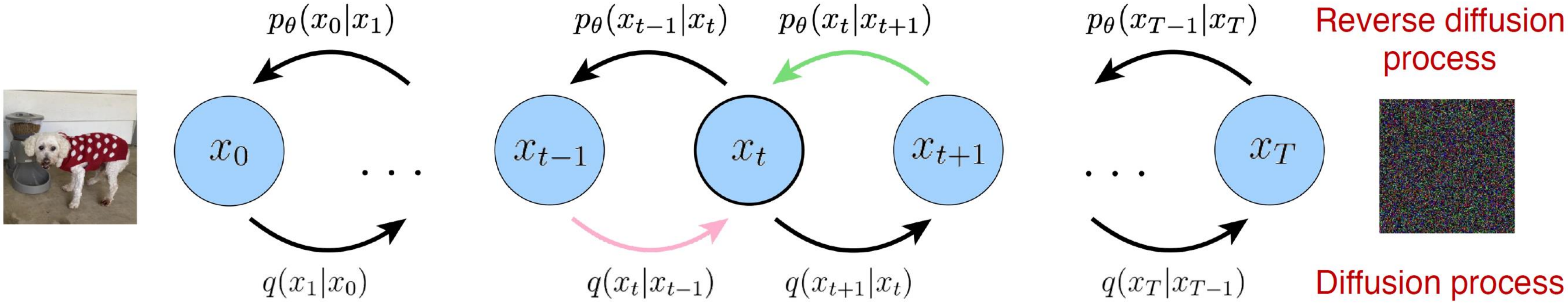


Similar to variational autoencoder, but:

1. The latent dimension is exactly equal to the data dimension.
2. Encoder q is not learned, but pre-defined as a Gaussian distribution centered around the output of previous timestep.
3. Gaussian parameters of latent encoders vary over time such that distribution of final latent is a standard Gaussian.

Learning Diffusion Models

Key idea: use variational inference



$$\log p(\boldsymbol{x}) \geq \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log \frac{p(\boldsymbol{x}_{0:T})}{q(\boldsymbol{x}_{1:T} \mid \boldsymbol{x}_0)}\right]$$

Our old friend the ELBO

$$= \underbrace{\mathbb{E}_{q(\boldsymbol{x}_1|\boldsymbol{x}_0)}\left[\log p_{\boldsymbol{\theta}}(\boldsymbol{x}_0 \mid \boldsymbol{x}_1)\right]}_{\text{reconstruction term}} - \underbrace{\mathcal{D}_{\mathrm{KL}}(q(\boldsymbol{x}_T \mid \boldsymbol{x}_0) \,||\, p(\boldsymbol{x}_T))}_{\text{prior matching term}}$$

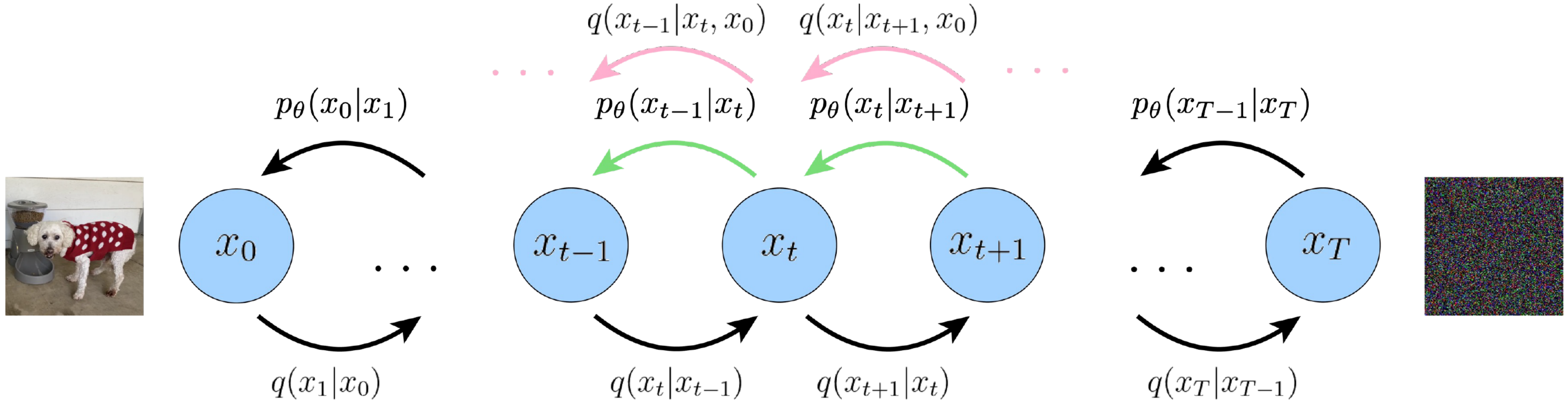
Multi-level VAE!

$$- \sum_{t=2}^{T} \underbrace{\mathbb{E}_{q(\boldsymbol{x}_t|\boldsymbol{x}_0)}\left[\mathcal{D}_{\mathrm{KL}}(q(\boldsymbol{x}_{t-1} \mid \boldsymbol{x}_t, \boldsymbol{x}_0) \,||\, p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1} \mid \boldsymbol{x}_t))\right]}_{\text{denoising matching term}}$$

[Tutorial by Calvin Luo and Yang Song]

Learning Diffusion Models

Key idea: use variational inference



Intuition: Neural network to predict cleaner image x_{t-1} from noisy image x_t at time t, consistent with the noise adding process.

Use Bayes rule to reverse, proportional to a Gaussian

Also parameterize as Gaussian, use reparameteriztion trick

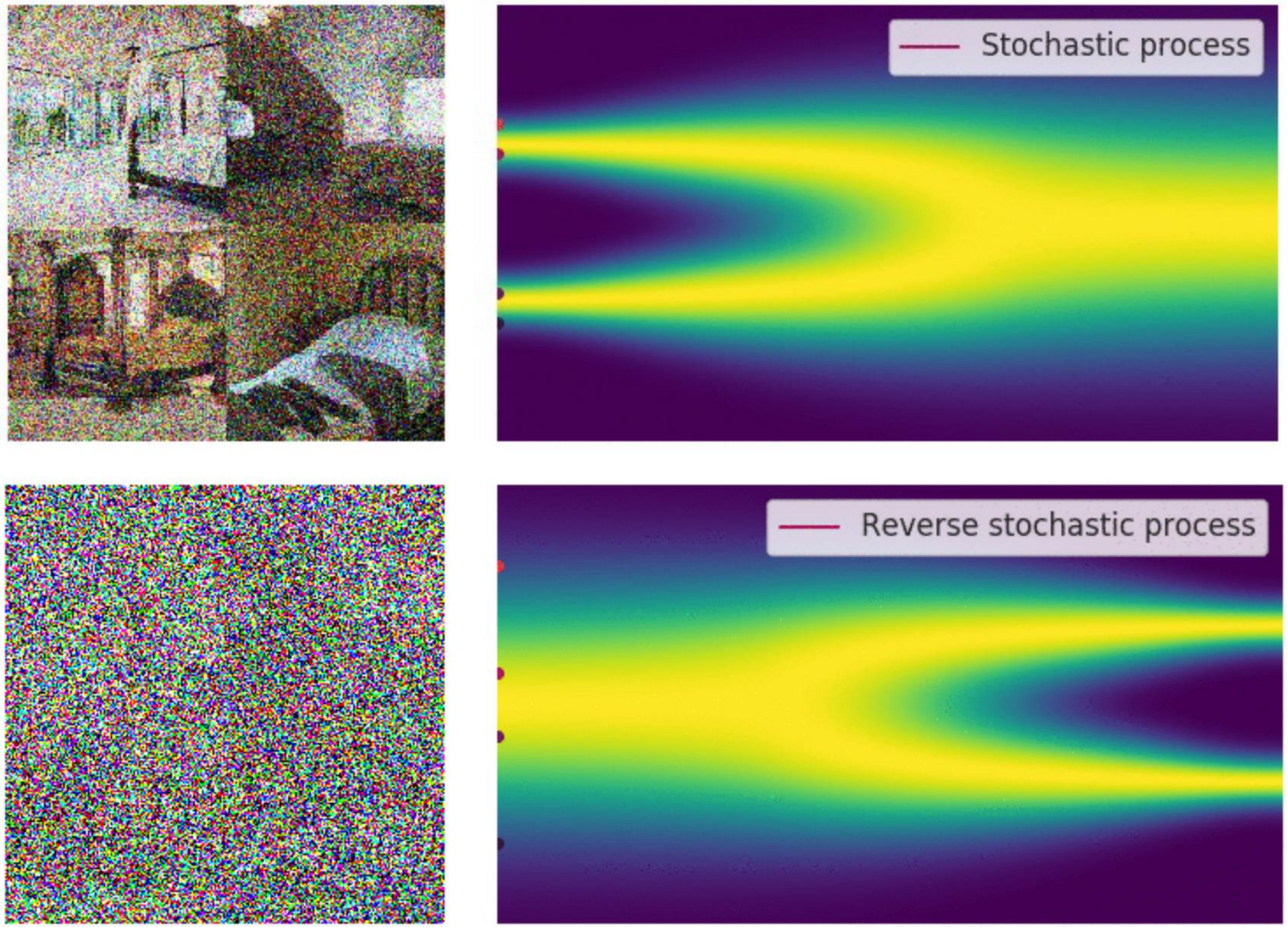
$$-\sum_{t=2}^{T} \underbrace{\mathbb{E}_{q(\boldsymbol{x}_t|\boldsymbol{x}_0)}\left[\mathcal{D}_{\mathrm{KL}}(q(\boldsymbol{x}_{t-1} \mid \boldsymbol{x}_t, \boldsymbol{x}_0) \mid\mid p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1} \mid \boldsymbol{x}_t))\right]}_{\text{denoising matching term}}$$

[Tutorial by Calvin Luo and Yang Song]

