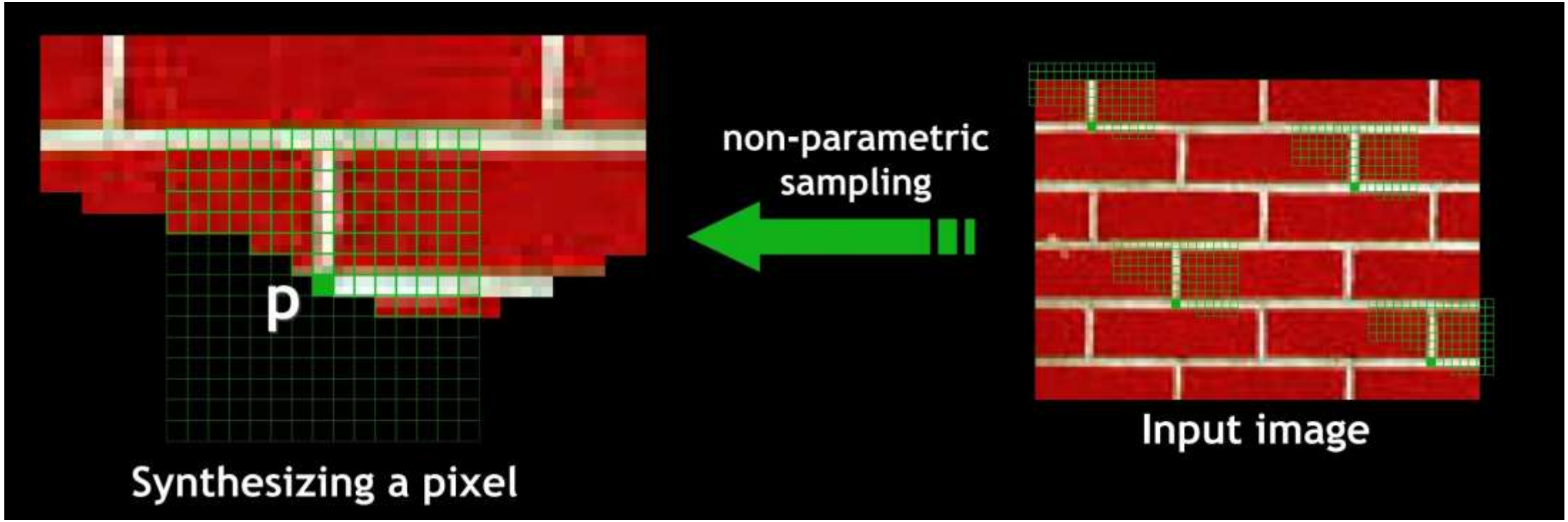
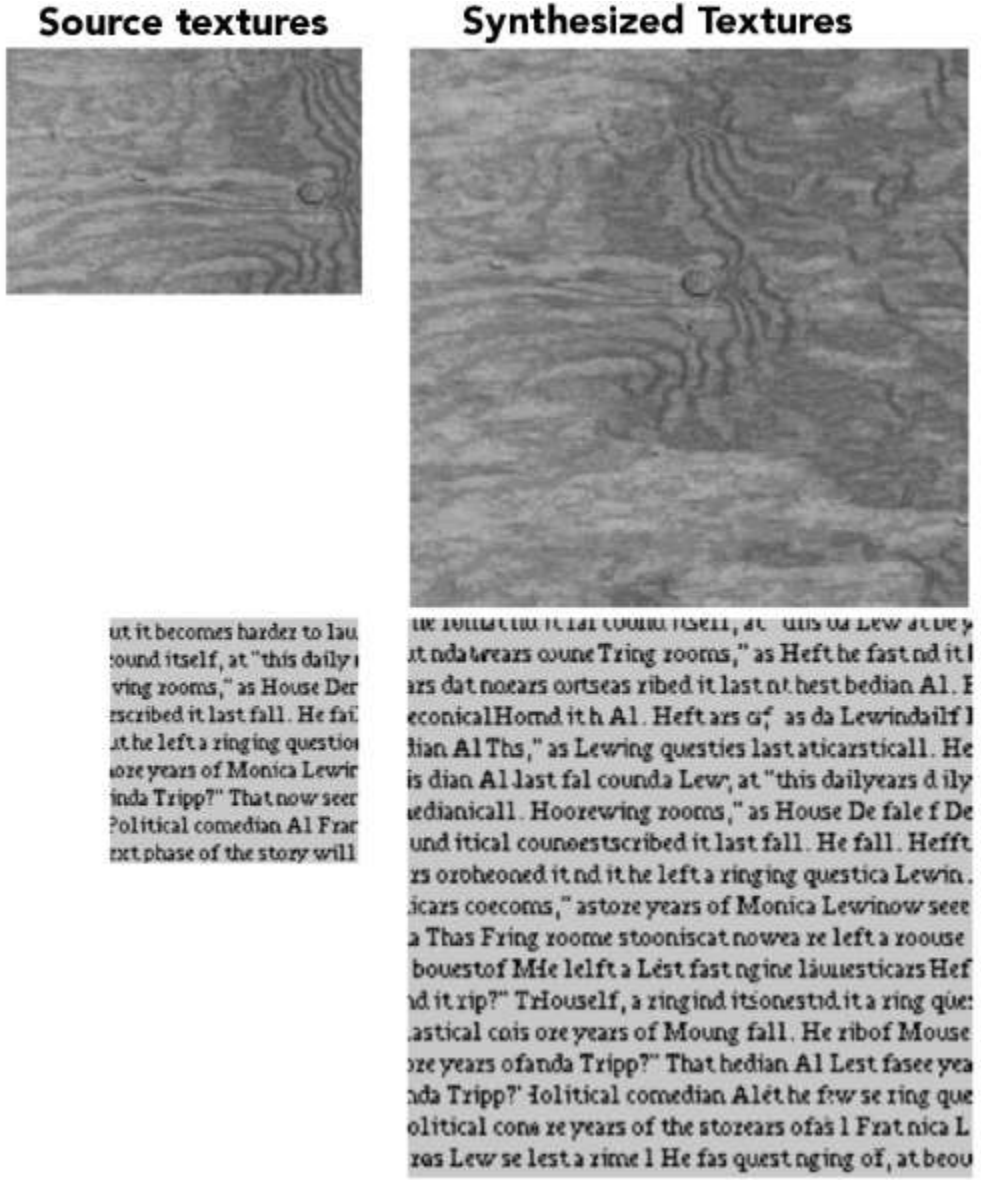
Recap.

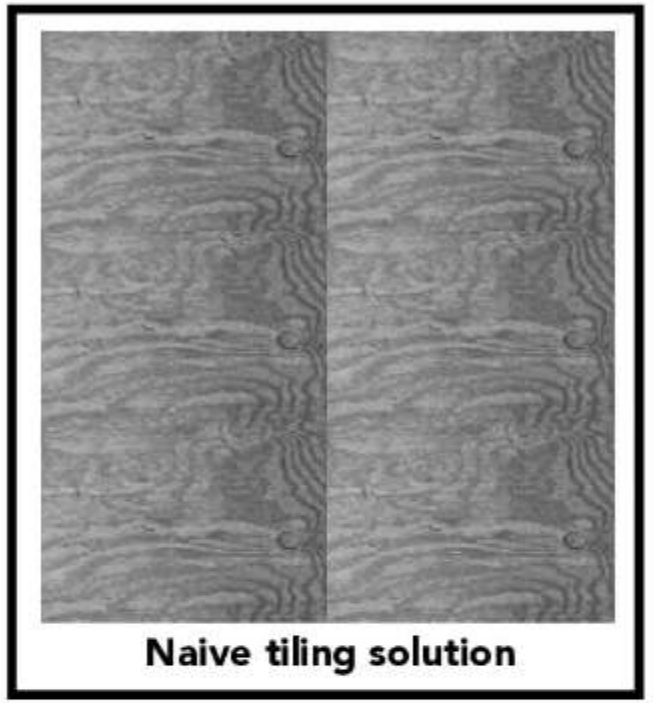
Generative Models before the “GenAI” Era



Texture Synthesis by Non-parametric Sampling, ICCV 1999

Generative Models before the “GenAI” Era



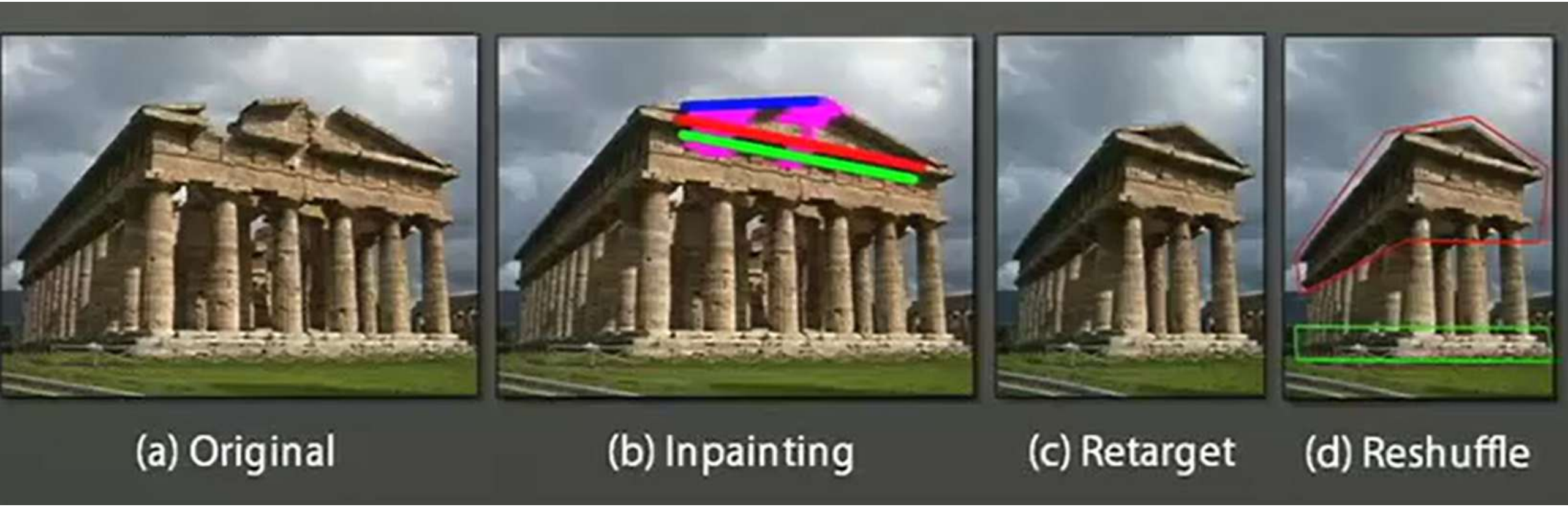


[Efros and Leung 99]

Texture Synthesis by Non-parametric Sampling, ICCV 1999

PatchMatch

* C. Barnes, E. Shechtman, A. Finkelstein, and D. Goldman. Patchmatch: a randomized correspondence algorithm for structural image editing. TOG, 2009.



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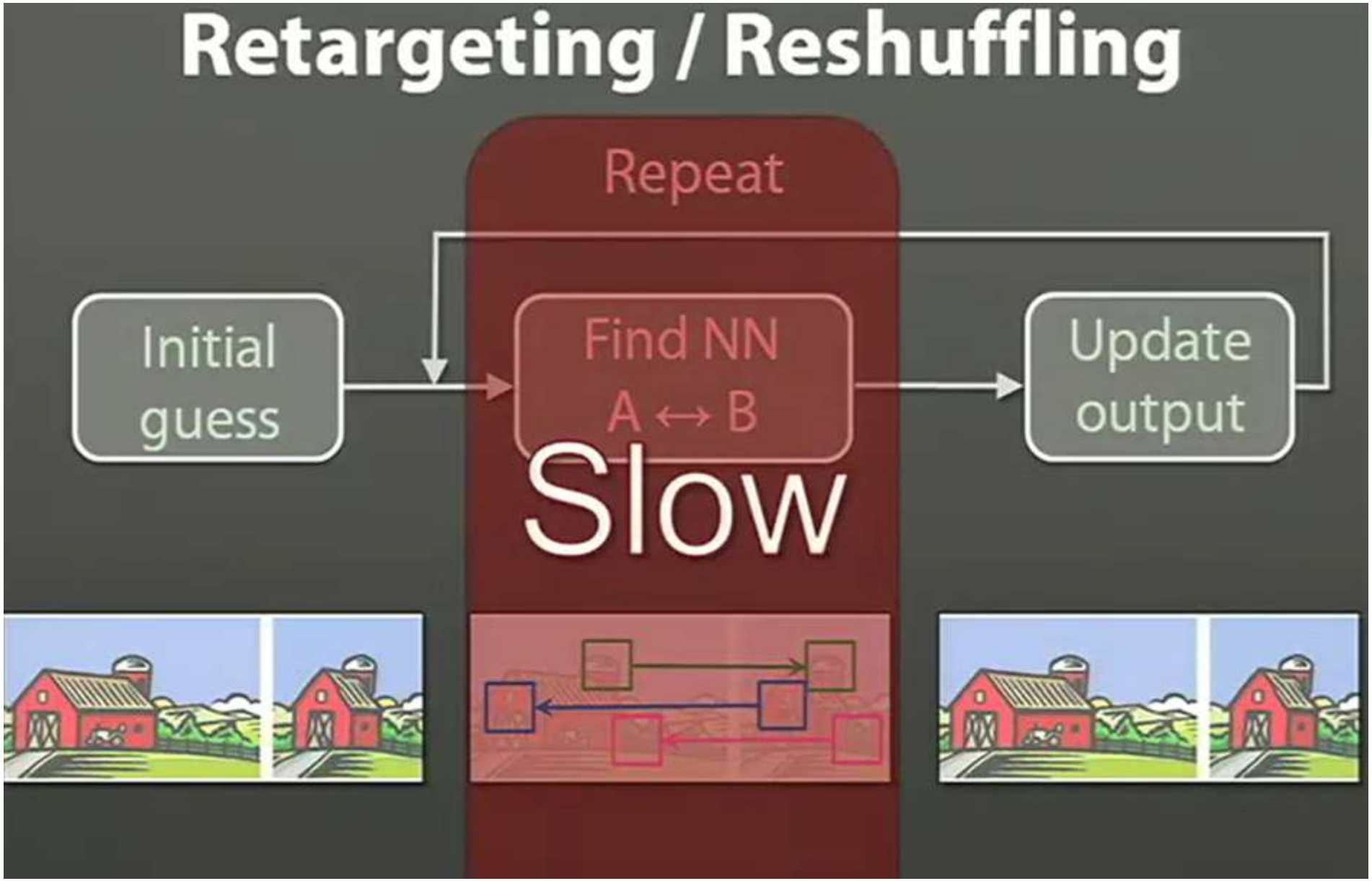

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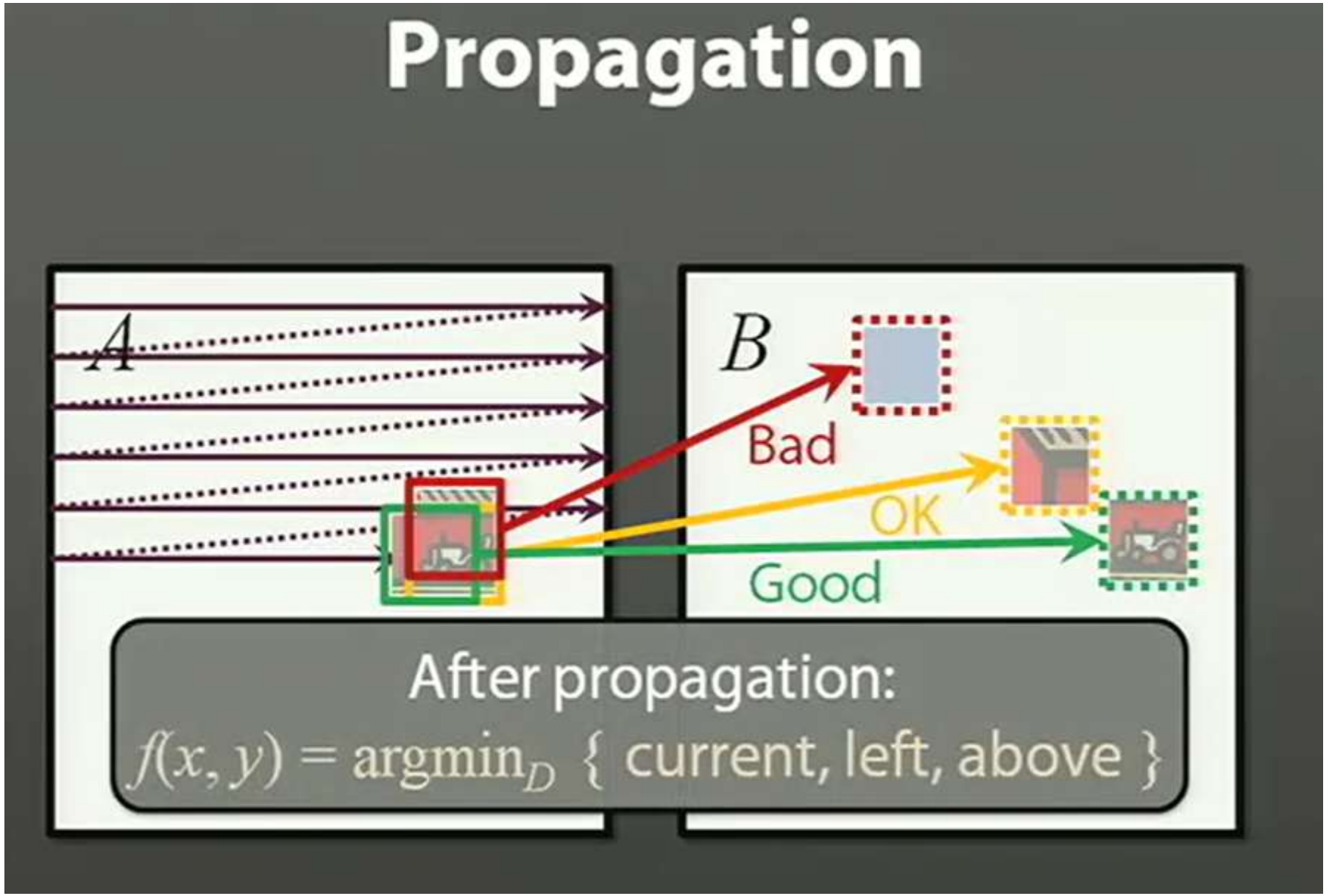

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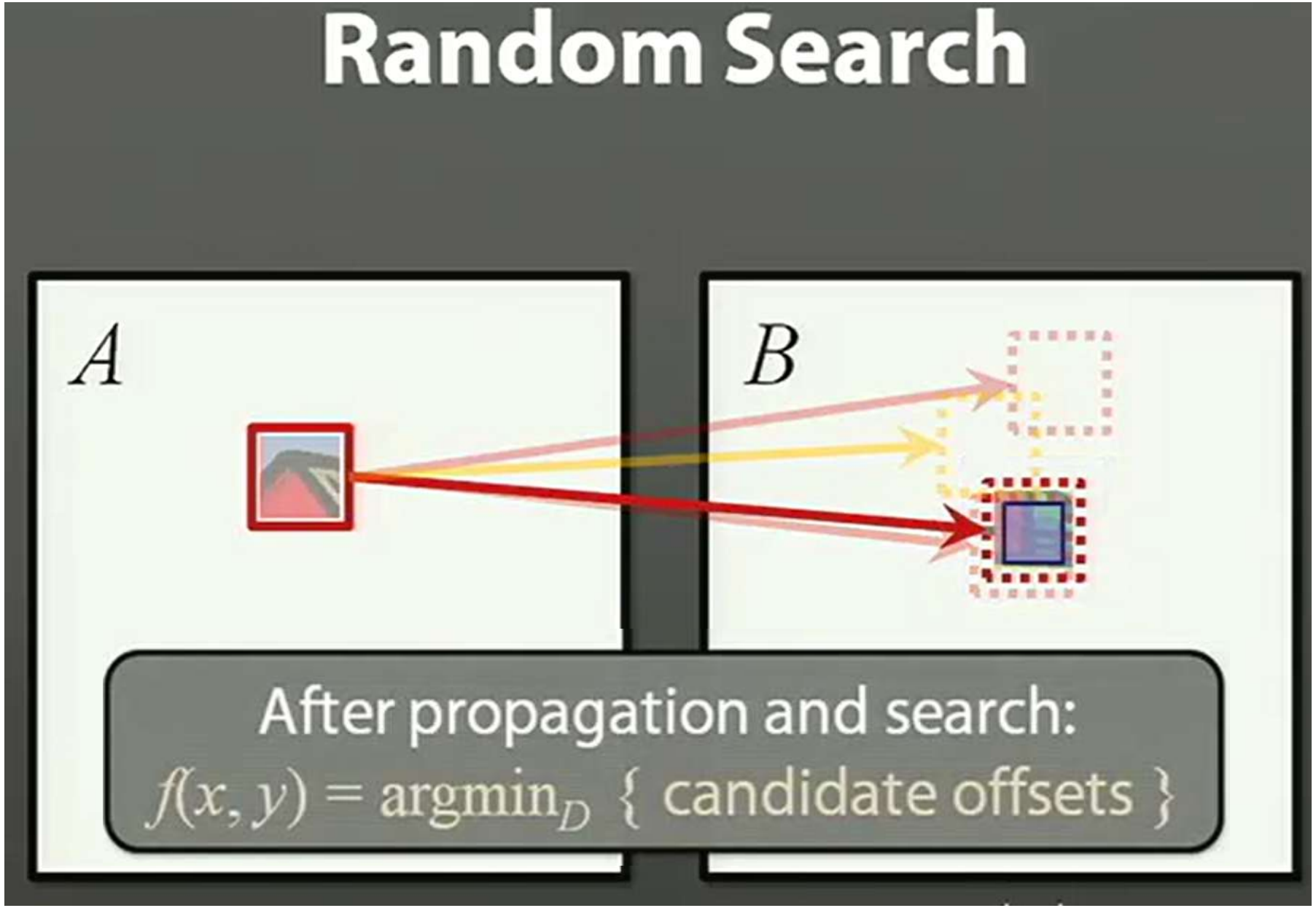

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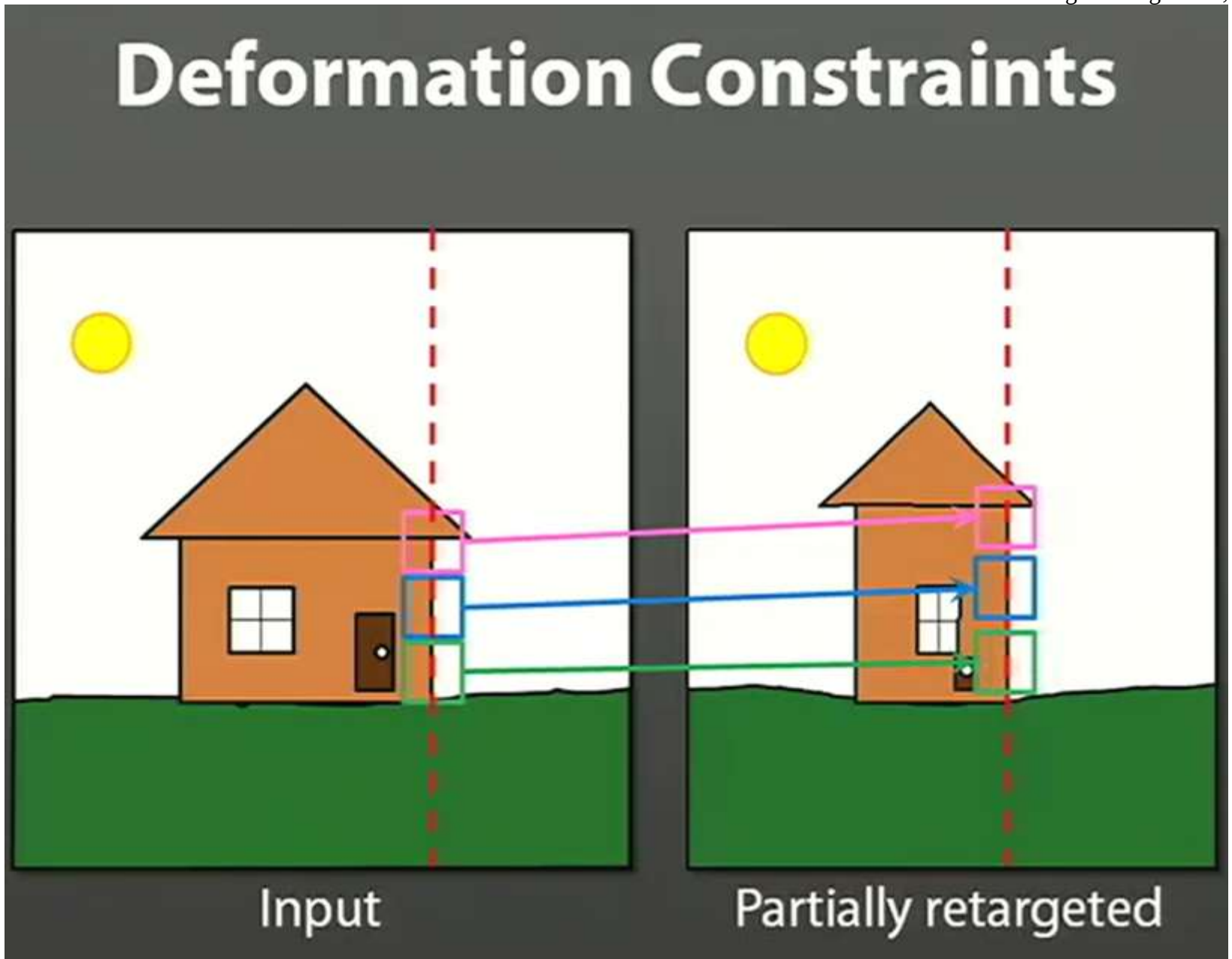
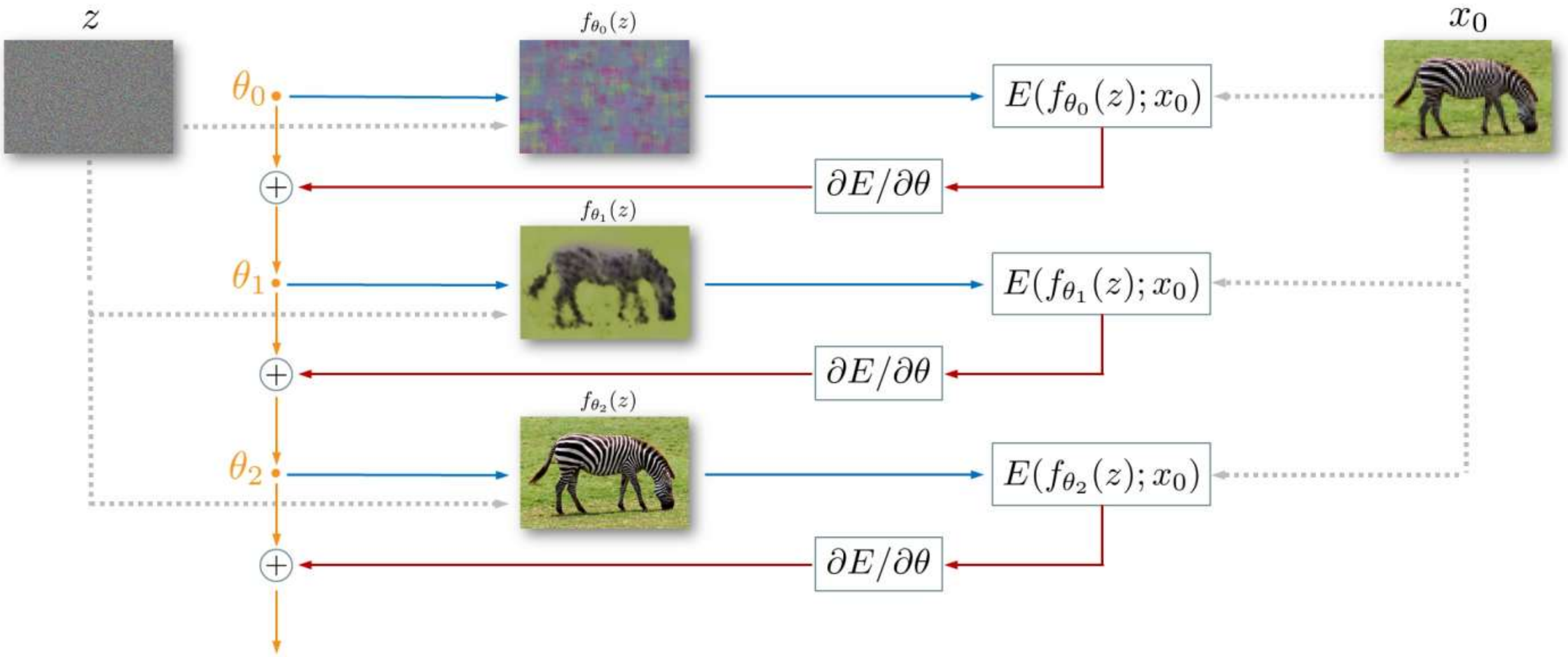


Deep Image Prior

Ulyanov, Dmitry, Andrea Vedaldi, and Victor Lempitsky. "Deep image prior." Proceedings of the IEEE conference on computer vision and pattern recognition. 2018.



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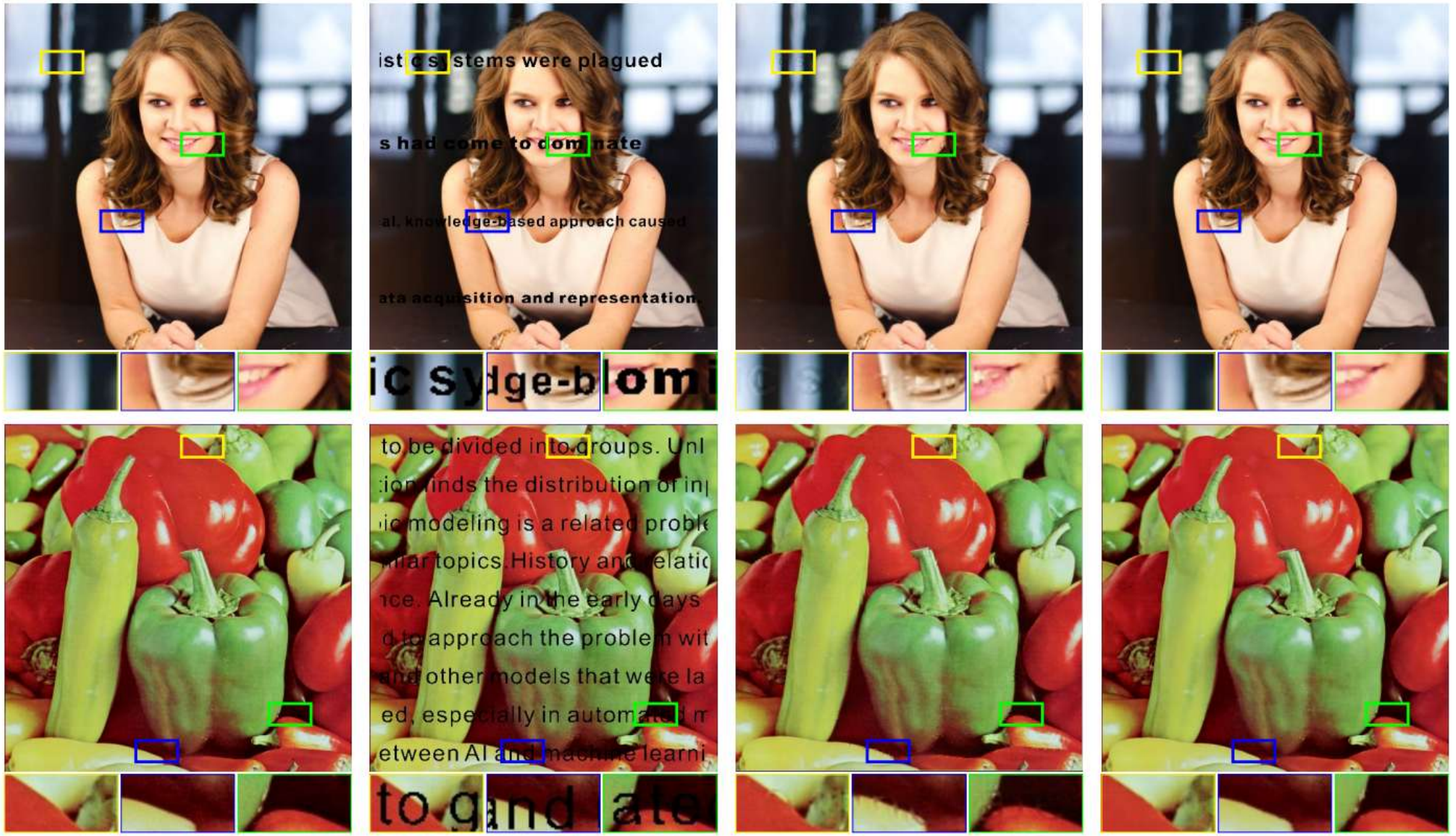

(a) Original image (b) Corrupted image (c) Shepard networks [44] (d) Deep Image Prior

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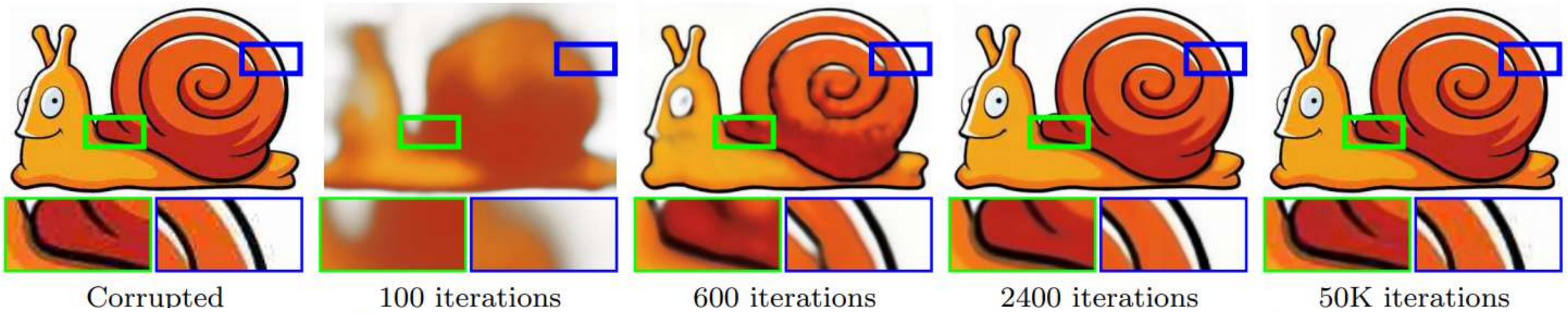
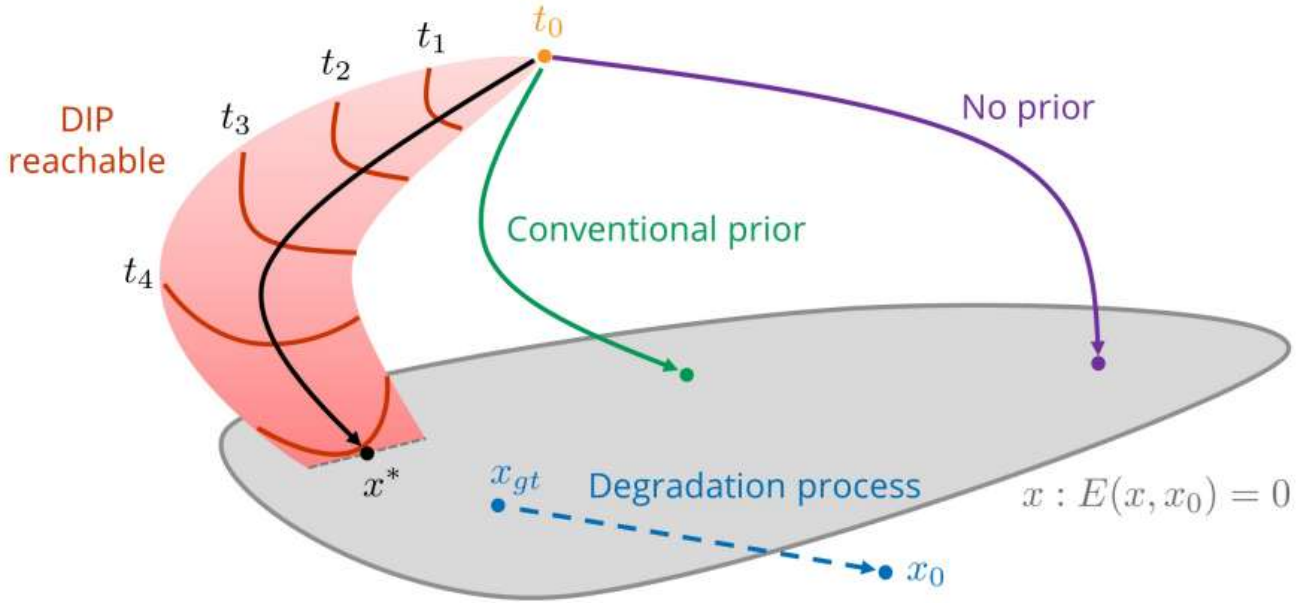
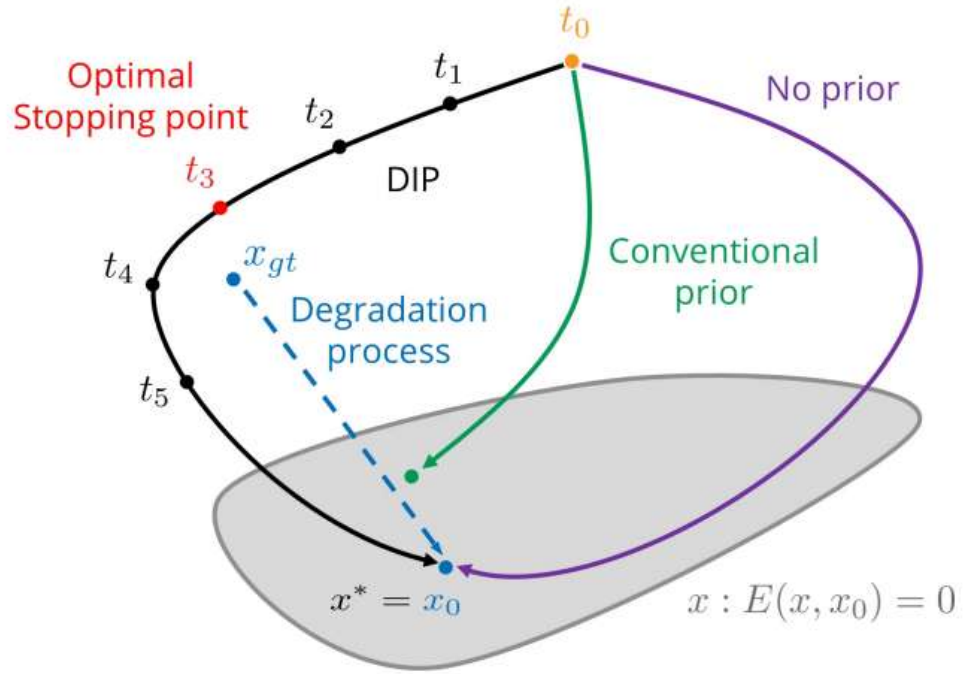






Create New Content

- Patchmatch and Deep Image Prior can’t provide new images
  - PatchMatch: borrow new content from other images
  - DIP: new noise? Totally out of control

- How?

