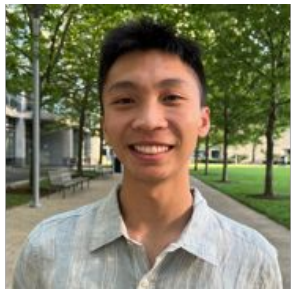
CS294-158 Deep Unsupervised Learning

Lecture 4 Latent Variable Models -- Variational AutoEncoder (VAE)

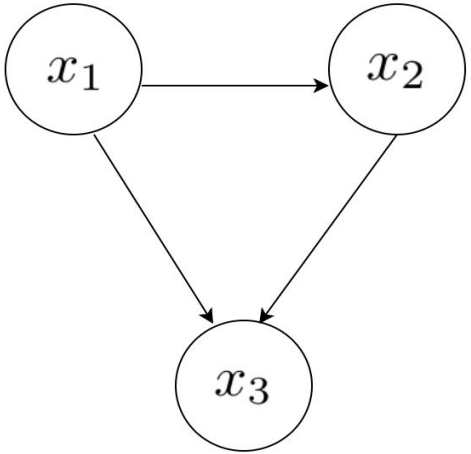


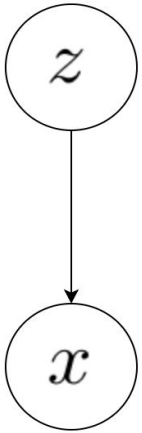



Pieter Abbeel, Wilson Yan, Kevin Frans, Philipp Wu

Latent Variable Models

- Autoregressive models + Flows
  - All random variables are observed
- Latent Variable Models (LVMs):
  - Some random variables are hidden - we do not get to observe





Why Latent Variable Models?

- Simpler, lower-dimensional representations of data often possible
  - Latent variable models hold the promise of automatically identifying those hidden representations

Why Latent Variable Models?

- AR models are slow to sample because all pixels (observation dims) are assumed to be dependent on each other
- We can make part of observation space independent *conditioned on some latent variables*
  - Latent variable models *can* have faster sampling by exploiting statistical patterns

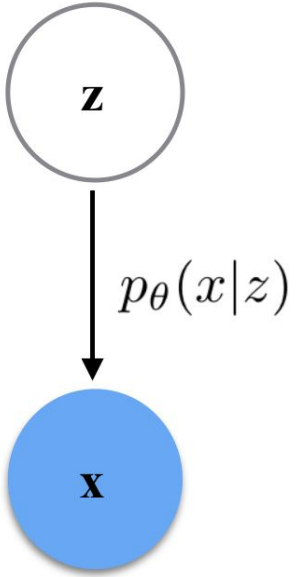
Latent Variable Models

- Sometimes, it's possible to design a latent variable model with an understanding of the causal process that generates data
- In general, we don't know what are the latent variables and how they interact with observations
  - Most popular models make little assumption about what are the latent variables
  - Best way to specify latent variables is still an active area of research

Example latent variable model

$$z = (z_1, z_2, \cdots, z_K) \sim p(z; \beta) = \prod_{k=1}^{K} \beta_k^{z_k} (1 - \beta_k)^{1 - z_k}$$

$$x = (x_1, x_2, \cdots, x_L) \sim p_\theta(x|z) \Leftrightarrow \text{Bernoulli}(x_i; \text{DNN}(z))$$



Latent Variable Model

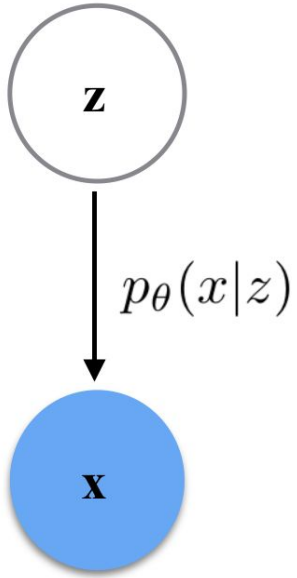
- Sample $z \sim p_Z(z)$

  $x \sim p_\theta(x \mid z)$

- Evaluate likelihood $p_\theta(x) = \sum_z p_Z(z) p_\theta(x \mid z)$

- Train $\max_\theta \sum_i \log p_\theta(x^{(i)}) = \sum_i \log \sum_z p_Z(z) p_\theta(x^{(i)} \mid z)$