Diffusion Models as Differential Equations

From discrete diffusion process to continuous diffusion process

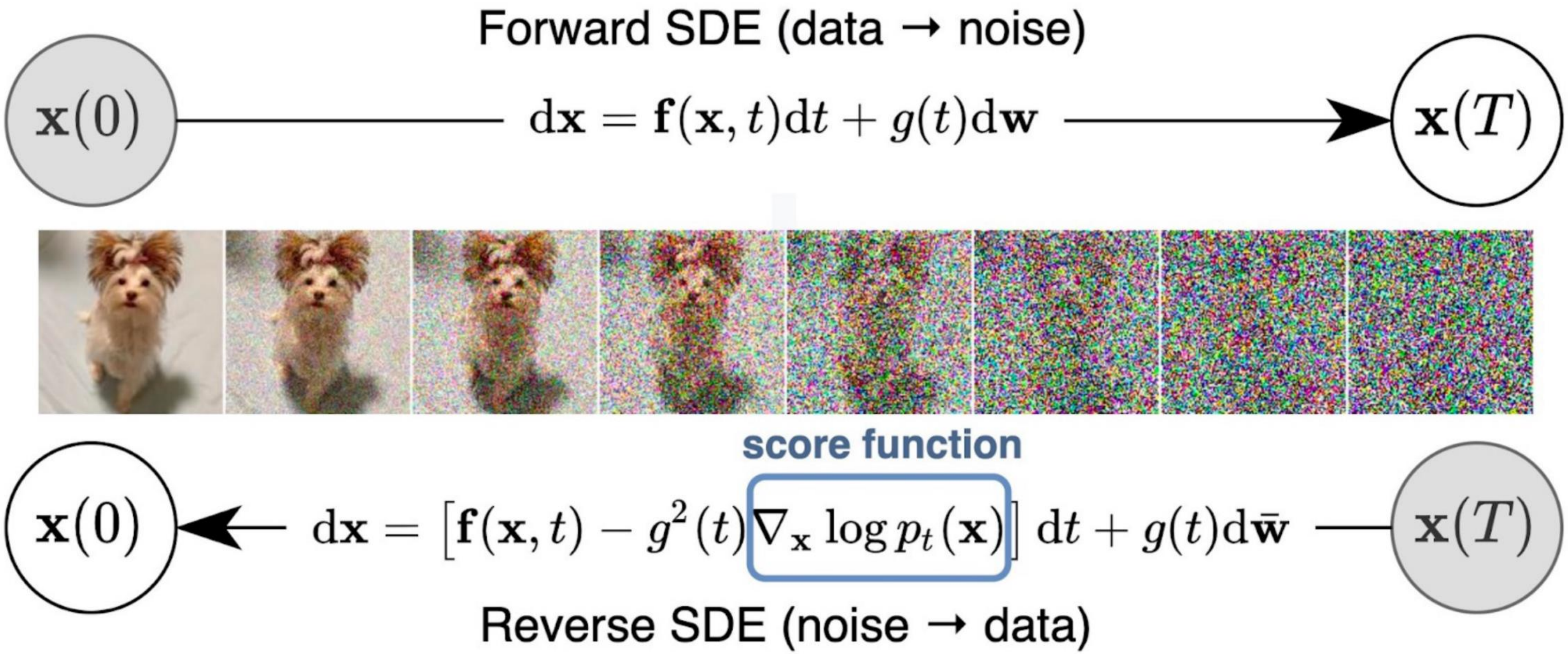
- Higher quality samples
- Exact log-likelihood
- Controllable generation



[Tutorial by Yang Song]

Diffusion Models as Differential Equations

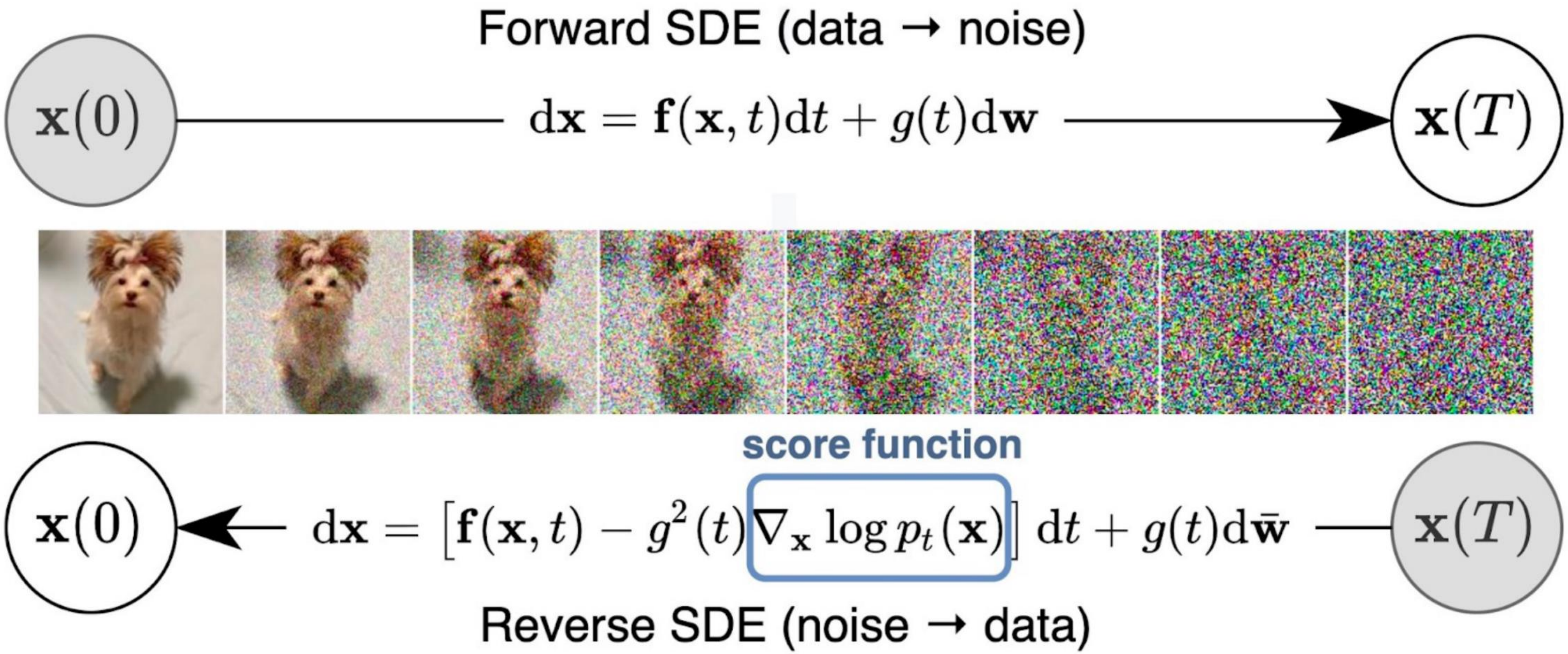
From discrete diffusion process to continuous diffusion process



Think ‘infinite-layer’ latent variable model

Diffusion Models as Differential Equations

From discrete diffusion process to continuous diffusion process



Think ‘infinite-layer’ latent variable model

Diffusion Models as Differential Equations

From discrete diffusion process to continuous diffusion process

Conditioning Diffusion Models on Text

- DALL-E 2 https://cdn.openai.com/papers/dall-e-2.pdf
- Diffusion on top of frozen CLIP

Imagen https://arxiv.org/pdf/2205.11487.pdf

Diffusion on top of frozen T5 embeddings

A black apple and a green backpack.

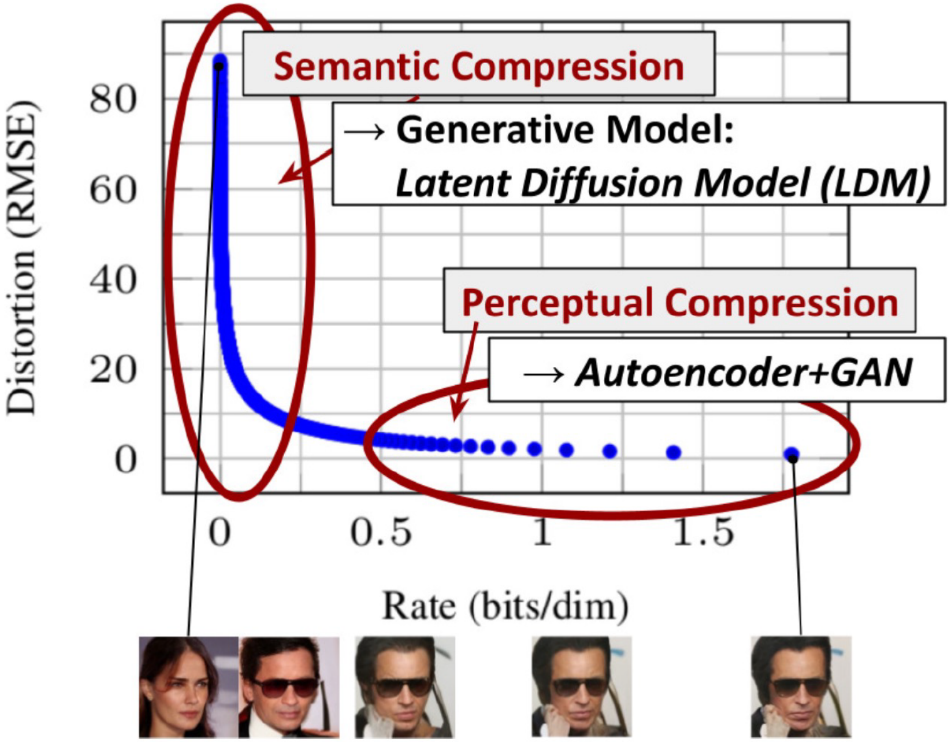
A horse riding an astronaut.