Variational Autoencoder (VAE)

Overview

- Variational Autoencoder (VAE)
- Relation to Expectation-Maximization (EM)
- Vector Quantized VAE (VQ-VAE)

Procedural graphics

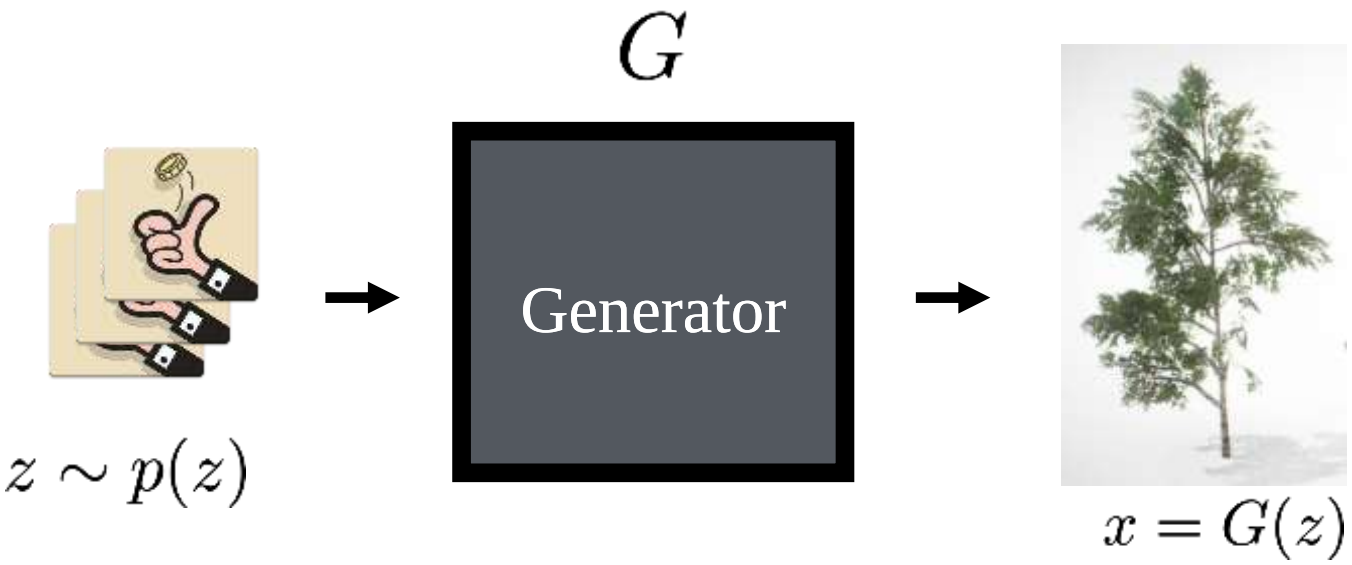
[Anders Scheil]

Aylean @Aylean · Nov 17

Made up a set of rules and rolled some dice to decide how this plant would grow. I never did get that five of a kind, as expected, but I was still hopeful! 🌱🍀🎉

52 1.1K 4.5K

Image synthesis from “noise”



Sampler

$$G : \mathcal{Z} \to \mathcal{X}$$

$$z \sim p(z)$$

$$x = G(z)$$

Recap: Deep Image Prior

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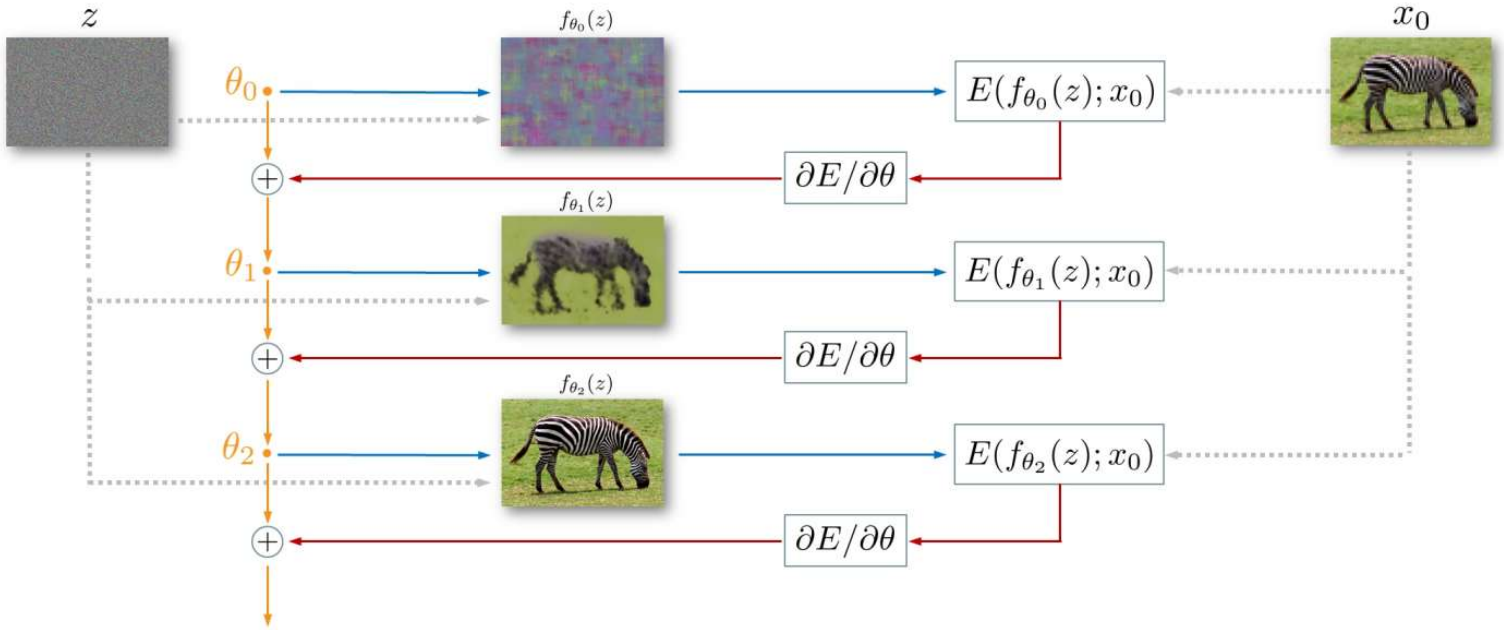
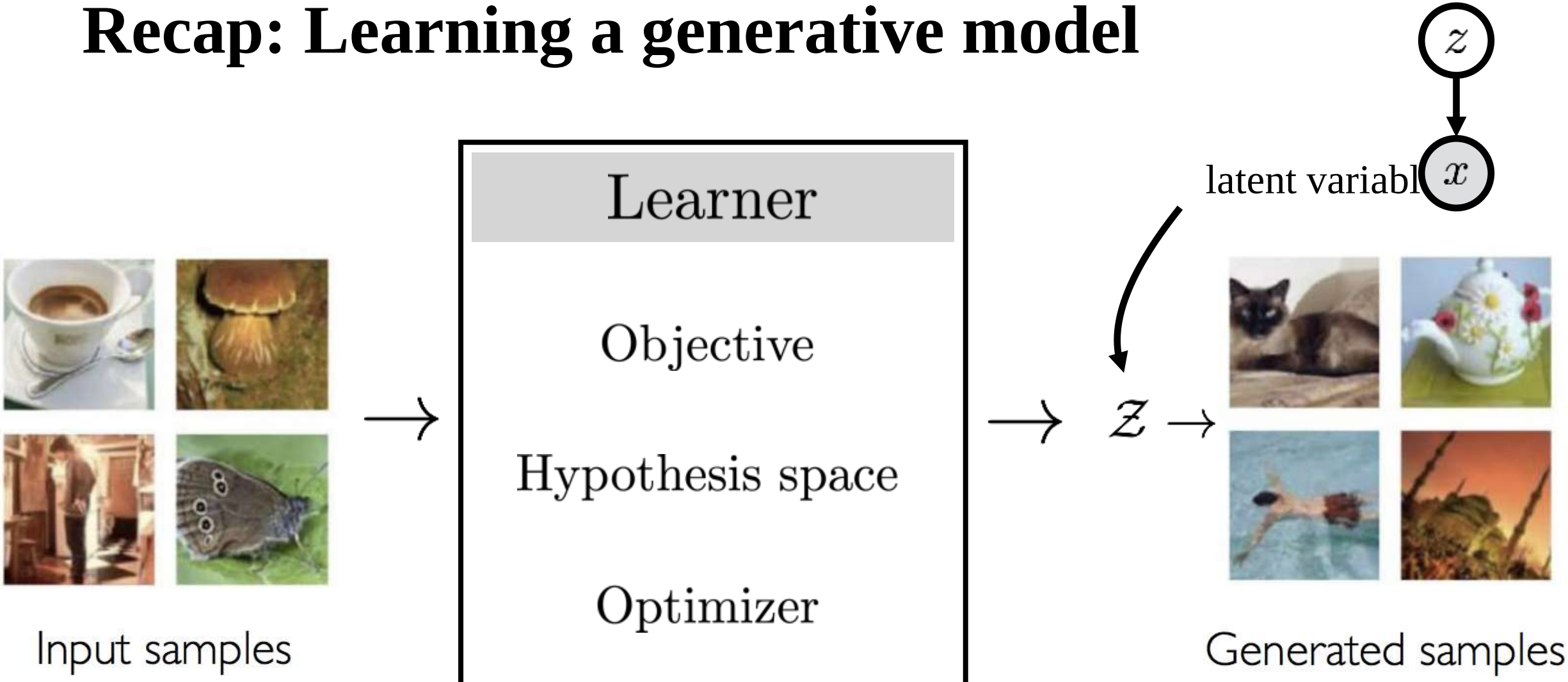
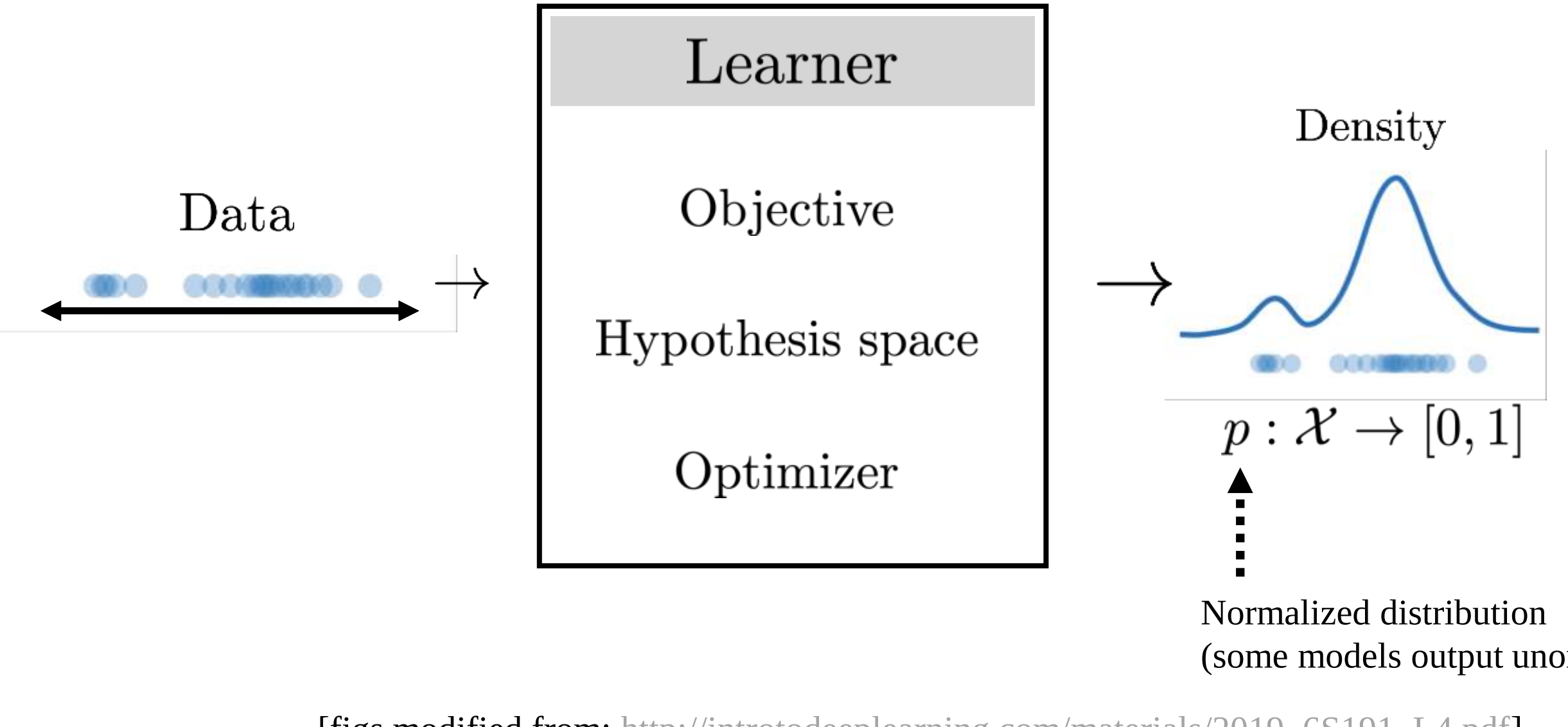


Recap: Learning a generative model



[figs modified from: http://introtodeeplearning.com/materials/2019_6S191_L4.pdf]

Recap: Learning a density model



[figs modified from: http://introtodeeplearning.com/materials/2019_6S191_L4.pdf]

Case study #1: Fitting a Gaussian to data

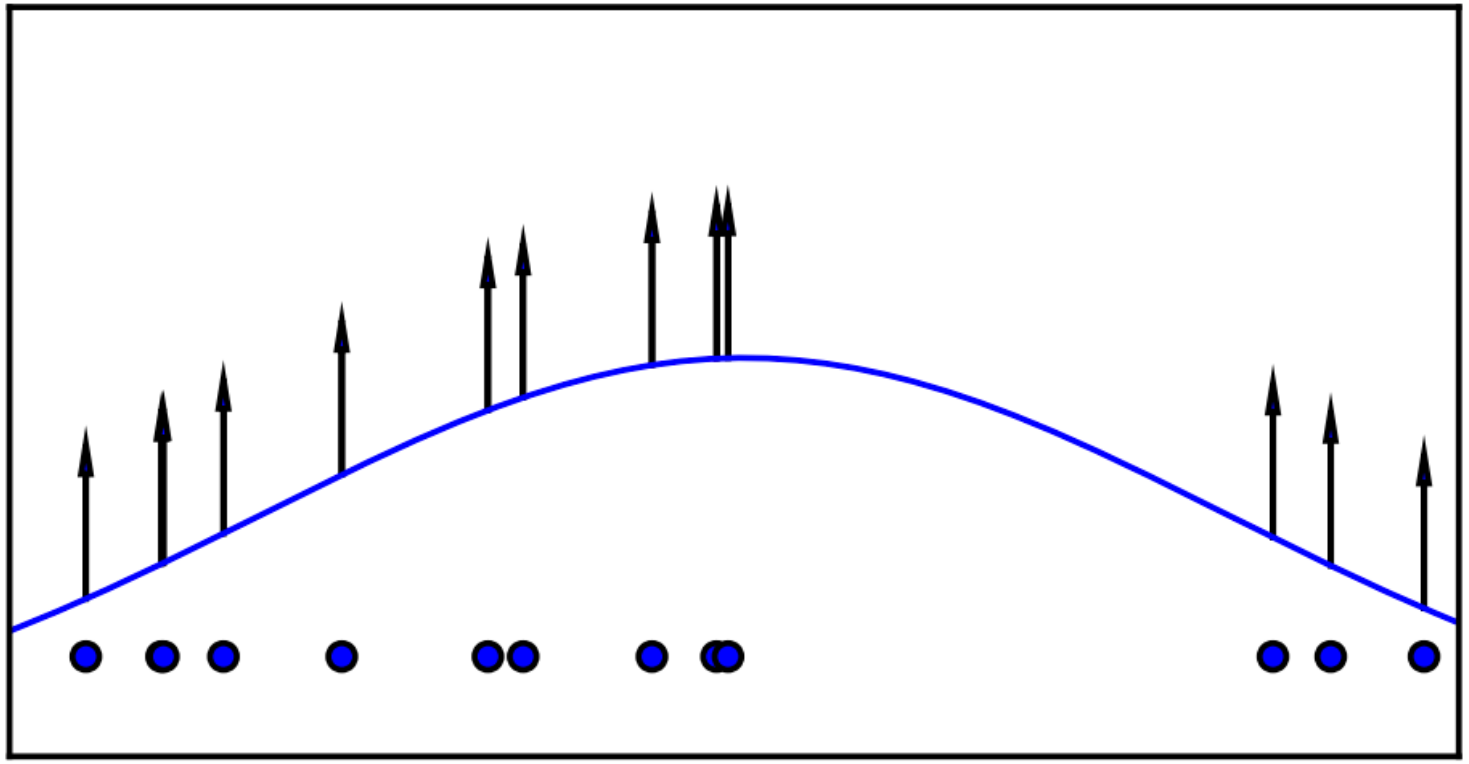


fig from [Goodfellow, 2016]

Max likelihood objective

$$\max_{\theta} \mathbb{E}_{x \sim p_{\text{data}}} [\log p_\theta(x)]$$

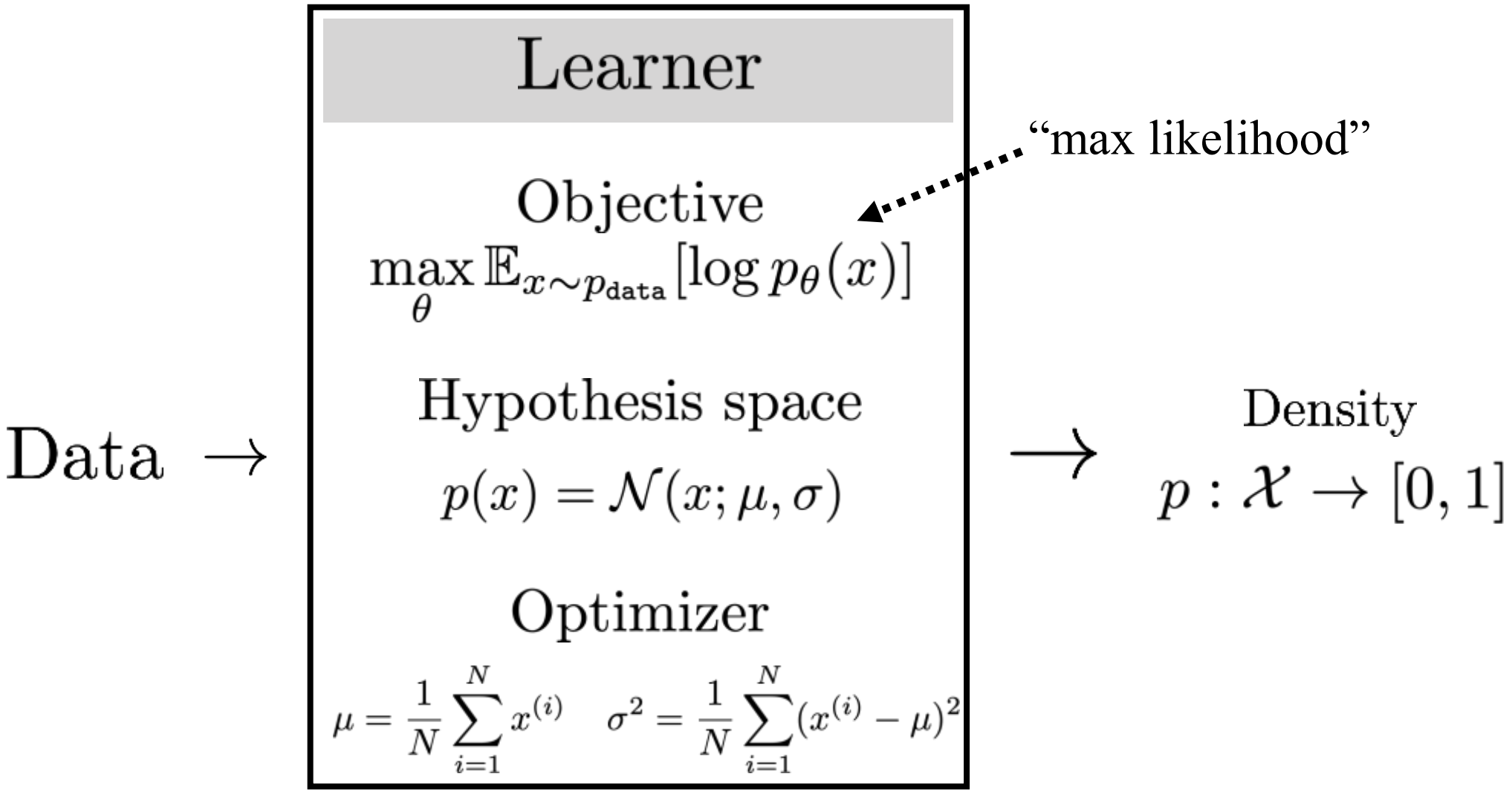
Considering only Gaussian fits

$$p_\theta(x) = \mathcal{N}(x; \mu, \sigma)$$
$$\theta = [\mu, \sigma]$$

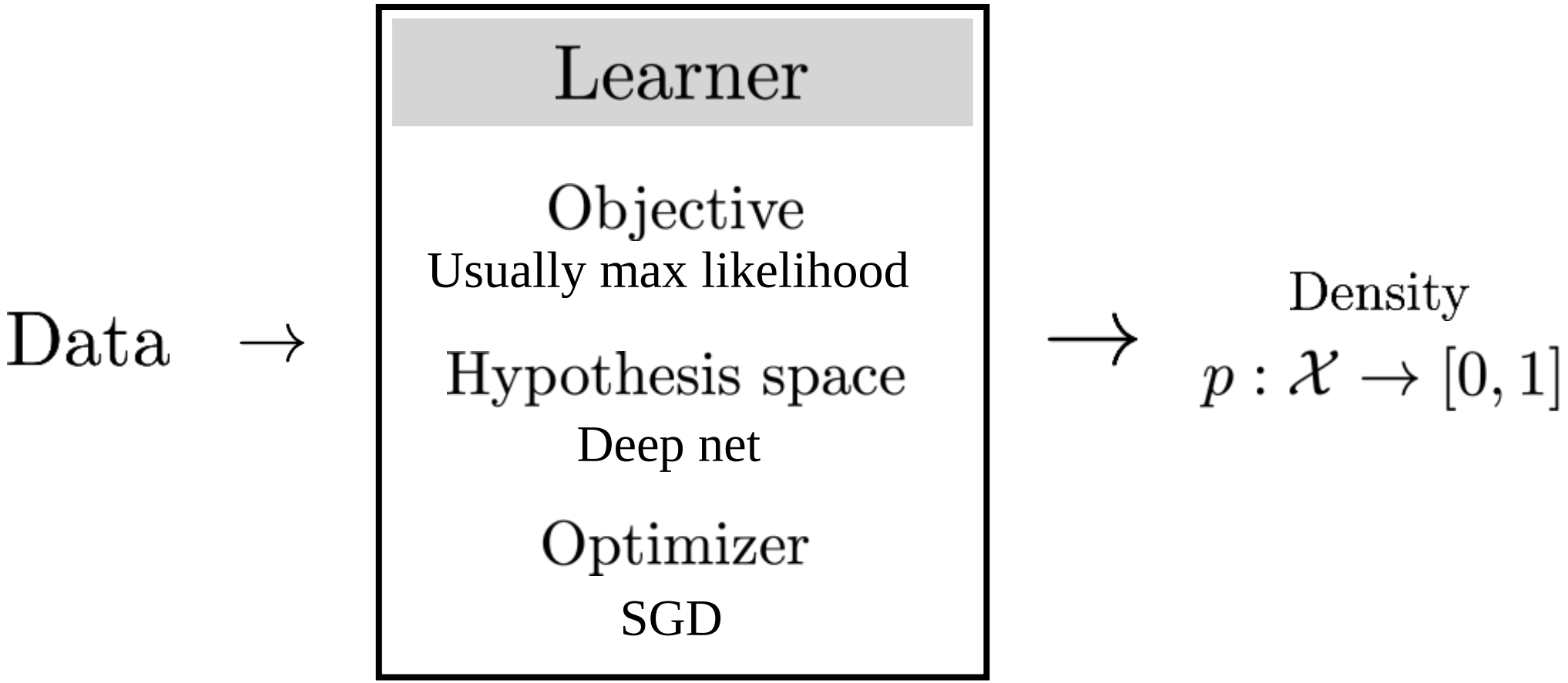
Closed form optimum:

$$\mu = \frac{1}{N} \sum_{i=1}^{N} x^{(i)} \quad \sigma^2 = \frac{1}{N} \sum_{i=1}^{N} (x^{(i)} - \mu)^2$$

Case study #1: Fitting a Gaussian to data



Case study #2: learning a deep generative model



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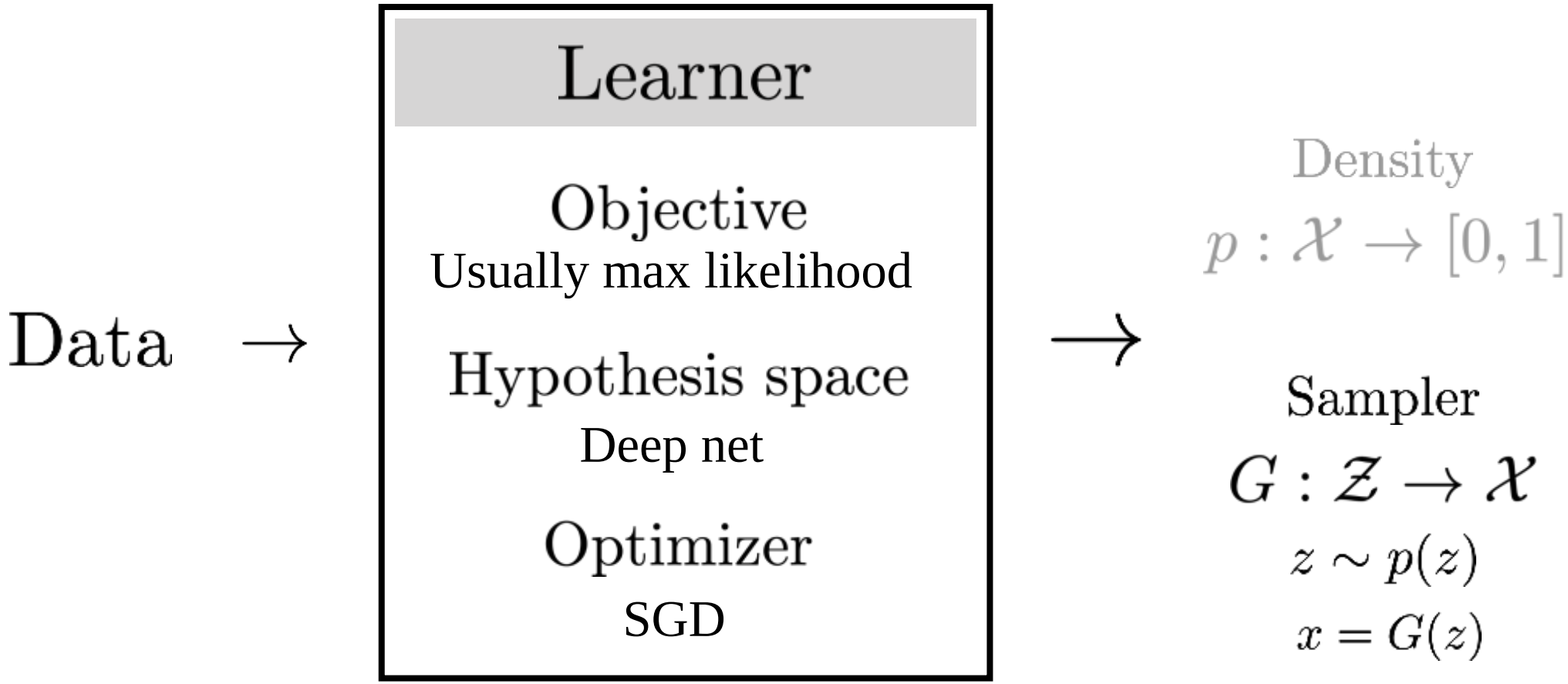
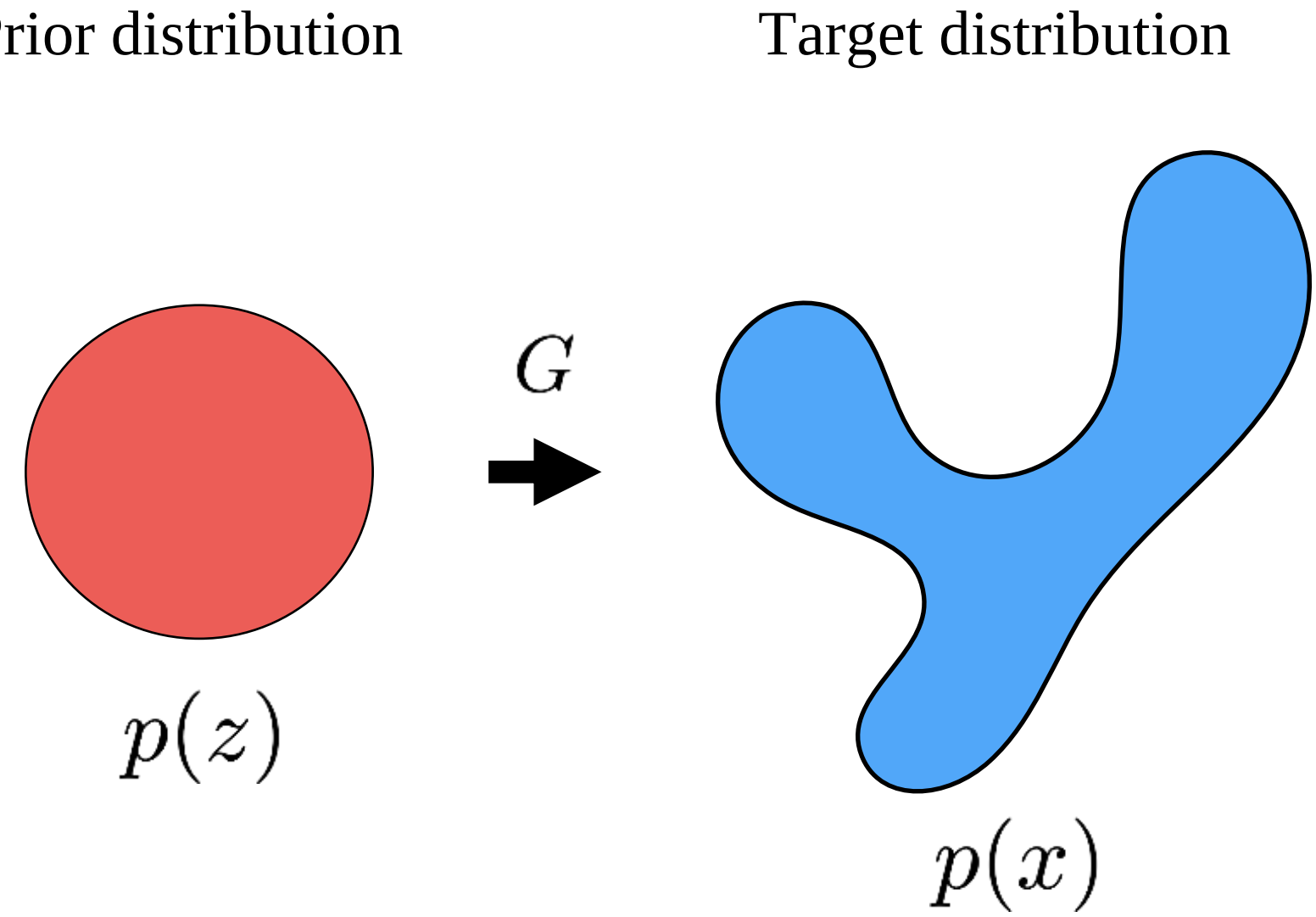
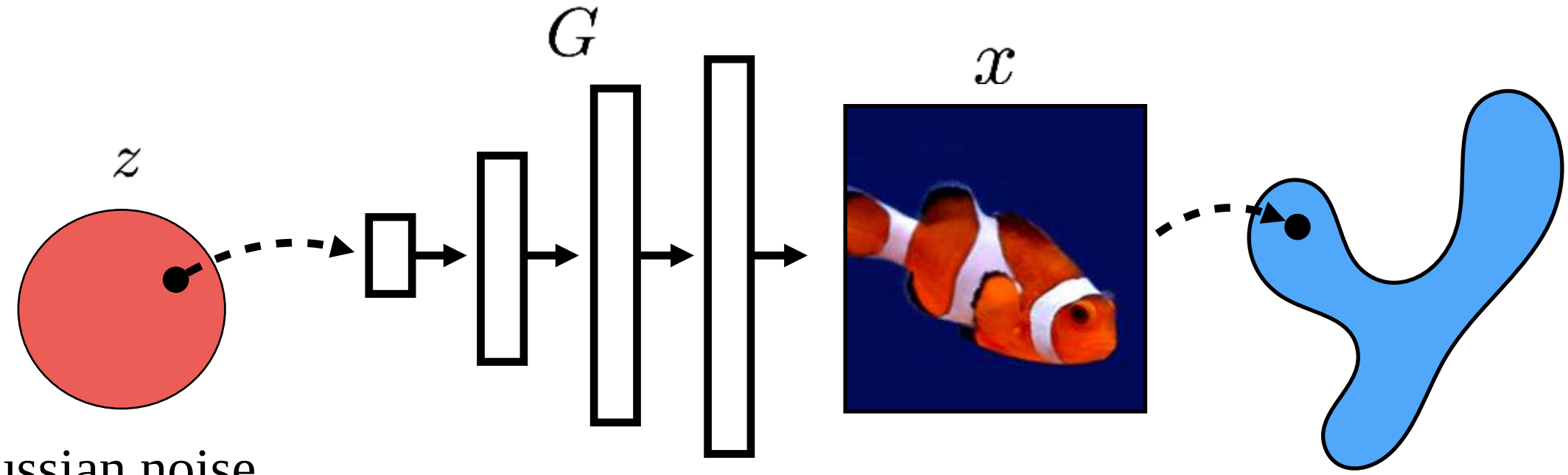


Models that provide a sampler but no density are called **implicit generative models**

Deep generative models are distribution transformers



Deep generative models are distribution transformers

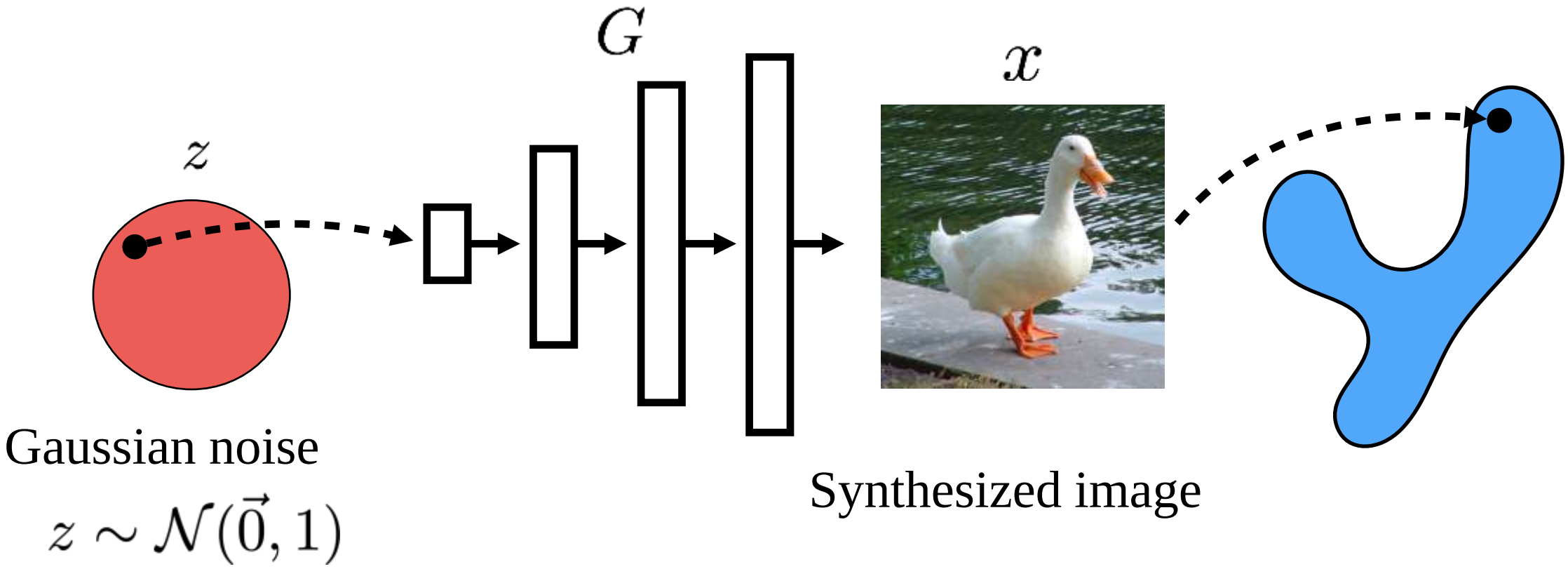


Gaussian noise

$z \sim \mathcal{N}(\vec{0}, 1)$

Synthesized image

Deep generative models are distribution transformers

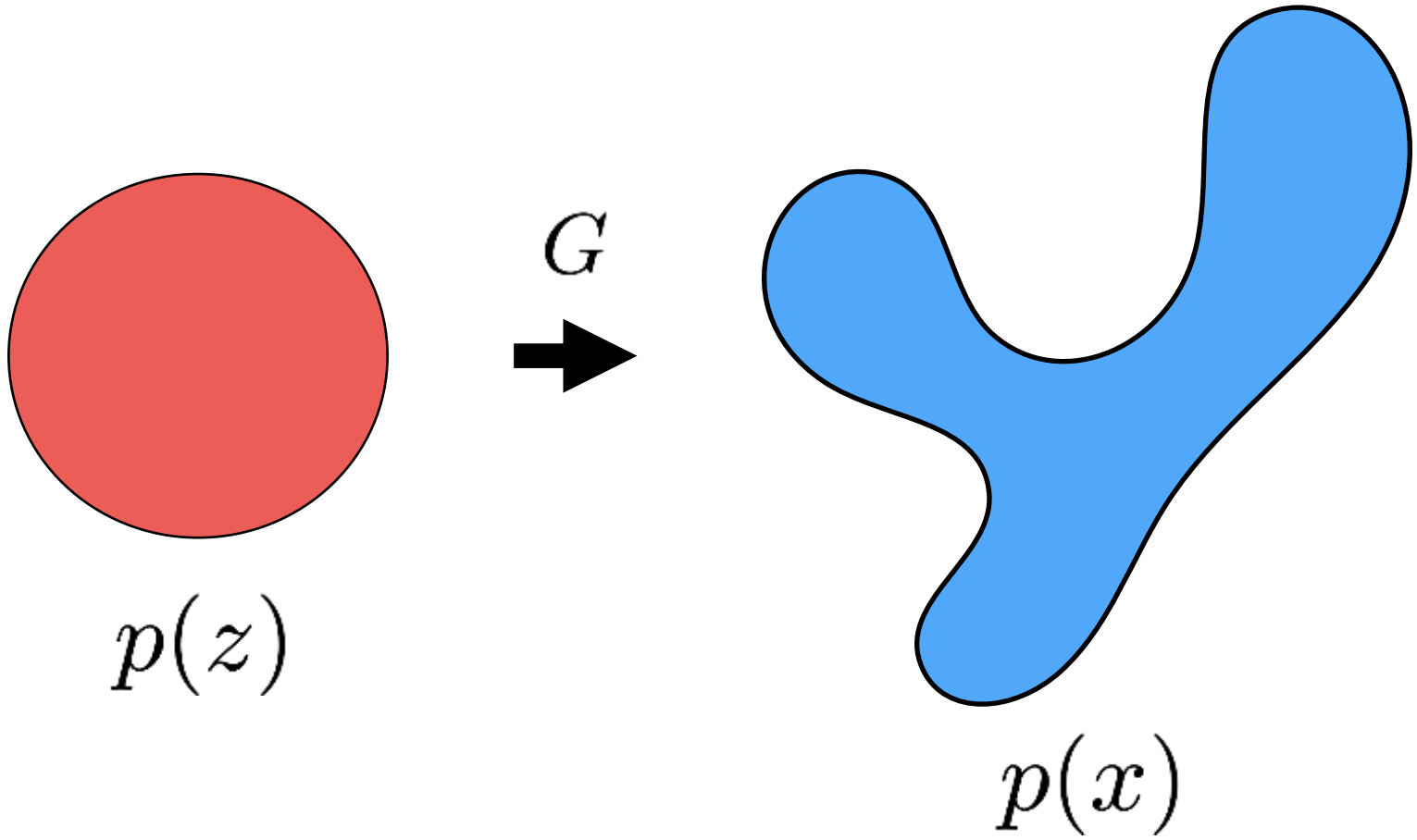


Variational Autoencoders (VAEs)

[Kingma & Welling, 2014; Rezende, Mohamed, Wierstra 2014]

Prior distribution

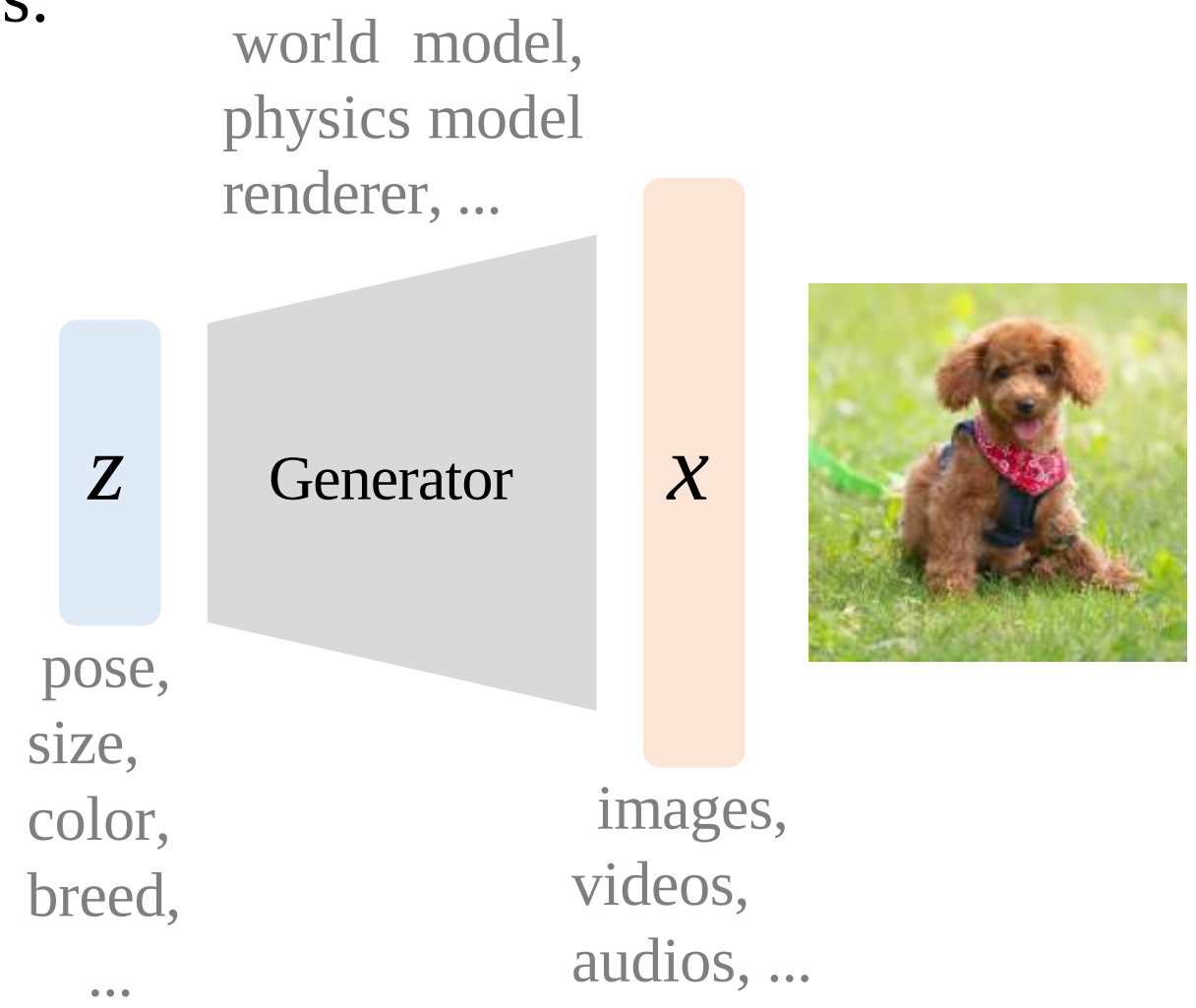
Target distribution



Latent Variable Models

Assuming a data generation process:

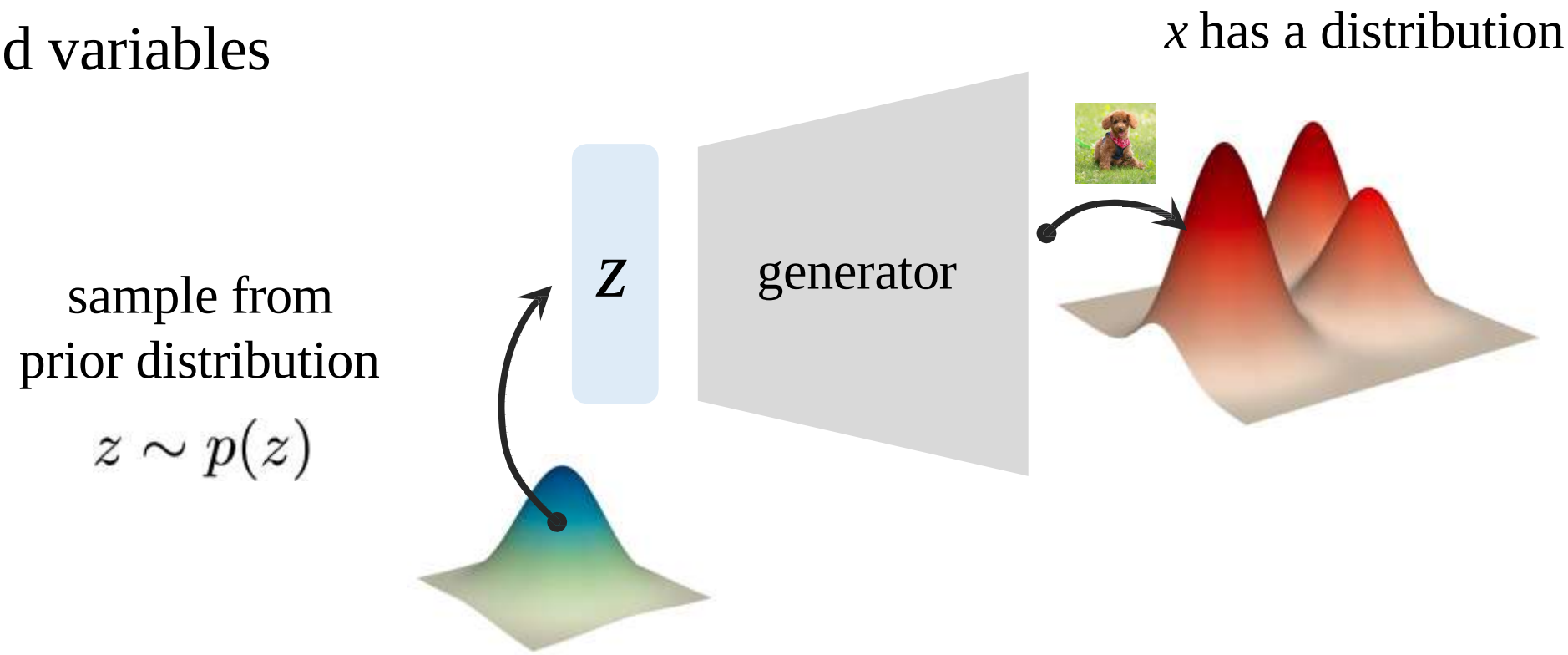
- z - latent variables
- x - observed variables



Latent Variable Models

Assuming a data generation process:

- z - latent variables
- x - observed variables



Latent Variable Models

Assuming a data generation process:

- z - latent variables
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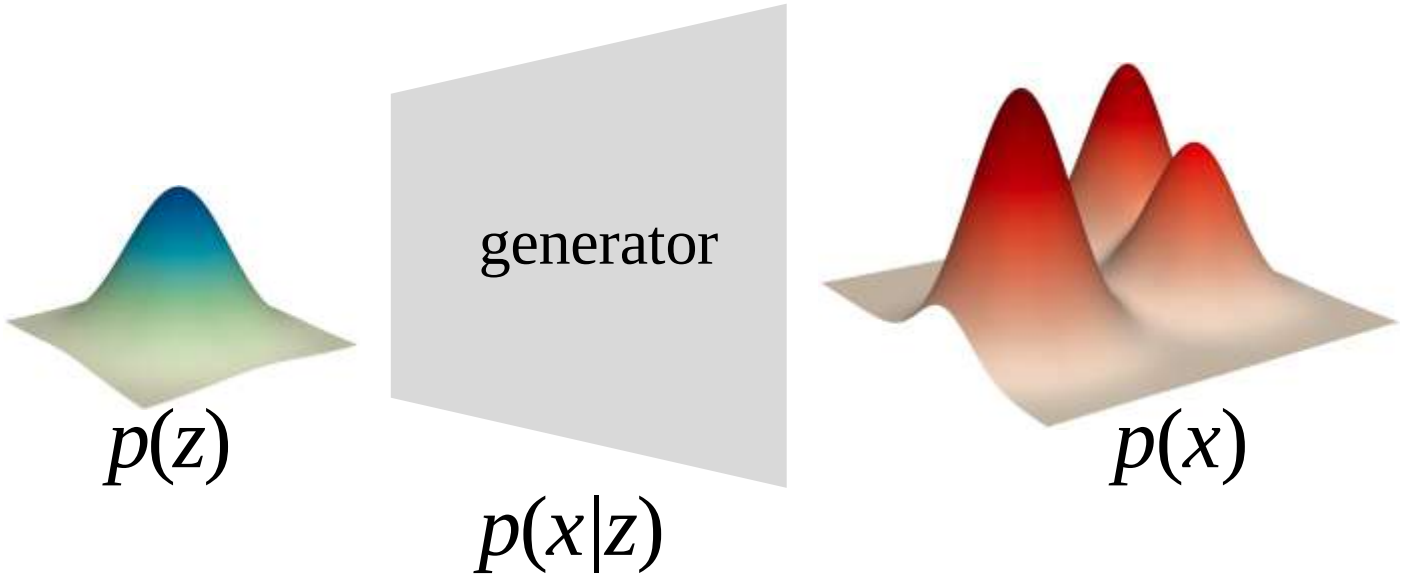
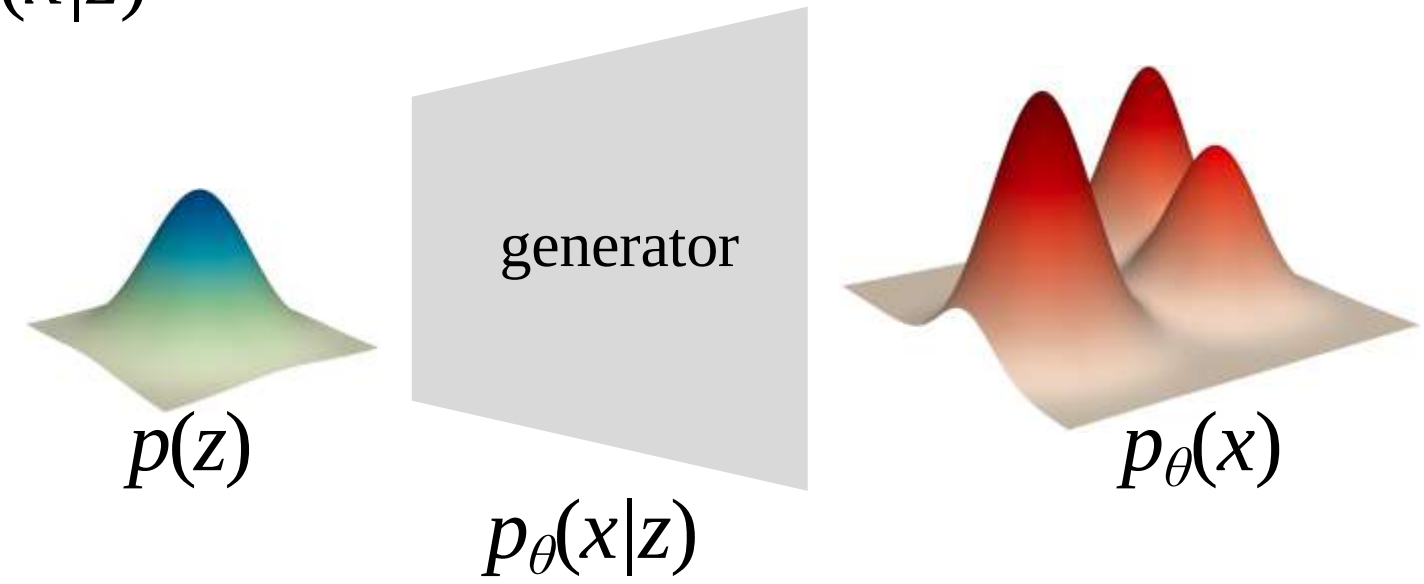


Latent Variable Models

Represent a distribution by a neural network

- θ - learnable parameters
- represent a function: $p_\theta(x|z)$



Measuring how good a distribution is ...