- Representation $x \rightarrow z$



Outline

- Motivation
- Training Latent Variable Models (including VAE and IWAE)
  - Objective
    - Exact
    - Prior Sampling
    - Importance Sampling
    - Variational Lower Bound (VLB) / Evidence Lower BOund (ELBO)
  - Optimization
    - Likelihood Ratio Gradients vs. Reparameterization Trick Gradients
    - Optimizing the VLB/ELBO
- Variations*:*
  - Different priors p(z)
  - SOTA: VQ-VAE, VQ-VAE 2.0
  - Connection to other generative models
- Related ideas:
  - Mutual Information Estimation

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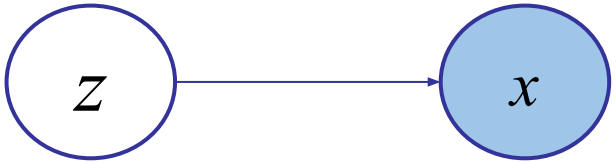
Training Latent Variable Models

- Objective:



$$\max_{\theta} \sum_{i} \log p_\theta(x^{(i)}) = \sum_{i} \log \sum_{z} p_Z(z) p_\theta(x^{(i)} \mid z)$$

- Scenario 1: z can only take on a small number of values → exact objective tractable

- Scenario 2: z can take on an impractical number of values to enumerate → approximate

How about optimizing $p_Z(z)$? = "learning the prior" and sometimes done [more later]

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Exact Likelihood Objective

Example: mixture of 3 Gaussians, with uniform prior over components

$$p_\theta(x) = \sum_z p_Z(z) p_\theta(x \mid z)$$

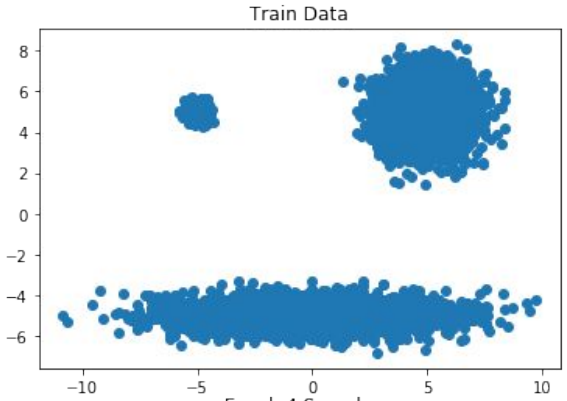
$$p_Z(z = A) = p_Z(z = B) = p_Z(z = C) = \frac{1}{3}$$

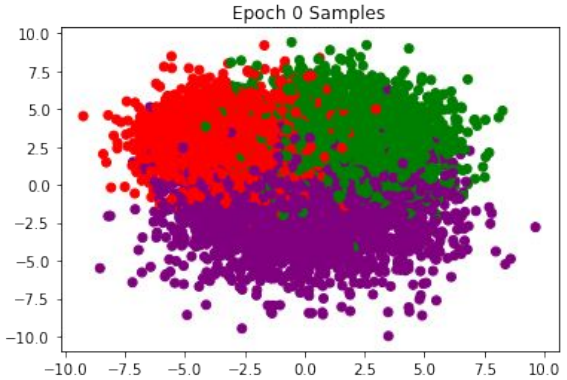
$$p_\theta(x \mid z = k) = \frac{1}{(2\pi)^{\frac{n}{2}} |\Sigma_k|^{\frac{1}{2}}} \exp\left(-\frac{1}{2}(x - \mu_k)^\top \Sigma_k^{-1}(x - \mu_k)\right)$$