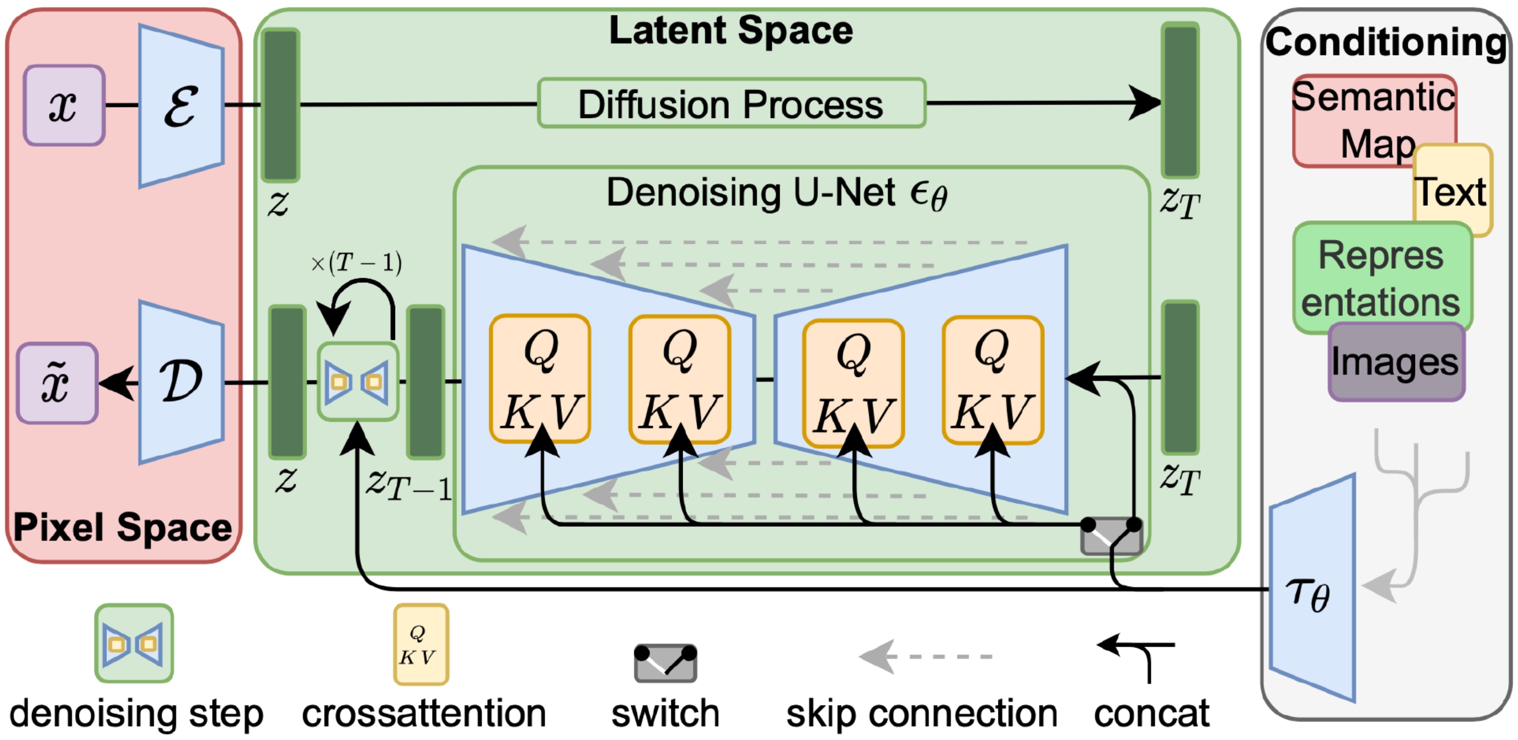
Text-to-Image Generation with Latent Diffusion

1. Directly training diffusion models with conditional information

Diffusion process in latent space instead of pixel space – faster training and inference.

Use autoencoder for perceptual compression, diffusion model for semantic compression.



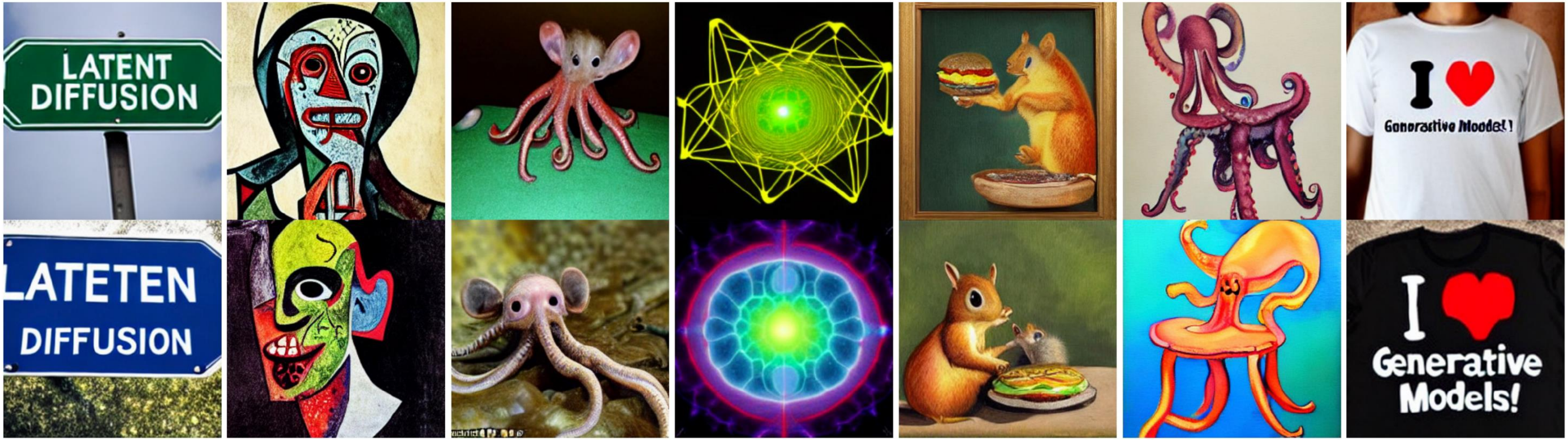


[Rombach et al., High-Resolution Image Synthesis with Latent Diffusion Models. CVPR 2022]

Text-to-Image Generation with Latent Diffusion

Text-to-Image Synthesis on LAION. 1.45B Model.

'A street sign that reads "Latent Diffusion" '	'A zombie in the style of Picasso'	'An image of an animal half mouse half octopus'	'An illustration of a slightly conscious neural network'	'A painting of a squirrel eating a burger'	'A watercolor painting of a chair that looks like an octopus'	'A shirt with the inscription: "I love generative models!" '



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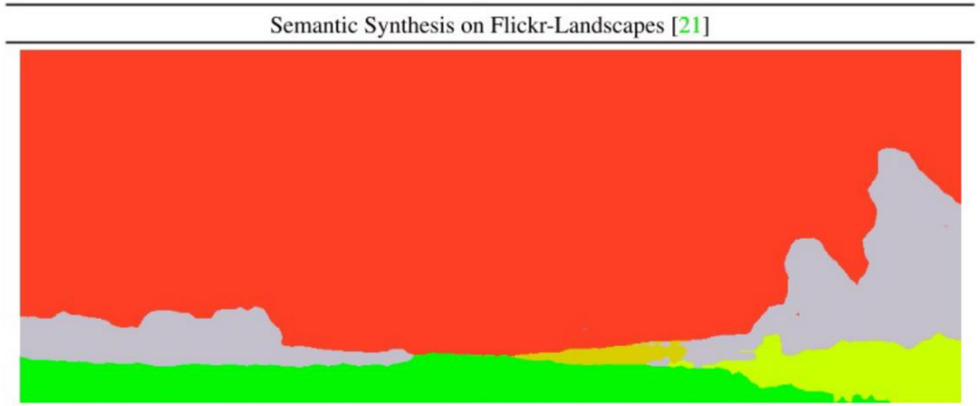