Minimize Kullback–Leibler (KL) divergence:

$$\min_\theta \; \mathcal{D}_{\mathrm{KL}}(\, p_{data} \, || \, p_\theta \,)$$

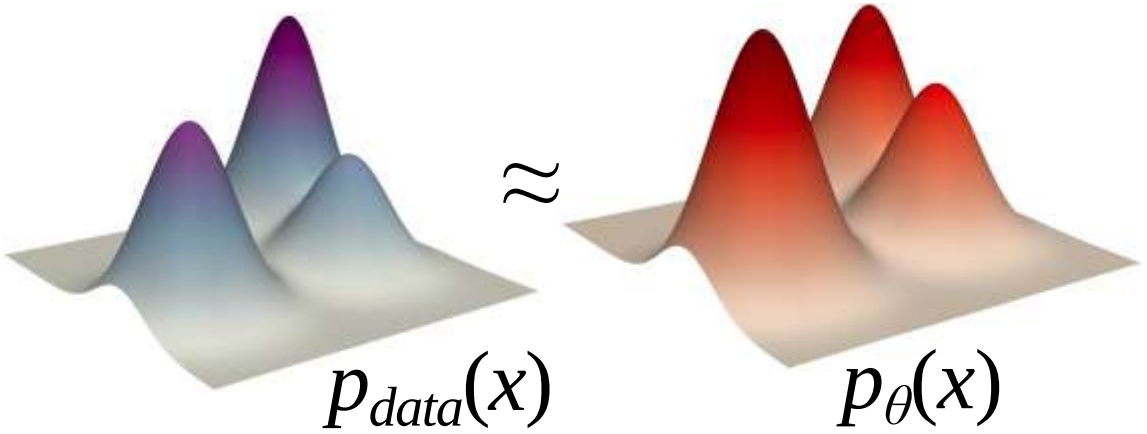
Note: consider other criteria than KL?

⇒ Maximize likelihood:

$$\max_\theta \; \mathbb{E}_{x \sim p_{data}} \log p_\theta(x)$$

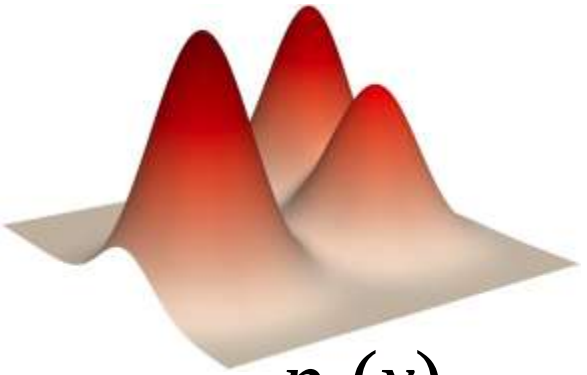
$\arg\min_\theta \; \mathcal{D}_{\mathrm{KL}}(\, p_{data} \, || \, p_\theta \,)$ tl; dr

$$\begin{aligned}
&= \arg\min_\theta \sum_x p_{data}(x) \log \frac{p_{data}(x)}{p_\theta(x)} \\
&= \arg\min_\theta \sum_x -p_{data}(x) \log p_\theta(x) + const \\
&= \arg\max_\theta \sum_x p_{data}(x) \log p_\theta(x) \\
&= \arg\max_\theta \; \mathbb{E}_{x \sim p_{data}} \log p_\theta(x)
\end{aligned}$$



Latent Variable Models

We want to maximize $\mathbb{E}_{x \sim p_{data}} \log p_\theta(x)$



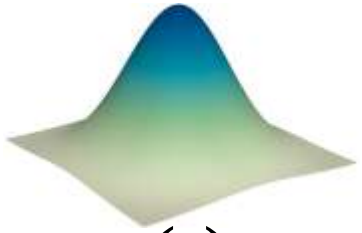
$p_\theta(x)$

Latent Variable Models

We want to maximize $\mathbb{E}_{x \sim p_{data}} \log p_\theta(x)$

with $p_\theta(x)$ represented as:

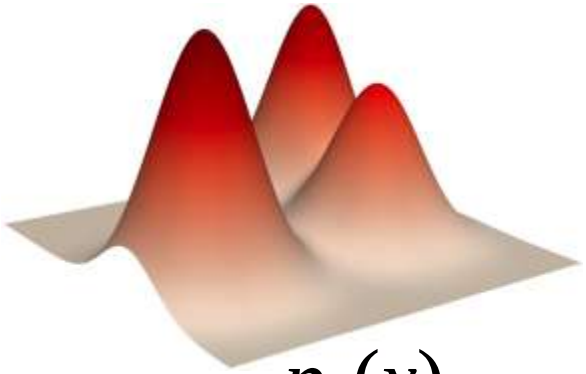
$$p_\theta(x) = \int_z p_\theta(x|z)p(z)dz$$



$p(z)$

generator

$p_\theta(x|z)$



$p_\theta(x)$

Latent Variable Models

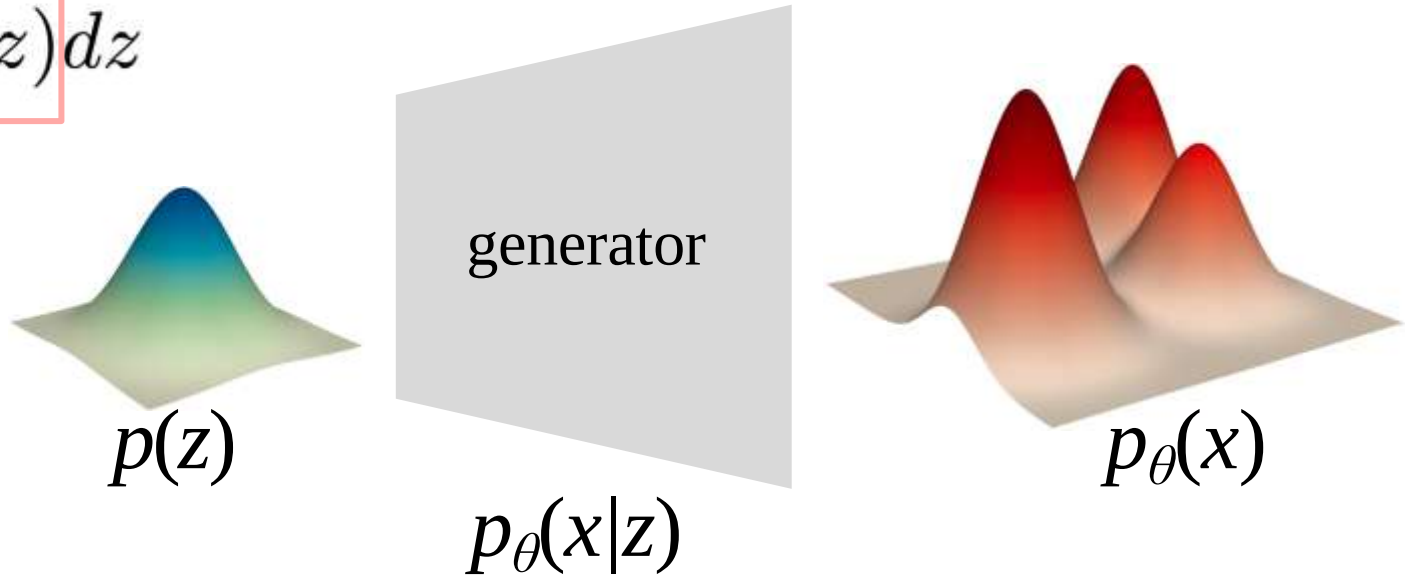
We want to maximize $\mathbb{E}_{x \sim p_{data}} \log p_\theta(x)$

with $p_\theta(x)$ represented as:

$$p_\theta(x) = \int_z p_\theta(x|z)p(z)dz$$

Two sets of unknowns:

- We need to optimize for θ
- We can't control "**true**" $p(z)$



Idea: introduce a "controllable" distribution $q(z)$

Latent Variable Models

$$\log p_\theta(x)$$

Rewrite log likelihood by latent z

$$= \int_z q(z) \log p_\theta(x) dz$$

- for any distribution $q(z)$

$$= \int_z q(z) \log \left(\frac{p_\theta(x|z) p_\theta(z)}{p_\theta(z|x)} \right) dz$$

- Bayes' rule

$$= \int_z q(z) \log \left(\frac{p_\theta(x|z) p_\theta(z)}{p_\theta(z|x)} \frac{q(z)}{q(z)} \right) dz$$

$$= \int_z q(z) \left(\log p_\theta(x|z) + \log \frac{p_\theta(z)}{q(z)} + \log \frac{q(z)}{p_\theta(z|x)} \right) dz$$

$$= \mathbb{E}_{z \sim q(z)} \left[\log p_\theta(x|z) \right] - \mathcal{D}_{\mathrm{KL}} \left(q(z) || p_\theta(z) \right) + \mathcal{D}_{\mathrm{KL}} \left(q(z) || p_\theta(z|x) \right)$$

Latent Variable Models

$$\log p_\theta(x)$$

$$= \int_z q(z) \log p_\theta(x) dz$$

$$= \int_z q(z) \log \left(\frac{p_\theta(x|z) p_\theta(z)}{p_\theta(z|x)} \right) dz$$

$$= \int_z q(z) \log \left(\frac{p_\theta(x|z) p_\theta(z)}{p_\theta(z|x)} \frac{q(z)}{q(z)} \right) dz$$

$$= \int_z q(z) \left(\log p_\theta(x|z) + \log \frac{p_\theta(z)}{q(z)} + \log \frac{q(z)}{p_\theta(z|x)} \right) dz$$

$$= \mathbb{E}_{z \sim q(z)} \left[\log p_\theta(x|z) \right] - \mathcal{D}_{\mathrm{KL}} \left(q(z) || p_\theta(z) \right) + \mathcal{D}_{\mathrm{KL}} \left(q(z) || p_\theta(z|x) \right)$$

Rewrite log likelihood by latent *z*

- for any distribution $q(z)$
- Bayes' rule
- just algebra
- just algebra

Latent Variable Models

$$\log p_\theta(x)$$

$$= \int_z q(z) \log p_\theta(x) dz$$

$$= \int_z q(z) \log \left(\frac{p_\theta(x|z) p_\theta(z)}{p_\theta(z|x)} \right) dz$$

$$= \int_z q(z) \log \left(\frac{p_\theta(x|z) p_\theta(z)}{p_\theta(z|x)} \frac{q(z)}{q(z)} \right) dz$$

$$= \int_z q(z) \left(\log p_\theta(x|z) + \log \frac{p_\theta(z)}{q(z)} + \log \frac{q(z)}{p_\theta(z|x)} \right) dz$$

$$= \mathbb{E}_{z \sim q(z)} \left[\log p_\theta(x|z) \right] - \mathcal{D}_{\mathrm{KL}} \left(q(z) || p_\theta(z) \right) + \mathcal{D}_{\mathrm{KL}} \left(q(z) || p_\theta(z|x) \right)$$

Rewrite log likelihood by latent z

- for any distribution $q(z)$
- Bayes' rule
- just algebra
- just algebra

Latent Variable Models

$$
\begin{aligned}
& \log p_\theta(x) \\
= & \int_z q(z) \log p_\theta(x) dz \\
= & \int_z q(z) \log \left(\frac{p_\theta(x|z) p_\theta(z)}{p_\theta(z|x)} \right) dz \\
= & \int_z q(z) \log \left(\frac{p_\theta(x|z) p_\theta(z)}{p_\theta(z|x)} \frac{q(z)}{q(z)} \right) dz \\
= & \int_z q(z) \left(\log p_\theta(x|z) + \log \frac{p_\theta(z)}{q(z)} + \log \frac{q(z)}{p_\theta(z|x)} \right) dz \\
= & \mathbb{E}_{z \sim q(z)} \left[\log p_\theta(x|z) \right] - \mathcal{D}_{\mathrm{KL}} \left(q(z) || p_\theta(z) \right) + \mathcal{D}_{\mathrm{KL}} \left(q(z) || p_\theta(z|x) \right)
\end{aligned}
$$

Rewrite log likelihood by latent z

- for any distribution $q(z)$
- Bayes' rule
- just algebra
- just algebra

Latent Variable Models

$$
\begin{aligned}
& \log p_\theta(x) \\
= & \int_z q(z) \log p_\theta(x) dz \\
= & \int_z q(z) \log \left(\frac{p_\theta(x|z) p_\theta(z)}{p_\theta(z|x)} \right) dz \\
= & \int_z q(z) \log \left(\frac{p_\theta(x|z) p_\theta(z)}{p_\theta(z|x)} \frac{q(z)}{q(z)} \right) dz \\
= & \int_z q(z) \left(\log p_\theta(x|z) + \log \frac{p_\theta(z)}{q(z)} + \log \frac{q(z)}{p_\theta(z|x)} \right) dz \\
= & \mathbb{E}_{z \sim q(z)} \Big[\log p_\theta(x|z) \Big] - \mathcal{D}_{\mathrm{KL}} \Big(q(z) || p_\theta(z) \Big) + \mathcal{D}_{\mathrm{KL}} \Big(q(z) || p_\theta(z|x) \Big)
\end{aligned}
$$

Rewrite log likelihood by latent z

- for any distribution $q(z)$
- Bayes' rule
- just algebra
- just algebra

Latent Variable Models

intractable

$$\log p_\theta(x)$$

Rewrite log likelihood by latent z

- for any distribution $q(z)$
- Bayes' rule

$$= \int_z q(z) \log p_\theta(x) dz$$

$$= \int_z q(z) \log \left(\frac{p_\theta(x|z) p_\theta(z)}{p_\theta(z|x)} \right) dz$$

$$= \int_z q(z) \log \left(\frac{p_\theta(x|z) p_\theta(z)}{p_\theta(z|x)} \frac{q(z)}{q(z)} \right) dz$$

$$= \int_z q(z) \left(\log p_\theta(x|z) + \log \frac{p_\theta(z)}{q(z)} + \log \frac{q(z)}{p_\theta(z|x)} \right) dz$$

$$= \mathbb{E}_{z \sim q(z)} \left[\log p_\theta(x|z) \right] - \mathcal{D}_{\mathrm{KL}} \left(q(z) || p_\theta(z) \right) + \mathcal{D}_{\mathrm{KL}} \left(q(z) || p_\theta(z|x) \right)$$

tractable tractable intractable

Latent Variable Models

intractable $\log p_\theta(x) - \mathcal{D}_{\mathrm{KL}}\left(q(z)||p_\theta(z|x)\right)$ intractable

$= \mathbb{E}_{z\sim q(z)}\left[\log p_\theta(x|z)\right] - \mathcal{D}_{\mathrm{KL}}\left(q(z)||p_\theta(z)\right)$

tractable tractable

Latent Variable Models

intractable $\log p_\theta(x) - \mathcal{D}_{\mathrm{KL}}\left(q(z)||p_\theta(z|x)\right)$ intractable

$= \underbrace{\mathbb{E}_{z\sim q(z)}\left[\log p_\theta(x|z)\right] - \mathcal{D}_{\mathrm{KL}}\left(q(z)||p_\theta(z)\right)}$

tractable tractable

- This is called Evidence Lower Bound (ELBO)
- Lower bound of $\log p_\theta(x)$

- This equation holds for <u>any</u> distribution $q(z)$

Latent Variable Models

$q_\varphi(z|x)$ $\qquad\qquad$ $q_\varphi(z|x)$

$$\mathbb{E}_{z\sim q(z)}\left[\log p_\theta(x|z)\right] - \mathcal{D}_{\mathrm{KL}}\left(q(z)||p_\theta(z)\right)$$

tractable $\qquad$ tractable

- This is called Evidence Lower Bound (ELBO)
- Lower bound of $\log p_\theta(x)$

- This equation holds for <u>any</u> distribution $q(z)$

- Parameterize $q(z)$ by $q_\varphi(z|x)$

Latent Variable Models

$q_\varphi(z|x)$ $\quad$ $q_\varphi(z|x)$ $\quad$ $p(z)$

$$\mathbb{E}_{z\sim q(z)}\left[\log p_\theta(x|z)\right] - \mathcal{D}_{\mathrm{KL}}\left(q(z)||p_\theta(z)\right)$$

tractable $\quad$ tractable

- This is called Evidence Lower Bound (ELBO)
- Lower bound of $\log p_\theta(x)$

- This equation holds for <u>any</u> distribution $q(z)$

- Parameterize $q(z)$ by $q_\varphi(z|x)$
- let $p_\theta(z)$ be a simple known prior $p(z)$

Variational Autoencoder

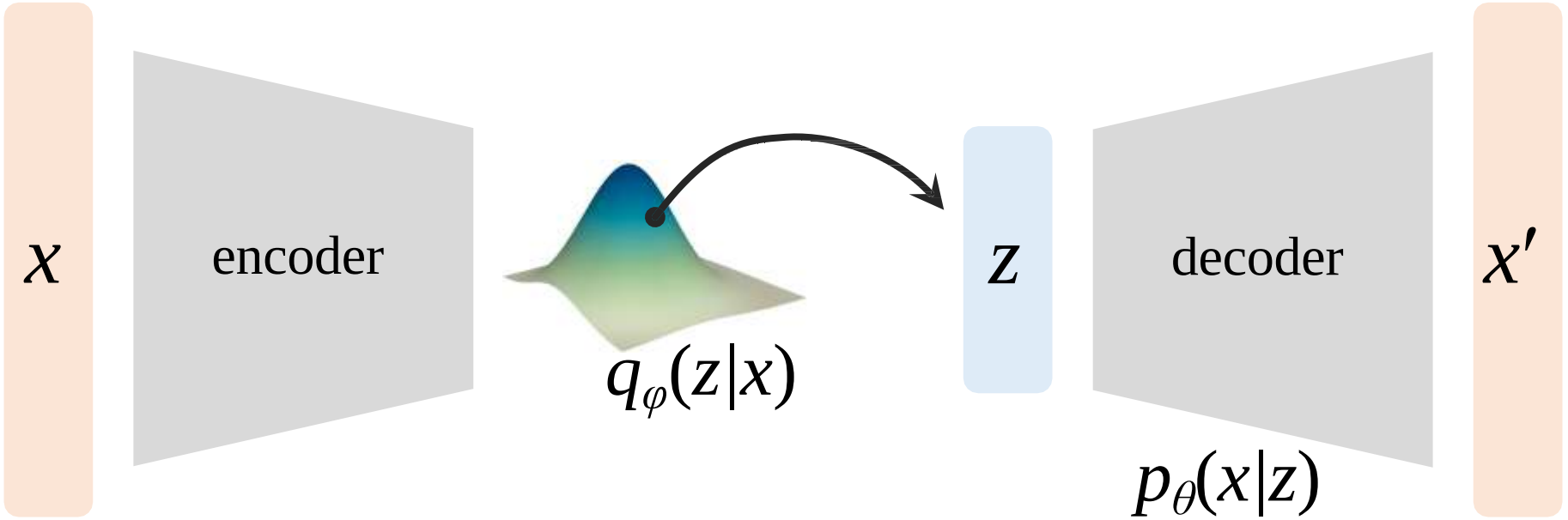
Maximize ELBO ⇒ minimize an objective:

$$\mathcal{L}_{\theta,\phi}(x) = -\mathbb{E}_{z\sim q_\phi(z|x)}\Big[\log p_\theta(x|z)\Big] + \mathcal{D}_{\mathrm{KL}}\Big(q_\phi(z|x)||p(z)\Big)$$

Variational Autoencoder

Maximize ELBO ⇒ minimize an objective:

$$\mathcal{L}_{\theta,\phi}(x) = -\mathbb{E}_{z\sim q_\phi(z|x)}\Big[\log p_\theta(x|z)\Big] + \mathcal{D}_{\mathrm{KL}}\Big(q_\phi(z|x)||p(z)\Big)$$



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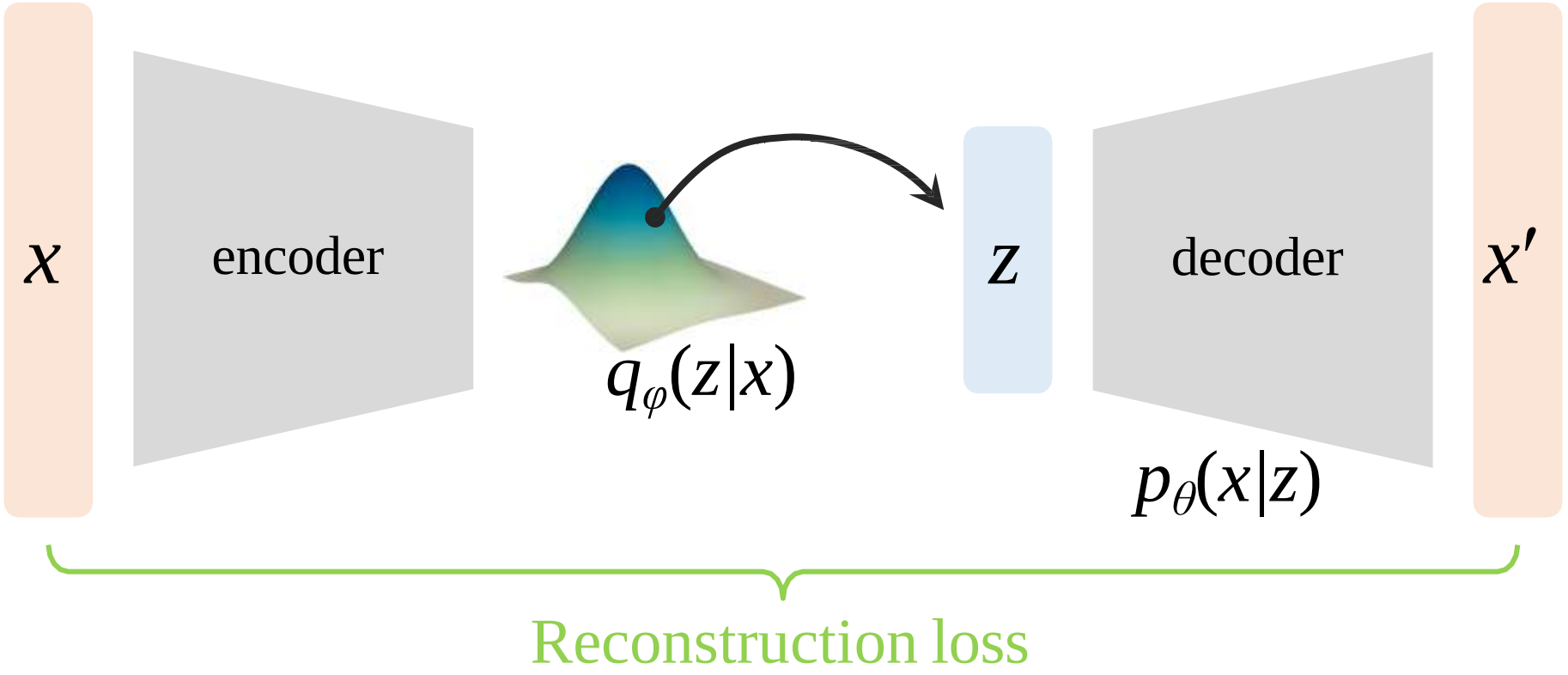

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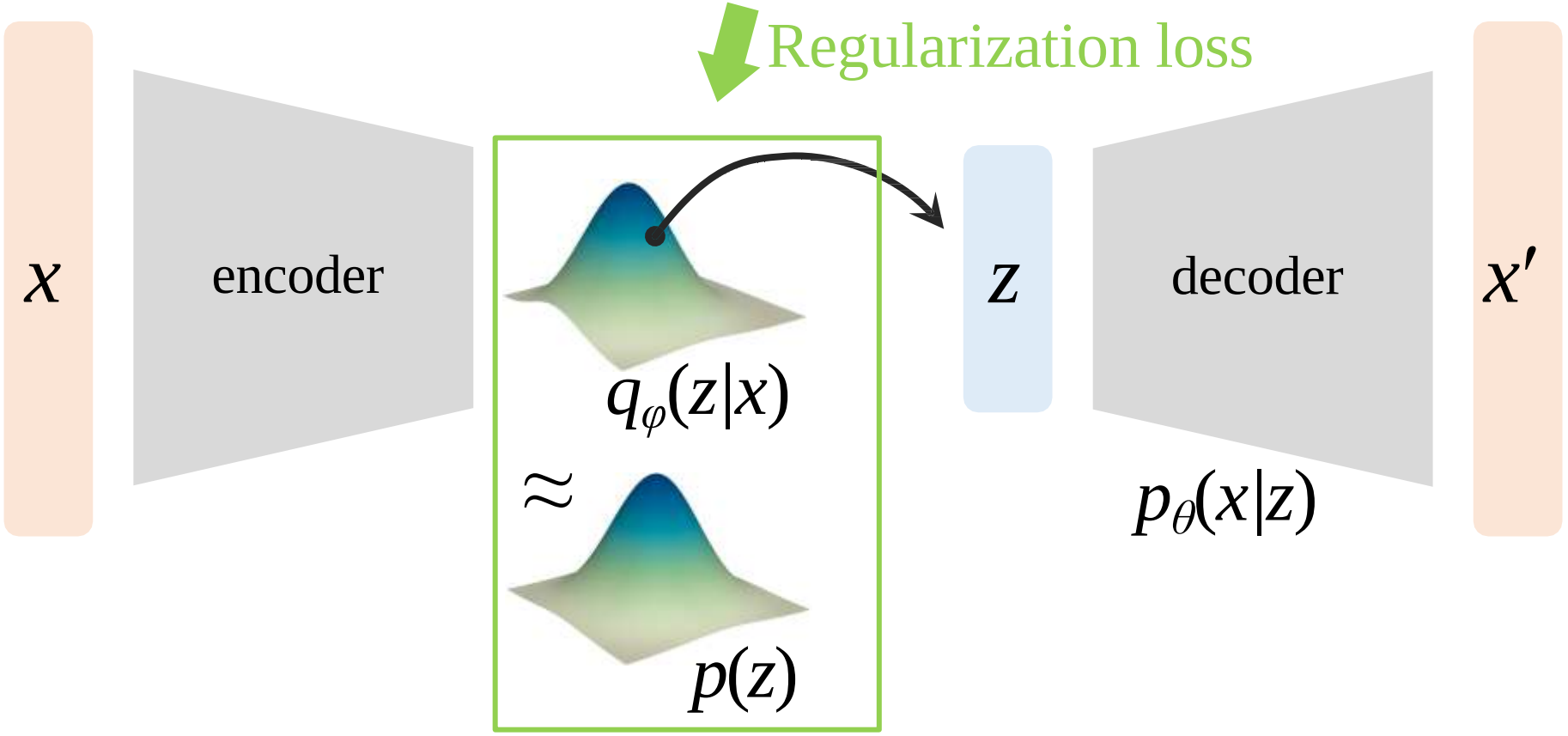
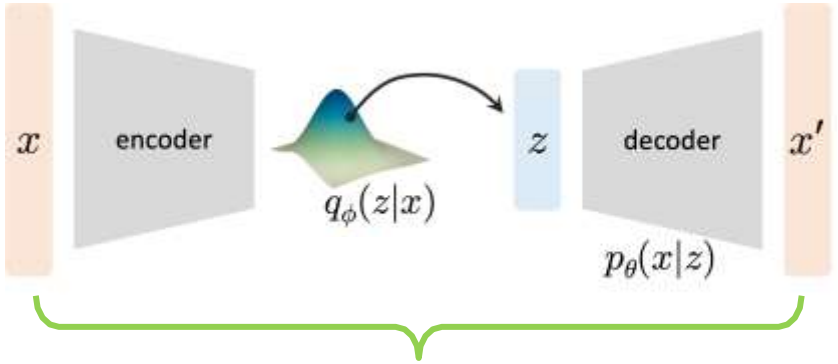


Variational Autoencoder



Reconstruction loss

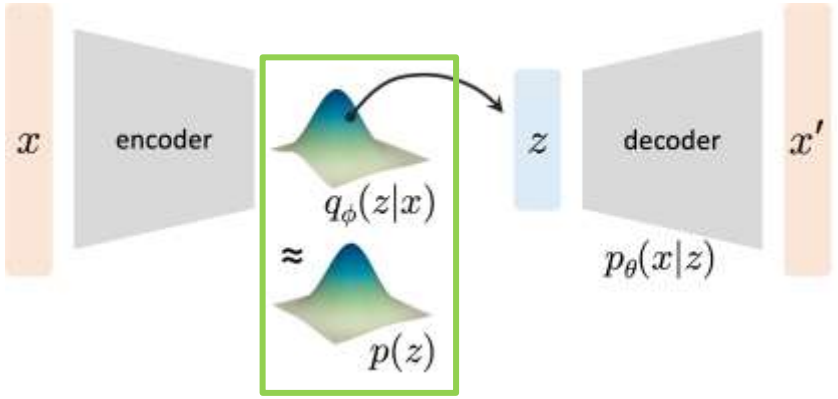
$$\mathcal{L}_{\theta,\phi}(x) = \boxed{-\mathbb{E}_{z\sim q_\phi(z|x)}\Big[\log p_\theta(x|z)\Big]} + \mathcal{D}_{\mathrm{KL}}\Big(q_\phi(z|x)||p(z)\Big)$$

Example: L2 loss

- one-step Monte Carlo: $z \sim q_\phi(z|x)$
- map *z* by decoder net: $\boxed{g_\theta(z) \to x'}$ network estimates distribution's parameters
- model $p_\theta(x|z)$ by Gaussian: $p_\theta(x|z) = \mathcal{N}(x \mid x', \sigma_0^2)$ (assume fixed std)
- negative log likelihood: $\frac{1}{2\sigma_0^2}||x - x'||^2 + const$

- L2 loss ⇒ a Gaussian neighborhood around data point *x*

Variational Autoencoder



Regularization loss

$$\mathcal{D}_{\mathrm{KL}}\Big(q_\phi(z|x)||p(z)\Big)$$

Example: Gaussian prior

- let $p(z) = \mathcal{N}(z \mid 0, \mathbf{I})$
- model $q_\phi(z|x)$ by Gaussian: $\mathcal{N}(z \mid \mu, \sigma)$
- map *x* by encoder net: $f_\phi(x) \rightarrow \mu, \sigma$

again, network estimates distribution's parameters

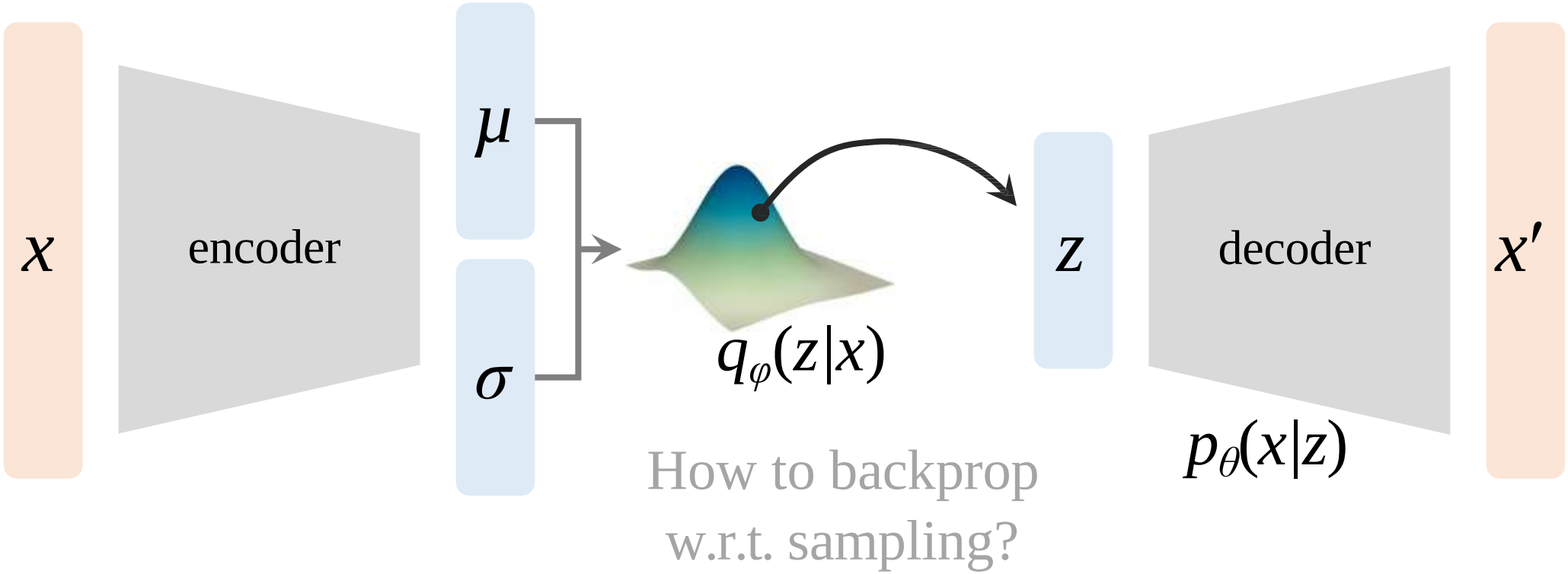
- compute loss analytically: $\mathcal{D}_{\mathrm{KL}}\Big(\mathcal{N}(z \mid \mu, \sigma) \,||\, \mathcal{N}(z \mid 0, \mathbf{I})\Big)$

- fixed covariance ⇒ L2 loss on μ

Variational Autoencoder

Maximize ELBO ⇒ minimize an objective:

$$\mathcal{L}_{\theta,\phi}(x) = -\mathbb{E}_{z\sim q_\phi(z|x)}\left[\log p_\theta(x|z)\right] + \mathcal{D}_{\mathrm{KL}}\left(q_\phi(z|x)||p(z)\right)$$



Variational Autoencoder

Maximize ELBO ⇒ minimize an objective:

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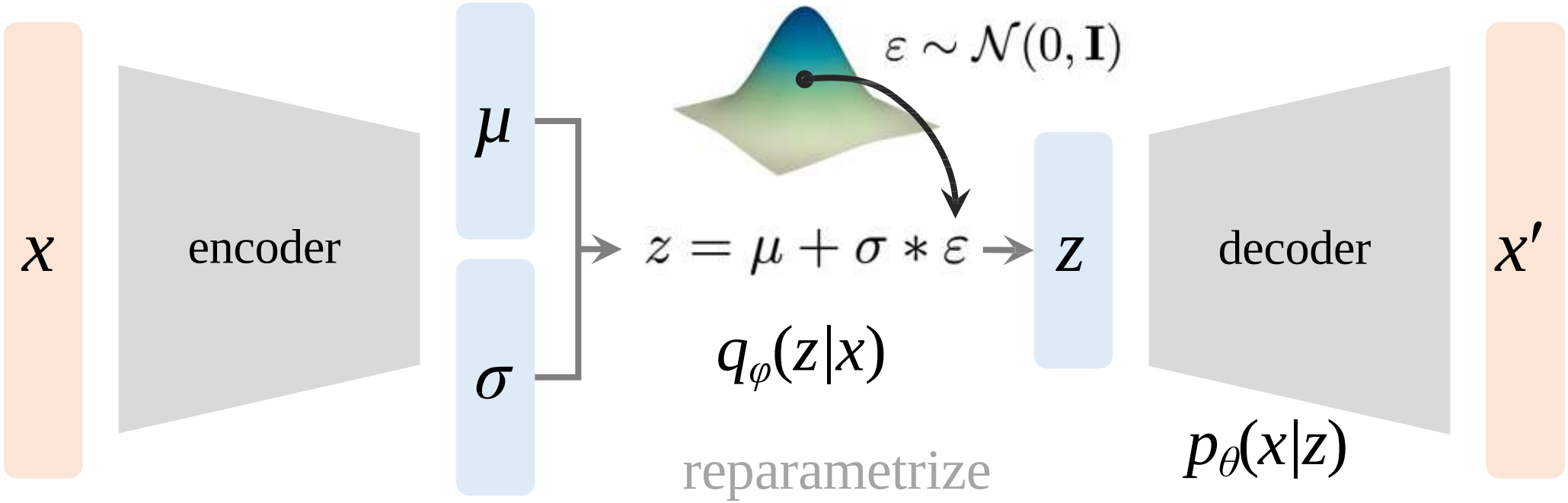


Variational Autoencoder

... so far, we have discussed an objective on one x:

$$\mathcal{L}_{\theta,\phi}(x) = -\mathbb{E}_{z\sim q_\phi(z|x)}\Big[\log p_\theta(x|z)\Big] + \mathcal{D}_{\mathrm{KL}}\Big(q_\phi(z|x)||p(z)\Big)$$

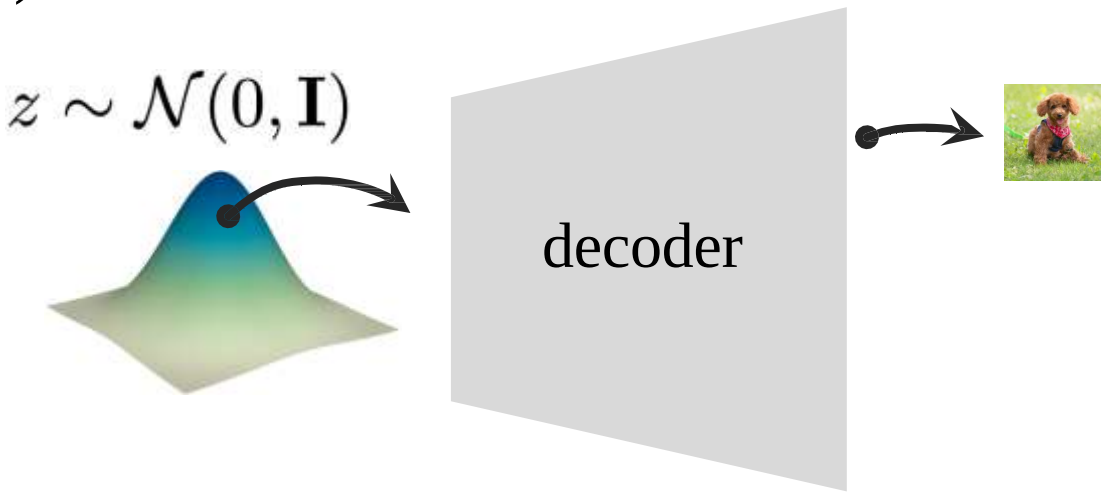
Overall loss is expectation over data:

$$\mathcal{L}_{\theta,\phi} = \mathbb{E}_{x\sim p_{data}(x)}\Big[-\mathbb{E}_{z\sim q_\phi(z|x)}\Big[\log p_\theta(x|z)\Big] + \mathcal{D}_{\mathrm{KL}}\Big(q_\phi(z|x)||p(z)\Big)\Big]$$

Variational Autoencoder

Inference (generation):

- sample z from: $\mathcal{N}(0, \mathbf{I})$
- map z by decoder net: $g_\theta(z)$