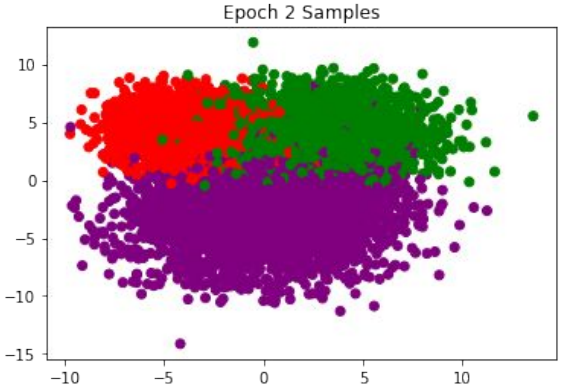
Training objective: $\max_\theta \sum_i \log p_\theta(x^{(i)})$

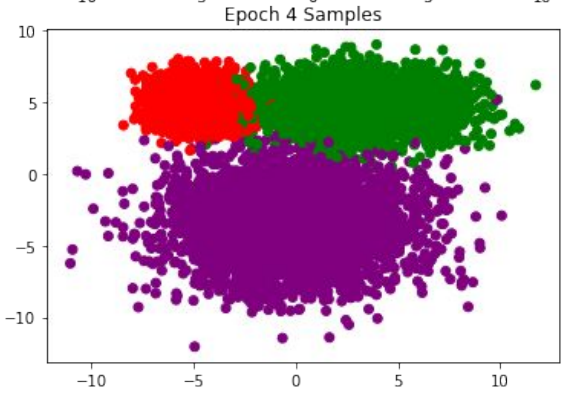
$$= \max_{\mu,\Sigma} \sum_i \log\Big[\frac{1}{3} \frac{1}{(2\pi)^{\frac{n}{2}} |\Sigma_A|^{\frac{1}{2}}} \exp\left(-\tfrac{1}{2}(x^{(i)} - \mu_A)^\top \Sigma_A^{-1}(x^{(i)} - \mu_A)\right)$$
$$+ \frac{1}{3} \frac{1}{(2\pi)^{\frac{n}{2}} |\Sigma_B|^{\frac{1}{2}}} \exp\left(-\tfrac{1}{2}(x^{(i)} - \mu_B)^\top \Sigma_B^{-1}(x^{(i)} - \mu_B)\right)$$
$$+ \frac{1}{3} \frac{1}{(2\pi)^{\frac{n}{2}} |\Sigma_C|^{\frac{1}{2}}} \exp\left(-\tfrac{1}{2}(x^{(i)} - \mu_C)^\top \Sigma_C^{-1}(x^{(i)} - \mu_C)\right)\Big]$$

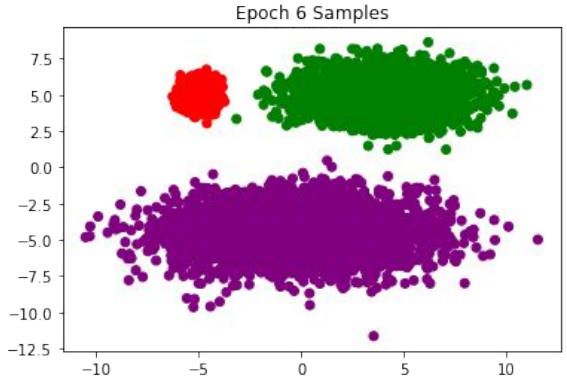
2-D Mixture of Gaussians

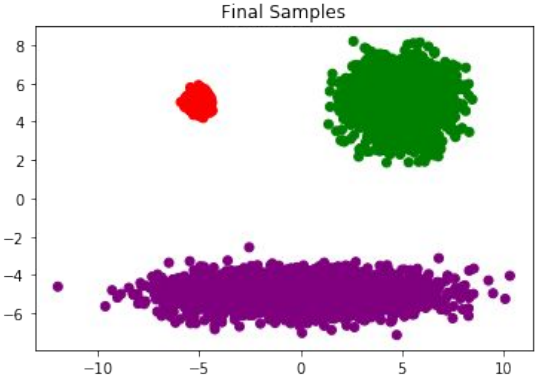












Prior Sampling

Main idea: if z can take on many values $\rightarrow$ sample z

$$\sum_i \log \sum_z p_Z(z) p_\theta(x^{(i)} \mid z) \approx \sum_i \log \frac{1}{K} \sum_{k=1}^{K} p_\theta(x^{(i)} \mid z_k^{(i)}) \qquad z_k^{(i)} \sim p_Z(z)$$

$\rightarrow$ run Stochastic Gradient Descent (SGD) on the approximate objective

Prior Sampling -- Example + Challenge

Consider data in N clusters:

Sampling z uniformly results in only in only 1/N terms being useful.