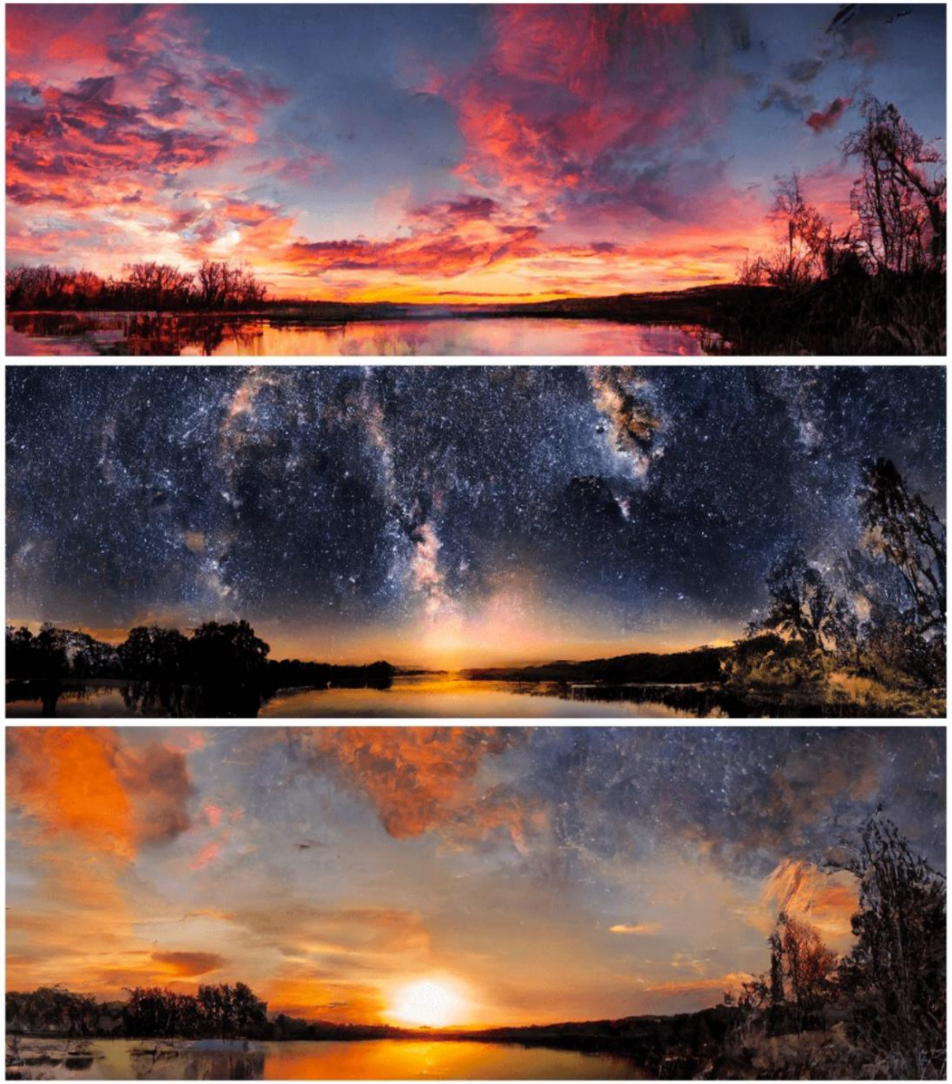

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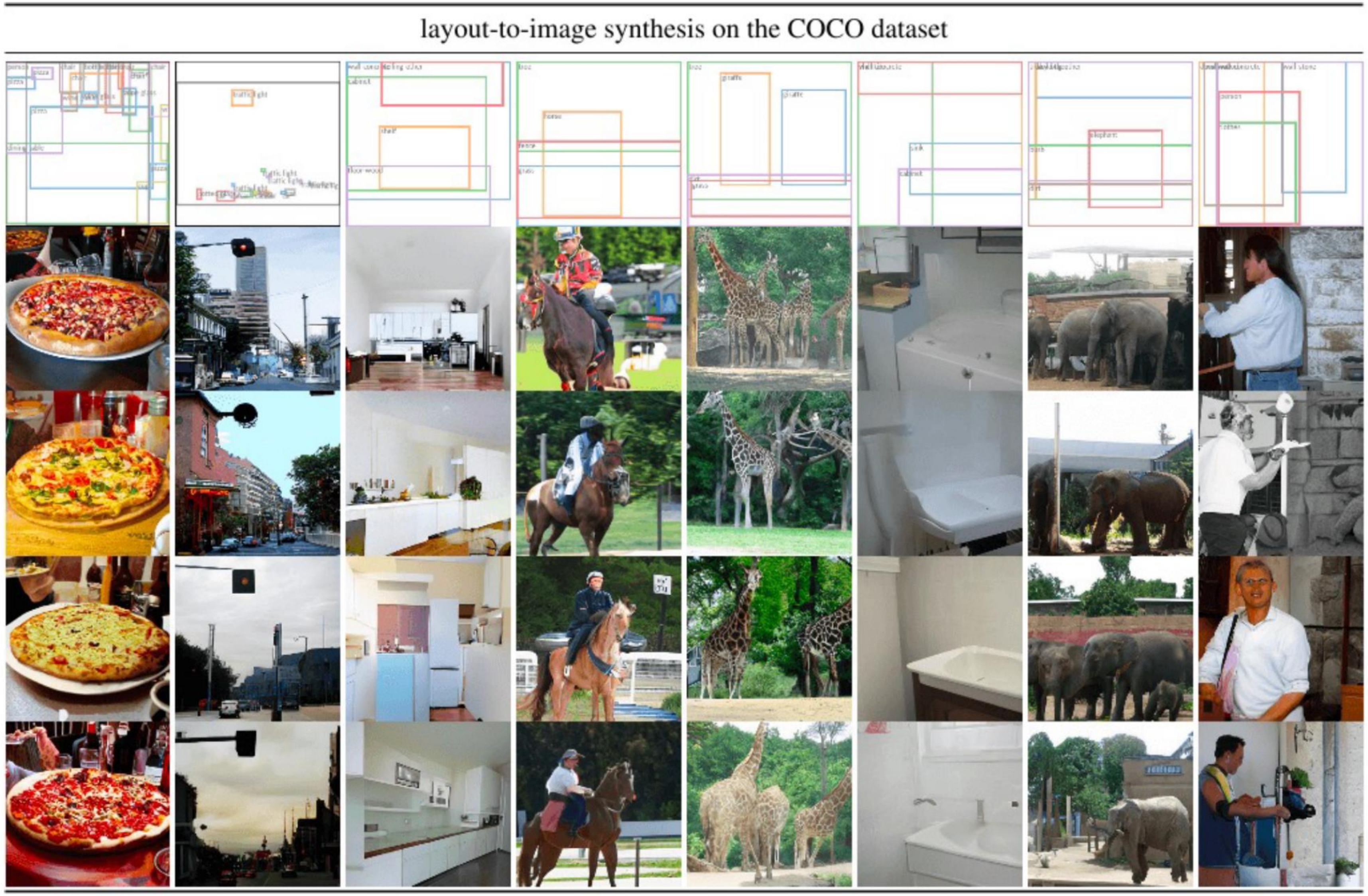

[Rombach et al., High-Resolution Image Synthesis with Latent Diffusion Models. CVPR 2022]

Summary: Diffusion Models

Likelihood-based

1. Autoregressive models – exact inference via chain rule	Easy to train, exact likelihood	Slow to sample from
2. VAEs – approximate inference via evidence lower bound	Fast & easy to train	Lower generation quality
3. Diffusion model – approximate inference via modeling noise	High generation quality	Slow to sample from

Generative Models

① Latent Variable Models

② Autoregressive Models

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④ Generative Adversarial Networks

⑤ Normalizing Flows

So Far…

PixelRNN/CNNs define tractable density function, optimize likelihood of training data:

$$p_\theta(x) = \prod_{i=1}^{n} p_\theta(x_i | x_1, ..., x_{i-1})$$

VAEs define intractable density function with latent **z**:

$$p_\theta(x) = \int p_\theta(z) p_\theta(x|z) dz$$

Cannot optimize directly, derive and optimize lower bound on likelihood instead

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What if we give up on explicitly modeling density, and just want ability to sample?

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What if we give up on explicitly modeling density, and just want ability to sample?

GANs: not modeling any explicit density function!

Generative Adversarial Networks

Problem: Want to sample from complex, high-dimensional training distribution. No direct way to do this!

Solution: Sample from a simple distribution we can easily sample from, e.g. random noise. Learn transformation to training distribution.

Generative Adversarial Networks

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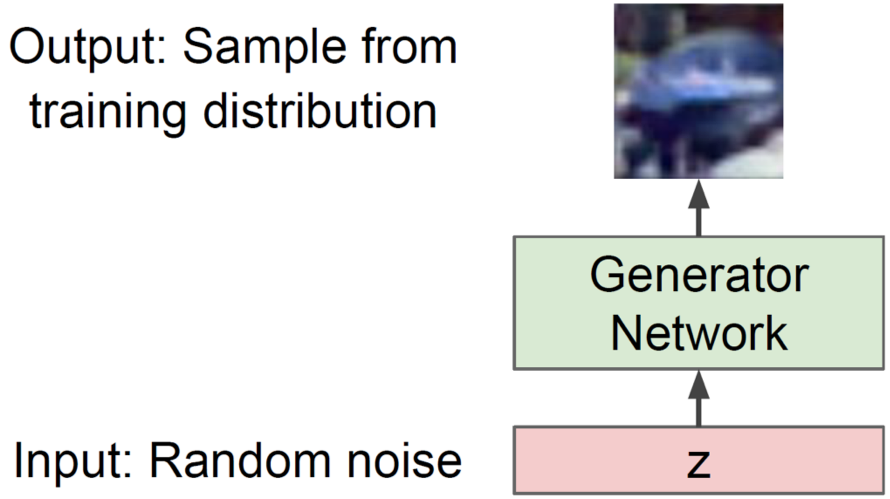

Ian Goodfellow et al., “Generative Adversarial Nets”, NIPS 2014

Generative Adversarial Networks

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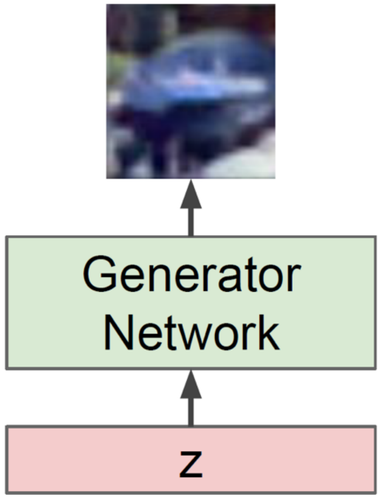
Solution: Sample from a simple distribution we can easily sample from, e.g. random noise. Learn transformation to training distribution.