Variational Autoencoder

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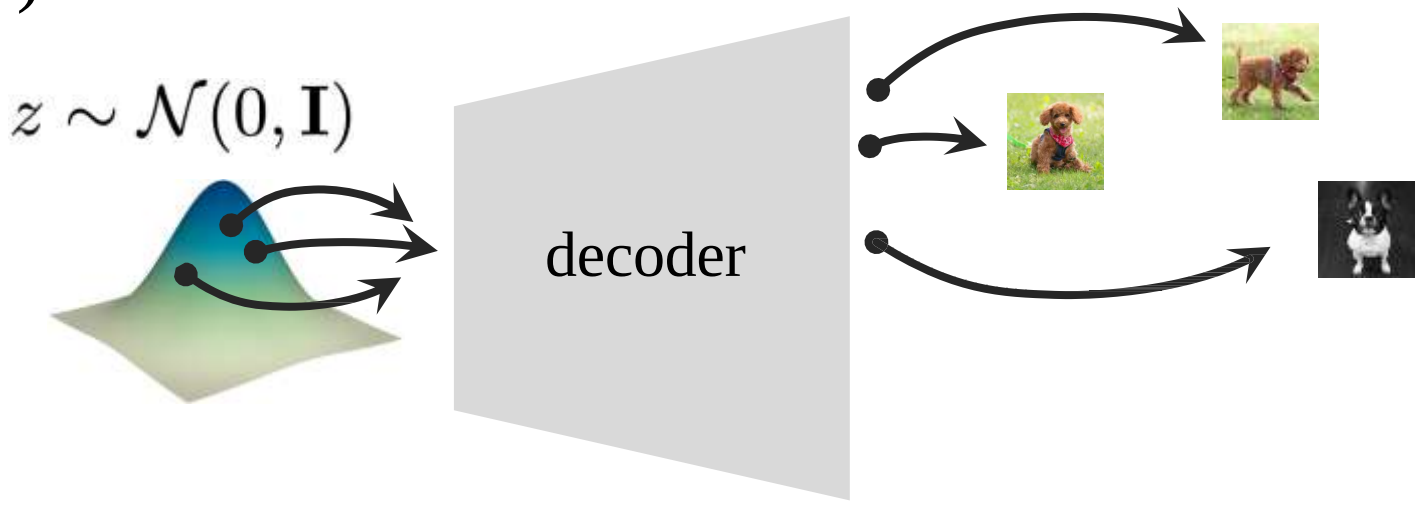

Variational Autoencoder

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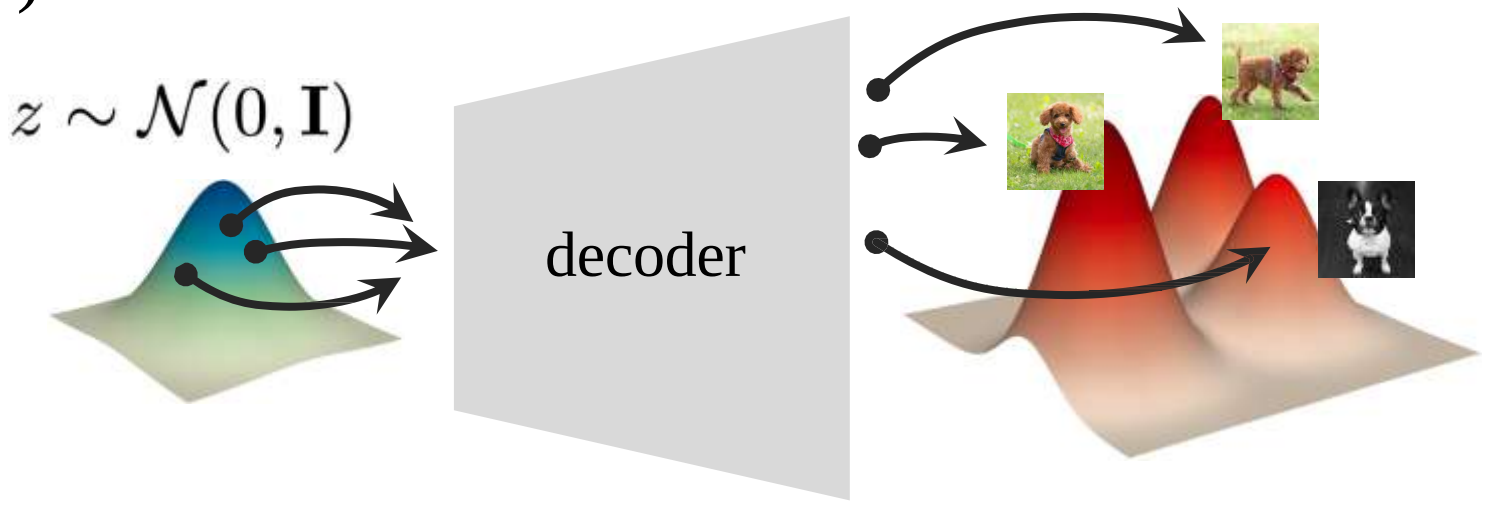

Variational Autoencoder

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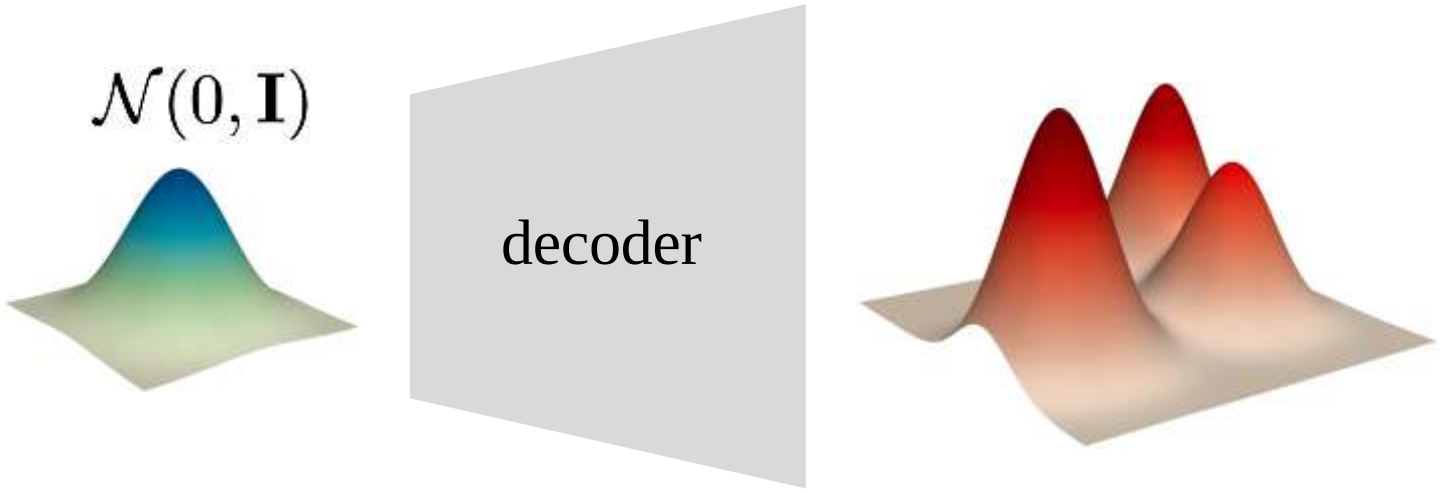
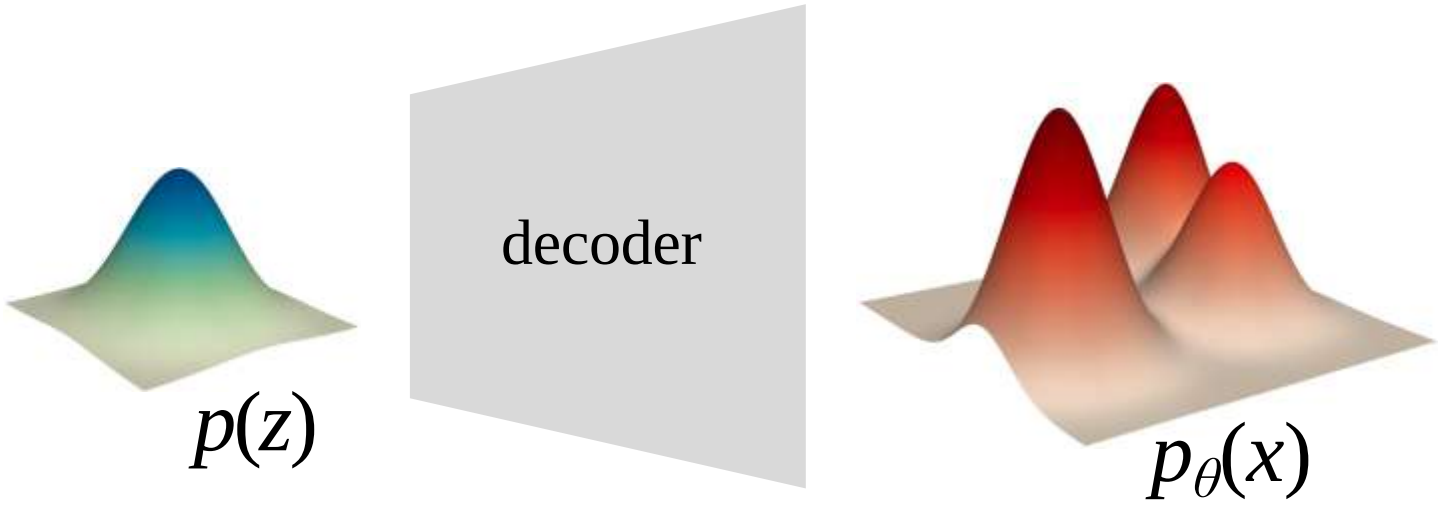
- map z by decoder net: $g_\theta(z)$



Decoder is a deterministic mapping from one distribution to another.

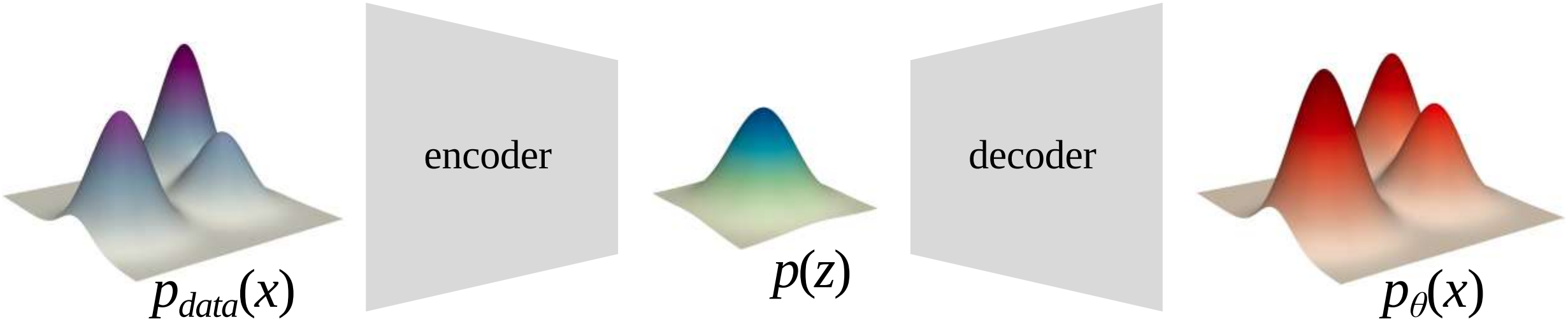
A view of “Autoencoding Distributions”

- decoder: maps latent distribution to data distribution



A view of “Autoencoding Distributions”

- encoder: maps data distribution to latent distribution
- decoder: maps latent distribution to data distribution



A view of “Autoencoding Distributions”

- encoder: maps data distribution to latent distribution
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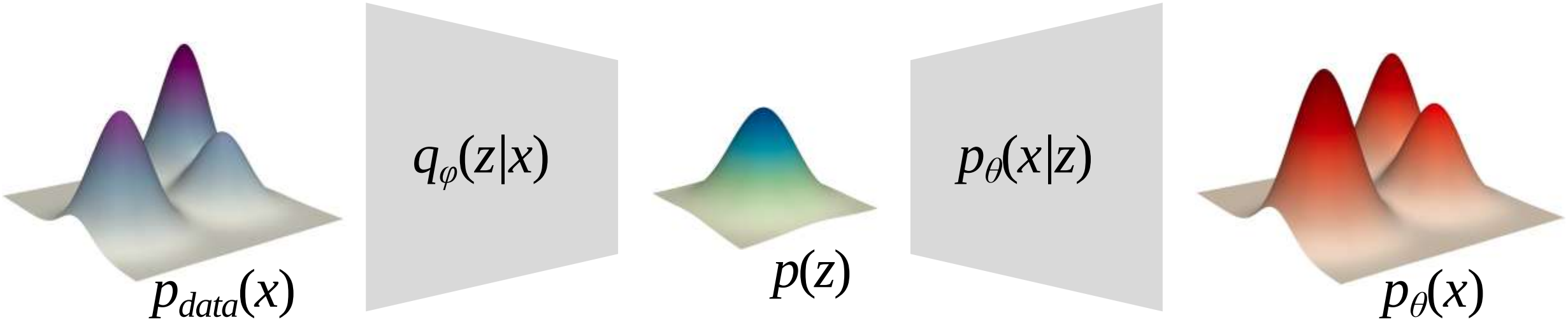
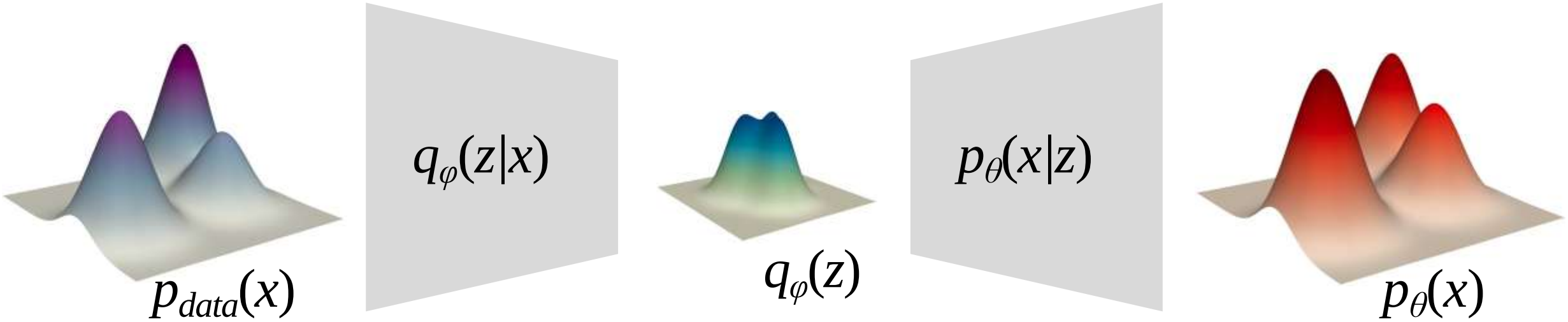


A view of “Autoencoding Distributions”

- encoded latent distribution: $q_\phi(z) = \int_x q_\phi(z|x) p_{data}(x) dx$



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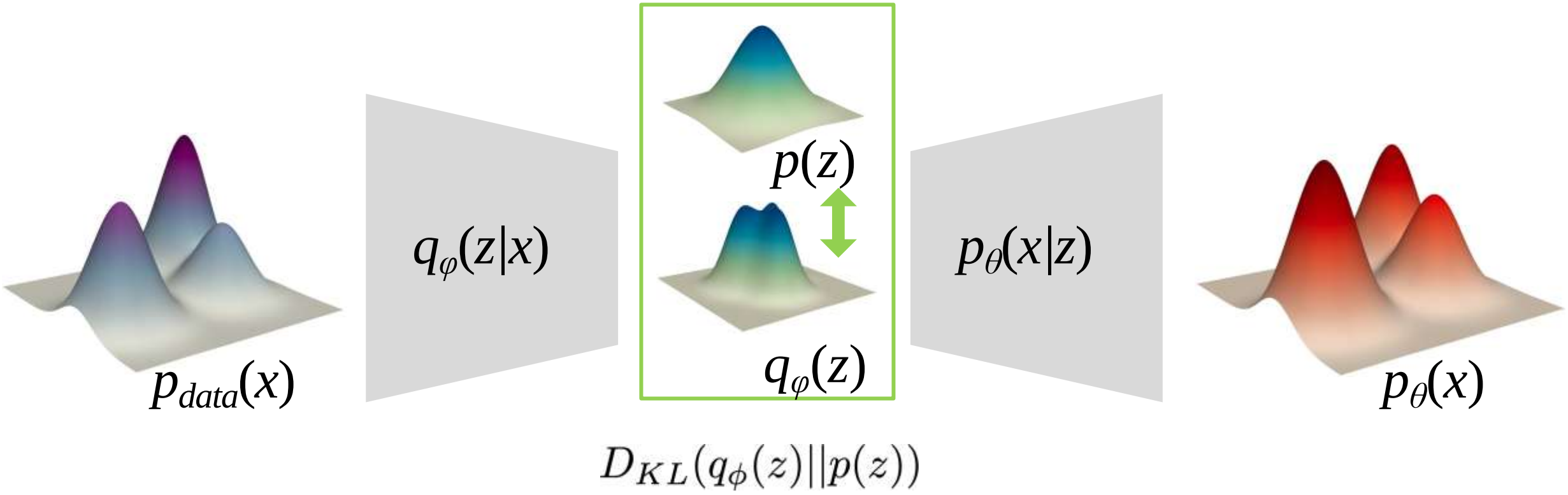
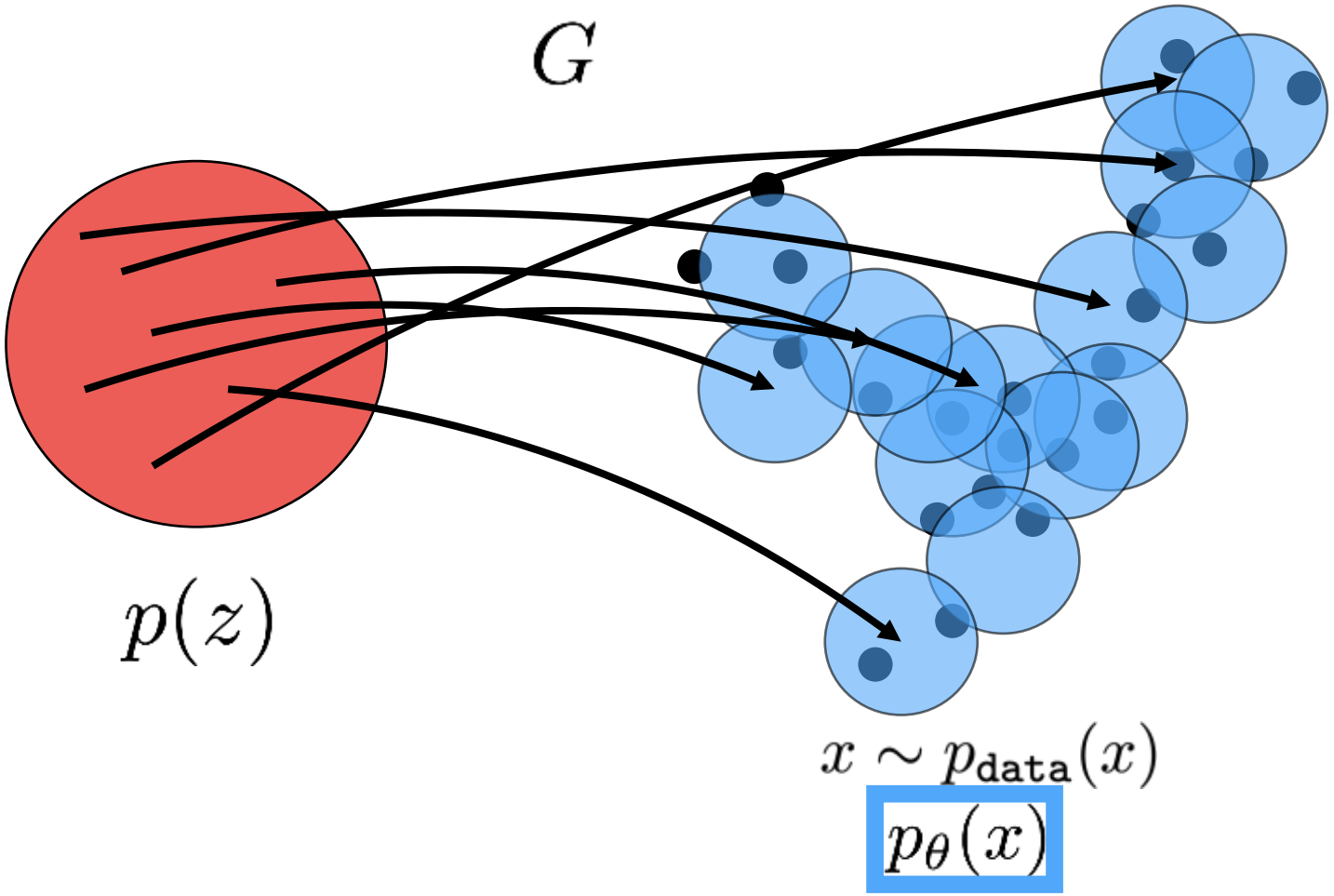


E.g., see "*InfoVAE: Information Maximizing Variational Autoencoders*", 2017

Variational Autoencoders (VAEs)

[Kingma & Welling, 2014; Rezende, Mohamed, Wierstra 2014]

Prior distribution Target distribution



Density model:

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

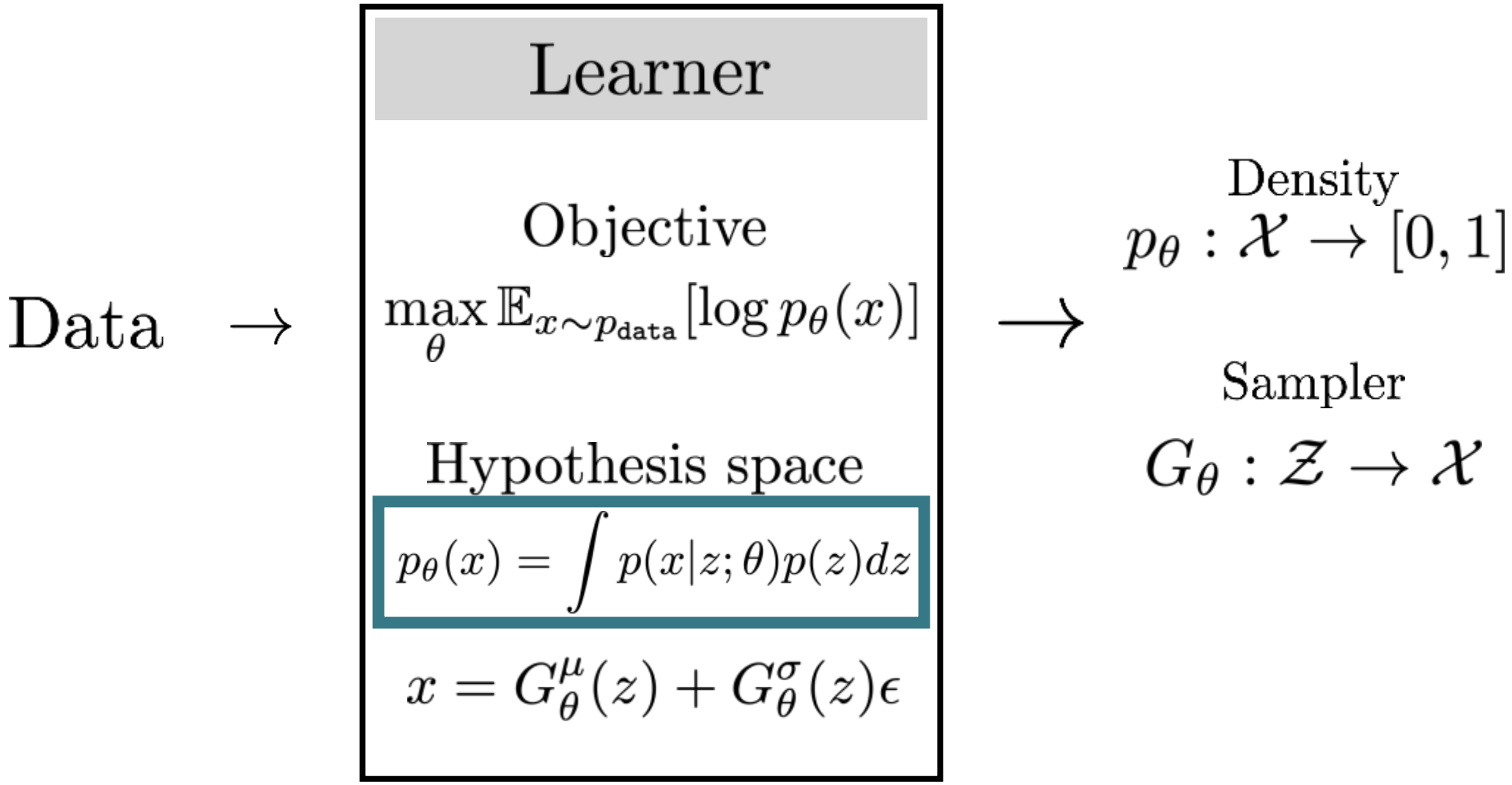
$$p(x|z;\theta) \sim \mathcal{N}(x; G^\mu_\theta(x), G^\sigma_\theta(x))$$

Sampling:

$$z \sim p(z) \quad \epsilon \sim \mathcal{N}(0,1)$$

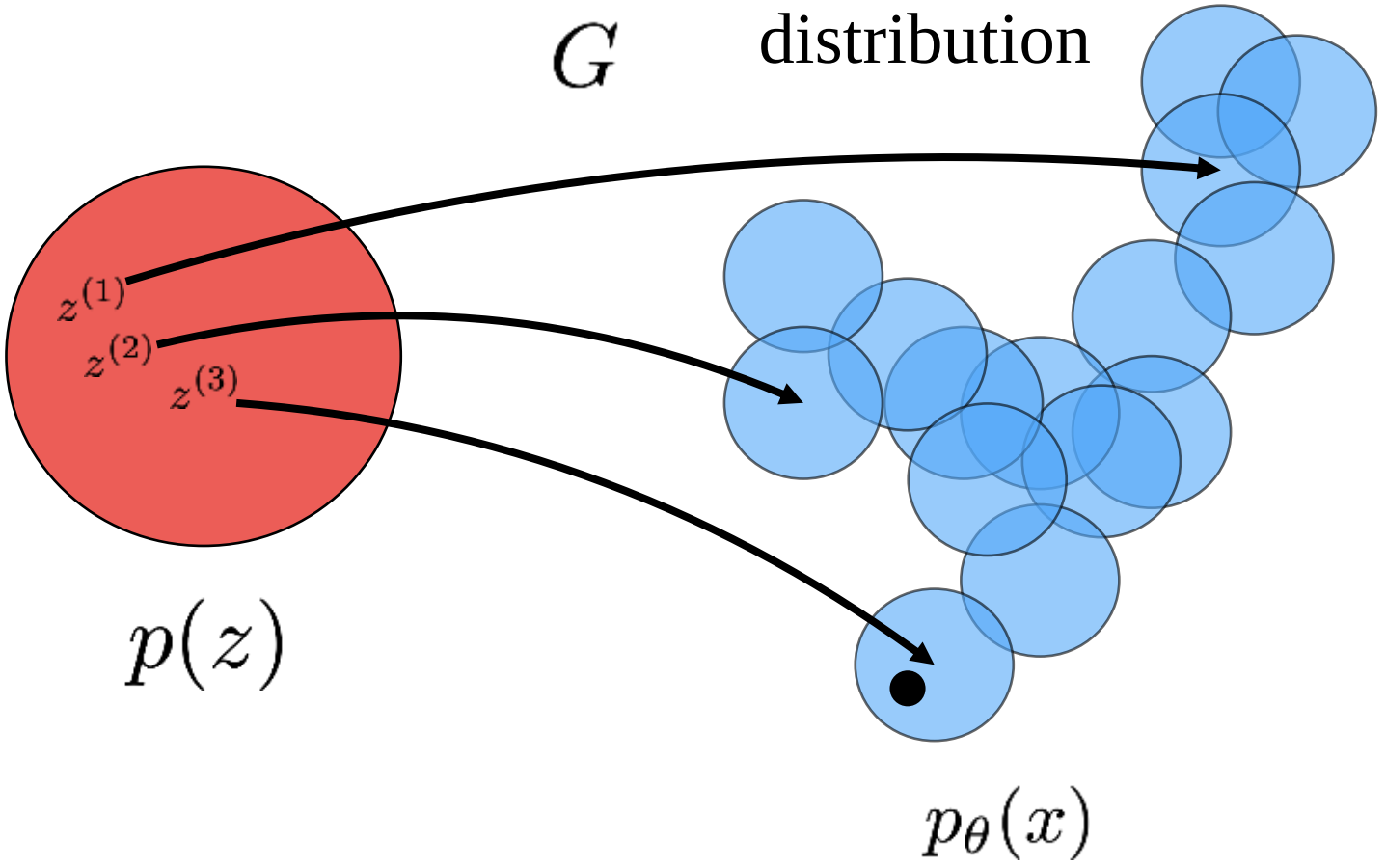
$$x = G^\mu_\theta(z) + G^\sigma_\theta(z)\epsilon$$

Variational Autoencoder (VAE)



Prior distribution

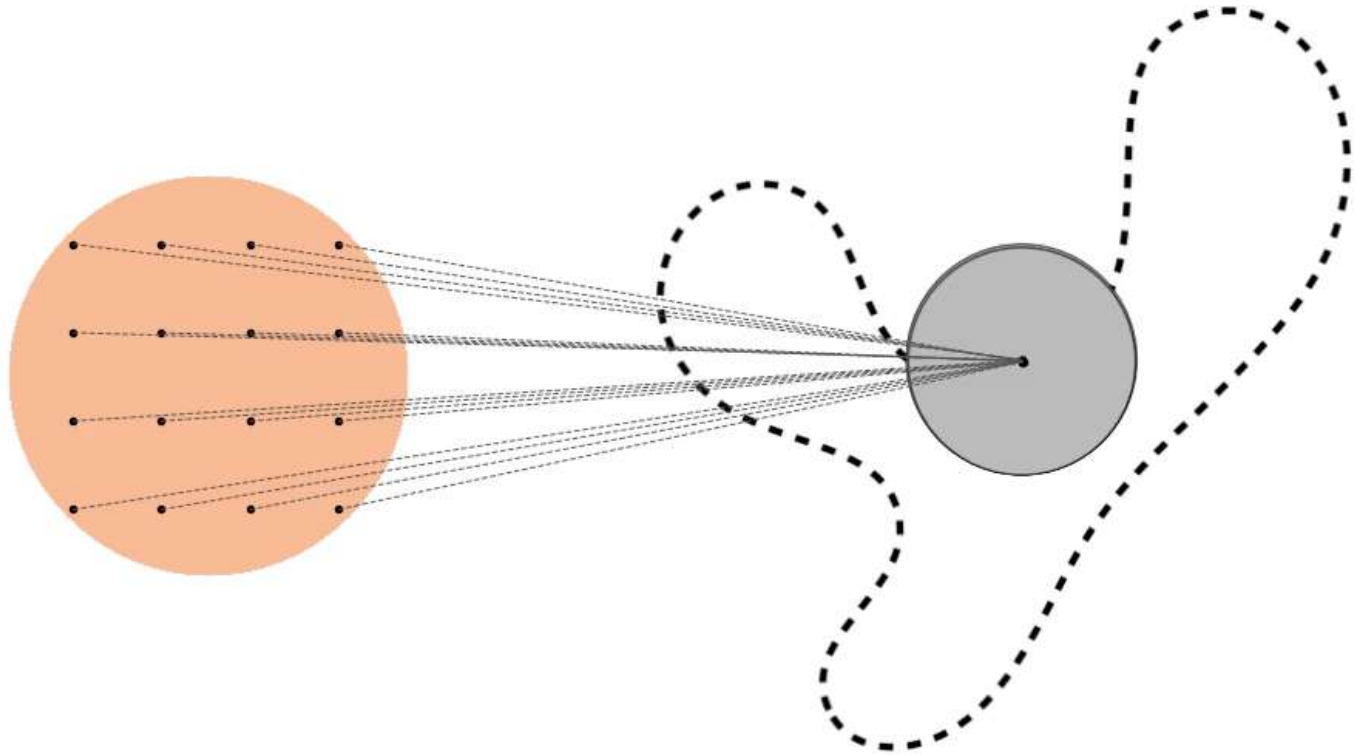
Current model of target distribution



In order to optimize our model, we need to measure the likelihood it assigns to each datapoint x

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

$$= p(x|z^{(1)})p(z^{(1)})dz +$$
$$p(x|z^{(2)})p(z^{(2)})dz +$$
$$p(x|z^{(3)})p(z^{(3)})dz + \ldots$$



Prior distribution

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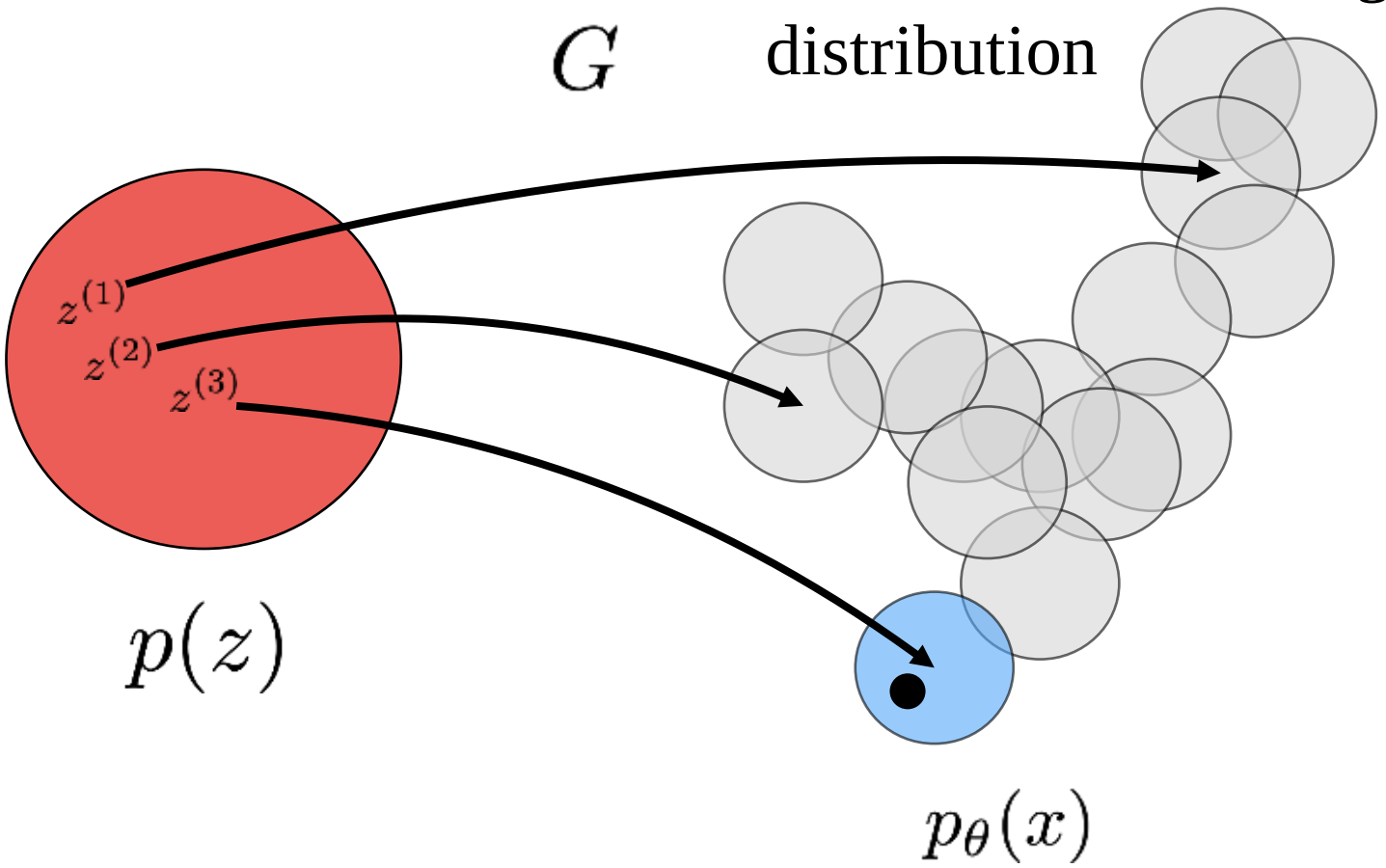


In order to optimize our model, we need to measure the likelihood it assigns to each datapoint x

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

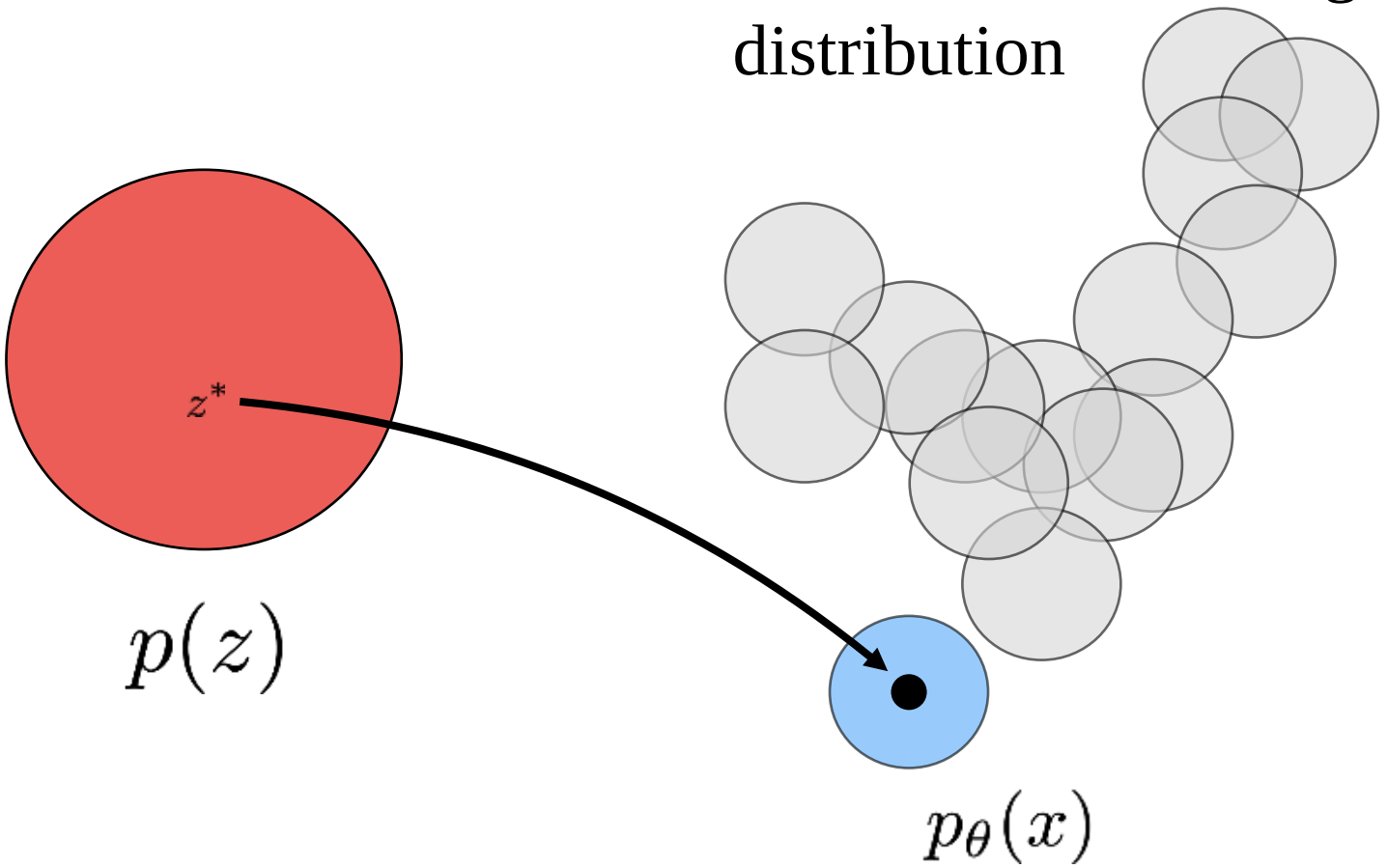
$$= \sim 0+$$

$$\sim 0+$$

$$p(x|z^{(3)})p(z^{(3)})dz + \ldots$$

Prior distribution

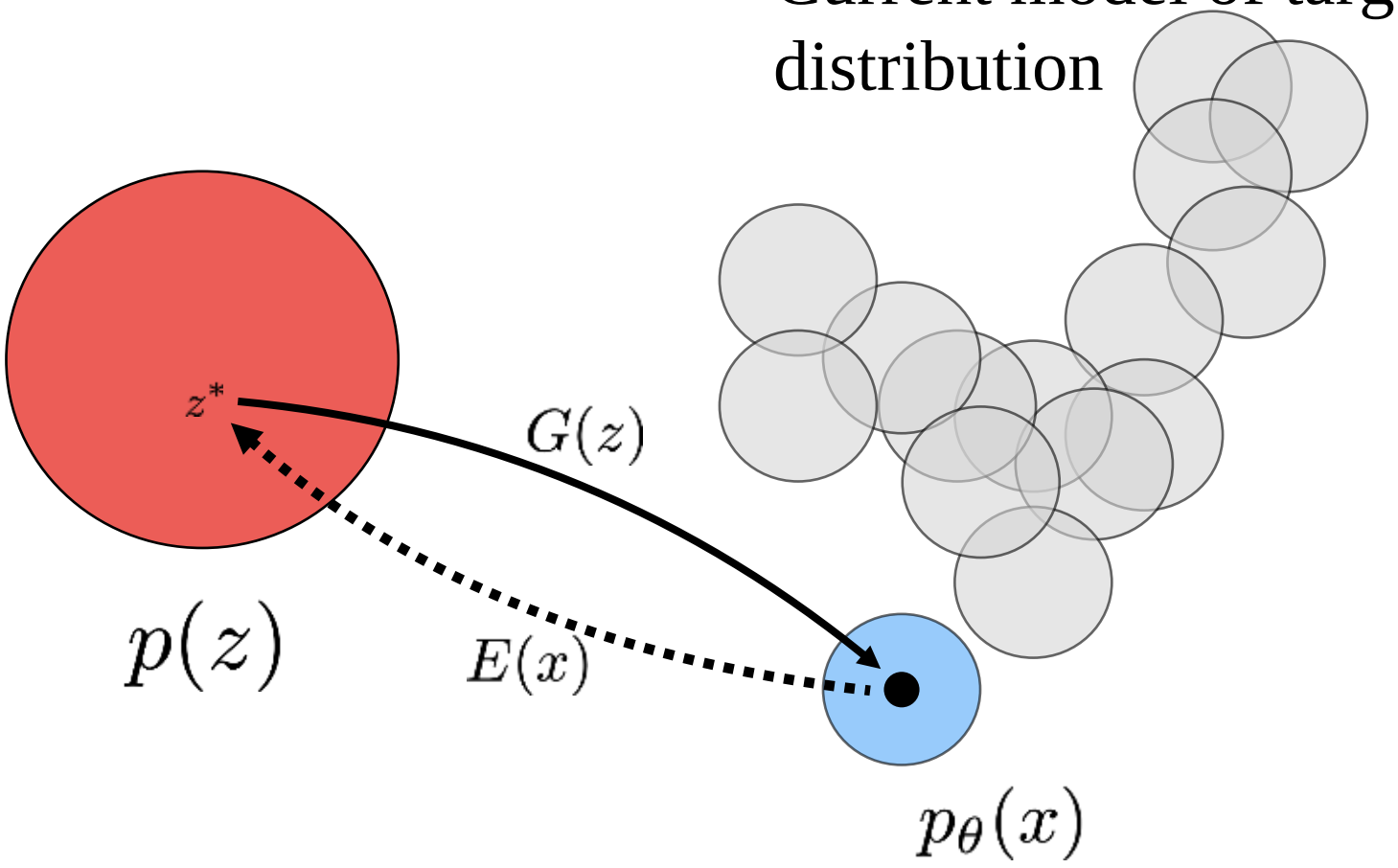
Current model of target distribution



If only we knew z*, we wouldn't need the integral…

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

$$\approx p(x|z^*;\theta)p(z^*)$$



Technical note: for the continuous math to actually work out, z ~ E(x) needs to be a distribution (typically set to Gaussian), but here we (incorrectly) treat it as deterministic for simplicity.*

If only we knew z*, we wouldn't need the integral…

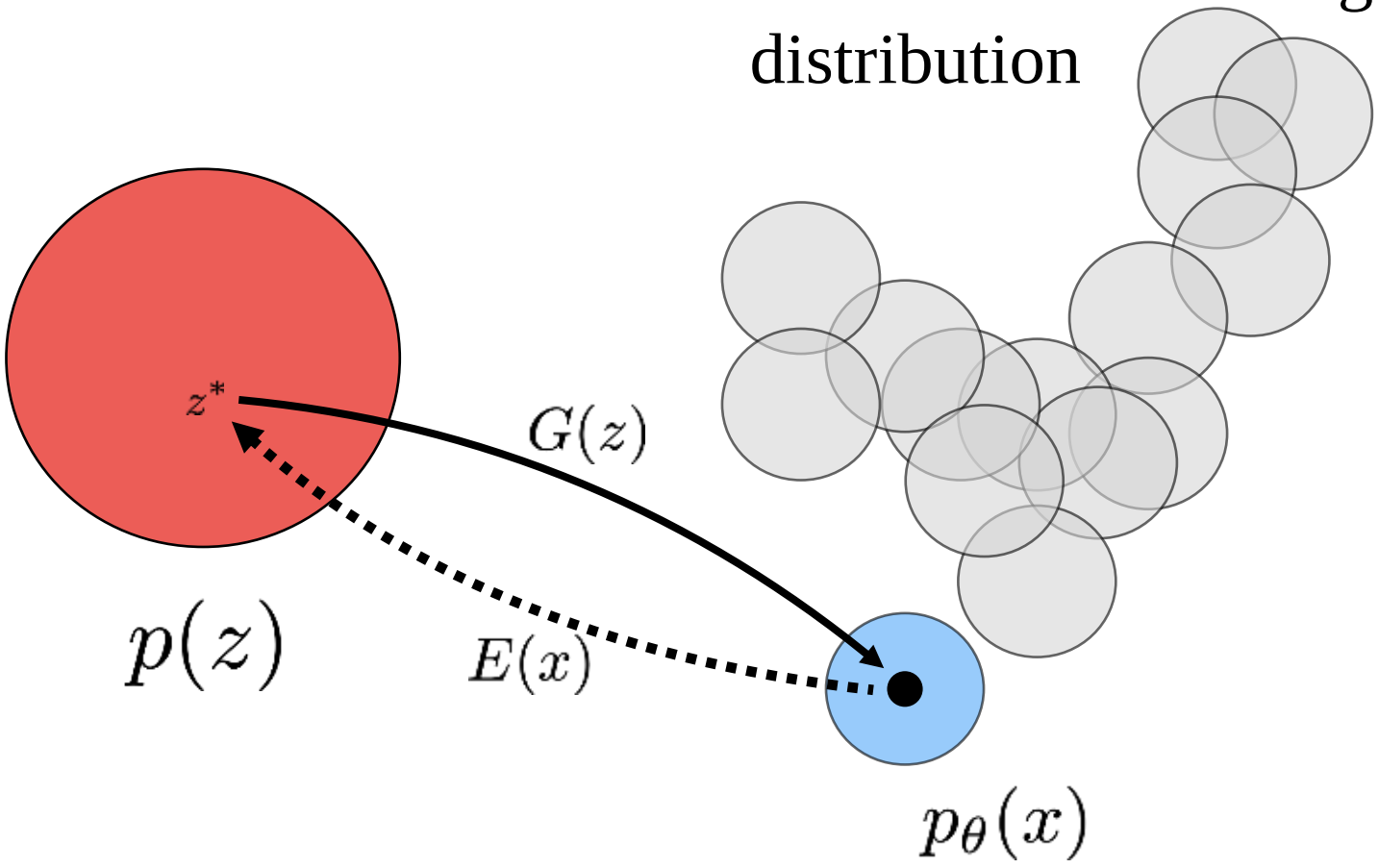
$$p_\theta(x) = \int p(x|z;\theta)p(z)dz$$

$$\approx p(x|z^*;\theta)p(z^*)$$

So, we simply try to predict z* for the given x!

$$z^* = E(x)$$

$$\arg\max_E p(x|E(x);\theta)p(E(x))$$



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$$\approx p(x|z^*;\theta)p(z^*)$$

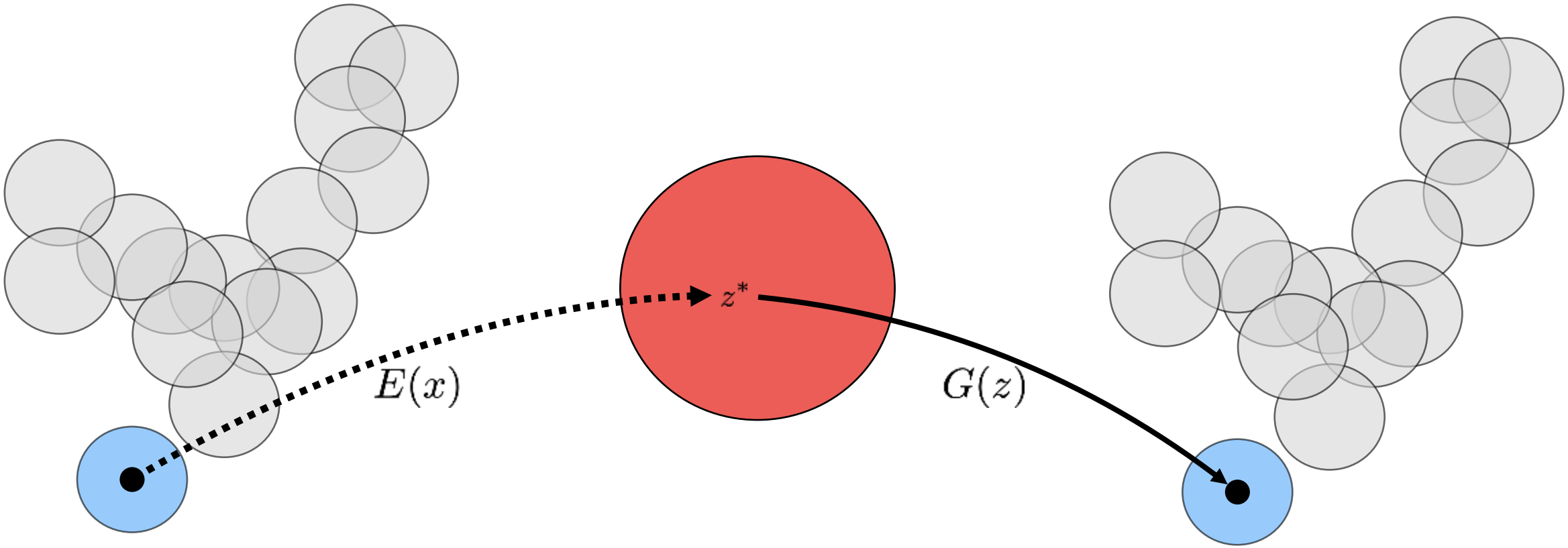
So, we simply try to predict z* for the given x!