Recall: z might correspond to many high level properties, e.g., 100 high level properties, probability of correct z for given x: 0.5^{100}

Issue: When going to higher dimensional data, it becomes near impossible to be lucky enough that a sampled z is a good match for a data point $x^{(i)}$

Importance Sampling -- Motivation / Background

Problem setting:

Want to compute $\mathbb{E}_{z \sim p_Z(z)}\left[f(z)\right]$

But: (1) hard to sample from $p_Z(z)$

and/or (2) samples from $p_Z(z)$ are not very informative

Example of (2):

Note: our Latent Variable Model objective is also example of (2)

Importance Sampling -- Algorithm

Formulation:

$$
\begin{aligned}
\mathbb{E}_{z\sim p_Z(z)}\left[f(z)\right] &= \sum_z p_Z(z) f(z) \\
&= \sum_z \frac{q(z)}{q(z)} p_Z(z) f(z) \\
&= \mathbb{E}_{z\sim q(z)}\left[\frac{p_Z(z)}{q(z)} f(z)\right] \\
&\approx \frac{1}{K}\sum_{k=1}^{K} \frac{p_Z(z^{(k)})}{q(z^{(k)})} f(z^{(k)}) \quad \text{with} \quad z^{(k)} \sim q(z)
\end{aligned}
$$

→ Can sample from q to compute expectation w.r.t. p

Importance Sampling for Latent Variable Model

Training Objective:

$$\sum_i \log \sum_z p_Z(z) p_\theta(x^{(i)} \mid z) \approx \sum_i \log \frac{1}{K} \sum_{k=1}^{K} \frac{p_Z(z_k^{(i)})}{q(z_k^{(i)})} p_\theta(x^{(i)} \mid z_k^{(i)}) \quad \text{with} \quad z_k^{(i)} \sim q(z_k^{(i)}))$$

Good proposal distribution q(z)?

We want samples compatible with $x^{(i)}$

→ How about $q(z) = p_\theta(z \mid x^{(i)}) = \frac{p_\theta(x^{(i)} \mid z) p_Z(z)}{p_\theta(x^{(i)})}$

Issue: not clear how to sample from this distribution...

Importance Sampling Proposal Distribution

General Principle of Variational Approach:

We can't directly use $\boldsymbol{p}$ we want

So, instead, we propose a parameterized distribution $\boldsymbol{q}$ we know we can work with easily (in this case, sample from easily), and try to find a parameter setting that makes it as good as possible.

E.g. find $q(z) = \mathcal{N}(z; \mu, \sigma^2)$ as close as possible to $p_\theta(z \mid x^{(i)}) = \dfrac{p_\theta(x^{(i)} \mid z) p_Z(z)}{p_\theta(x^{(i)})}$

Importance Sampling Proposal Distribution

$\longrightarrow$ optimize to find q

$$\min_{q(z)} \mathrm{KL}(q(z) \| p_\theta(z \mid x^{(i)})$$

$$= \min_{q(z)} \mathbb{E}_{z \sim q(z)} \log \left(\frac{q(z)}{p_\theta(z|x^{(i)})} \right)$$

$$= \min_{q(z)} \mathbb{E}_{z \sim q(z)} \log \left(\frac{q(z)}{p_\theta(x^{(i)}|z) p_Z(z) / p_\theta(x^{(i)})} \right)$$

$$= \min_{q(z)} \mathbb{E}_{z \sim q(z)} \left[\log q(z) - \log p_Z(z) - \log p_\theta(x^{(i)} \mid z) \right] + \log p_\theta(x^{(i)})$$

$$= \min_{q(z)} \mathbb{E}_{z \sim q(z)} \left[\log q(z) - \log p_Z(z) - \log p_\theta(x^{(i)} \mid z) \right] + \text{constant independent of z}$$

Note: all needed quantities in the objective readily computable

Amortized Inference

General Idea of Amortization: if same inference problem needs to be solved many times, can we parameterize a neural network to solve it?