But we don't know which sample z maps to which training image -> can't learn by reconstructing training images

Output: Sample from training distribution



Input: Random noise

Ian Goodfellow et al., "Generative Adversarial Nets", NIPS 2014

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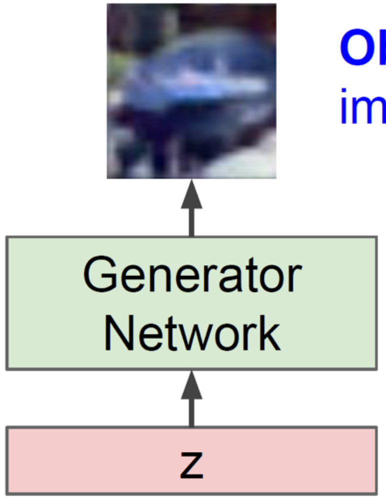
But we don't know which sample z maps to which training image -> can't learn by reconstructing training images

Output: Sample from training distribution



Input: Random noise

Objective: generated images should look "real"

Ian Goodfellow et al., "Generative Adversarial Nets", NIPS 2014

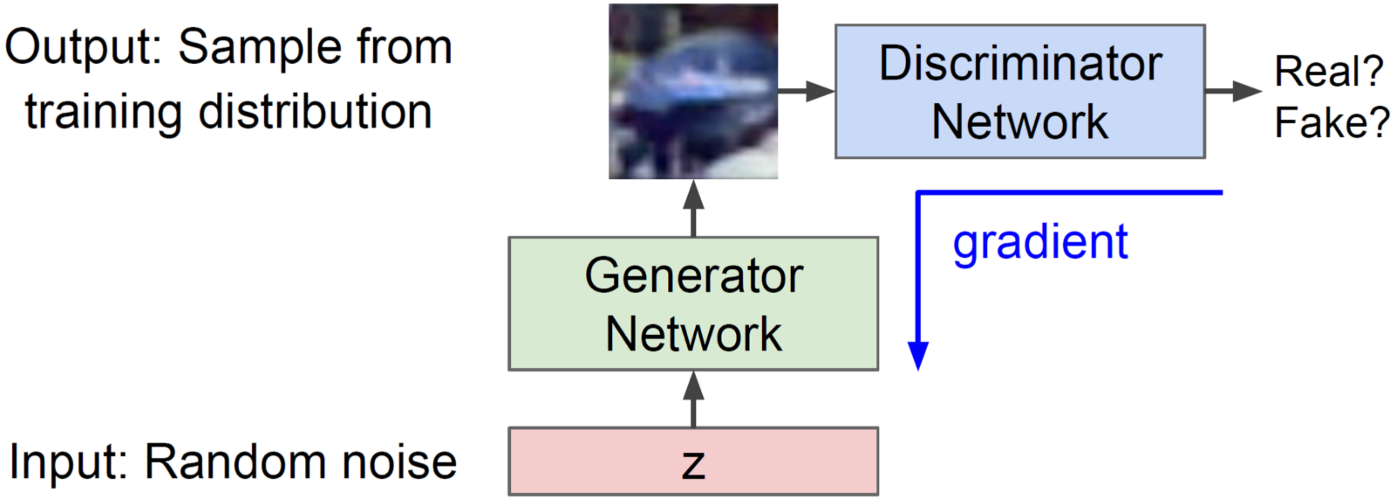
Generative Adversarial Networks

Problem: Want to sample from complex, high-dimensional training distribution. No direct way to do this!

Solution: Sample from a simple distribution we can easily sample from, e.g. random noise. Learn transformation to training distribution.

But we don't know which sample z maps to which training image -> can't learn by reconstructing training images

Solution: Use a discriminator network to tell whether the generate image is within data distribution ("real") or not



Ian Goodfellow et al., "Generative Adversarial Nets", NIPS 2014

Training GANs: Two-player game

Discriminator network: try to distinguish between real and fake images
Generator network: try to fool the discriminator by generating real-looking images

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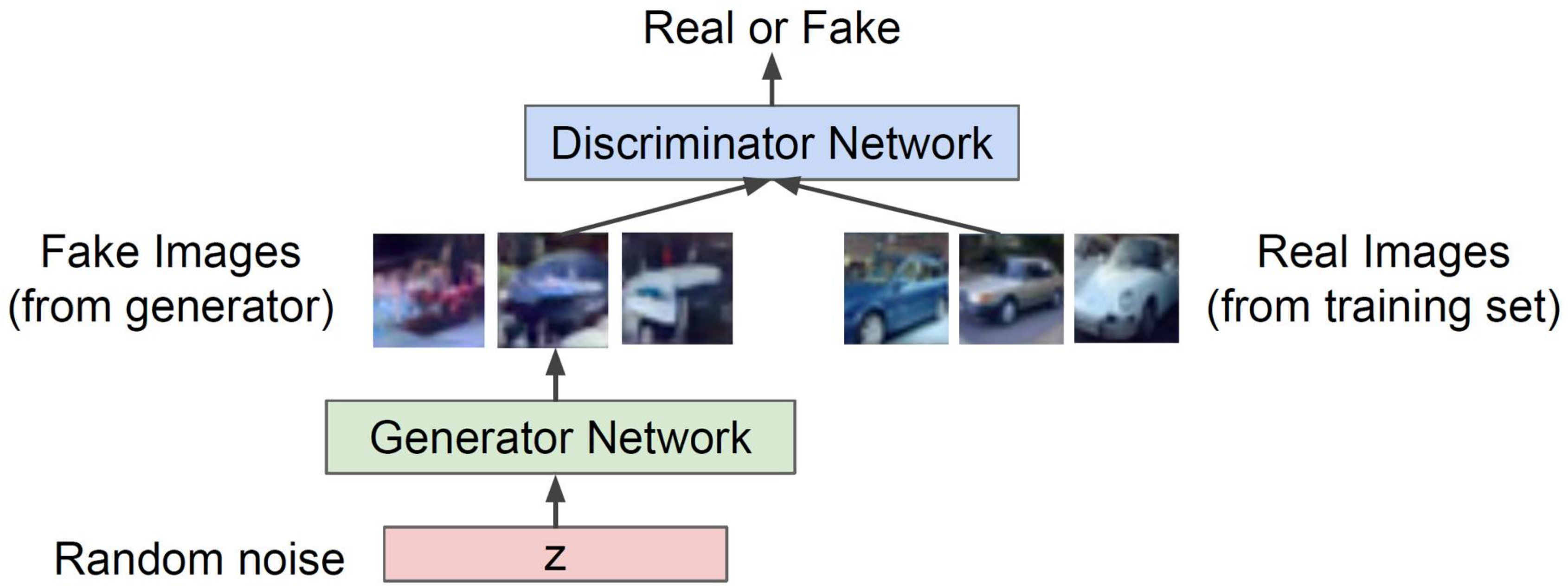

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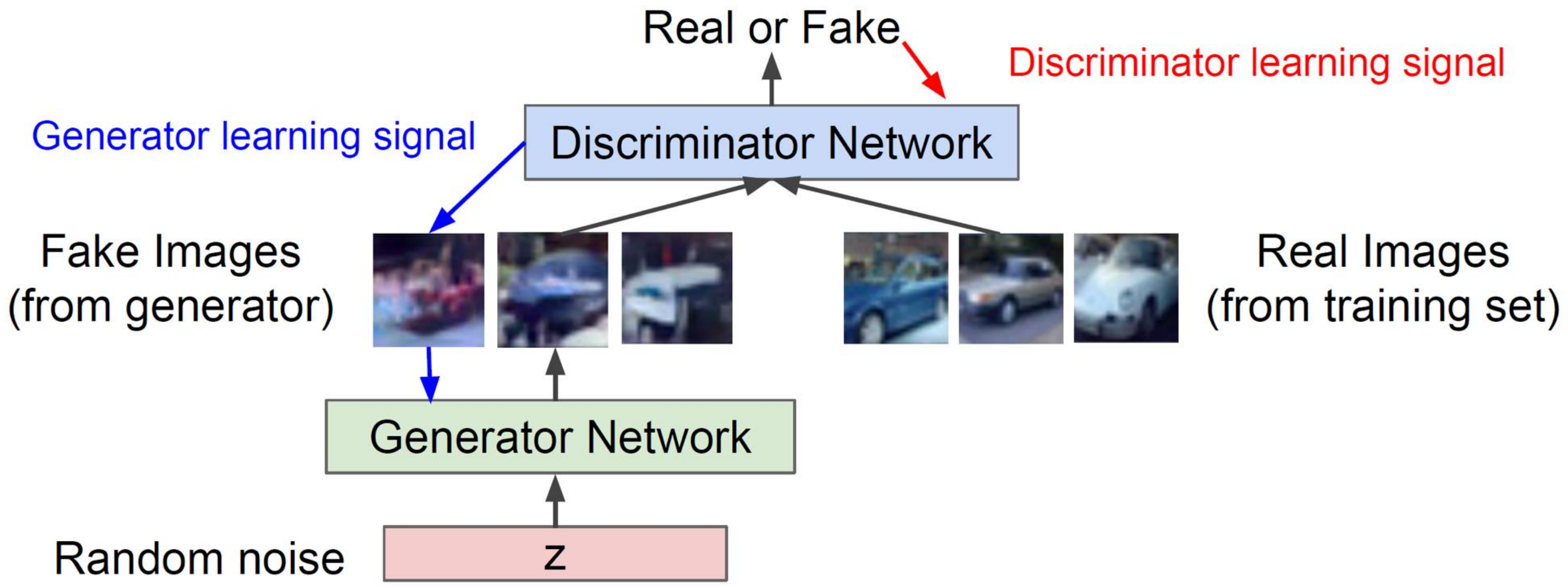

Ian Goodfellow et al., “Generative Adversarial Nets”, NIPS 2014

Training GANs: Two-player game

Discriminator network: try to distinguish between real and fake images
Generator network: try to fool the discriminator by generating real-looking images

Train jointly in **minimax game**

Minimax objective function:

$$\min_{\theta_g} \max_{\theta_d} \left[\mathbb{E}_{x \sim p_{data}} \log D_{\theta_d}(x) + \mathbb{E}_{z \sim p(z)} \log(1 - D_{\theta_d}(G_{\theta_g}(z))) \right]$$

Generator objective

Discriminator objective

Training GANs: Two-player game

Discriminator network: try to distinguish between real and fake images
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Minimax objective function:

Discriminator outputs likelihood in (0,1) of real image

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Discriminator output for real data x

Discriminator output for generated fake data G(z)

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$$\min_{\theta_g} \max_{\theta_d} \left[\mathbb{E}_{x \sim p_{data}} \log \underbrace{D_{\theta_d}(x)} + \mathbb{E}_{z \sim p(z)} \log(1 - \underbrace{D_{\theta_d}(G_{\theta_g}(z))}) \right]$$

Discriminator output for real data x

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Minimax objective function:

Discriminator outputs likelihood in (0,1) of real image

$$\min_{\theta_g} \max_{\theta_d} \left[\mathbb{E}_{x \sim p_{data}} \log \underbrace{D_{\theta_d}(x)}_{\text{Discriminator output for real data x}} + \mathbb{E}_{z \sim p(z)} \log(1 - \underbrace{D_{\theta_d}(G_{\theta_g}(z))}_{\text{Discriminator output for generated fake data G(z)}}) \right]$$

- Discriminator (θ_d) wants to **maximize objective** such that D(x) is close to 1 (real) and D(G(z)) is close to 0 (fake)
- Generator (θ_g) wants to **minimize objective** such that D(G(z)) is close to 1 (discriminator is fooled into thinking generated G(z) is real)

Ian Goodfellow et al., "Generative Adversarial Nets", NIPS 2014

Training GANs: Two-player game

Minimax objective function:

$$\min_{\theta_g} \max_{\theta_d} \left[\mathbb{E}_{x \sim p_{data}} \log D_{\theta_d}(x) + \mathbb{E}_{z \sim p(z)} \log(1 - D_{\theta_d}(G_{\theta_g}(z))) \right]$$

Alternate between:

1. **Gradient ascent** on discriminator

$$\max_{\theta_d} \left[\mathbb{E}_{x \sim p_{data}} \log D_{\theta_d}(x) + \mathbb{E}_{z \sim p(z)} \log(1 - D_{\theta_d}(G_{\theta_g}(z))) \right]$$

2. **Gradient descent** on generator

$$\min_{\theta_g} \mathbb{E}_{z \sim p(z)} \log(1 - D_{\theta_d}(G_{\theta_g}(z)))$$

Ian Goodfellow et al., “Generative Adversarial Nets”, NIPS 2014

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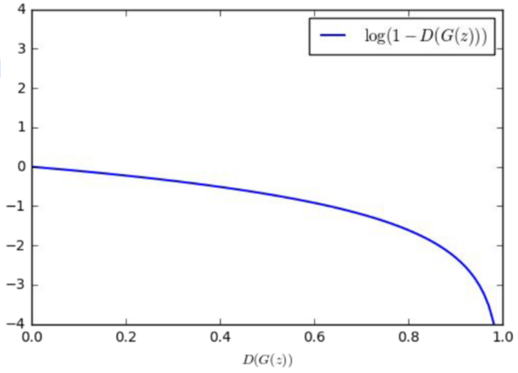
2. **Gradient descent** on generator

$$\min_{\theta_g} \mathbb{E}_{z \sim p(z)} \log(1 - D_{\theta_d}(G_{\theta_g}(z)))$$

In practice, optimizing this generator objective does not work well!

When sample is likely fake, want to learn from it to improve generator (move to the right on X axis).



Ian Goodfellow et al., "Generative Adversarial Nets", NIPS 2014

Training GANs: Two-player game

Minimax objective function:

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Alternate between:

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$$\max_{\theta_d} \left[\mathbb{E}_{x \sim p_{data}} \log D_{\theta_d}(x) + \mathbb{E}_{z \sim p(z)} \log(1 - D_{\theta_d}(G_{\theta_g}(z))) \right]$$

2. **Gradient descent** on generator

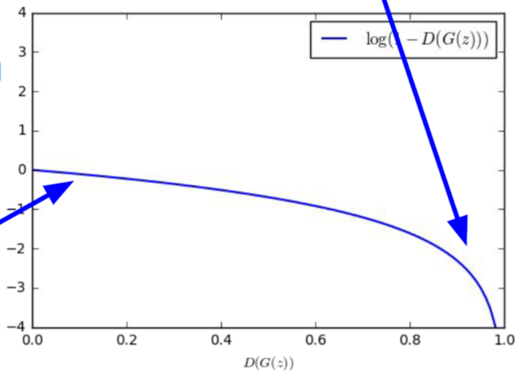
$$\min_{\theta_g} \mathbb{E}_{z \sim p(z)} \log(1 - D_{\theta_d}(G_{\theta_g}(z)))$$

In practice, optimizing this generator objective does not work well!

When sample is likely fake, want to learn from it to improve generator (move to the right on X axis).

But gradient in this region is relatively flat!

Gradient signal dominated by region where sample is already good



Ian Goodfellow et al., "Generative Adversarial Nets", NIPS 2014

Training GANs: Two-player game

Minimax objective function:

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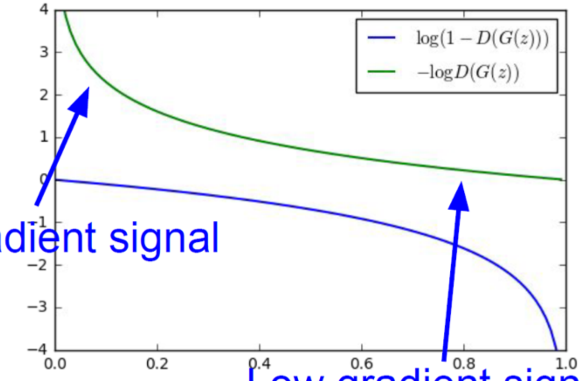
$$\max_{\theta_d} \left[\mathbb{E}_{x \sim p_{data}} \log D_{\theta_d}(x) + \mathbb{E}_{z \sim p(z)} \log(1 - D_{\theta_d}(G_{\theta_g}(z))) \right]$$

2. **Instead: Gradient ascent** on generator, different objective

$$\max_{\theta_g} \mathbb{E}_{z \sim p(z)} \log(D_{\theta_d}(G_{\theta_g}(z)))$$

Instead of minimizing likelihood of discriminator being correct, now maximize likelihood of discriminator being wrong.
Same objective of fooling discriminator, but now higher gradient signal for bad samples => works much better! Standard in practice.



High gradient signal

Low gradient signal

Ian Goodfellow et al., "Generative Adversarial Nets", NIPS 2014

Training GANs: Two-player game

Putting it together: GAN training algorithm

for number of training iterations **do**

  for k steps **do**

  - Sample minibatch of m noise samples $\{\boldsymbol{z}^{(1)}, \ldots, \boldsymbol{z}^{(m)}\}$ from noise prior $p_g(\boldsymbol{z})$.
  - Sample minibatch of m examples $\{\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(m)}\}$ from data generating distribution $p_{\text{data}}(\boldsymbol{x})$.
  - Update the discriminator by ascending its stochastic gradient:

$$\nabla_{\theta_d} \frac{1}{m} \sum_{i=1}^{m} \left[\log D_{\theta_d}(x^{(i)}) + \log(1 - D_{\theta_d}(G_{\theta_g}(z^{(i)}))) \right]$$

  end for

- Sample minibatch of m noise samples $\{\boldsymbol{z}^{(1)}, \ldots, \boldsymbol{z}^{(m)}\}$ from noise prior $p_g(\boldsymbol{z})$.
- Update the generator by ascending its stochastic gradient (improved objective):

$$\nabla_{\theta_g} \frac{1}{m} \sum_{i=1}^{m} \log(D_{\theta_d}(G_{\theta_g}(z^{(i)})))$$

end for

Ian Goodfellow et al., “Generative Adversarial Nets”, NIPS 2014

Training GANs: Two-player game

Putting it together: GAN training algorithm

for number of training iterations **do**
  for k steps **do**
  - Sample minibatch of m noise samples $\{\boldsymbol{z}^{(1)}, \ldots, \boldsymbol{z}^{(m)}\}$ from noise prior $p_g(\boldsymbol{z})$.
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  end for
  - Sample minibatch of m noise samples $\{\boldsymbol{z}^{(1)}, \ldots, \boldsymbol{z}^{(m)}\}$ from noise prior $p_g(\boldsymbol{z})$.
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$$\nabla_{\theta_g} \frac{1}{m} \sum_{i=1}^{m} \log(D_{\theta_d}(G_{\theta_g}(z^{(i)})))$$

end for

Some find k=1 more stable, others use k > 1, no best rule.

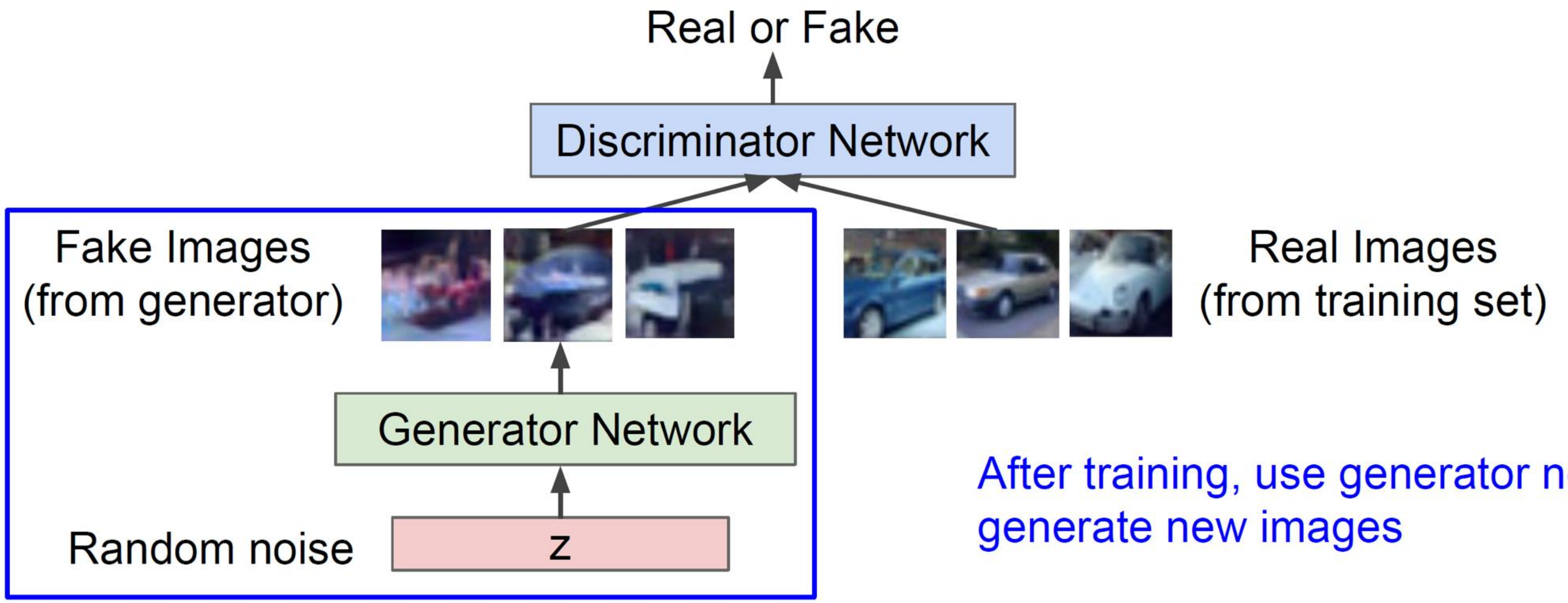
Followup work (e.g. Wasserstein GAN, BEGAN) alleviates this problem, better stability!