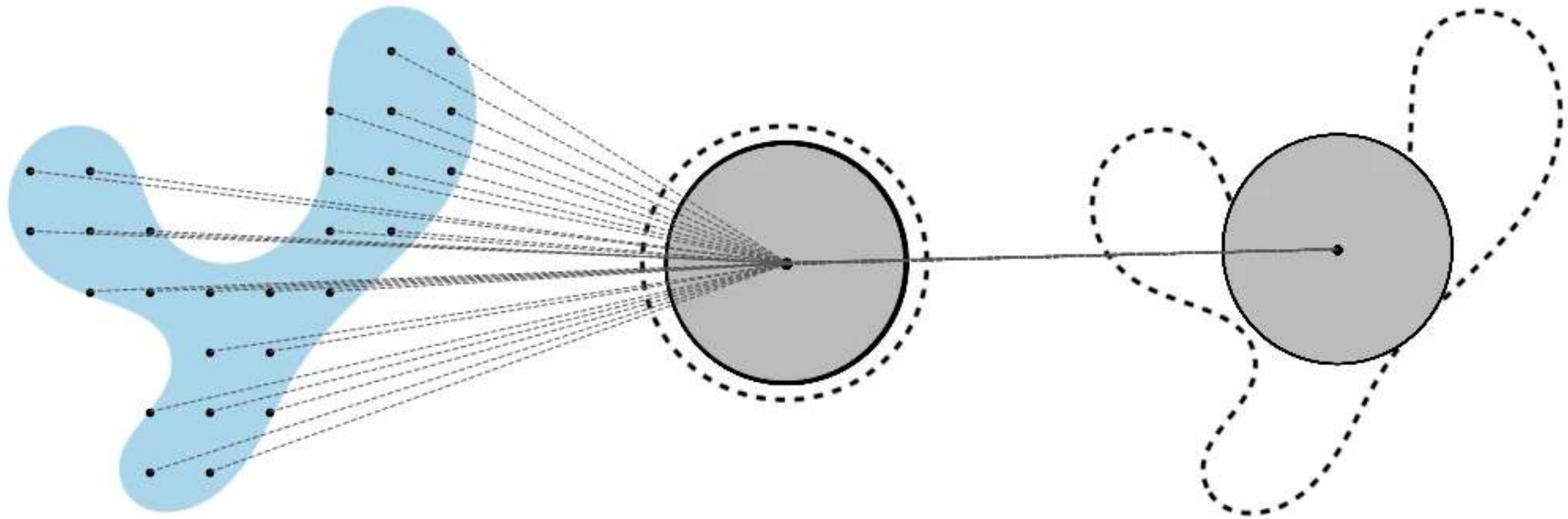
$$z^* = E(x)$$

(assuming unit Gaussian prior, isotropic Gaussian likelihood model) →

$$\arg\min_E \|G(E(x)) - x\|_2^2 + ||E(x)||_2^2$$

Autoencoder!





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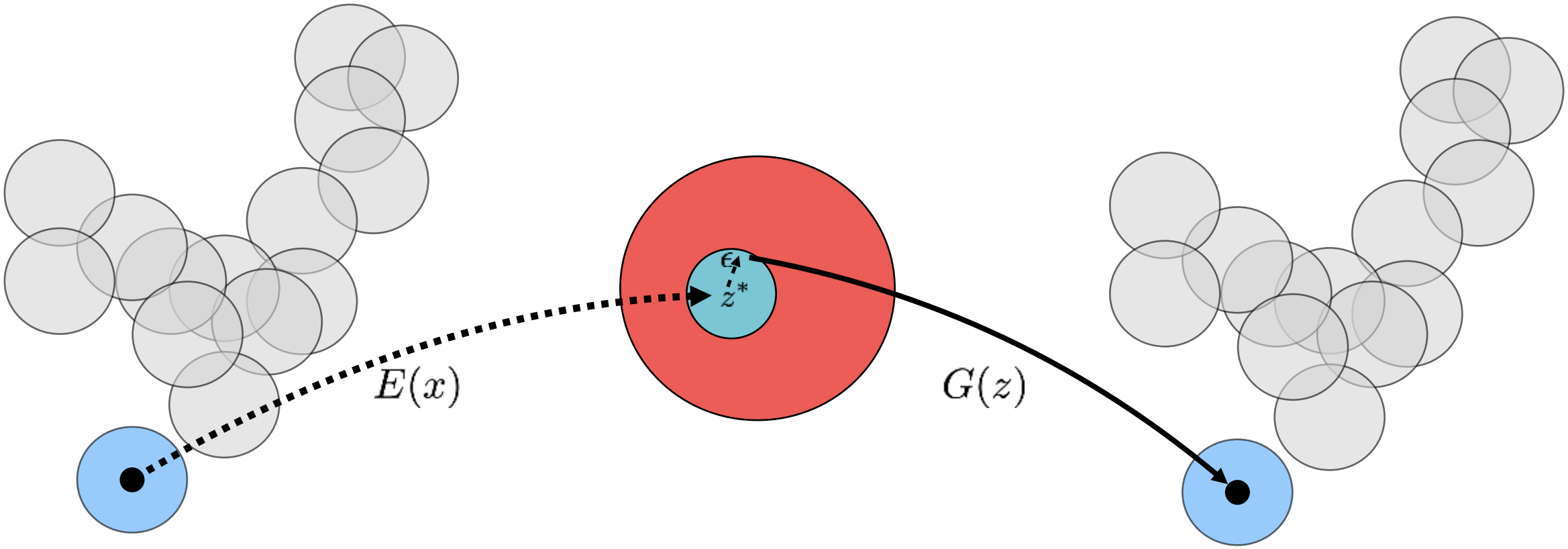
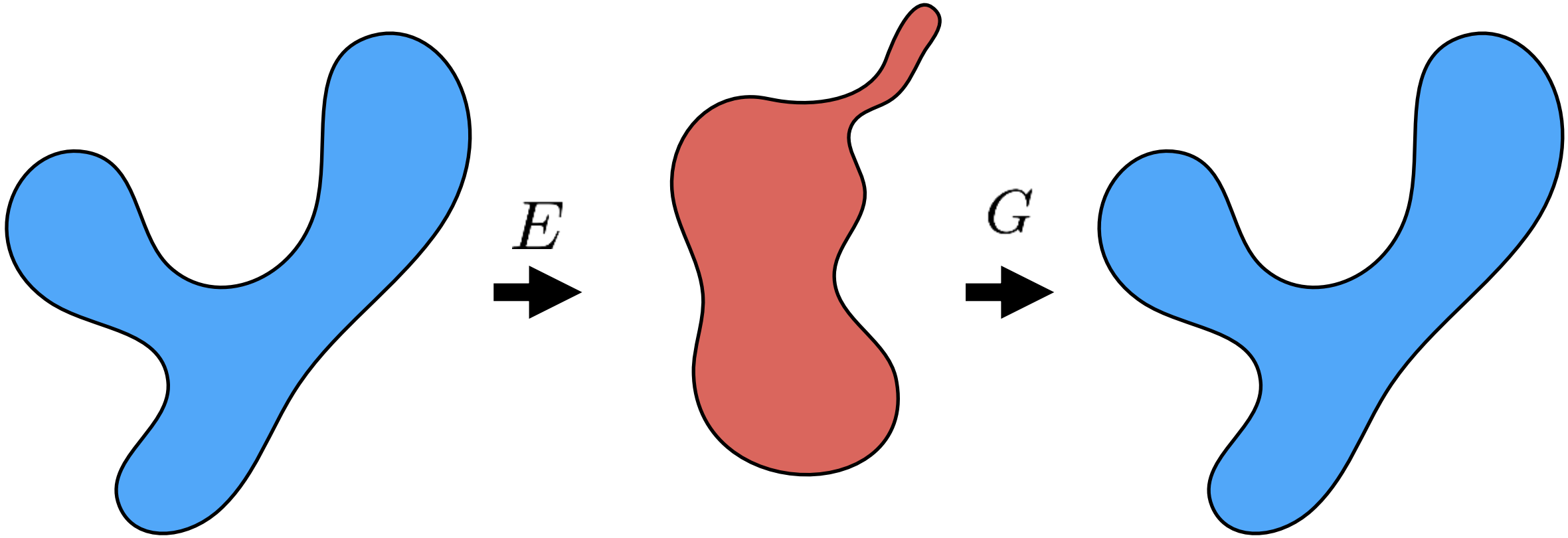


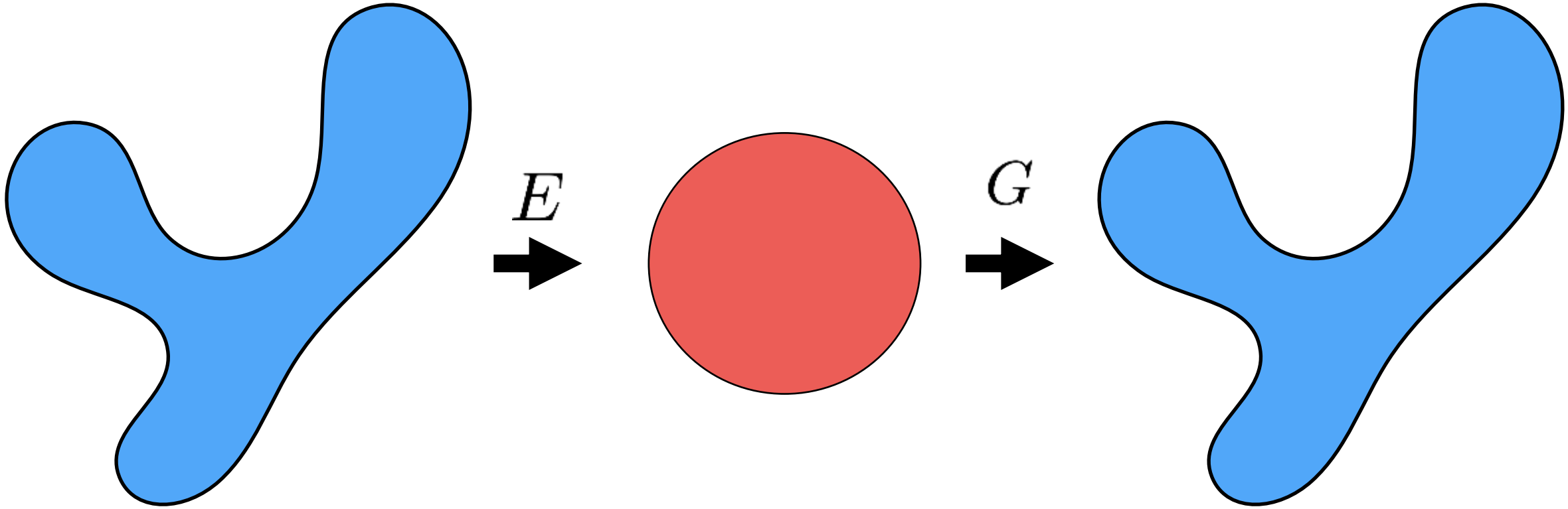
$$\arg\min_{G,E} \mathbb{E}_{x,\epsilon}[\|G(E(x+\epsilon)) - x\|_2^2 + \|E(x+\epsilon)\|_2^2]$$

Classical Autoencoder



$$\arg\min_{G,E} \mathbb{E}_x[\|G(E(x)) - x\|_2^2]$$

Variational Autoencoder

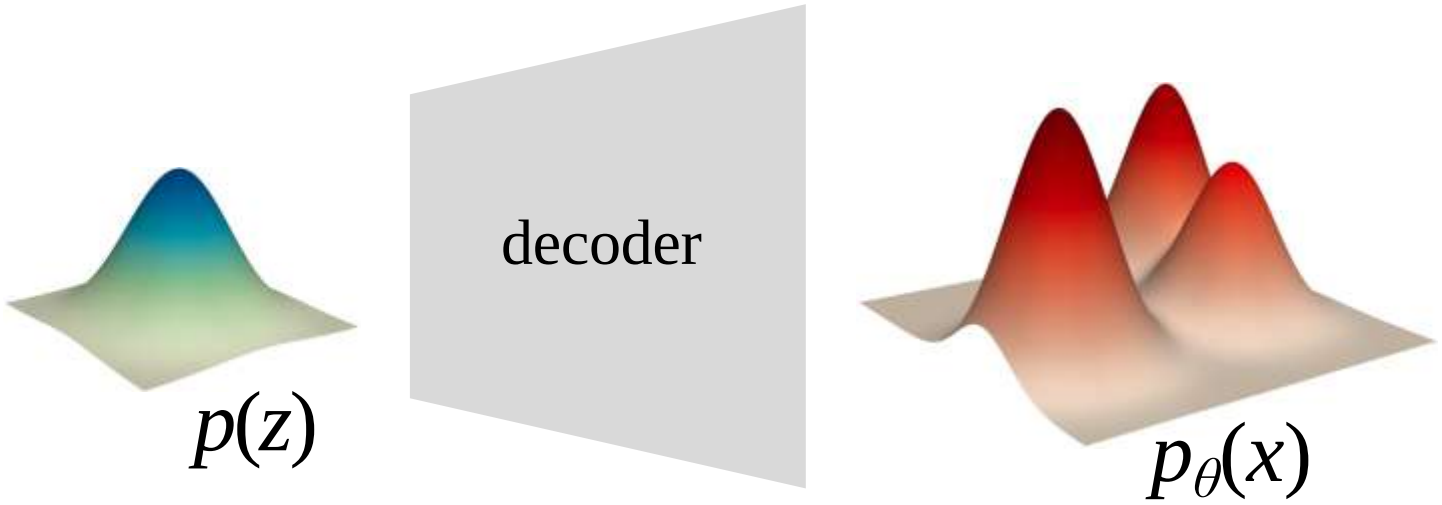


$$\arg\min_{G,E} \mathbb{E}_{x,\epsilon}[\|G(E(x+\epsilon)) - x\|_2^2 + \|E(x+\epsilon)\|_2^2]$$

Recap.

A view of “Autoencoding Distributions”

- decoder: maps latent distribution to data distribution



A view of “Autoencoding Distributions”

- encoder: maps data distribution to latent distribution
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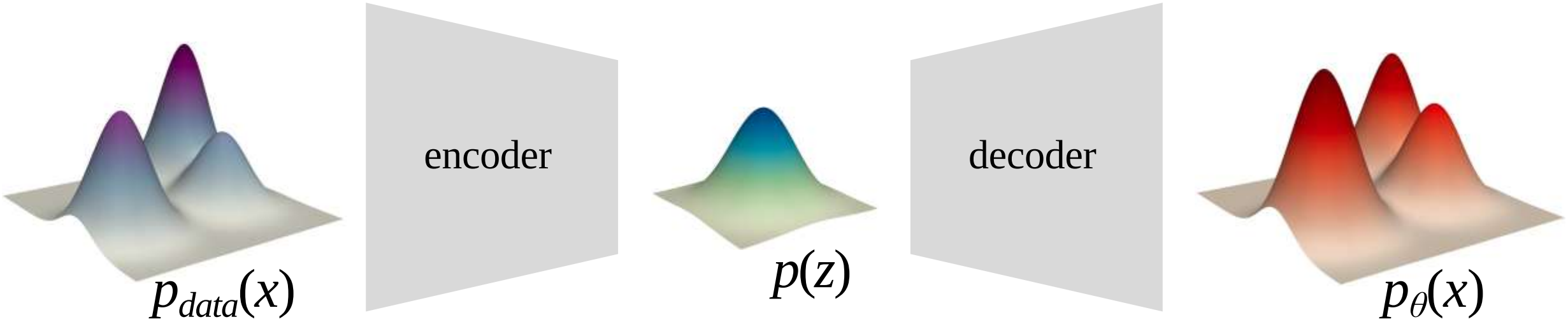

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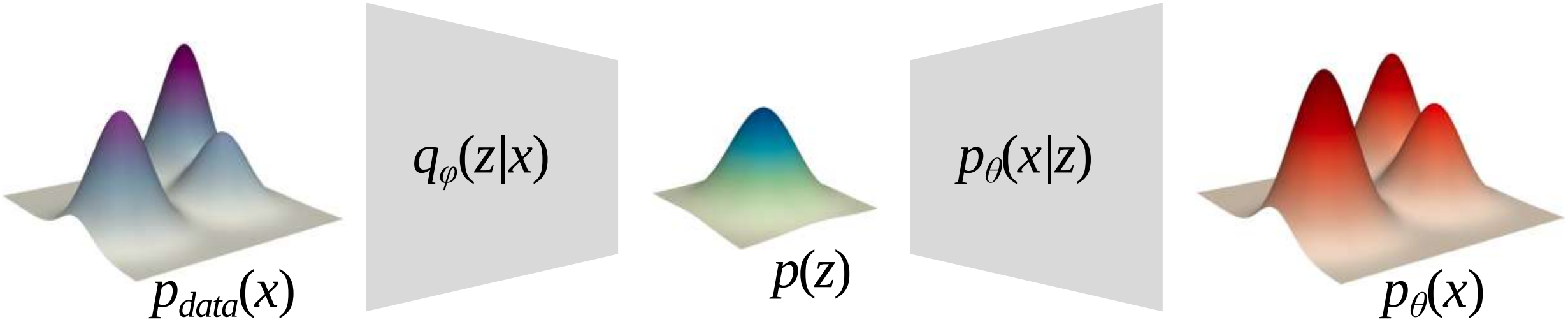
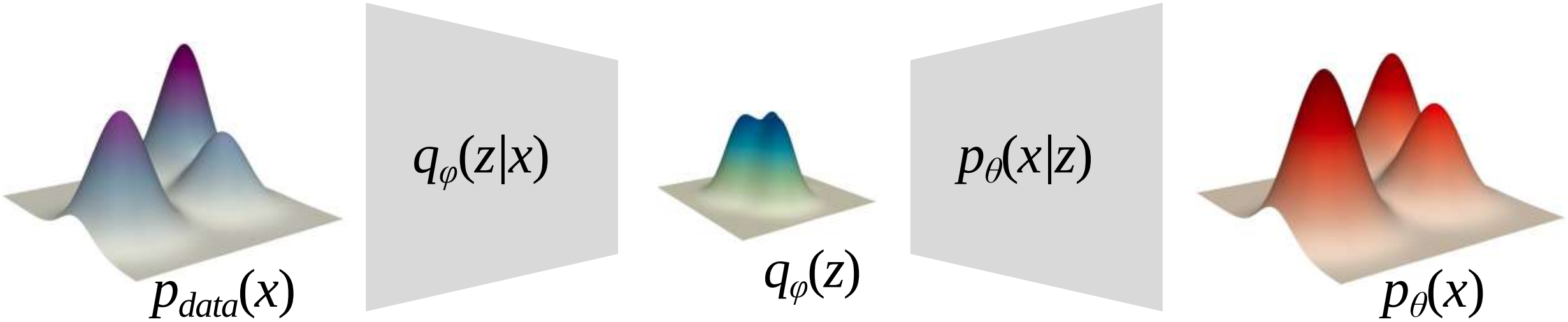


A view of “Autoencoding Distributions”

- encoded latent distribution: $q_\phi(z) = \int_x q_\phi(z|x) p_{data}(x) dx$



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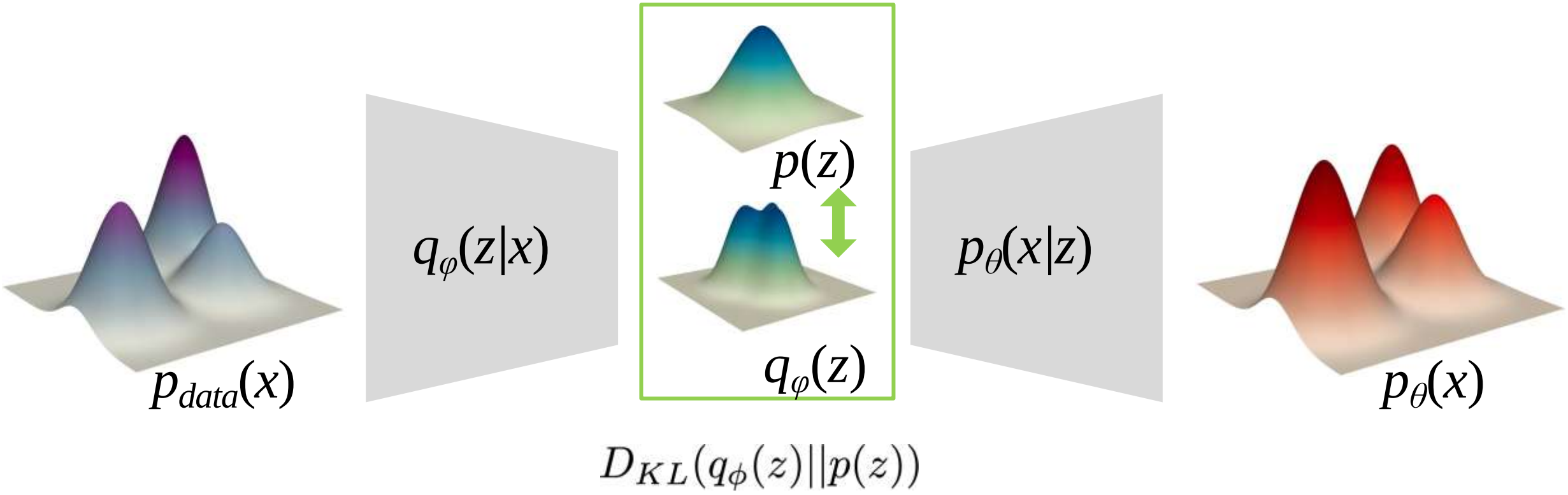

E.g., see "*InfoVAE: Information Maximizing Variational Autoencoders*", 2017

Illustration

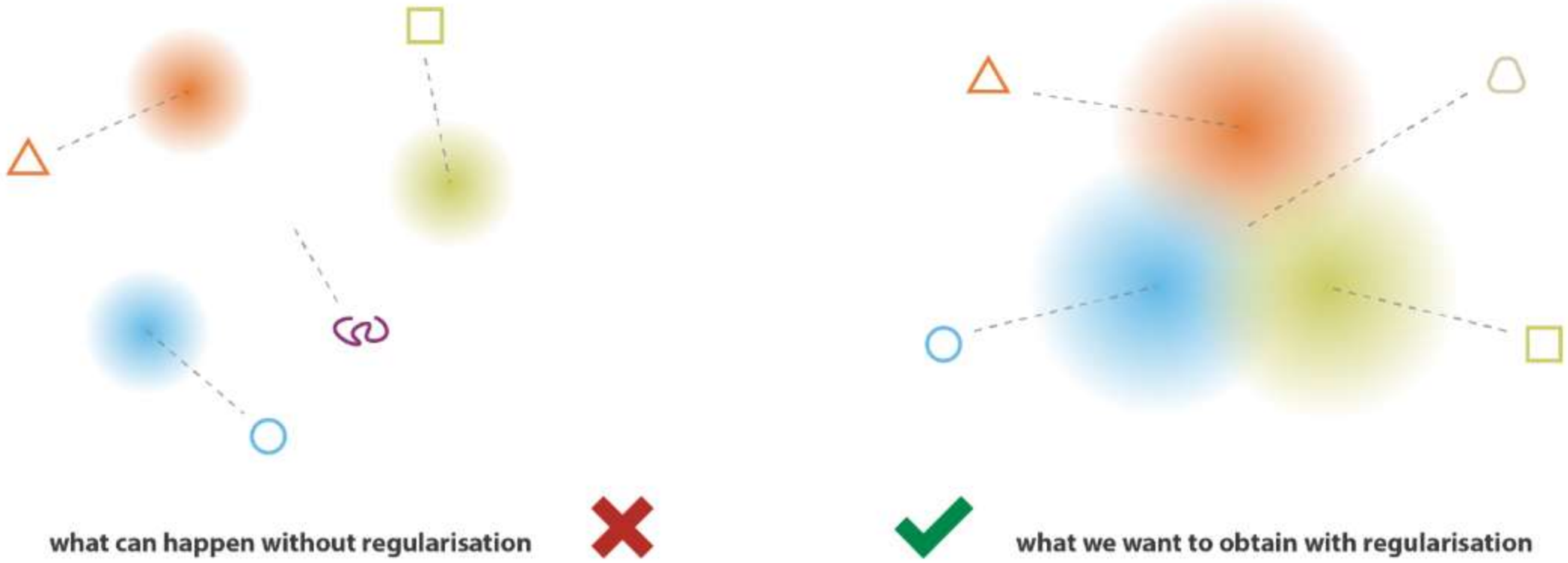

Figure adapted from: Joseph Rocca “Understanding Variational Autoencoders (VAEs)” https://towardsdatascience.com/understanding-variational-autoencoders-vaes-f70510919f73

Illustration

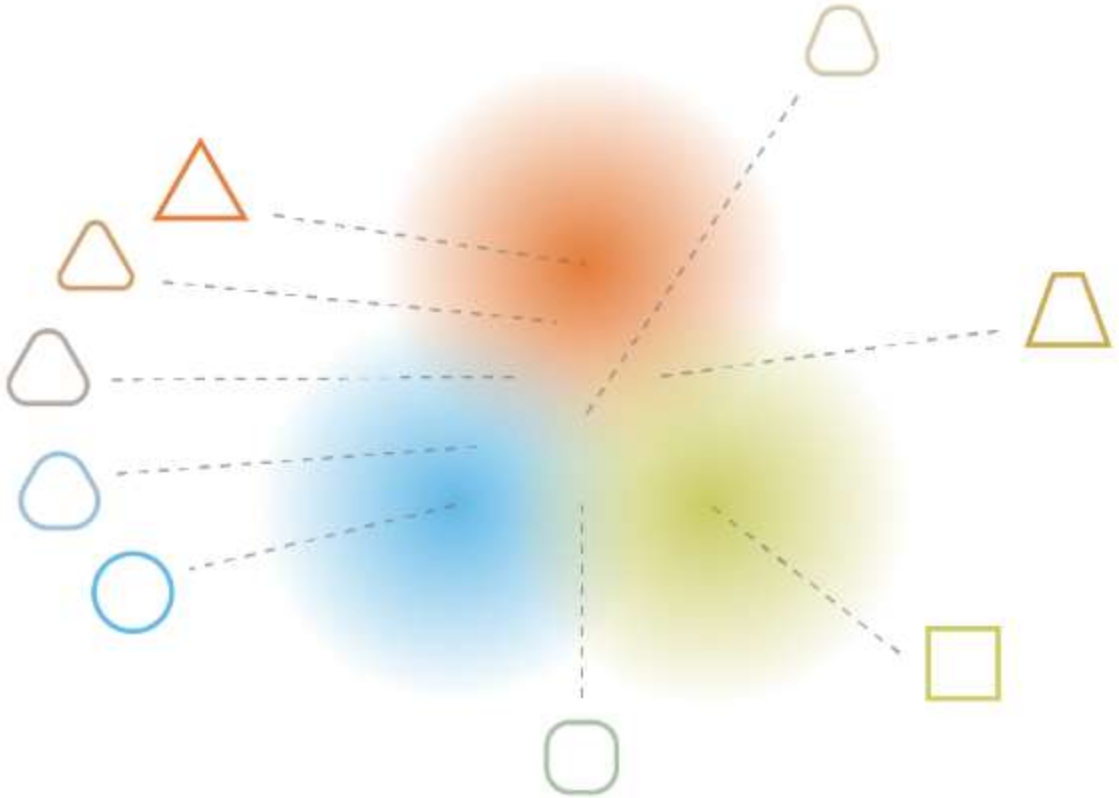

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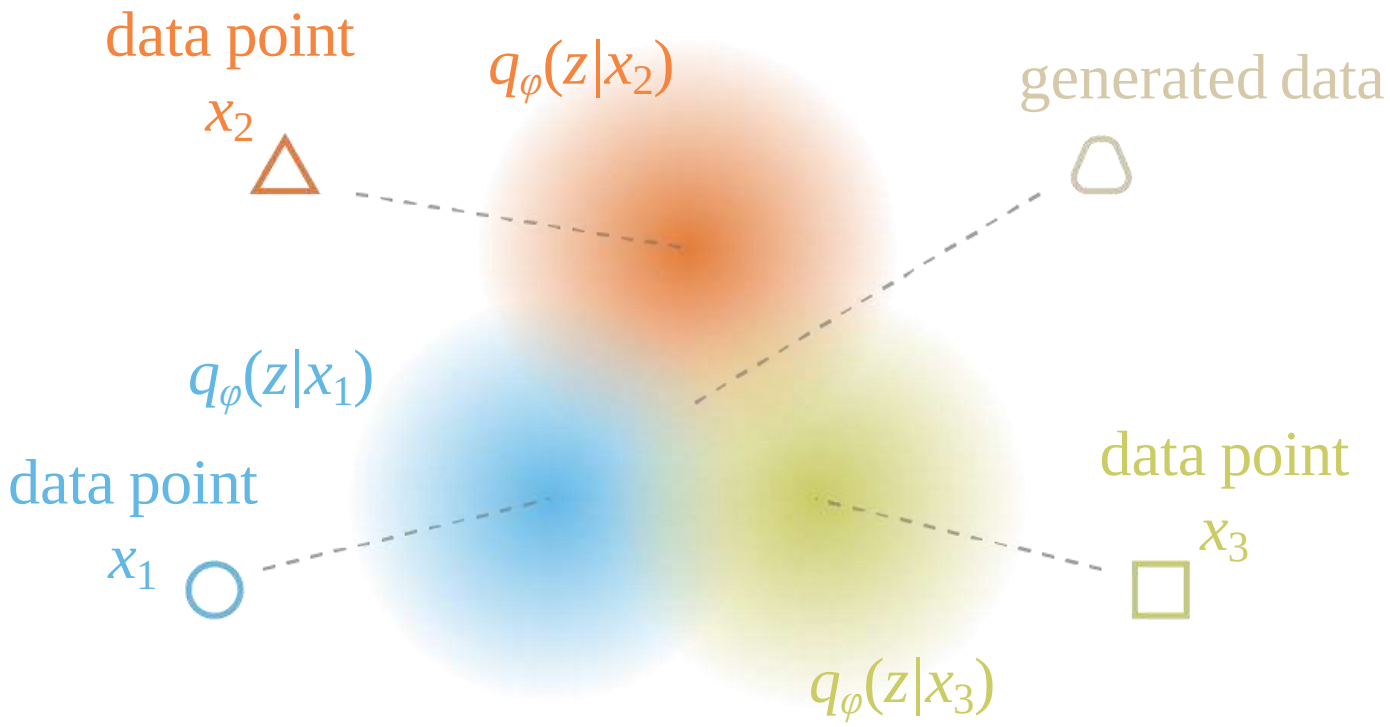
Illustration



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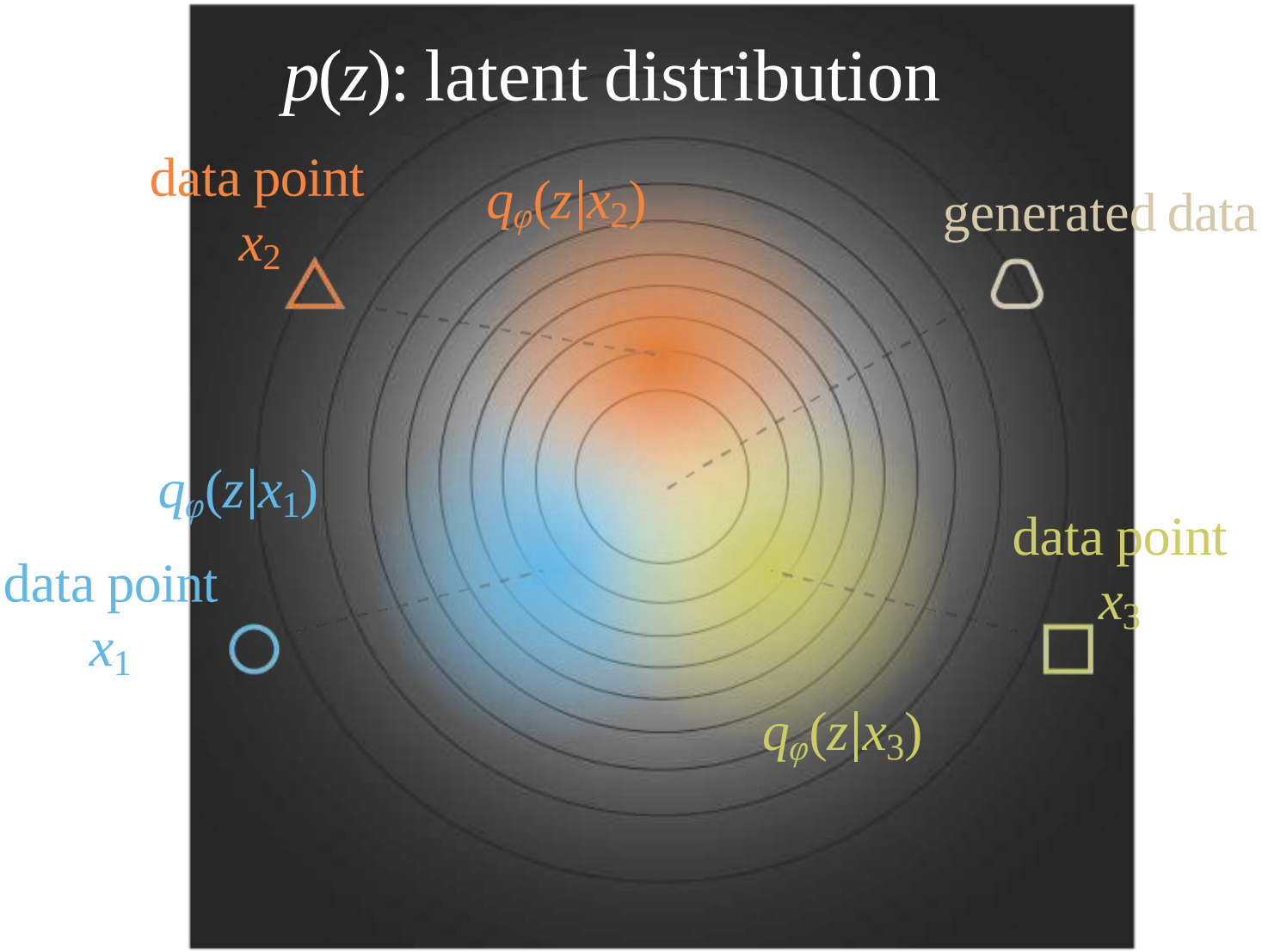