Our case: for all $x^{(i)}$ we want to solve:

$$\min_{q(z)} \mathrm{KL}(q(z) \| p_\theta(z \mid x^{(i)})$$

Amortized formulation:

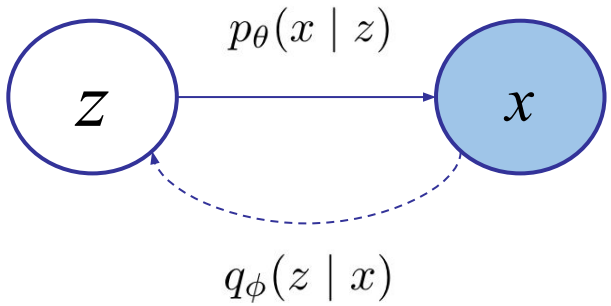
$$\min_{\phi} \sum_{i} \mathrm{KL}(q_\phi(z \mid x^{(i)}) \| p_\theta(z \mid x^{(i)}))$$

Trade-off: + : faster, regularization; - : not as precise

Amortized Inference

Amortized formulation:

$$\min_{\phi} \sum_{i} \mathrm{KL}(q_\phi(z \mid x^{(i)}) \| p_\theta(z \mid x^{(i)}))$$



E.g:

$$q_\phi(z \mid x) = \mathcal{N}(\mu_\phi(x), \sigma^2_\phi(x))$$

Equivalently: $z = \mu_\phi(x) + \varepsilon\sigma_\phi(x)$ with $\varepsilon \sim \mathcal{N}(0, I)$

Importance Weighted AutoEncoder (IWAE)

Objective:

$$\sum_i \log \frac{1}{K} \sum_{k=1}^{K} \frac{p_Z(z_k^{(i)})}{q(z_k^{(i)})} p_\theta(x^{(i)} \mid z_k^{(i)}) \quad \text{with} \quad z_k^{(i)} \sim q(z_k^{(i)}))$$

And:

$$\min_\phi \sum_i \mathrm{KL}(q_\phi(z \mid x^{(i)}) \| p_\theta(z \mid x^{(i)}))$$

$\rightarrow$ maximize term1 - term2

Importance Weighted AutoEncoder (IWAE)

Theorem 1. *For all k, the lower bounds satisfy*

$$\log p(\mathbf{x}) \geq \mathcal{L}_{k+1} \geq \mathcal{L}_k.$$

Moreover, if $p(\mathbf{h}, \mathbf{x})/q(\mathbf{h}|\mathbf{x})$ is bounded, then $\mathcal{L}_k$ approaches $\log p(\mathbf{x})$ as k goes to infinity.

[Burda et al., 2015]

VI as Importance Sampling [skip]

- We draw multiple z samples from q(z|x) and name them z_i
- Define w_i and L_k:

$$w_i = \frac{p(z_i, x)}{q(z_i|x)}$$

$$\mathcal{L}_k = \mathbb{E}\left[\log \frac{1}{k}\sum_{i=1}^{k} w_i\right] \leq \log \mathbb{E}\left[\frac{1}{k}\sum_{i=1}^{k} w_i\right] = \log p(\mathbf{x}),$$

[Burda et al., 2015]

Importance Weighted AutoEncoder (IWAE) [skip]