Arjovsky et al. "Wasserstein gan." arXiv preprint arXiv:1701.07875 (2017)
Berthelot, et al. "Began: Boundary equilibrium generative adversarial networks." arXiv preprint arXiv:1703.10717 (2017)

Ian Goodfellow et al., "Generative Adversarial Nets", NIPS 2014

Training GANs: Two-player game

Generator network: try to fool the discriminator by generating real-looking images
Discriminator network: try to distinguish between real and fake images



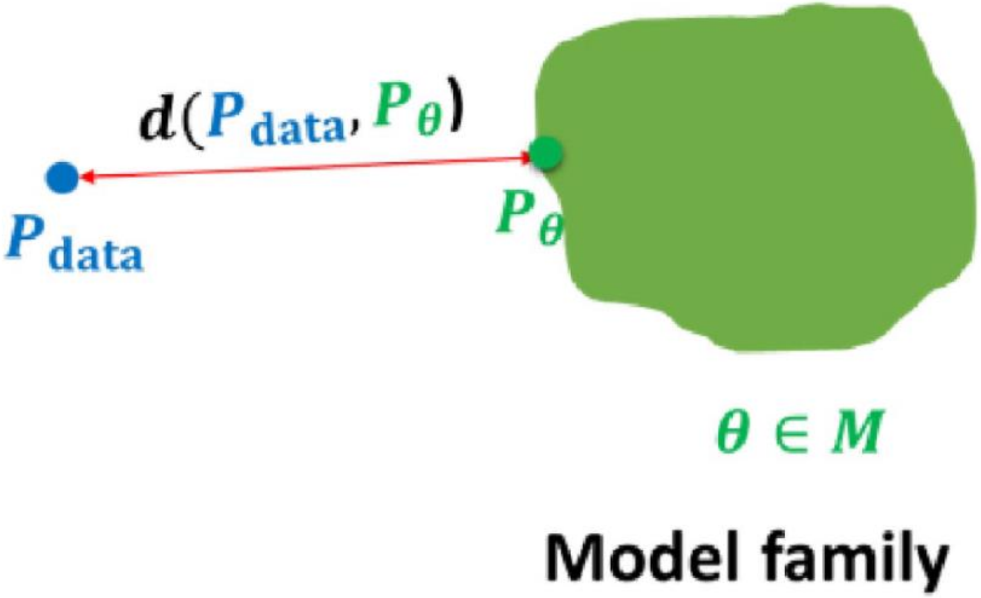
After training, use generator network to generate new images

Ian Goodfellow et al., “Generative Adversarial Nets”, NIPS 2014

Minimizing the distribution distance

Maximizing the discriminator is actually estimating the distribution distance between the data and the model!!!

$\mathbf{x}_i \sim P_{\text{data}}$
$i = 1, 2, \ldots, n$



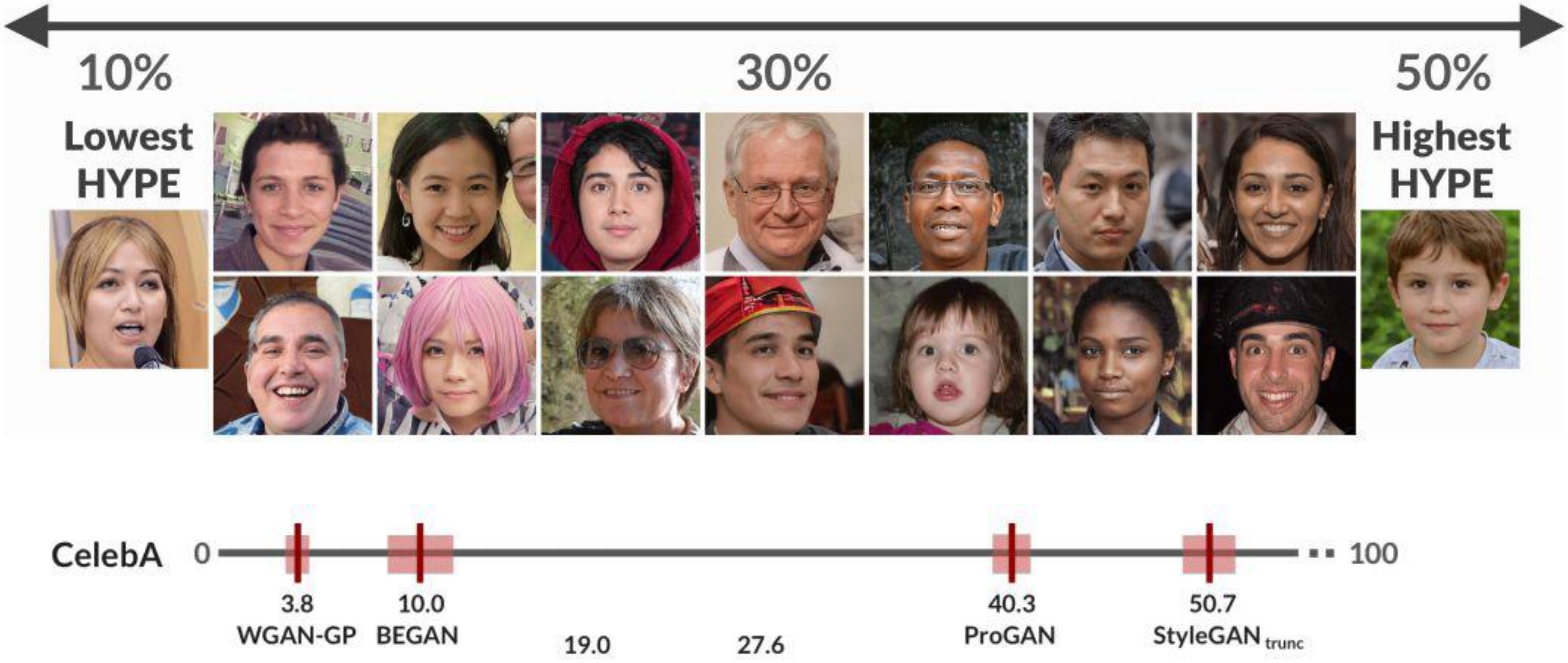
Ian Goodfellow et al., "Generative Adversarial Nets", NIPS 2014

Generative Adversarial Nets: Convolutional Architectures

Radford et al, ICLR 2016

2019: BigGAN

HYPE: Human eYe Perceptual Evaluations



hype.stanford.edu

Explosion of GANs

“The GAN Zoo”

- GAN - Generative Adversarial Networks
- 3D-GAN - Learning a Probabilistic Latent Space of Object Shapes via 3D Generative-Adversarial Modeling
- acGAN - Face Aging With Conditional Generative Adversarial Networks
- AC-GAN - Conditional Image Synthesis With Auxiliary Classifier GANs
- AdaGAN - AdaGAN: Boosting Generative Models
- AEGAN - Learning Inverse Mapping by Autoencoder based Generative Adversarial Nets
- AffGAN - Amortised MAP Inference for Image Super-resolution
- AL-CGAN - Learning to Generate Images of Outdoor Scenes from Attributes and Semantic Layouts
- ALI - Adversarially Learned Inference
- AM-GAN - Generative Adversarial Nets with Labeled Data by Activation Maximization
- AnoGAN - Unsupervised Anomaly Detection with Generative Adversarial Networks to Guide Marker Discovery
- ArtGAN - ArtGAN: Artwork Synthesis with Conditional Categorial GANs
- b-GAN - b-GAN: Unified Framework of Generative Adversarial Networks
- Bayesian GAN - Deep and Hierarchical Implicit Models
- BEGAN - BEGAN: Boundary Equilibrium Generative Adversarial Networks
- BiGAN - Adversarial Feature Learning
- BS-GAN - Boundary-Seeking Generative Adversarial Networks
- CGAN - Conditional Generative Adversarial Nets
- CaloGAN - CaloGAN: Simulating 3D High Energy Particle Showers in Multi-Layer Electromagnetic Calorimeters with Generative Adversarial Networks
- CCGAN - Semi-Supervised Learning with Context-Conditional Generative Adversarial Networks
- CatGAN - Unsupervised and Semi-supervised Learning with Categorical Generative Adversarial Networks
- CoGAN - Coupled Generative Adversarial Networks
- Context-RNN-GAN - Contextual RNN-GANs for Abstract Reasoning Diagram Generation
- C-RNN-GAN - C-RNN-GAN: Continuous recurrent neural networks with adversarial training
- CS-GAN - Improving Neural Machine Translation with Conditional Sequence Generative Adversarial Nets
- CVAE-GAN - CVAE-GAN: Fine-Grained Image Generation through Asymmetric Training
- CycleGAN - Unpaired Image-to-Image Translation using Cycle-Consistent Adversarial Networks
- DTN - Unsupervised Cross-Domain Image Generation
- DCGAN - Unsupervised Representation Learning with Deep Convolutional Generative Adversarial Networks
- DiscoGAN - Learning to Discover Cross-Domain Relations with Generative Adversarial Networks
- DR-GAN - Disentangled Representation Learning GAN for Pose-Invariant Face Recognition
- DualGAN - DualGAN: Unsupervised Dual Learning for Image-to-Image Translation
- EBGAN - Energy-based Generative Adversarial Network
- f-GAN - f-GAN: Training Generative Neural Samplers using Variational Divergence Minimization
- FF-GAN - Towards Large-Pose Face Frontalization in the Wild
- GAWWN - Learning What and Where to Draw
- GeneGAN - GeneGAN: Learning Object Transfiguration and Attribute Subspace from Unpaired Data
- Geometric GAN - Geometric GAN
- GoGAN - Gang of GANs: Generative Adversarial Networks with Maximum Margin Ranking
- GP-GAN - GP-GAN: Towards Realistic High-Resolution Image Blending
- IAN - Neural Photo Editing with Introspective Adversarial Networks
- iGAN - Generative Visual Manipulation on the Natural Image Manifold
- IcGAN - Invertible Conditional GANs for image editing
- ID-CGAN - Image De-raining Using a Conditional Generative Adversarial Network
- Improved GAN - Improved Techniques for Training GANs
- InfoGAN - InfoGAN: Interpretable Representation Learning by Information Maximizing Generative Adversarial Nets
- LAGAN - Learning Particle Physics by Example: Location-Aware Generative Adversarial Networks for Physics Synthesis
- LAPGAN - Deep Generative Image Models using a Laplacian Pyramid of Adversarial Networks