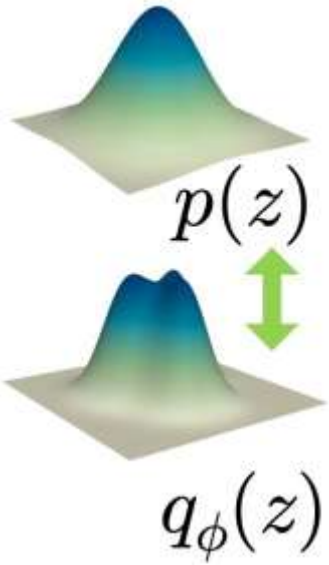

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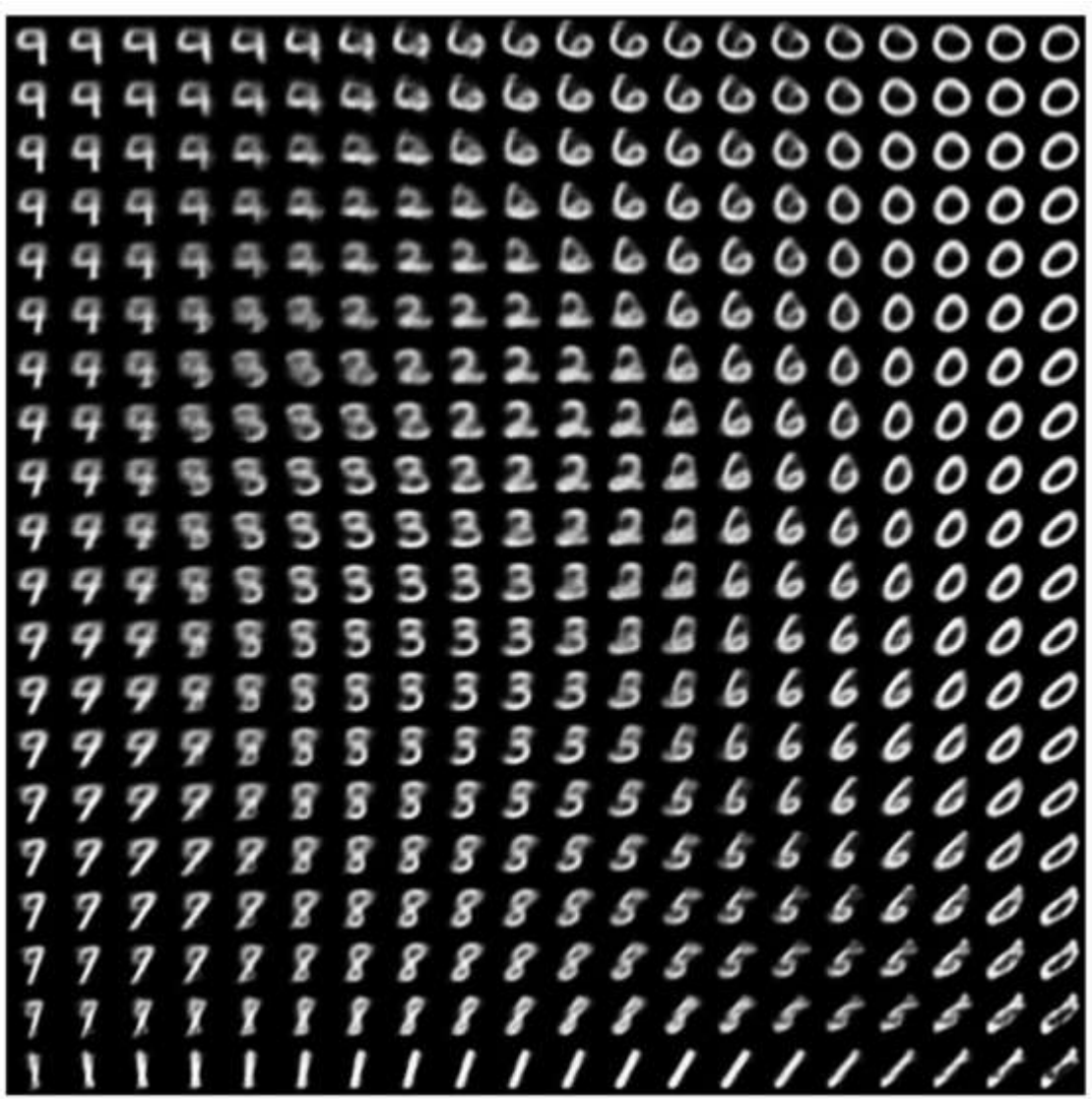
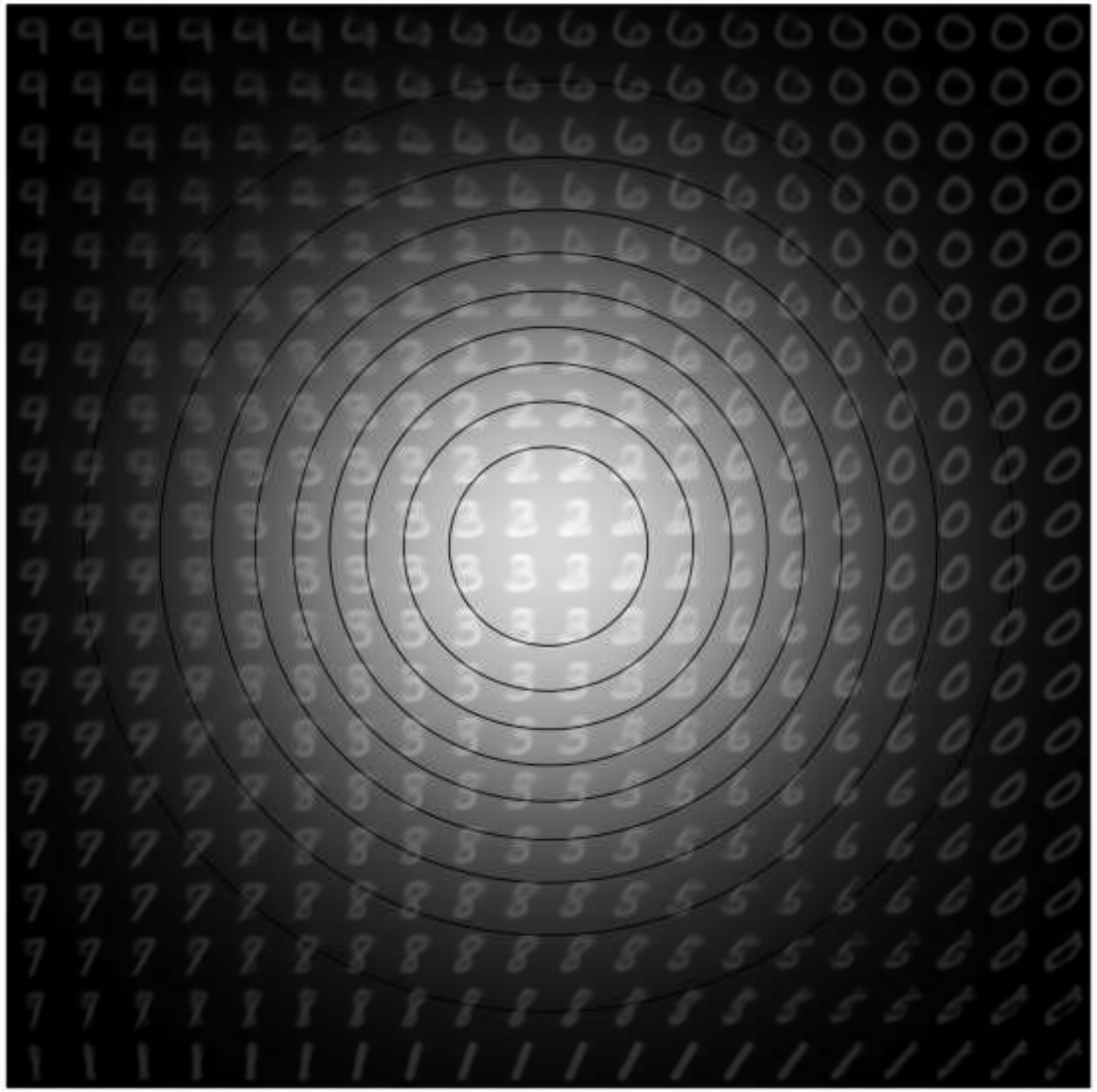
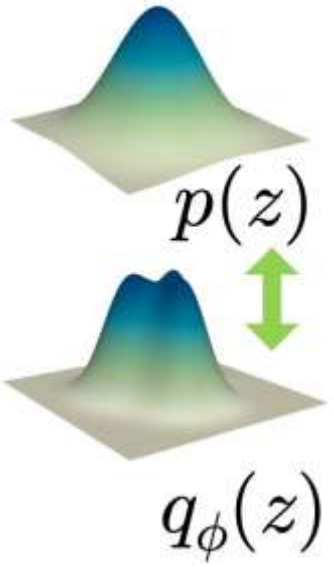
VAE: 2D latent space on MNIST



"Convolutional Variational Autoencoder"
https://colab.research.google.com/github/tensorflow/docs/blob/master/site/en/tutorials/generative/cvae.ipynb

VAE: 2D latent space on MNIST





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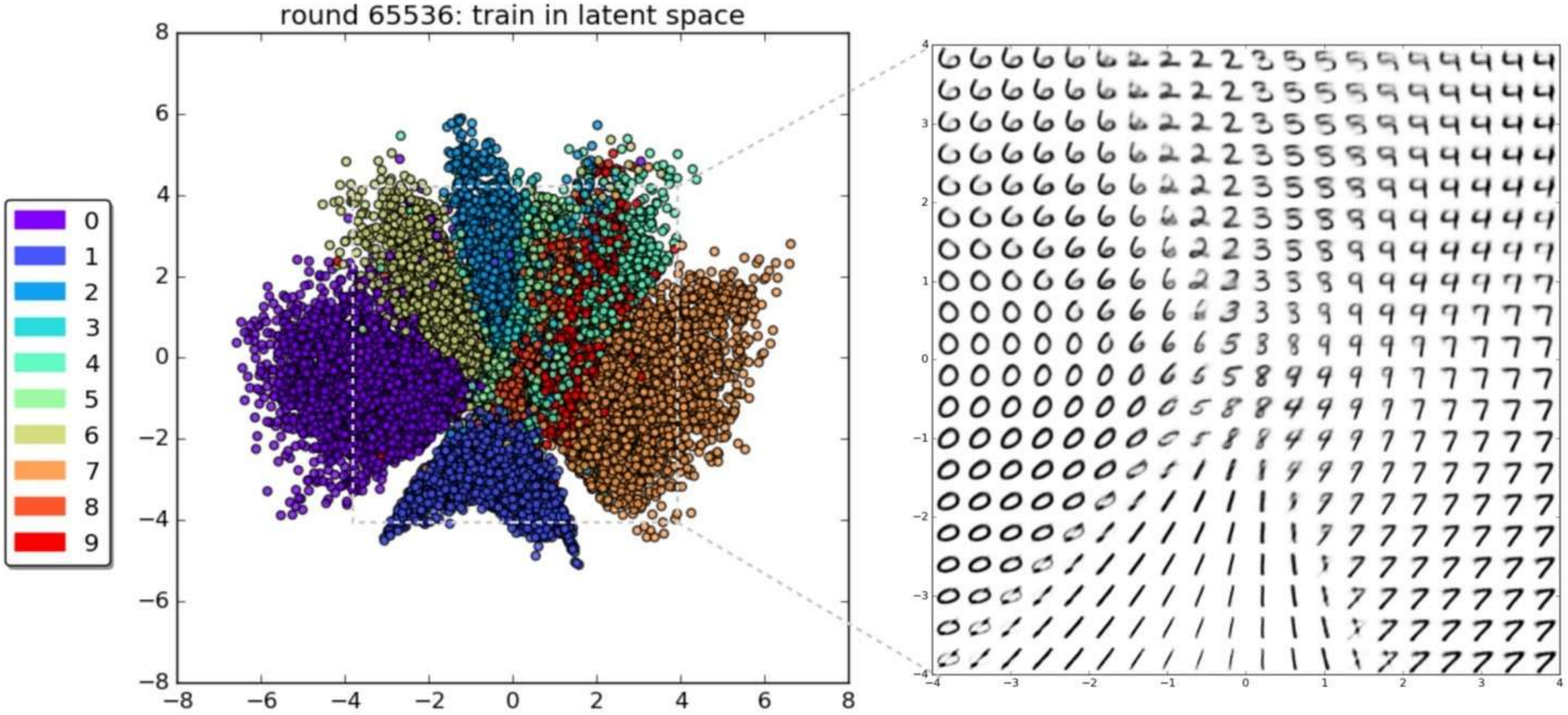
VAE: 2D latent space on MNIST



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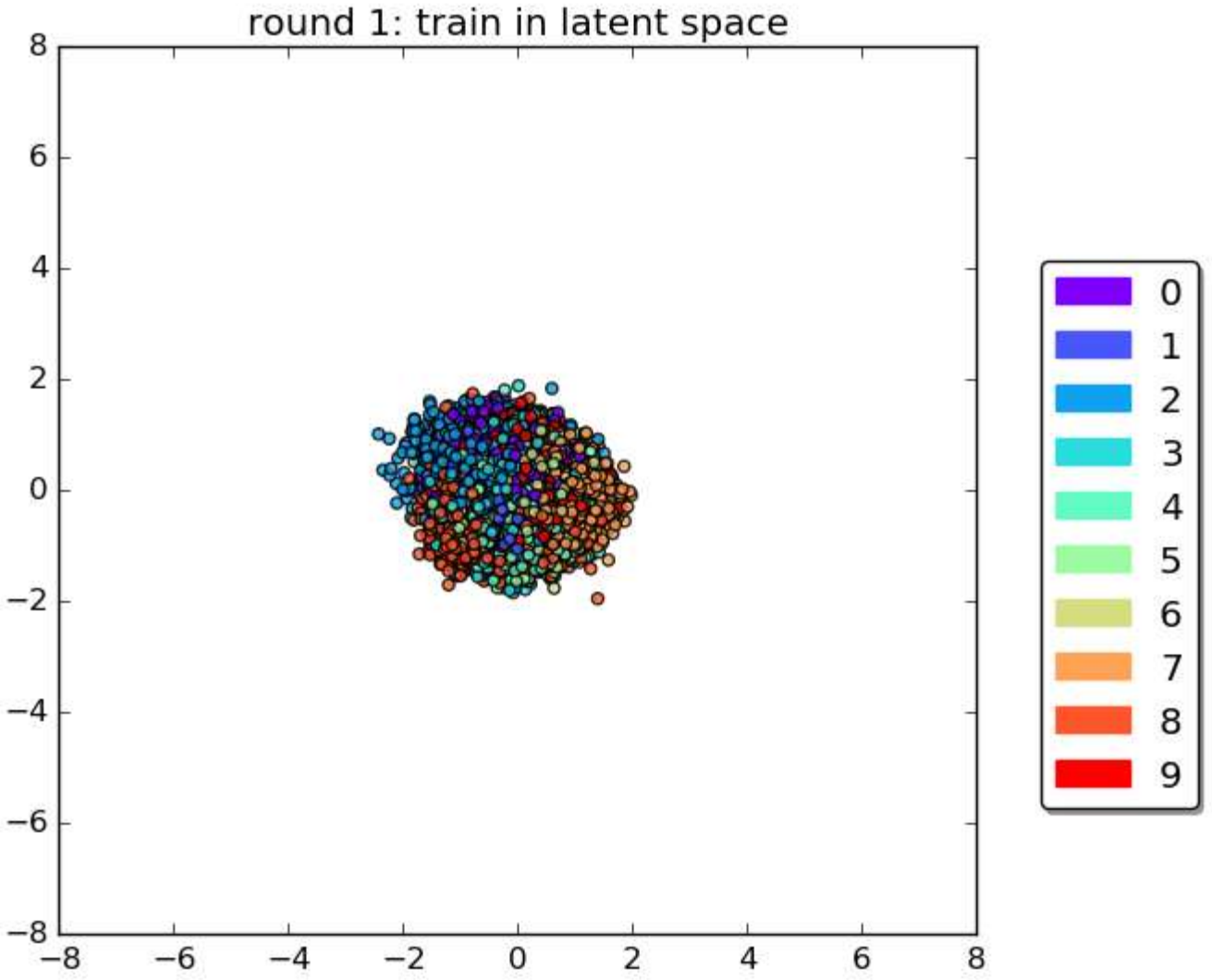
VAE: 2D latent space on MNIST



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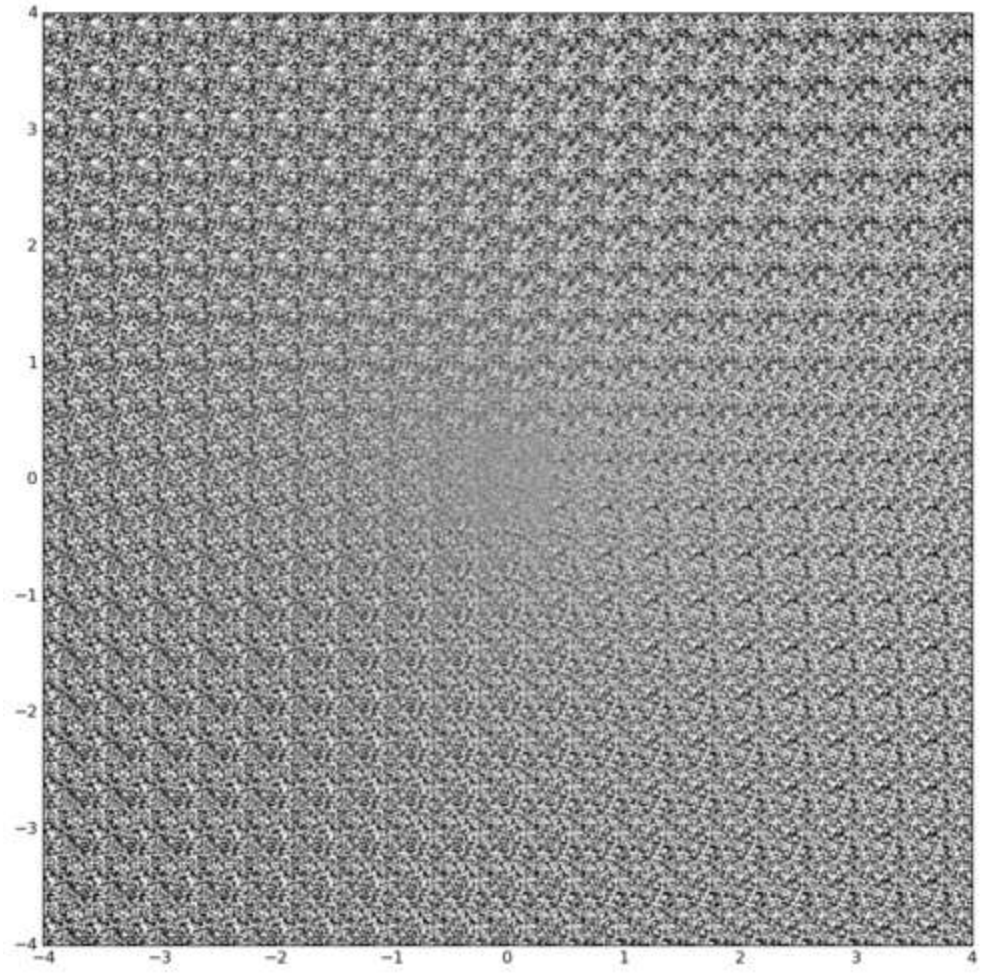
VAE: 2D latent space on MNIST



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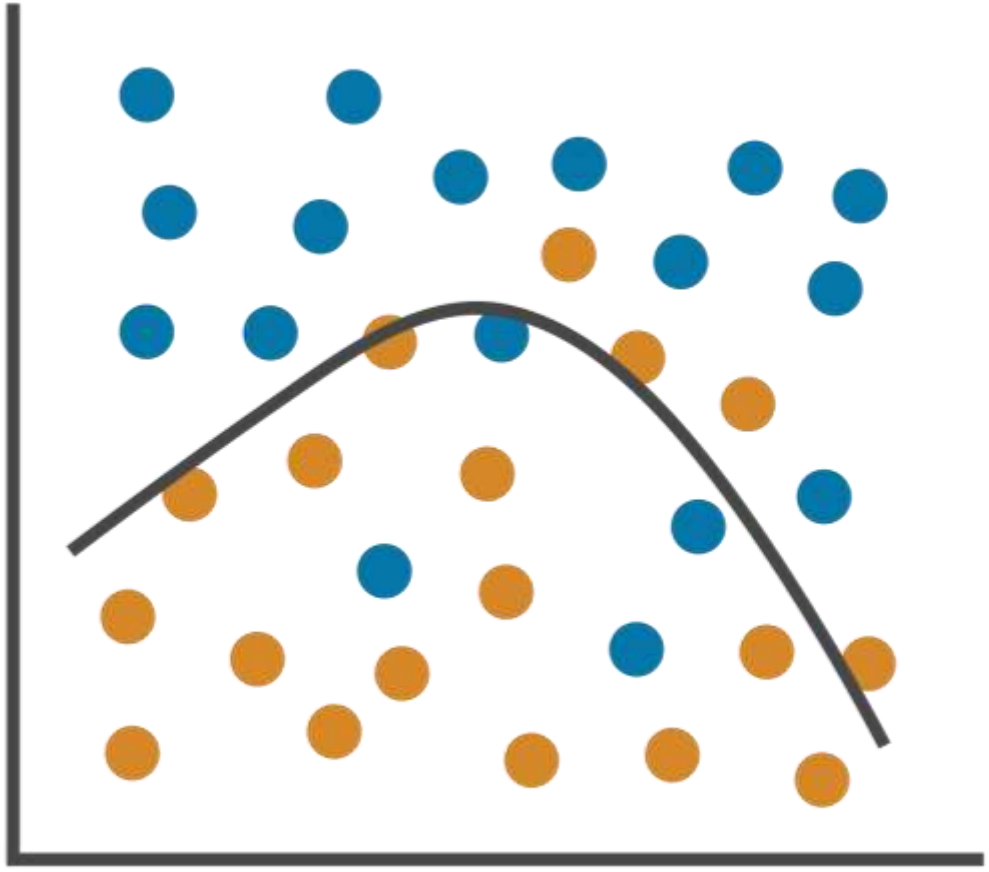
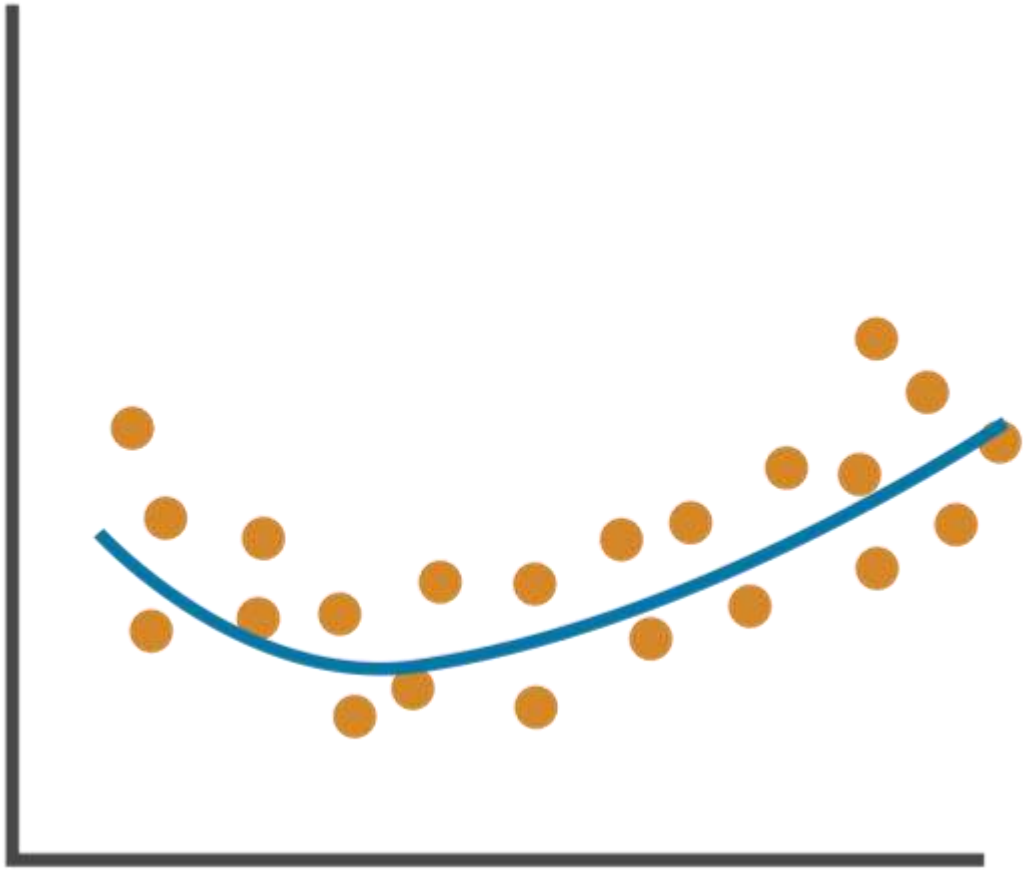
VAE: 2D latent space on “Frey Face” dataset

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

About How to Optimize





Two approaches:

- *Classification: Prob. Distribution*
- *Regression: Why we choose this approach? （self-supervised）*

Relation to Expectation-Maximization (EM)

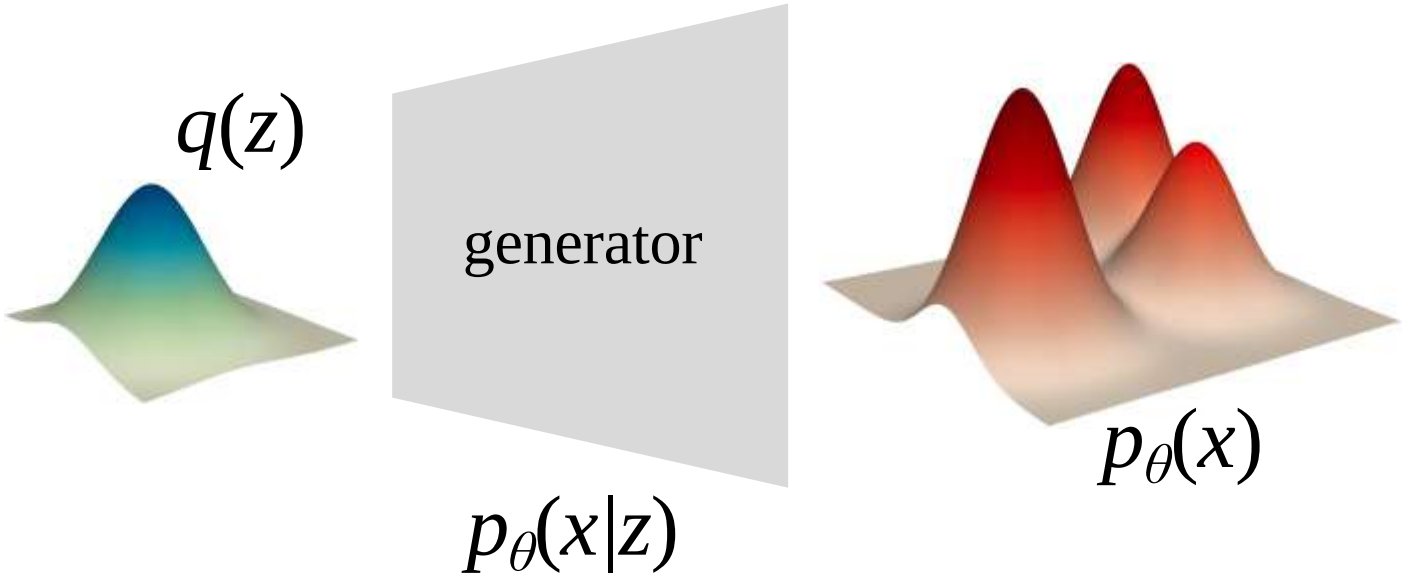
Recap: Latent Variable Models

Two sets of variables:

- q: distribution of latent
- θ: parameters of generator

VAE:

- parametrize q by a network
- stochastic gradient decent



Expectation-Maximization (EM):

- often parametrize q analytically
- coordinate descent (i.e., alternating optimization)

EM – A Match x

EM – Before Match q

EM – Before Match θ

EM – First Half x_t, q, θ

EM – Intermission $q^{(t)}$ and $p_\theta(z|x)$

EM – Second Half $p_\theta(x_{t+1}|z)$

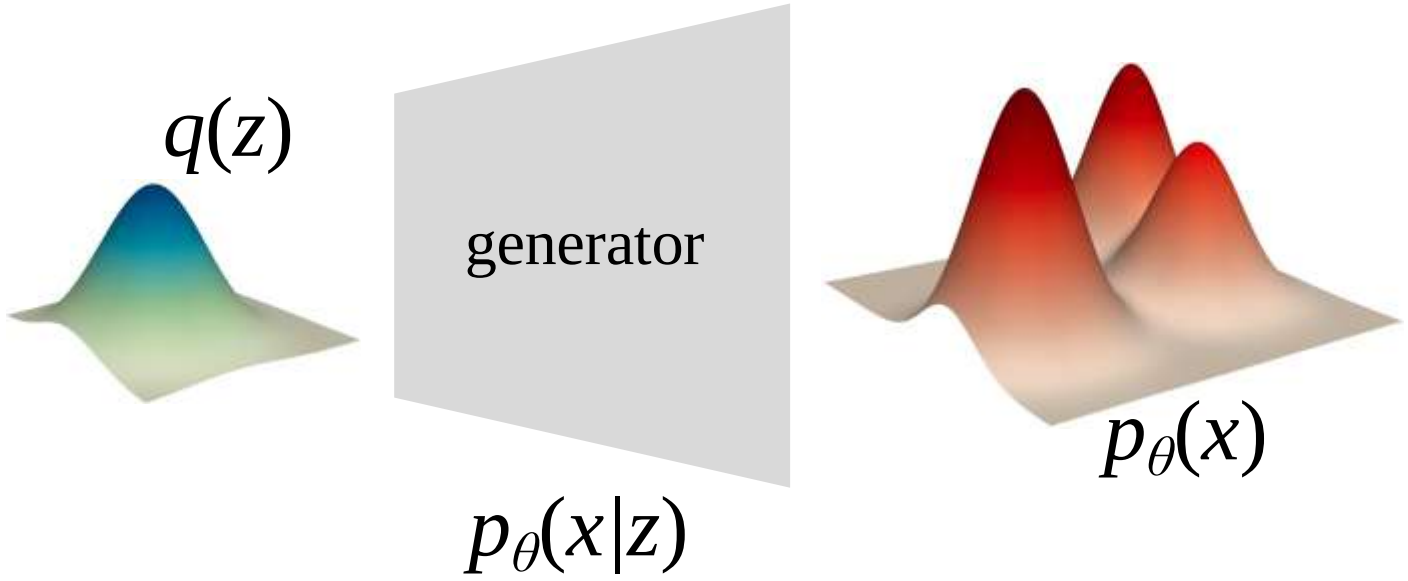
EM – Maximize $p_\theta(x)$

Posterior $p_\theta(z|x)$

Posterior $p_\theta(z|x)$

EM as A Max-Max Procedure

$$\text{ELBO} = \mathbb{E}_{x \sim p_{data}(x)} \Big[\mathbb{E}_{z \sim q(z|x)} \Big[\log p_\theta(x|z) \Big] - \mathcal{D}_{\text{KL}} \Big(q(z|x) || p(z) \Big) \Big]$$



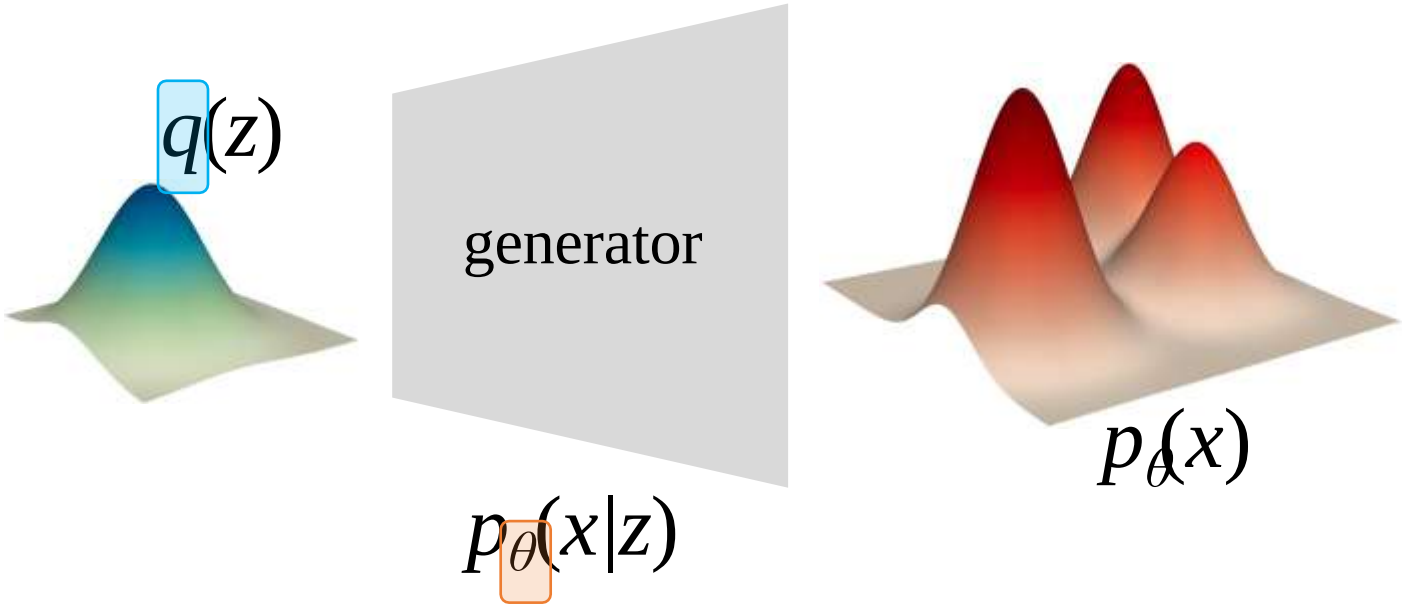
EM as A Max-Max Procedure

$$\text{ELBO} = \mathbb{E}_{x \sim p_{data}(x)} \left[\mathbb{E}_{z \sim q(z|x)} \left[\log p_\theta(x|z) \right] - \mathcal{D}_{\text{KL}} \left(q(z|x) || p(z) \right) \right]$$

$$\max_{\theta, q} \text{ELBO}(\theta, q(\cdot))$$

Two sets of variables:

- q - distribution of latent
- θ - parameters of generator



Coordinate descent:

- max-max procedure (GAN: max-min)

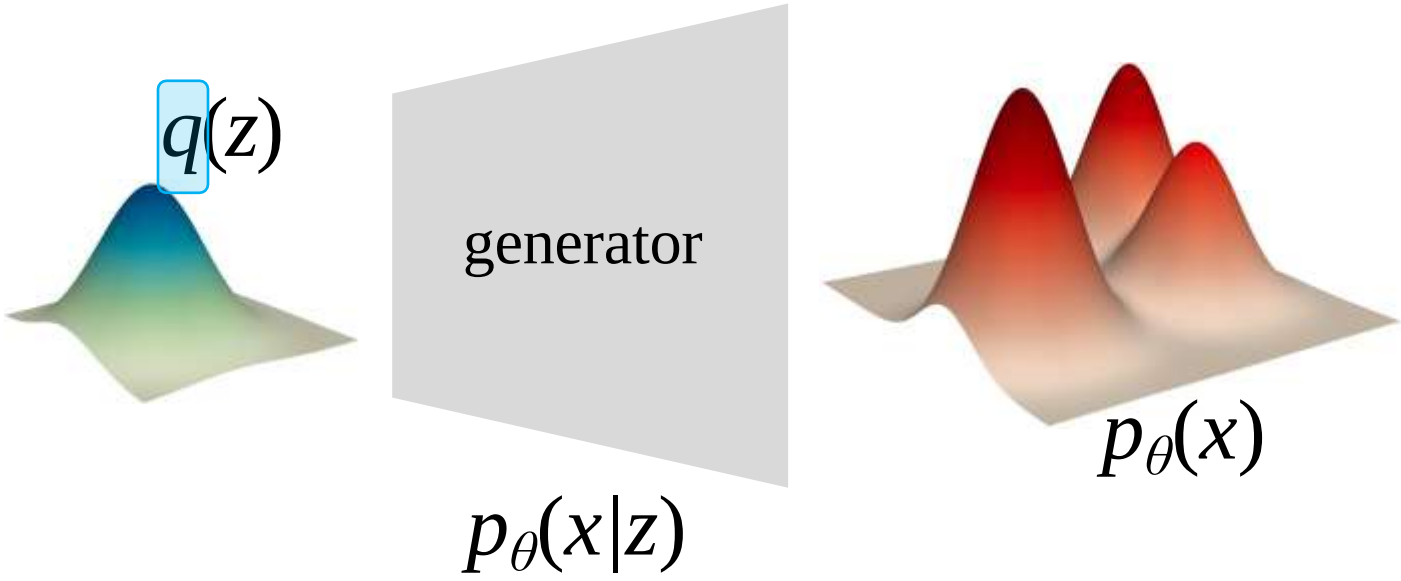
EM as A Max-Max Procedure

$$\text{ELBO} = \mathbb{E}_{x \sim p_{data}(x)} \left[\mathbb{E}_{z \sim q(z|x)} \left[\log p_\theta(x|z) \right] - \mathcal{D}_{\text{KL}} \left(q(z|x) || p(z) \right) \right]$$

$$\max_{\theta, q} \text{ELBO}(\theta, q(\cdot))$$

E-step: optimize for q

$$q^{(t)} = p_{\theta^{(t)}}(z|x)$$



Details can be found in: Hastie et al. “The Elements of Statistical Learning”.

EM as A Max-Max Procedure

$$\text{ELBO} = \mathbb{E}_{x \sim p_{data}(x)} \Big[\mathbb{E}_{z \sim q(z|x)} \big[\log p_\theta(x|z) \big] - \mathcal{D}_{\text{KL}} \big(q(z|x) || p(z) \big) \Big]$$

$$\max_{\theta, q} \text{ELBO}(\theta, q(\cdot))$$

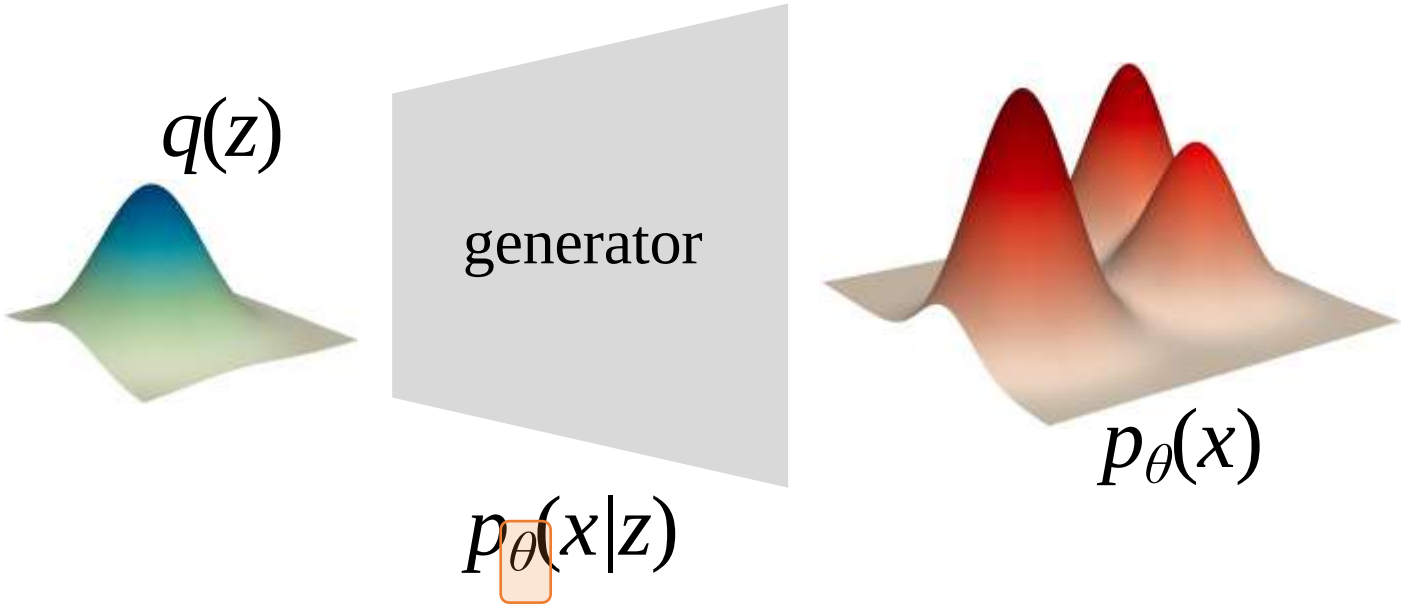
E-step: optimize for q

$$q^{(t)} = p_{\theta^{(t)}}(z|x)$$

M-step: optimize for θ

$$\theta^{(t+1)} = \arg\max_{\theta} Q(\theta|\theta^{(t)})$$

with sub-objective defined as: $Q(\theta|\theta^{(t)}) = \mathbb{E}_{p_{data}(x)} \mathbb{E}_{p_{\theta^{(t)}}(z|x)} [\log p_\theta(x, z)]$



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EM as A Max-Max Procedure

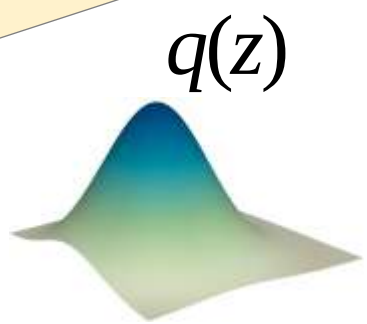
$$\text{ELBO} = \mathbb{E}_{x \sim p_{data}(x)} \left[\mathbb{E}_{z \sim q(z|x)} \left[\log p_\theta \right. \right.$$

$$\max_{\theta, q} \text{ELBO}(\theta, q(\cdot))$$

q: often in analytical forms
- Gaussian Mixtures
- **K-means**

E-step: optimize for q

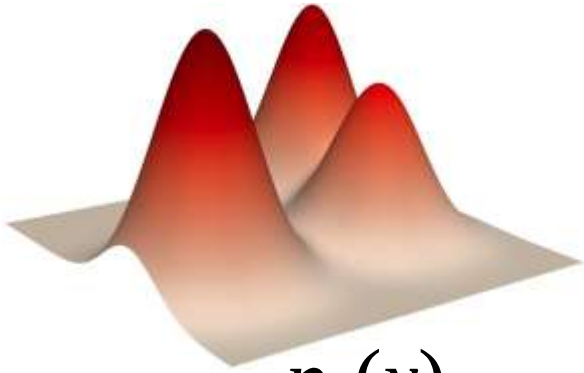
$$q^{(t)} = p_{\theta^{(t)}}(z|x)$$



$q(z)$

generator

$p_\theta(x|z)$



$p_\theta(x)$

M-step: optimize for θ

$$\theta^{(t+1)} = \arg\max_\theta Q(\theta|\theta^{(t)})$$

with sub-objective defined as: $Q(\theta|\theta^{(t)}) = \mathbb{E}_{p_{data}(x)} \mathbb{E}_{p_{\theta^{(t)}}(z|x)} [\log p_\theta(x, z)]$

Details can be found in: Hastie et al. “The Elements of Statistical Learning”.

A running example of EM: K-means

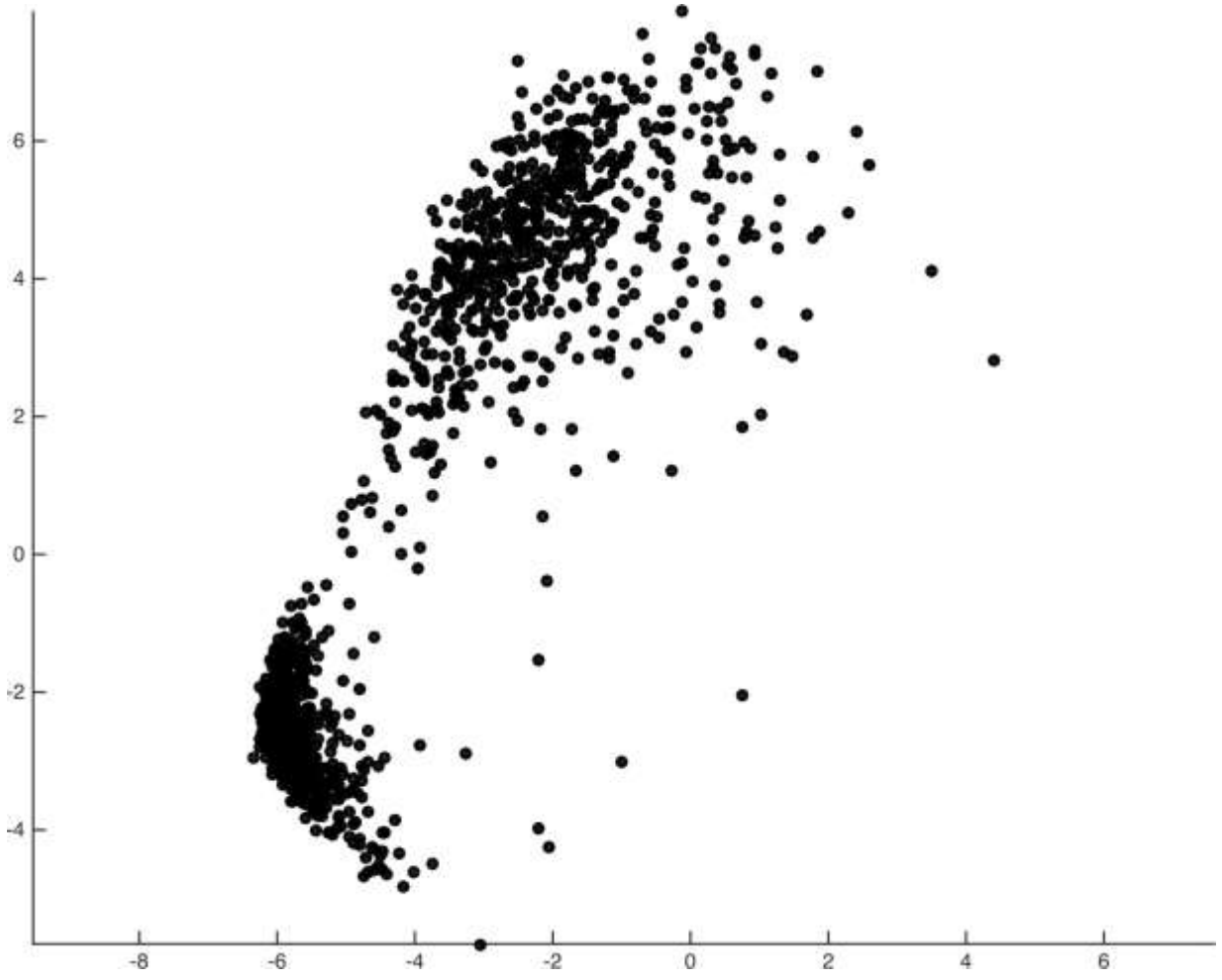
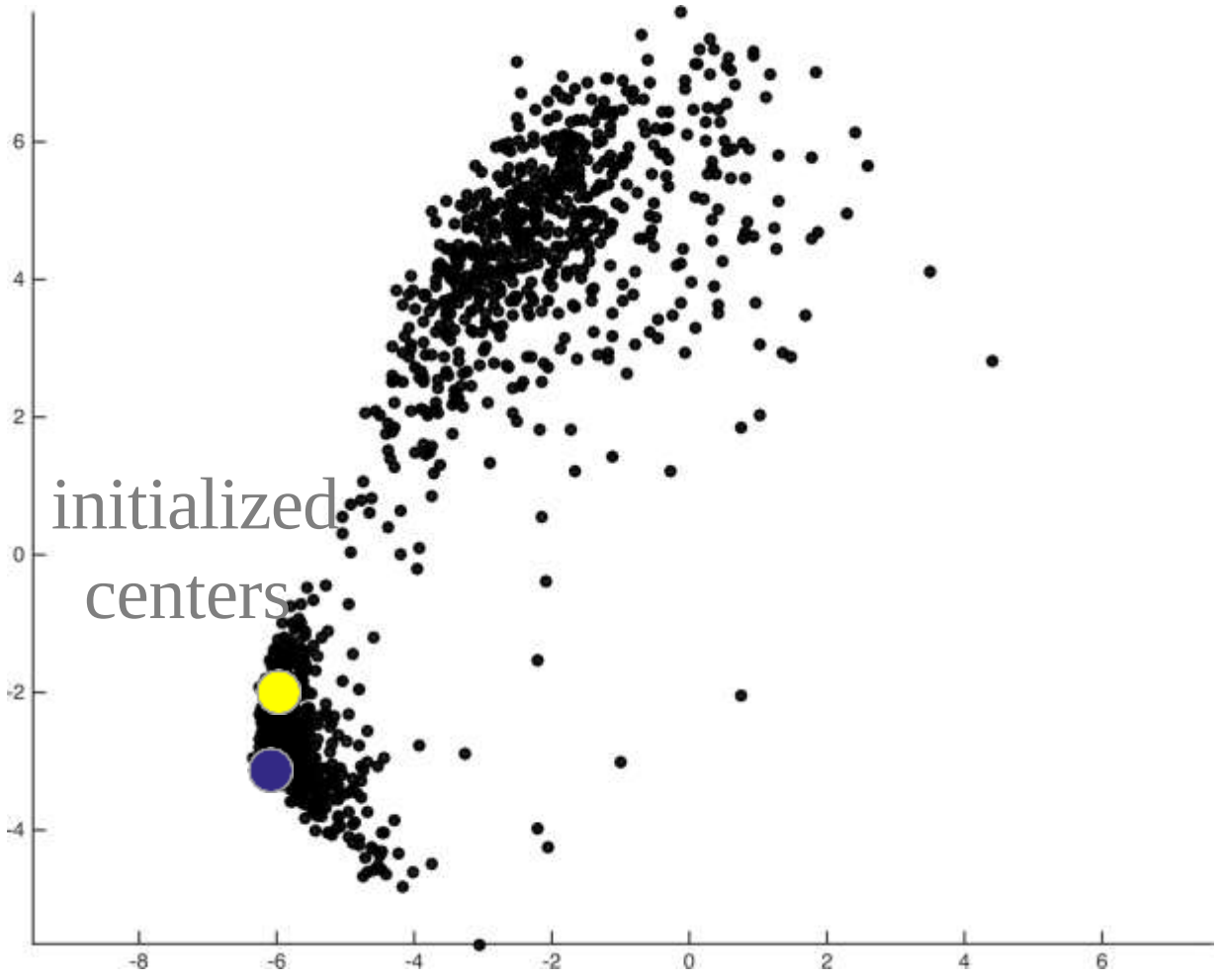


Figure adapted from: Marion Neumann, https://www.cse.wustl.edu/~m.neumann/sp2016/cse517/lecturenotes/lecturenote20.html

A running example of EM: K-means

- cluster centers: θ



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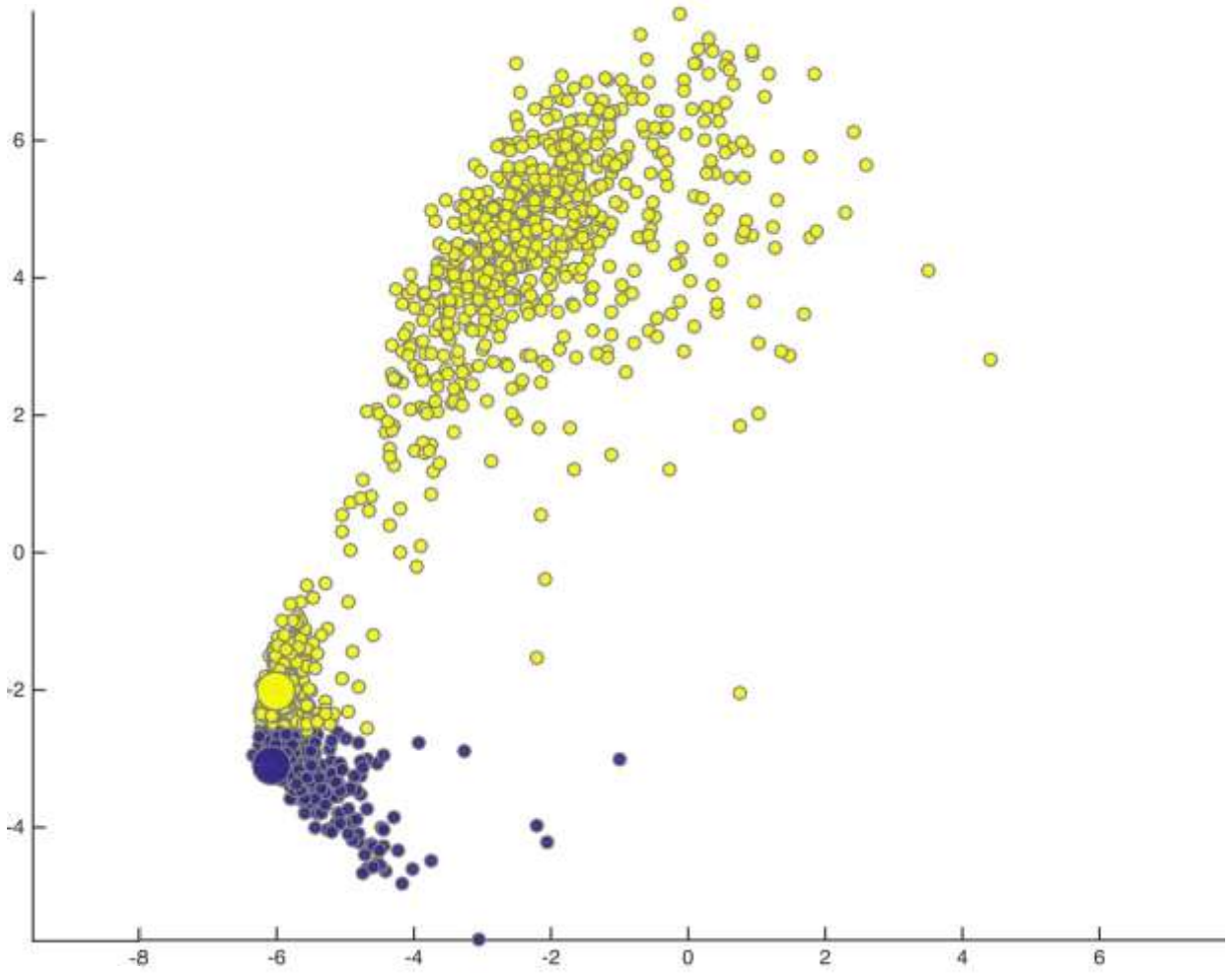
A running example of EM: K-means

- cluster centers: θ
- assignment:



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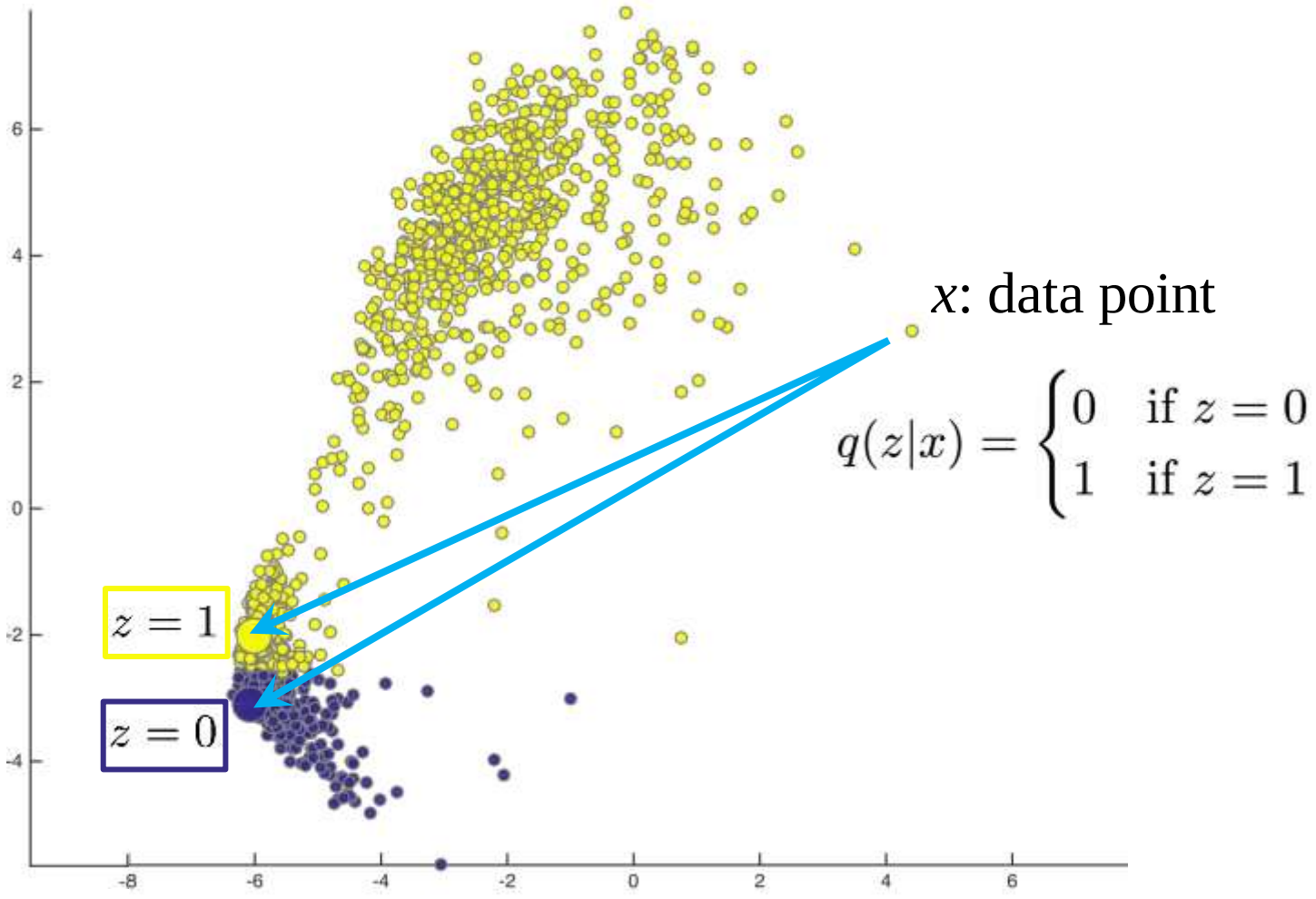
A running example of EM: K-means

- cluster centers: θ
- assignment: E-step



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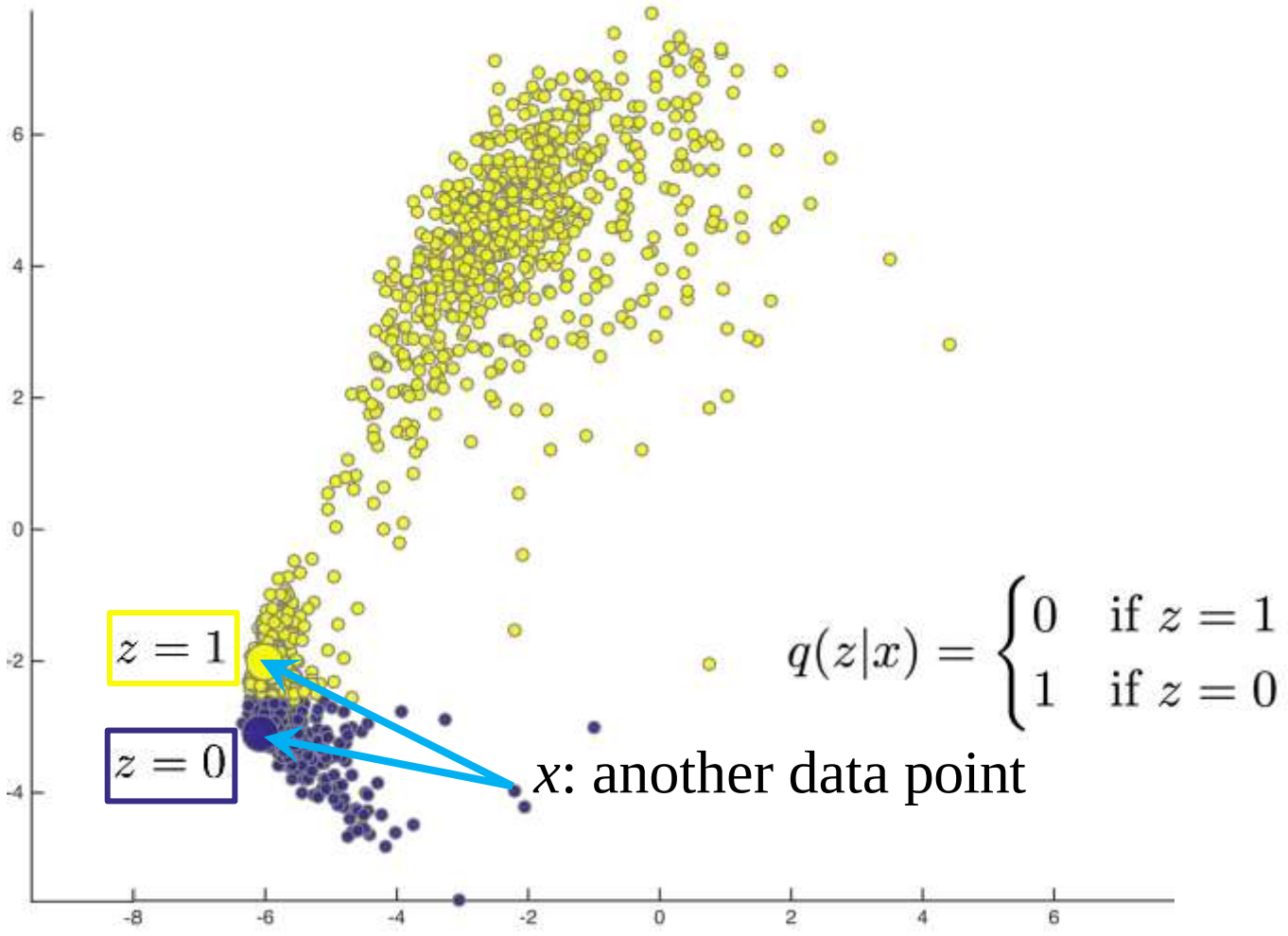
A running example of EM: K-means

- cluster centers: θ
- assignment: E-step



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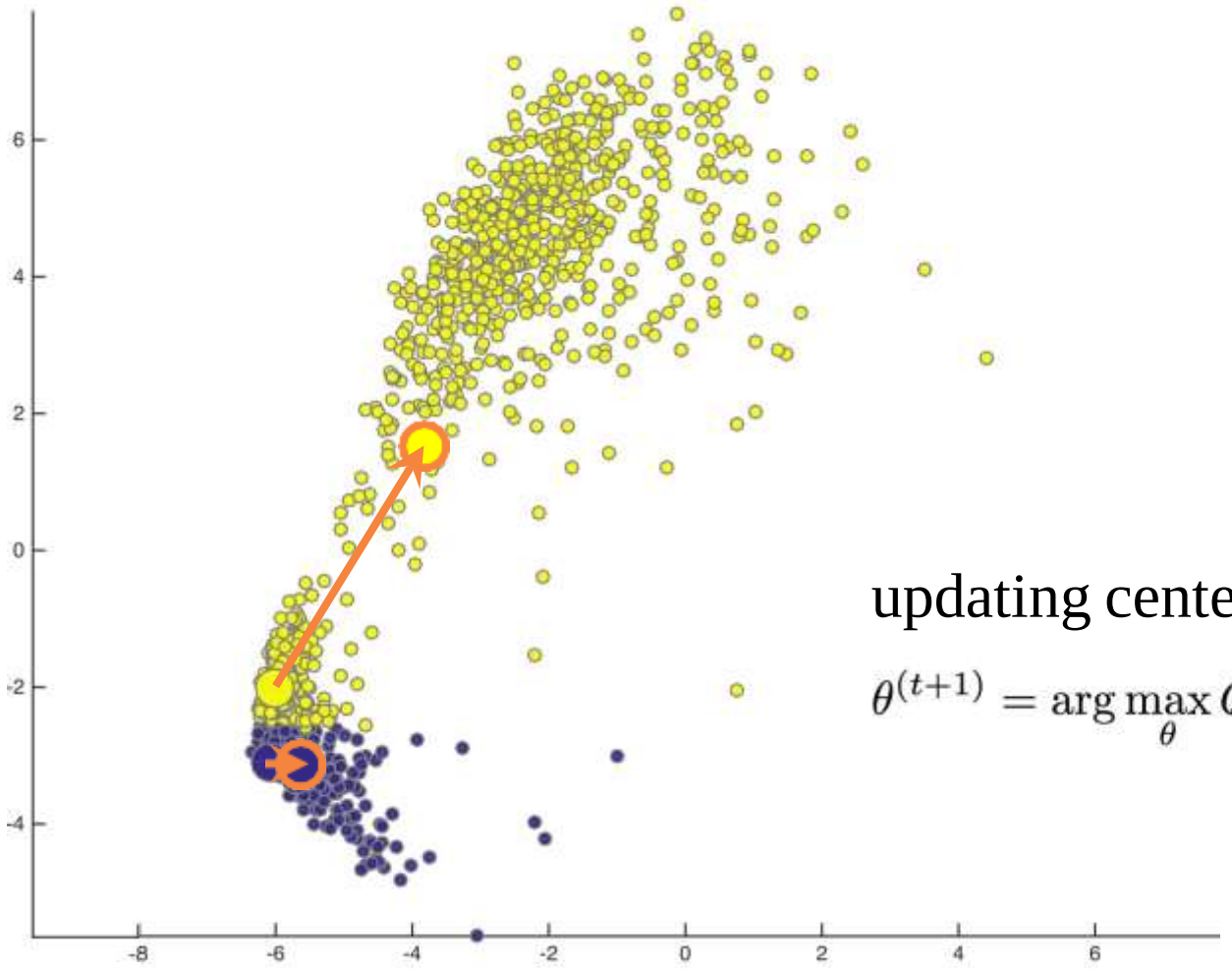
A running example of EM: K-means

- cluster centers: θ
- assignment: E-step
- update: M-step



updating centers by:

$$\theta^{(t+1)} = \arg\max_{\theta} Q(\theta|\theta^{(t)})$$

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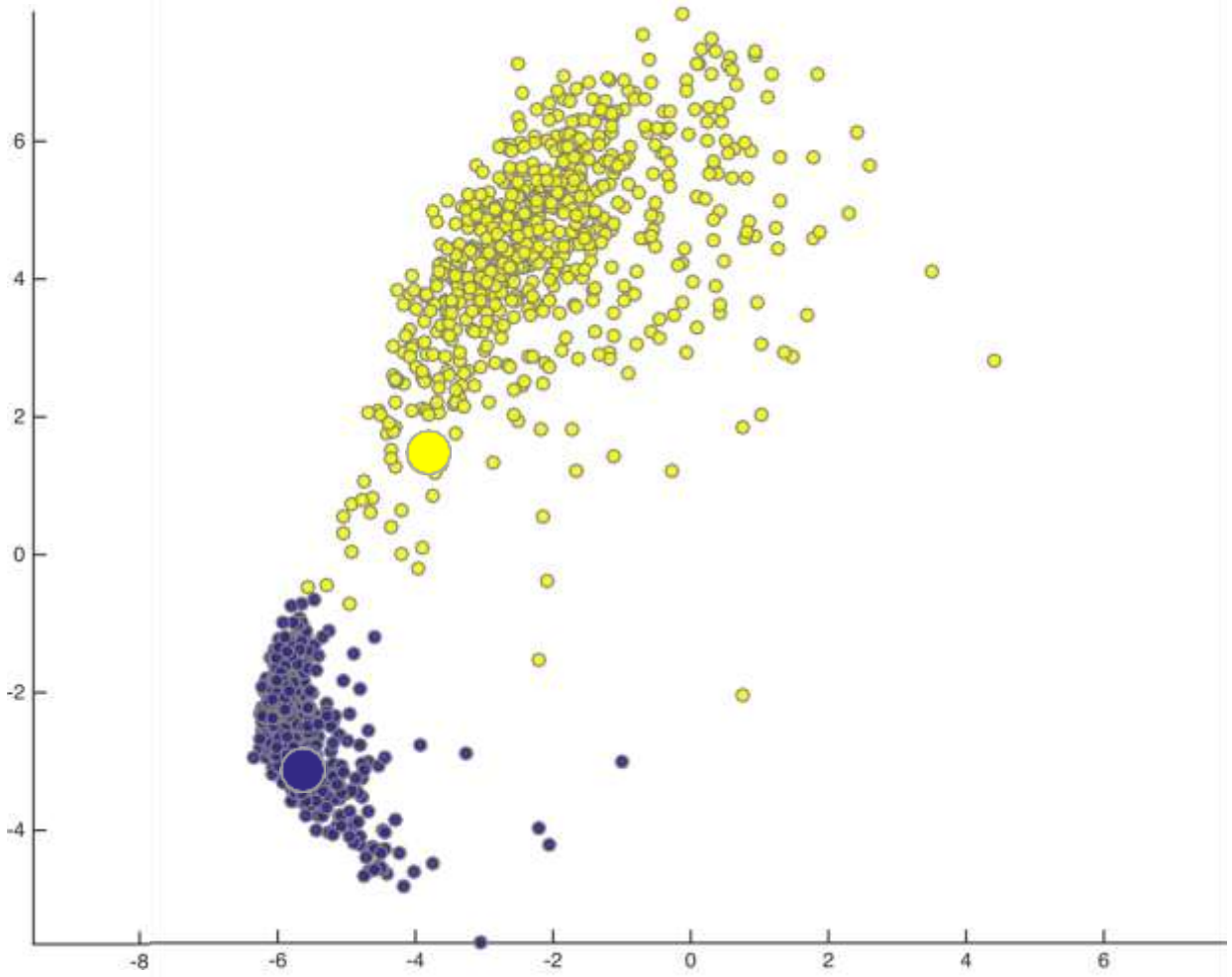
A running example of EM: K-means

- cluster centers: θ
- assignment: E-step
- update: M-step



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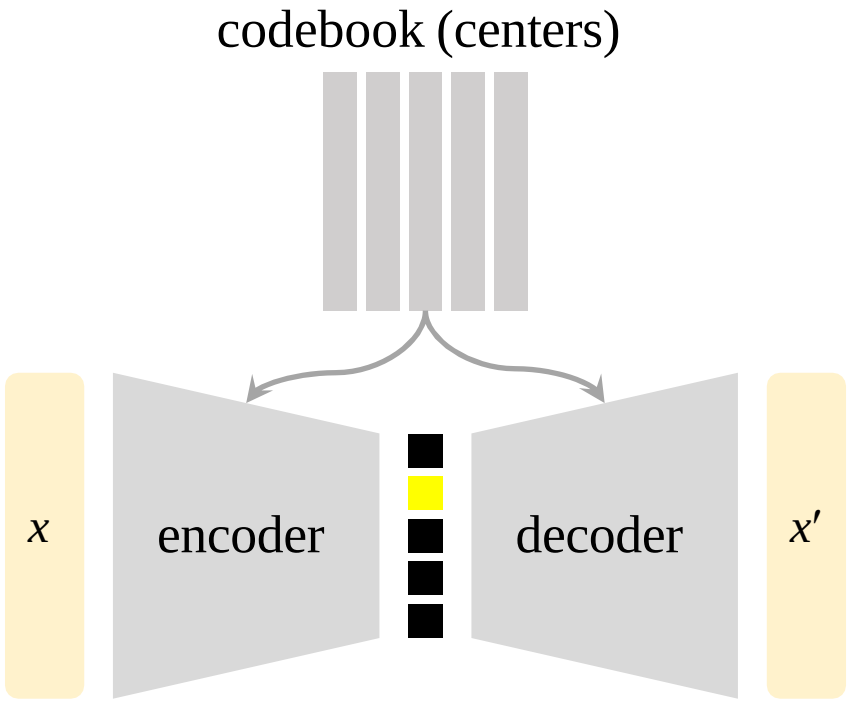
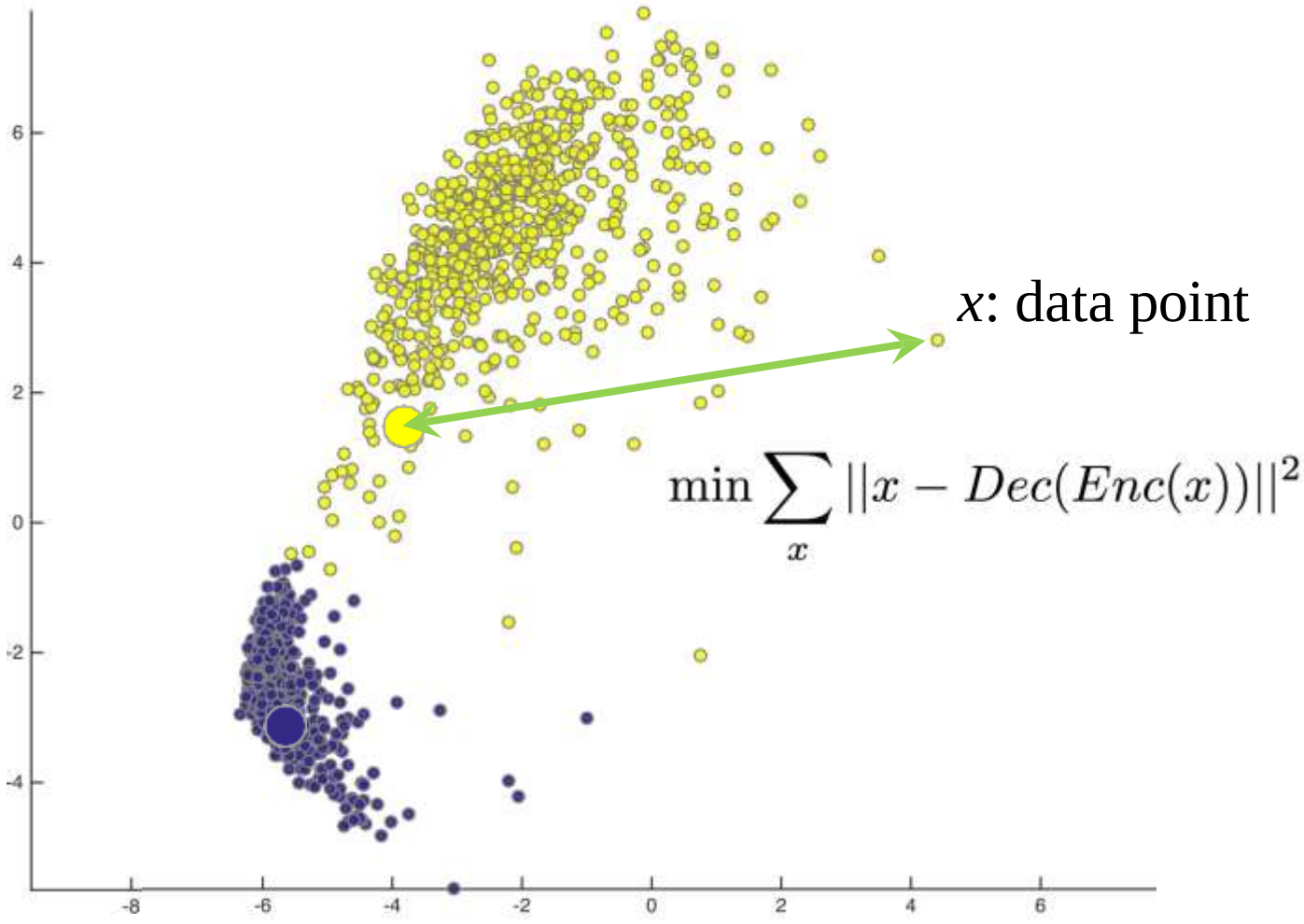
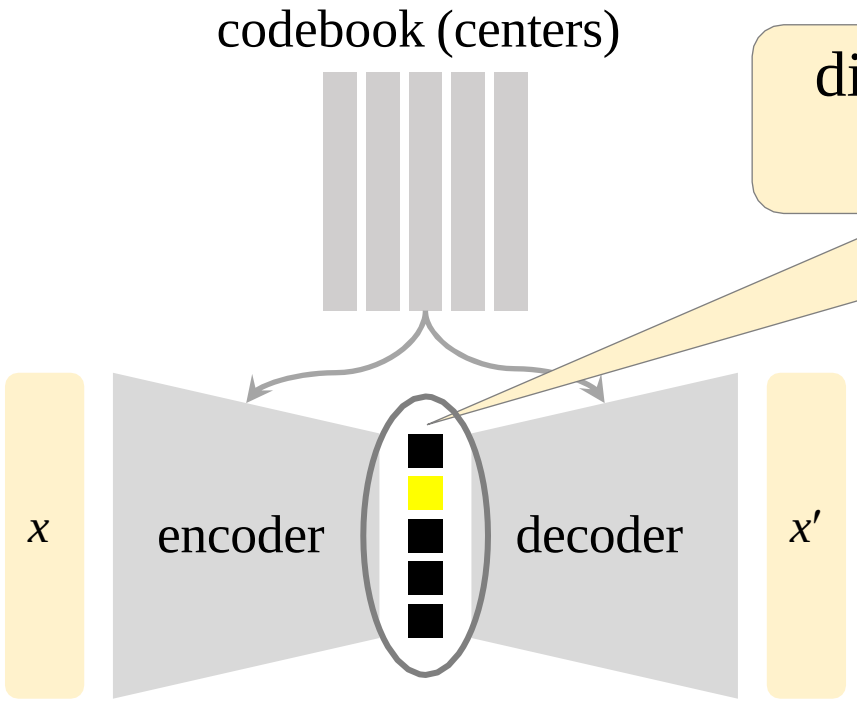
K-means as **Autoencoder**

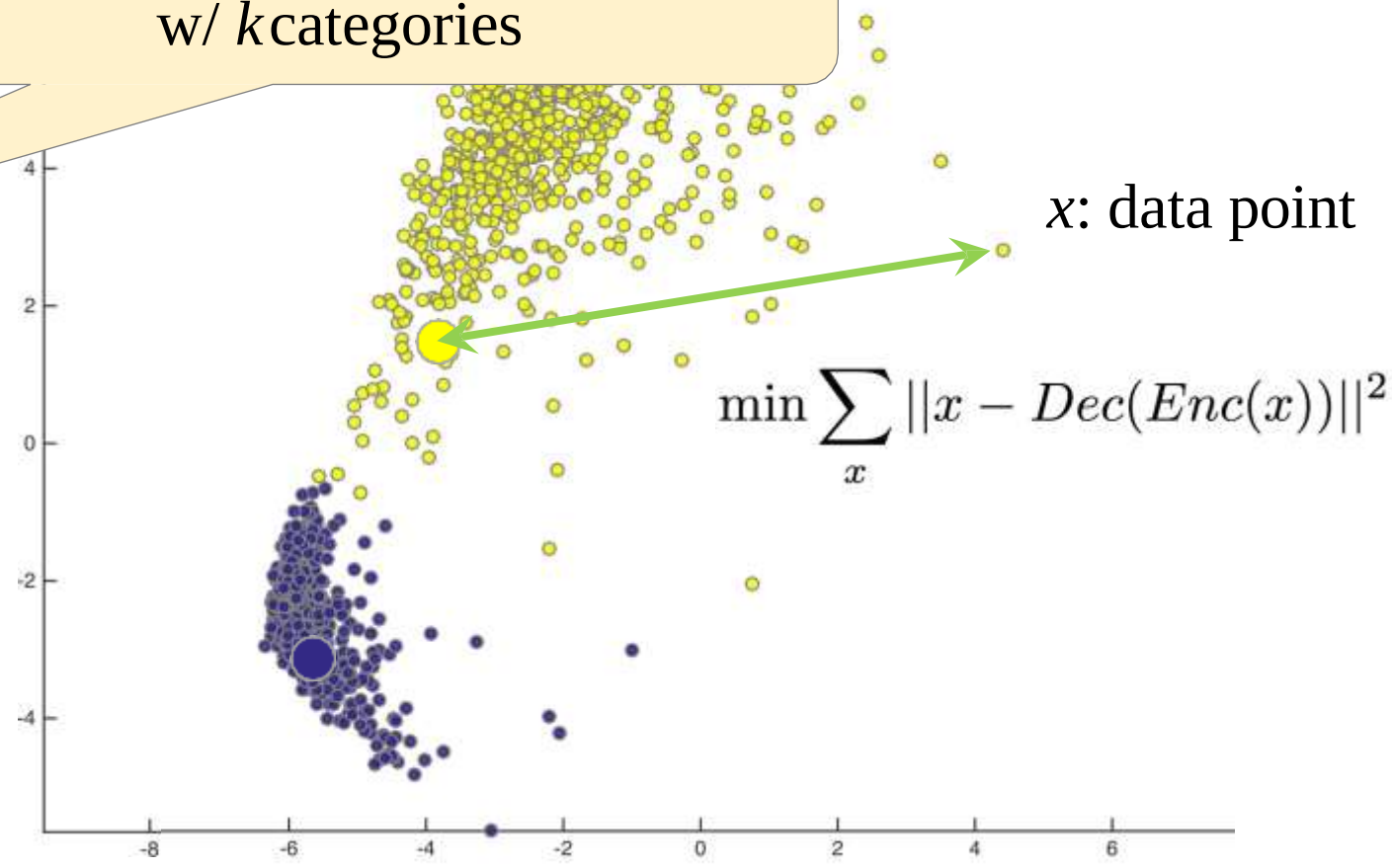


- encode: map x to one-hot
- decode: map one-hot to x'
- x' is a center



K-means as **Autoencoder**





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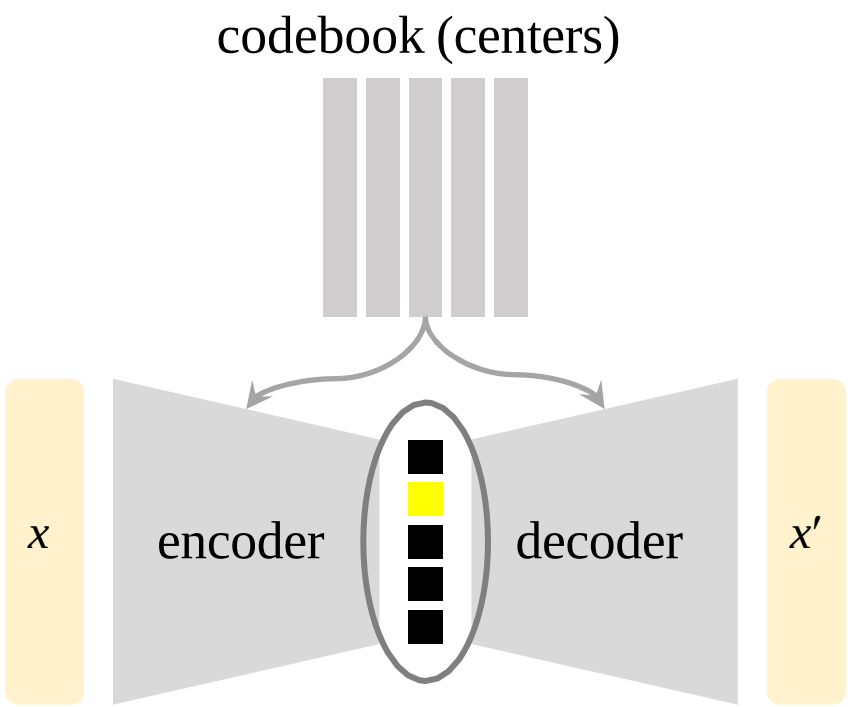
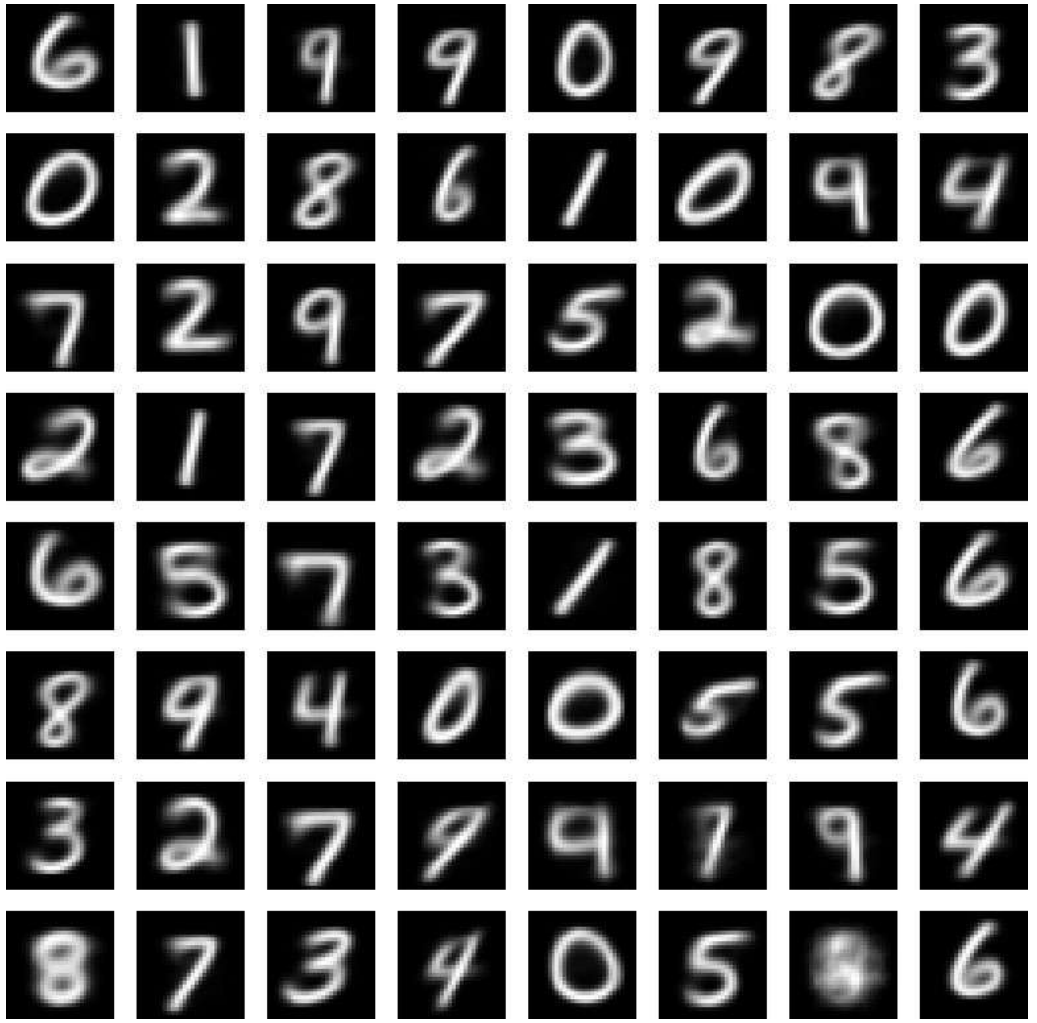
K-means as **Autoencoder**



- encode: map x to one-hot
- decode: map one-hot to x'
- x' is a center

codebook on MNIST, $k = 64$

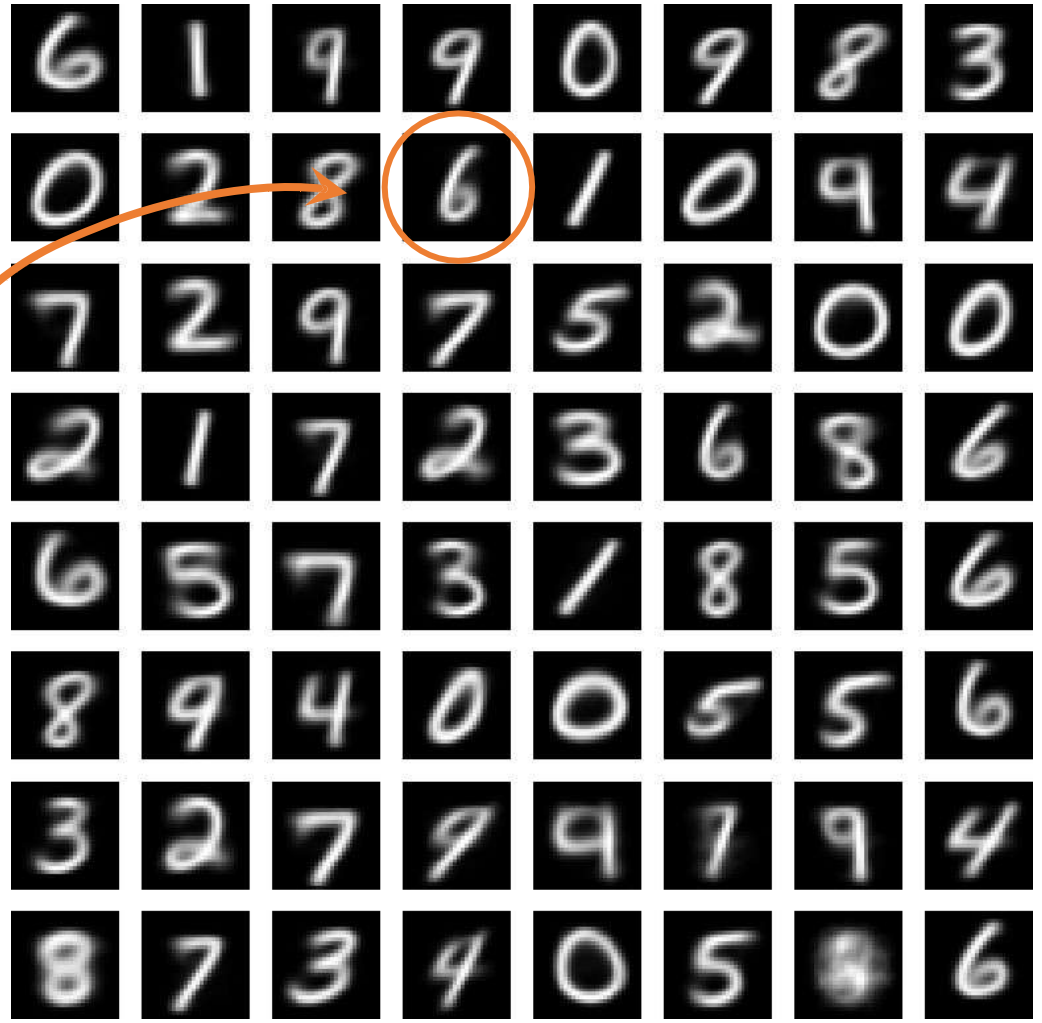


K-means as **Generative Models**

- randomly sample: $z \sim \mathcal{U}[0, k)$
- map z by the decoder
- generation result is one codeword

$z = 11$

codebook on MNIST, $k = 64$



- this is a valid generative model
- but not a “good” one
- but a good thought model

thus far, ...