https://github.com/hindupuravinash/the-gan-zoo

Generative Models

① Latent Variable Models

② Autoregressive Models

③ Diffusion Models

④ Generative Adversarial Networks

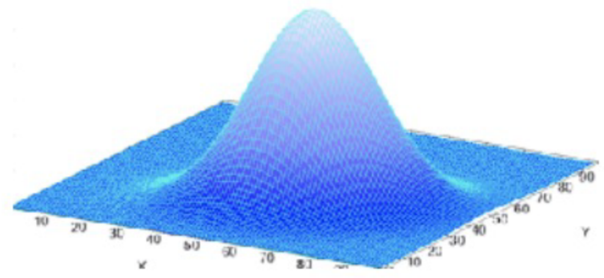
⑤ Normalizing Flows

Normalizing Flows

Model families so far:

- **Autoregressive models** provide tractable likelihoods but no direct mechanism for learning features.
- **Variational autoencoders** can learn feature representations (via latent variables z) but have intractable marginal likelihoods.

Can we do both?



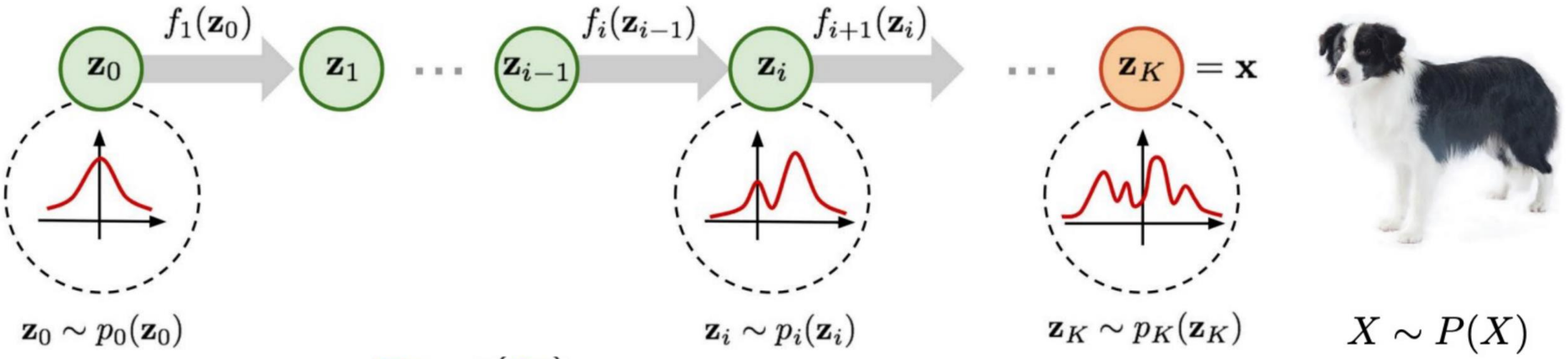
$$X = f(Z)$$

$$Z = f^{-1}(X)$$

$Z \sim N(0, I)$

$X \sim P(X)$

Normalizing Flows



$$\boldsymbol{z}_0 \sim p(\boldsymbol{z}_0)$$
$$\boldsymbol{x} = \boldsymbol{z}_K = f_K \circ f_{K-1} \circ \cdots \circ f_1(\boldsymbol{z}_0)$$

inference: $\boldsymbol{z}_i = f_i^{-1}(\boldsymbol{z}_{i-1})$

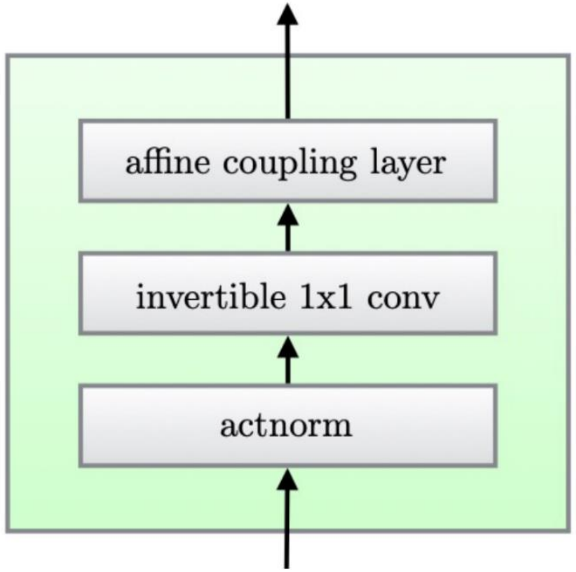
density: $p(\boldsymbol{z}_i) = p(\boldsymbol{z}_{i-1}) \left|\det \frac{d\boldsymbol{z}_{i-1}}{d\boldsymbol{z}_i}\right|$

training: maximizes data log-likelihood

$$\log p(\boldsymbol{x}) = \log p(\boldsymbol{z}_0) + \sum_{i=1}^{K} \log \left|\det \frac{d\boldsymbol{z}_{i-1}}{d\boldsymbol{z}_i}\right|$$

[Slides from Eric Xing]

Normalizing Flows



Description	Function	Reverse Function	Log-determinant
Actnorm. See Section 3.1.	$\forall i,j : \mathbf{y}_{i,j} = \mathbf{s} \odot \mathbf{x}_{i,j} + \mathbf{b}$	$\forall i,j : \mathbf{x}_{i,j} = (\mathbf{y}_{i,j} - \mathbf{b})/\mathbf{s}$	$h \cdot w \cdot \texttt{sum}(\log \lvert\mathbf{s}\rvert)$
Invertible 1×1 convolution. $\mathbf{W} : [c \times c]$. See Section 3.2.	$\forall i,j : \mathbf{y}_{i,j} = \mathbf{W}\mathbf{x}_{i,j}$	$\forall i,j : \mathbf{x}_{i,j} = \mathbf{W}^{-1}\mathbf{y}_{i,j}$	$h \cdot w \cdot \log \lvert\det(\mathbf{W})\rvert$ or $h \cdot w \cdot \texttt{sum}(\log \lvert\mathbf{s}\rvert)$ (see eq. (10))
Affine coupling layer. See Section 3.3 and (Dinh et al., 2014)	$\mathbf{x}_a, \mathbf{x}_b = \texttt{split}(\mathbf{x})$ $(\log \mathbf{s}, \mathbf{t}) = \texttt{NN}(\mathbf{x}_b)$ $\mathbf{s} = \exp(\log \mathbf{s})$ $\mathbf{y}_a = \mathbf{s} \odot \mathbf{x}_a + \mathbf{t}$ $\mathbf{y}_b = \mathbf{x}_b$ $\mathbf{y} = \texttt{concat}(\mathbf{y}_a, \mathbf{y}_b)$	$\mathbf{y}_a, \mathbf{y}_b = \texttt{split}(\mathbf{y})$ $(\log \mathbf{s}, \mathbf{t}) = \texttt{NN}(\mathbf{y}_b)$ $\mathbf{s} = \exp(\log \mathbf{s})$ $\mathbf{x}_a = (\mathbf{y}_a - \mathbf{t})/\mathbf{s}$ $\mathbf{x}_b = \mathbf{y}_b$ $\mathbf{x} = \texttt{concat}(\mathbf{x}_a, \mathbf{x}_b)$	$\texttt{sum}(\log(\lvert\mathbf{s}\rvert))$

[Kingma et al., Generative Flow with Invertible 1x1 Convolutions. NeurIPS 2018]

Summary: Normalizing Flows

- Relatively easy to train.
- Exact likelihood.

- Very constrained architecture.

Work combining VAEs, autoregressive models, and flow-based models, see https://lilianweng.github.io/posts/2018-10-13-flow-models/

Summary: Generative Models

Likelihood-based		
1. VAEs – approximate inference via evidence lower bound	Fast & easy to train	Lower generation quality
2. Autoregressive models – exact inference via chain rule	Easy to train, exact likelihood	Slow to sample from
3. Flows – exact inference via invertible transformations	Easy to train, exact likelihood	Constrained architecture
Likelihood-free		
1. GANs – discriminative real vs generated samples	High generation quality	Hard to train, can't get features

Summary: Generative Models

GAN: Adversarial training

VAE: maximize variational lower bound

Flow-based models: Invertible transform of distributions

Diffusion models: Gradually add Gaussian noise and then reverse