- **VAE**: maximize ELBO
  - parameterize q by network
  - optimize by Stochastic Gradient Descent

- **EM**: maximize ELBO
  - parameterize q analytically
  - optimize by Coordinate Descent

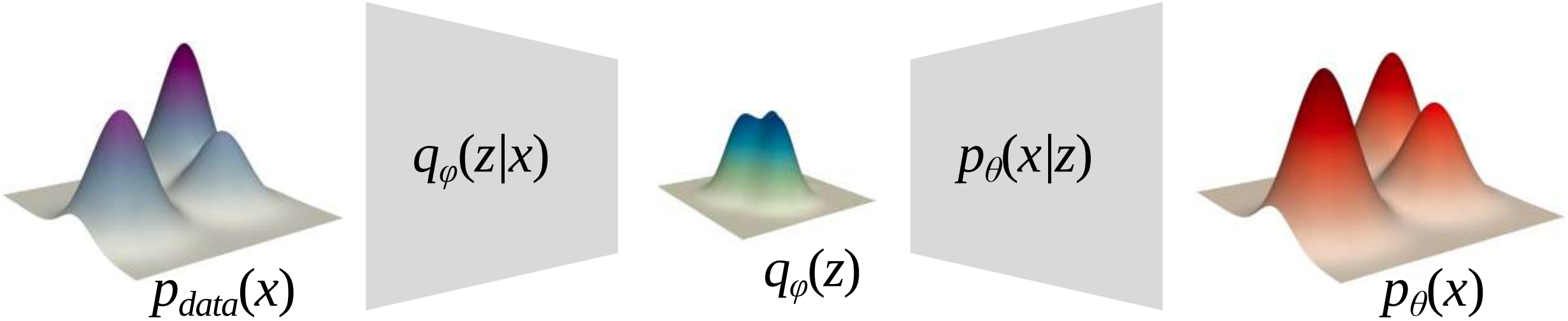
- **K-means**:
  - special case of EM; special case of AE
  - discrete distribution

- next: **VQ-VAE**

Vector Quantized VAE (VQ-VAE)

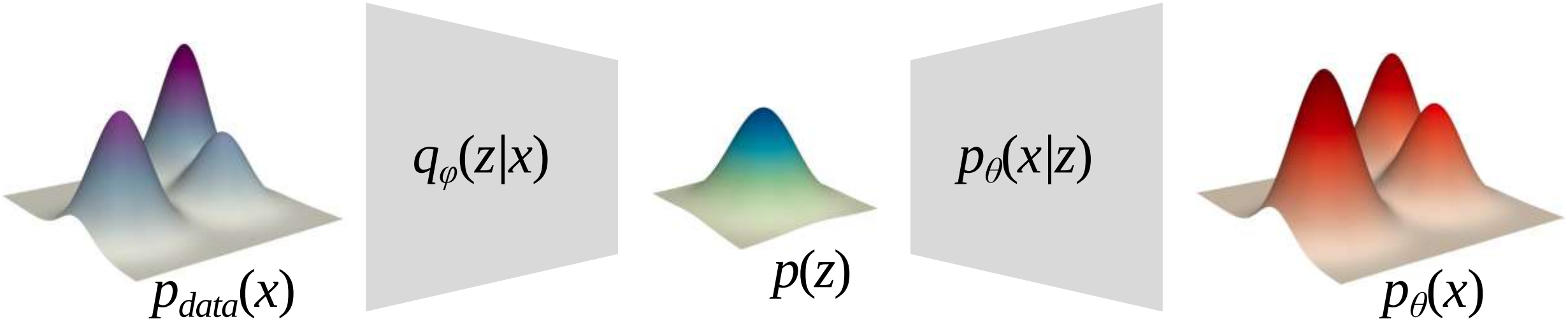
Recap

- Original VAE: latent variables are continuous



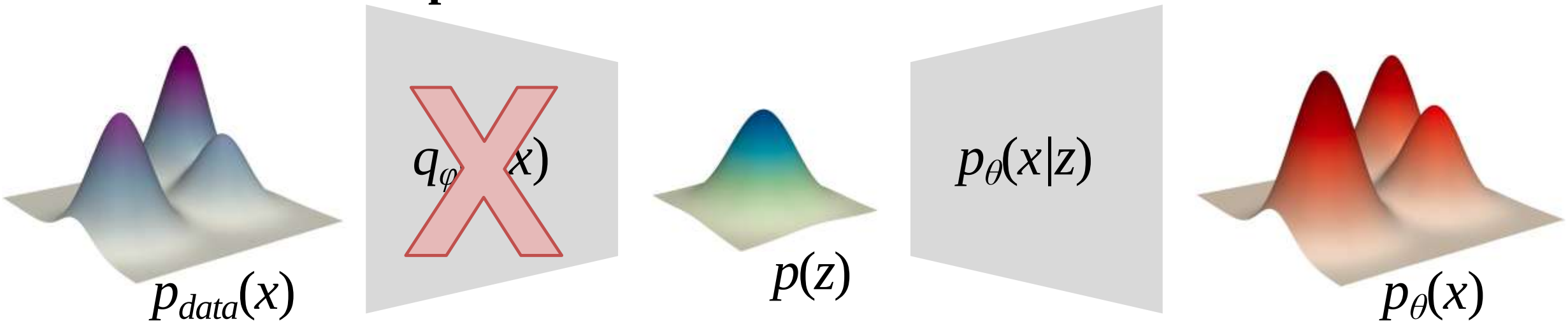
VAE

- encoder: maps data distribution to latent distribution
- decoder: maps latent distribution to data distribution



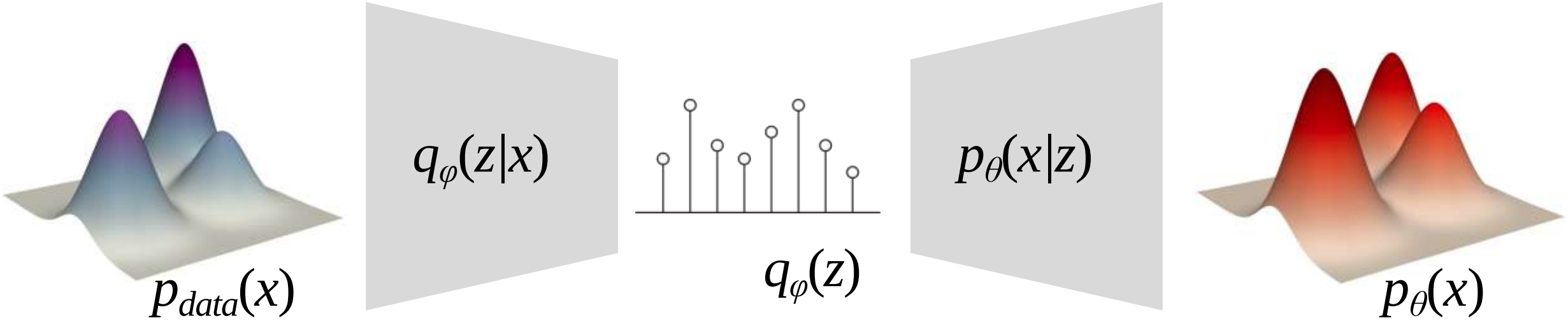
VAE

- encoder: maps data distribution to latent distribution
- decoder: maps latent distribution to data distribution
- **Posterior Collapse**



Discrete Latent Variables

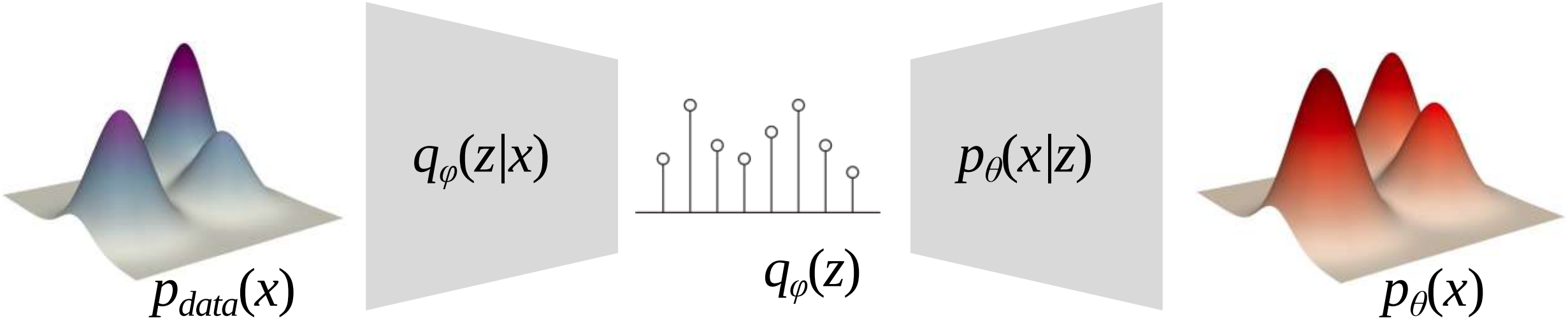
- model **multimodal** distributions
- **categorical**: no particular relation between numbers (SSN, zip code, ...)
- **symbolic**: language, speech, planning, ...



Discrete Latent Variables + VAE

Maximize ELBO

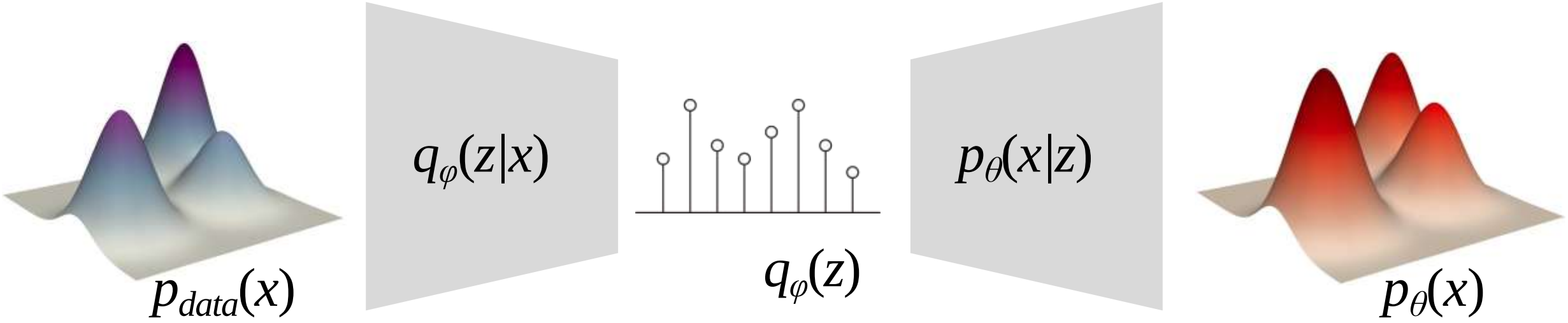
- Reconstruction loss: about x
- Regularization loss: about z (discrete)



Discrete Latent Variables + VAE

Reconstruction loss: about x

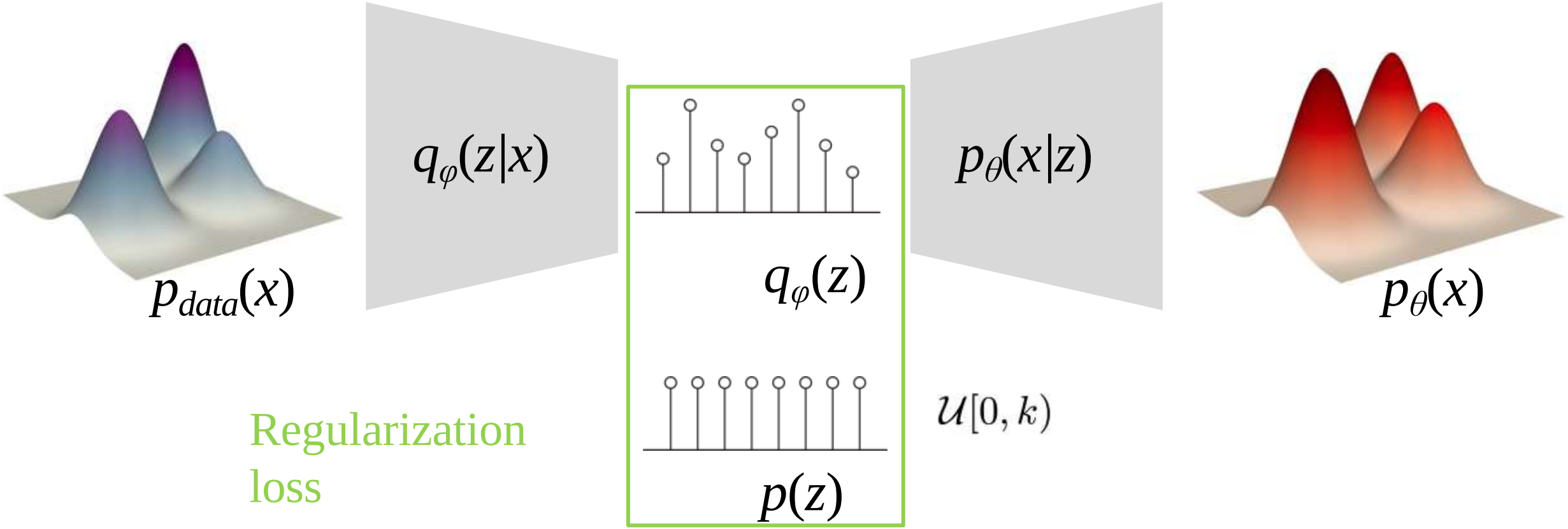
- same as VAE: $-\mathbb{E}_{z\sim q_\phi(z|x)}\left[\log p_\theta(x|z)\right]$



Discrete Latent Variables + VAE

Regularization loss: about z

- conceptually, same as VAE: $\mathcal{D}_{\mathrm{KL}}\left(q_\phi(z|x)||p(z)\right)$
- but how can we backprop w.r.t. discrete sampling?



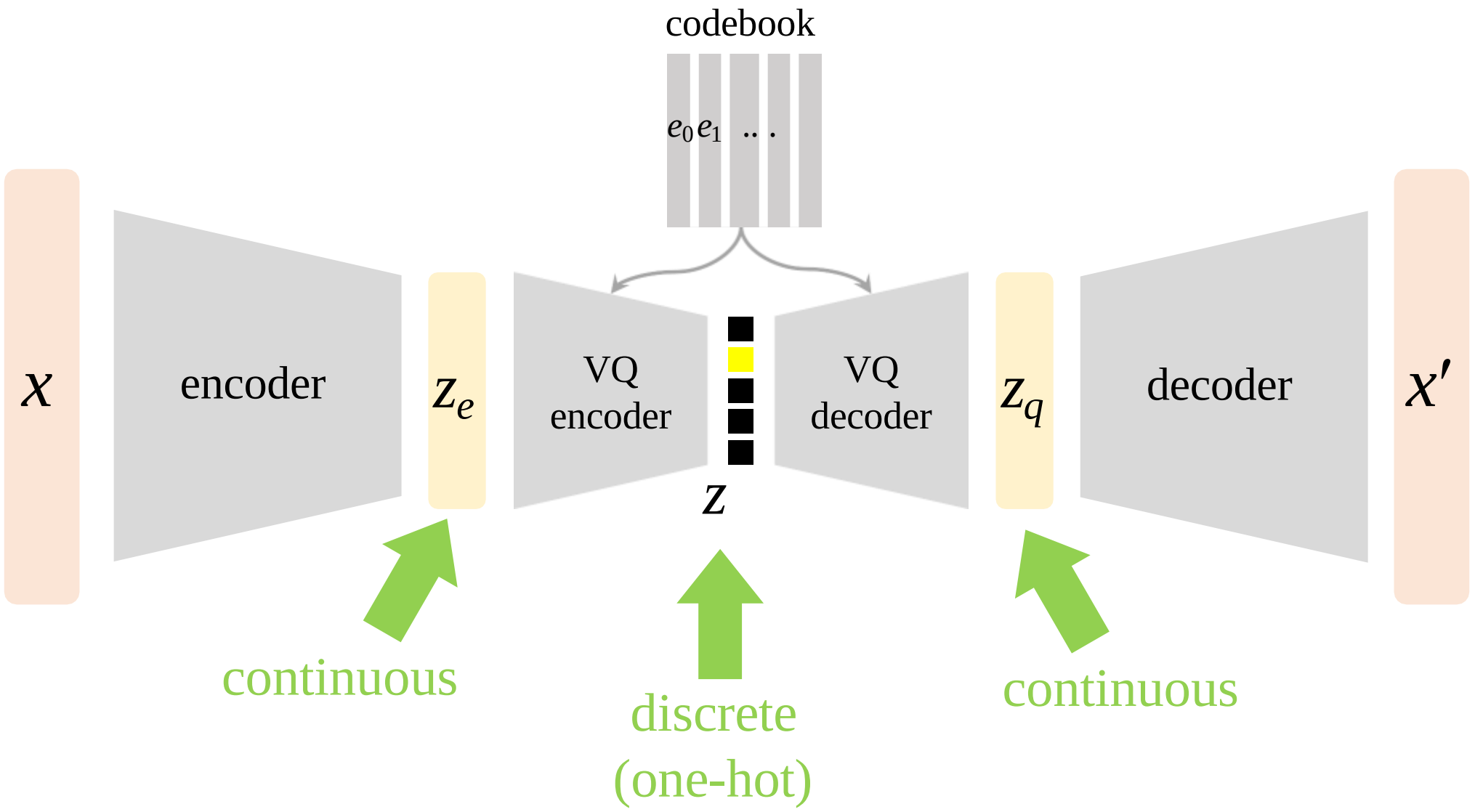
Discrete Latent Variables + VAE

Solution: K-means

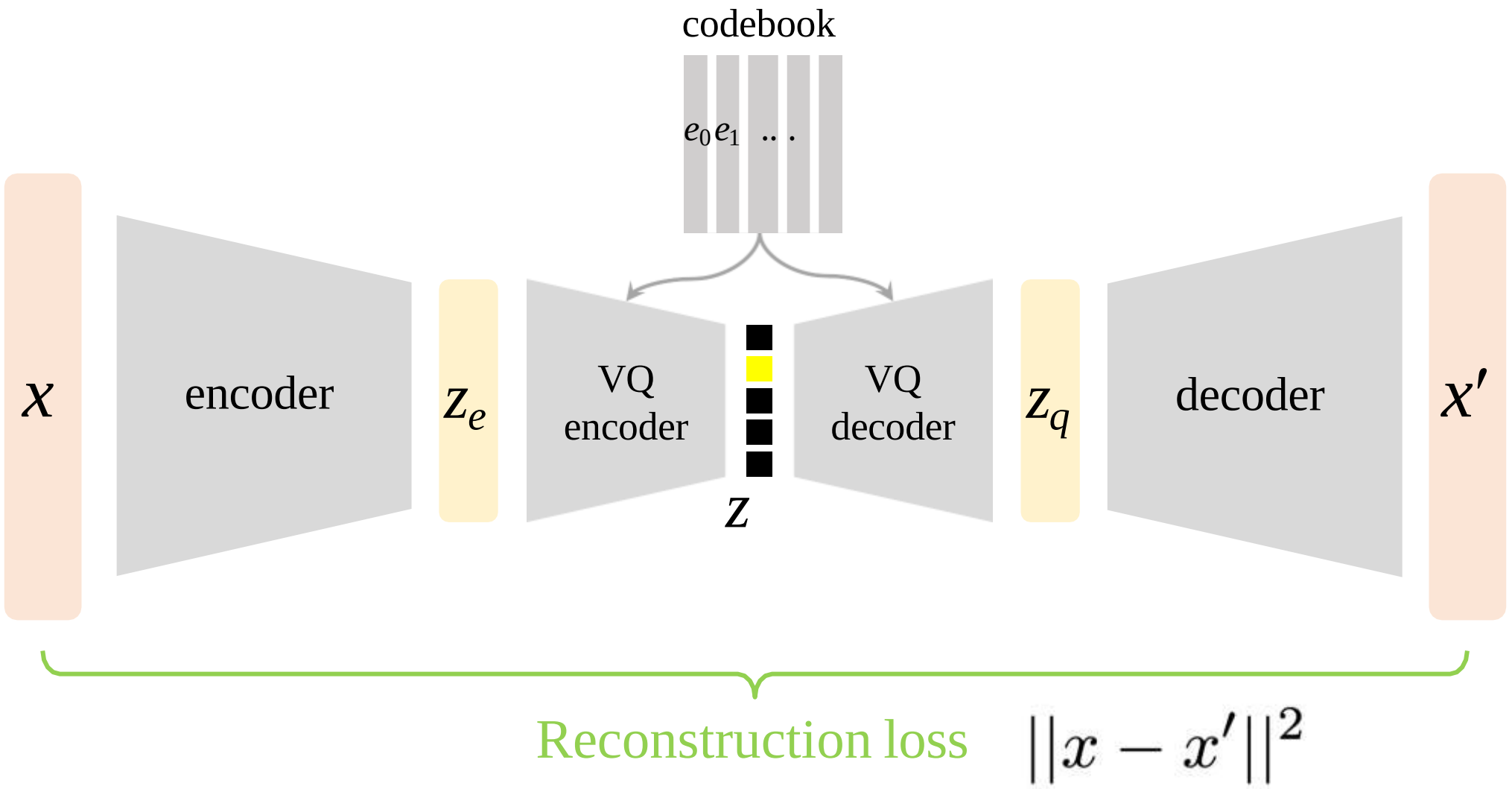
- K-means is autoencoding
- K-means has an objective function (reconstruction loss)
- K-means implicitly encourages codebook uniformity

This leads us to VQ-VAE ...

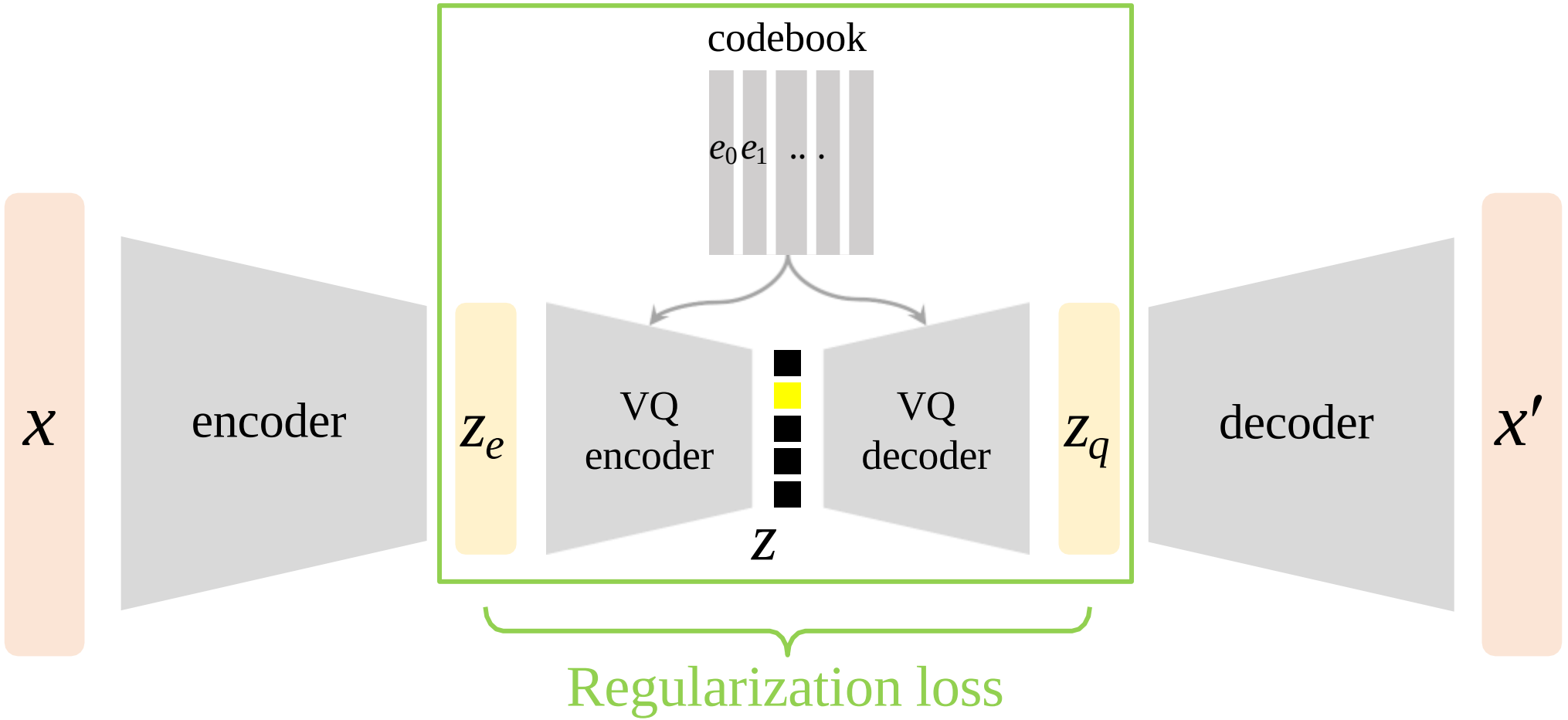
Vector Quantized VAE



Vector Quantized VAE



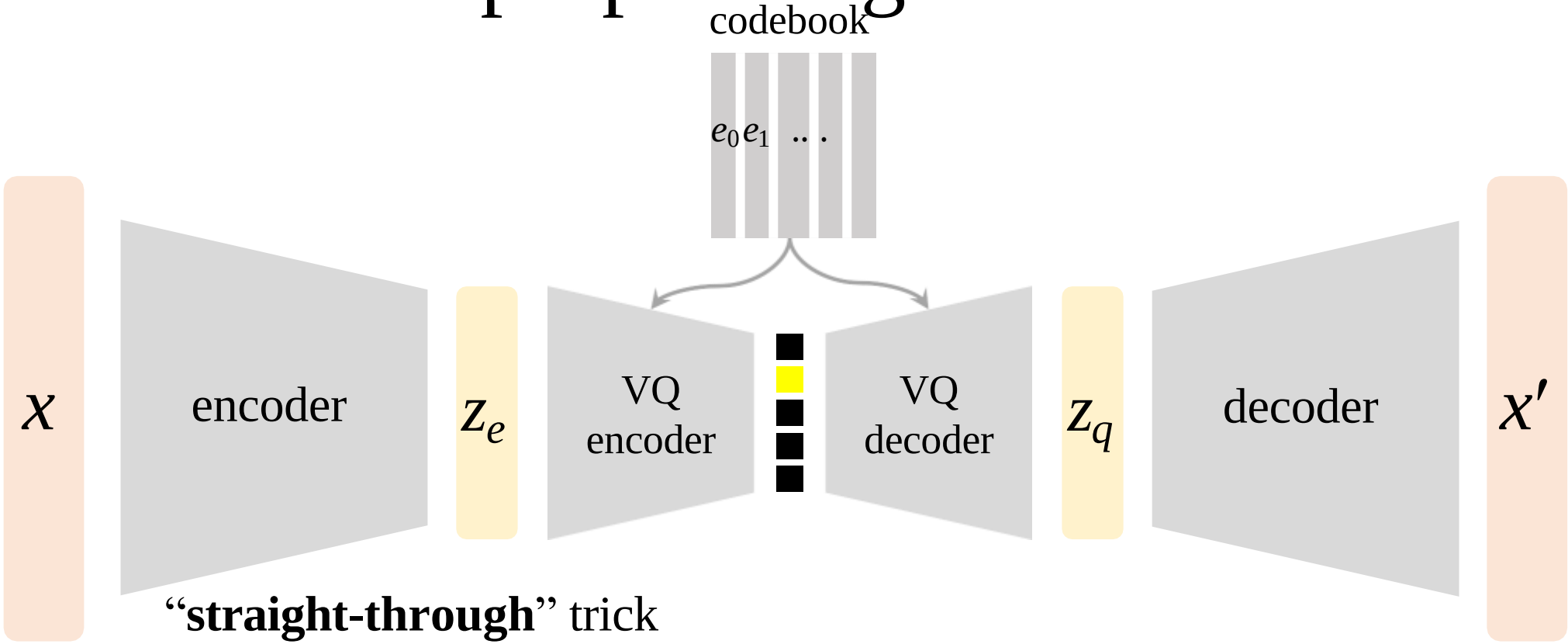
Vector Quantized VAE



conceptually, this is the K-means reconstruction loss: $\|z_e - z_q\|^2$

*The VQ-VAE paper uses $\|\text{sg}[z_e(x)] - e\|_2^2 + \beta\|z_e(x) - \text{sg}[e]\|_2^2$ which weights the gradients differently

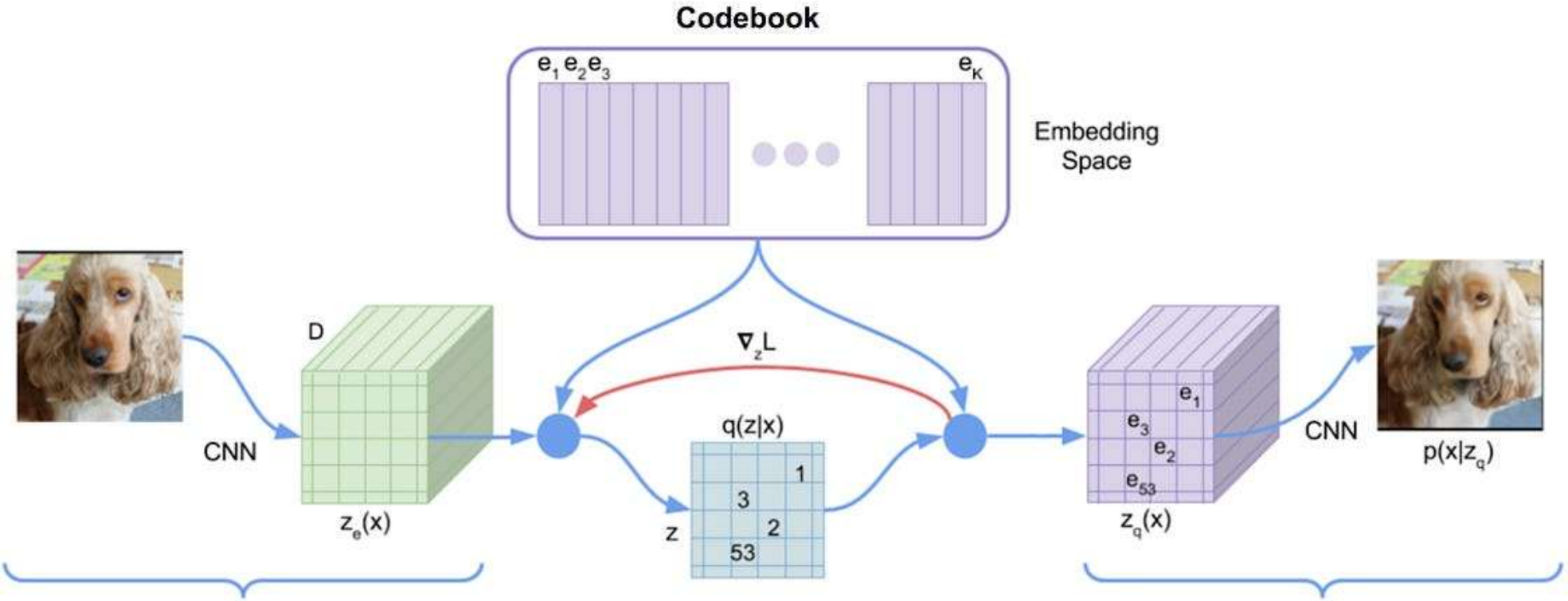
How to backprop through one-hot vector?

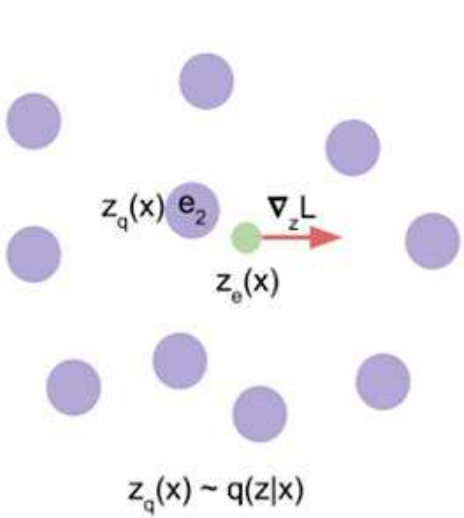


"**straight-through**" trick

- forward: hardmax's output (i.e., argmax and one-hot)
- backward: softmax's gradient
- in code: `stop_grad(hardmax(y) - softmax(y)) + softmax(y)`

VQ-VAE

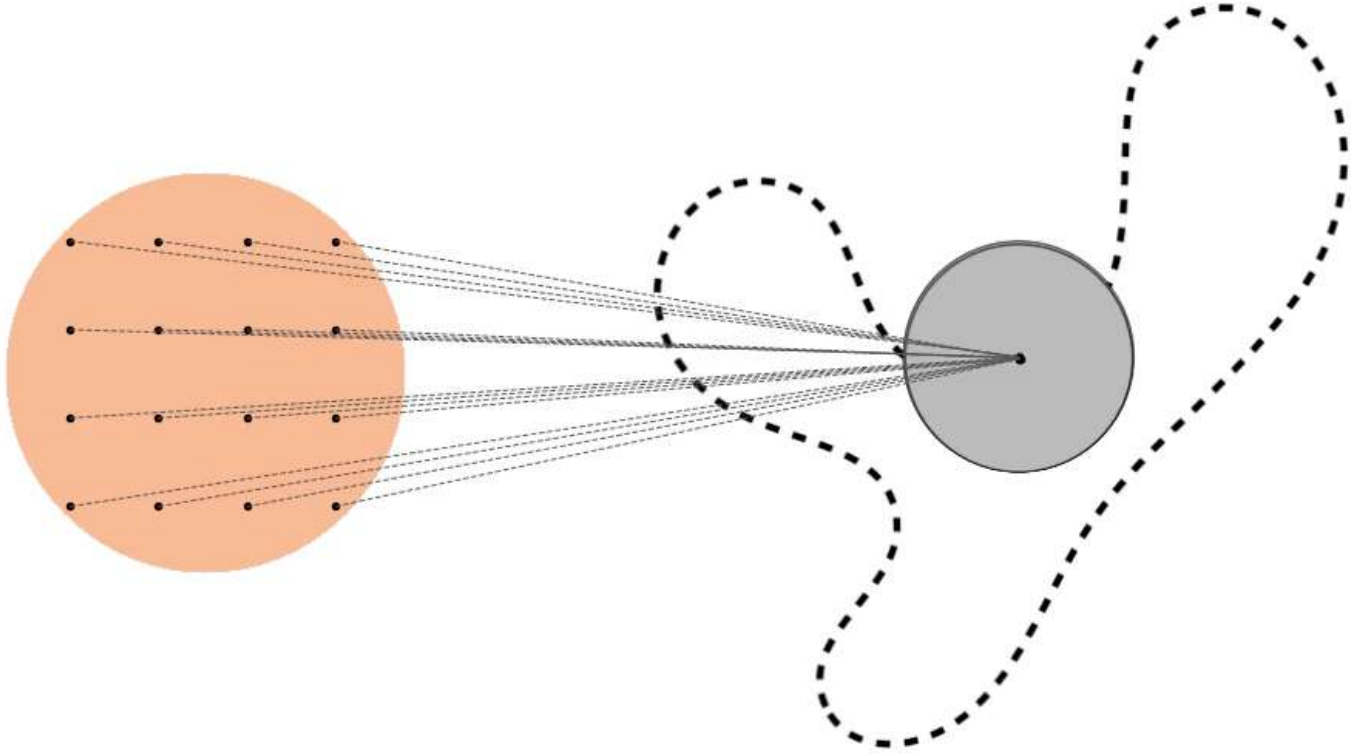




Posterior categorical distribution:

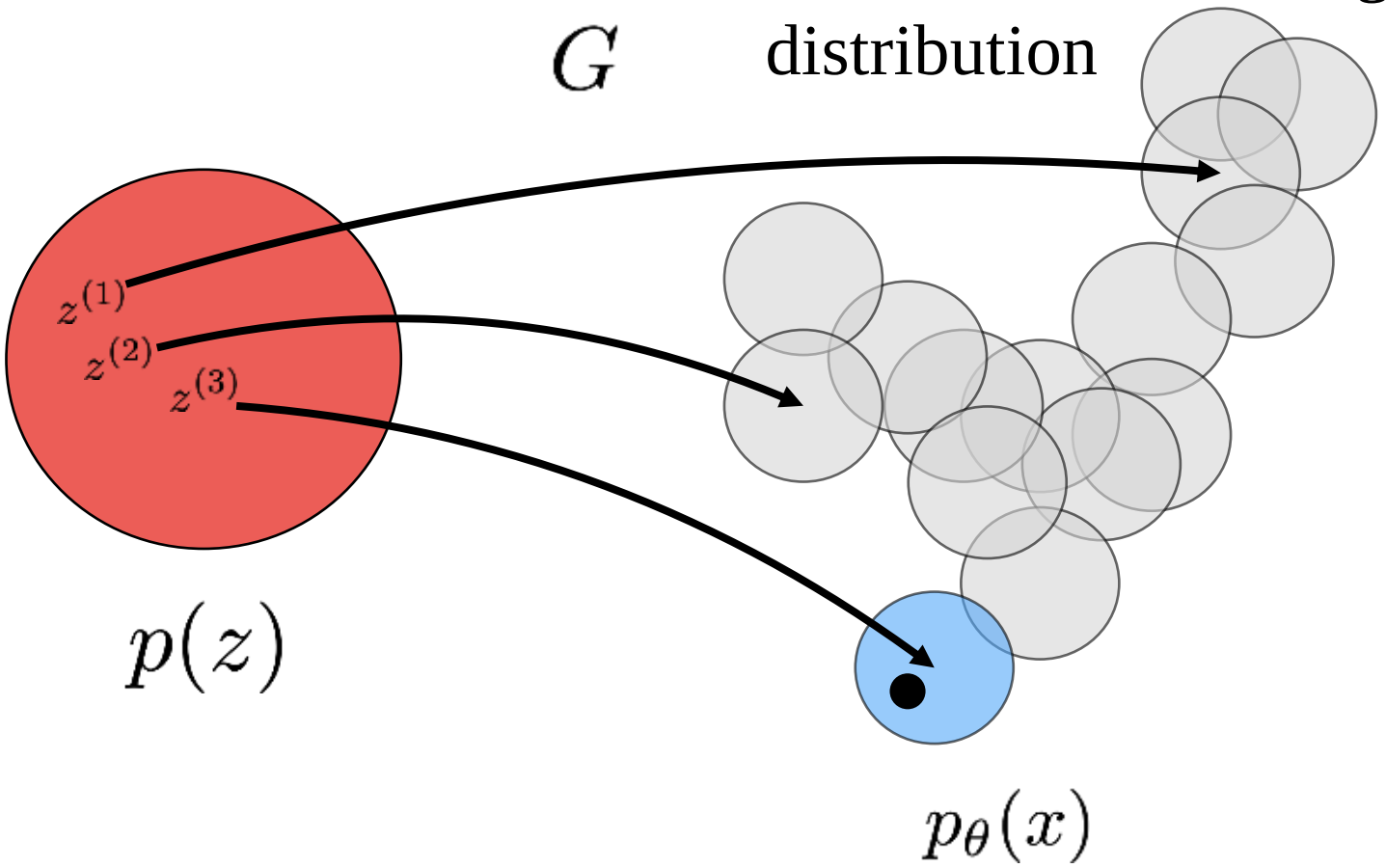
$$q(\mathbf{z}=\mathbf{e}_k|\mathbf{x}) = \begin{cases} 1 & \text{if } k = \arg\min_i \|\mathbf{z}_e(\mathbf{x}) - \mathbf{e}_i\|_2 \\ 0 & \text{otherwise.} \end{cases}$$

Recap. VAE



Prior distribution

Current model of target distribution



In order to optimize our model, we need to measure the likelihood it assigns to each datapoint x

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

$$= \sim 0+$$

$$\sim 0+$$

$$p(x|z^{(3)})p(z^{(3)})dz + \ldots$$

Vector Quantized VAE

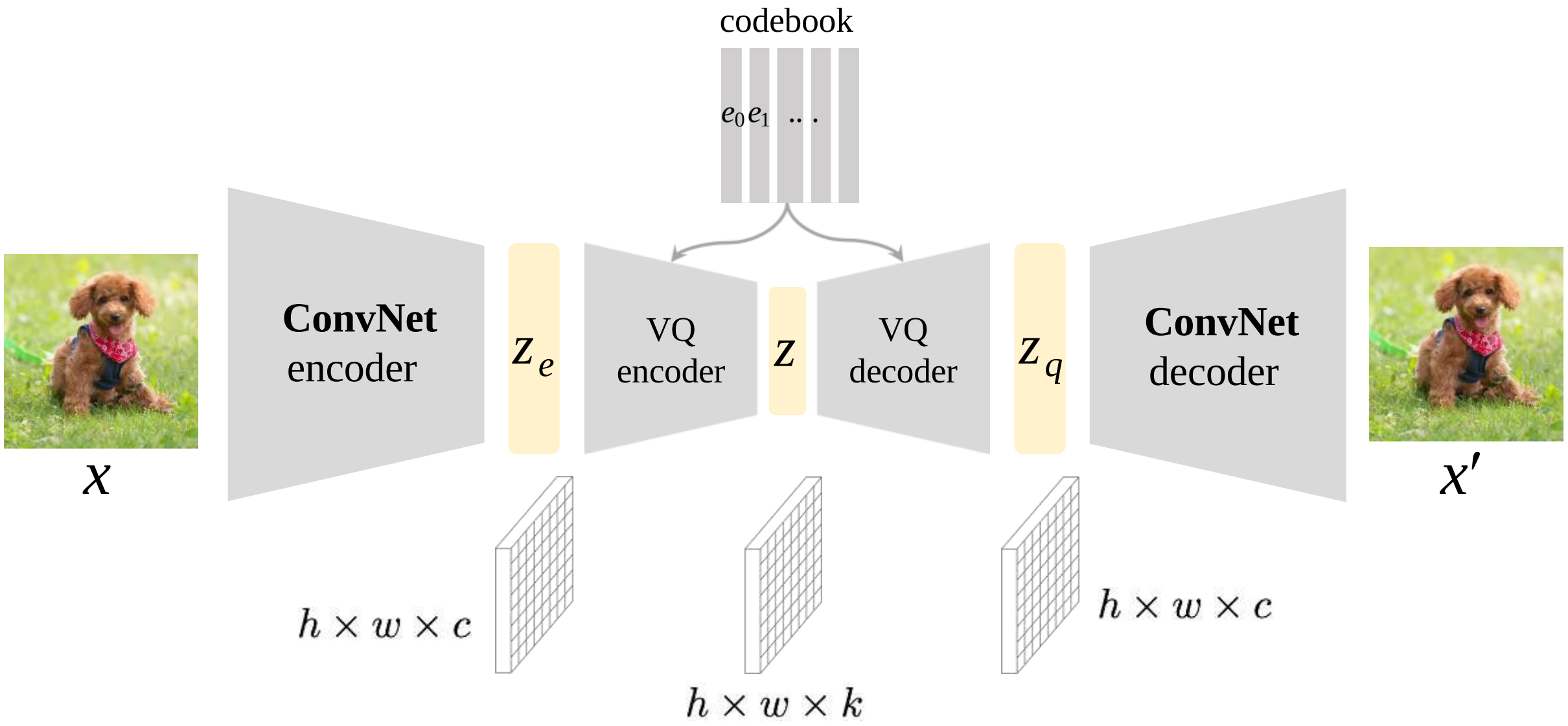
A single one-hot latent is not useful

- it's "deep K-means": with deep encoder/decoder
- a valid generative model; but not a "good" one

VQ-VAE: often used as "**tokenizers**"

- output multiple one-hot vectors
- don't reduce latent spatial/temporal size to 1
- use ConvNet/Transformer as encoder and decoder

VQ-VAE as Tokenizers



Notes

- Both VAE and VQ-VAE can be “tokenizers” (produce spatial latents).

But:

- prior $p(z)$ only models per-token (per-location) distribution
- prior $p(z)$ doesn’t model **joint** distribution across tokens
- spatial tokens are not **independent**
- at inference, we can’t sample from **i.i.d.** prior $p(z)$

Next: modeling joint distribution:

$$p(z) = p(z_1)p(z_2|z_1)p(z_3|z_1, z_2)p(z_4|z_1, z_2, z_3)\dots$$

- Autoregressive models
- Masked models
- Diffusion models

Main References

- Kingma and Welling. “Auto-Encoding Variational Bayes”, ICLR 2014
- Neal and Hinton. “A view of the EM algorithm that justifies incremental, sparse, and other variants”, 1999
- Hastie, et al. “The Elements of Statistical Learning”, 2001
- van den Oord, et al. “Neural Discrete Representation Learning”, NeurIPS 2017