$$
\begin{aligned}
\mathcal{L}_k &= \mathbb{E}_{\mathbf{h}_1,\ldots,\mathbf{h}_k}\left[\log \frac{1}{k}\sum_{i=1}^{k}\frac{p(\mathbf{x},\mathbf{h}_i)}{q(\mathbf{h}_i|\mathbf{x})}\right] \\
&= \mathbb{E}_{\mathbf{h}_1,\ldots,\mathbf{h}_k}\left[\log \mathbb{E}_{I=\{i_1,\ldots,i_m\}}\left[\frac{1}{m}\sum_{j=1}^{m}\frac{p(\mathbf{x},\mathbf{h}_{i_j})}{q(\mathbf{h}_{i_j}|\mathbf{x})}\right]\right] \\
&\geq \mathbb{E}_{\mathbf{h}_1,\ldots,\mathbf{h}_k}\left[\mathbb{E}_{I=\{i_1,\ldots,i_m\}}\left[\log \frac{1}{m}\sum_{j=1}^{m}\frac{p(\mathbf{x},\mathbf{h}_{i_j})}{q(\mathbf{h}_{i_j}|\mathbf{x})}\right]\right] \\
&= \mathbb{E}_{\mathbf{h}_1,\ldots,\mathbf{h}_m}\left[\log \frac{1}{m}\sum_{i=1}^{m}\frac{p(\mathbf{x},\mathbf{h}_i)}{q(\mathbf{h}_i|\mathbf{x})}\right] = \mathcal{L}_m
\end{aligned}
$$

[Burda et al., 2015]

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VLB: Derivation 1 (Jensen)

[live derivation]

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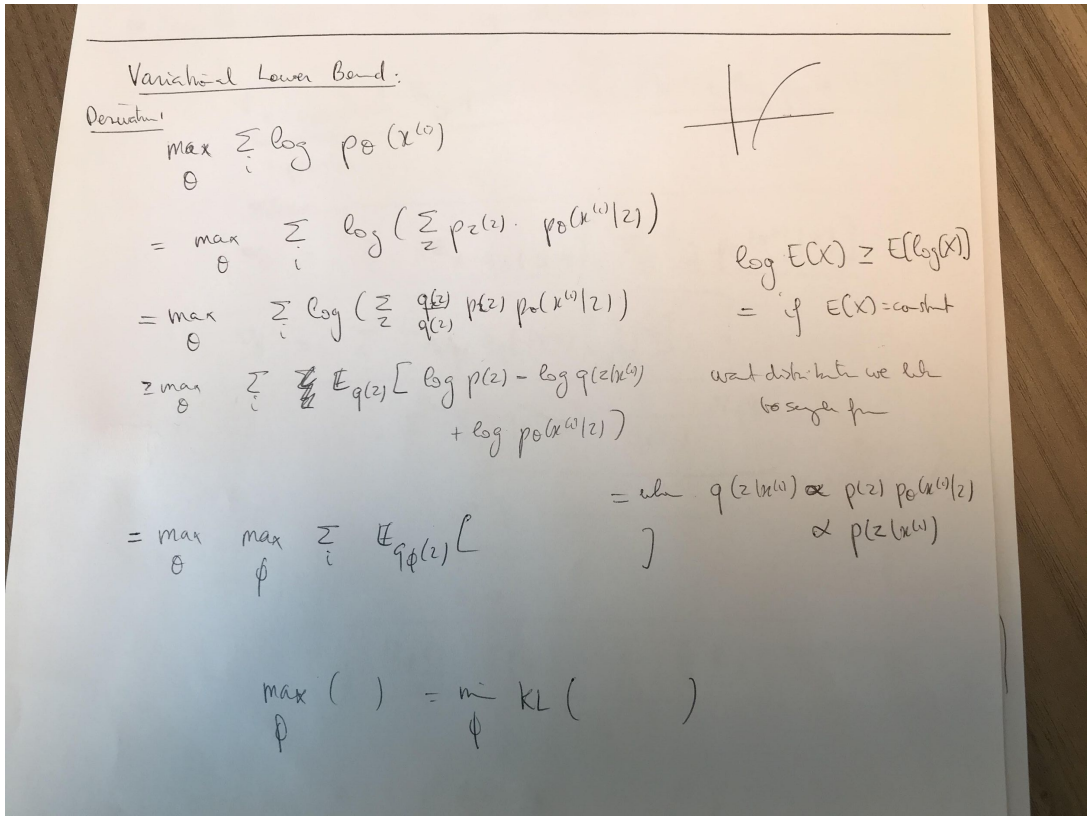
[live derivation]



VLB: Derivation 2 (KL)

$$
\begin{aligned}
D_{\mathrm{KL}}\left[q_x(z) \parallel p(z|x)\right] &= \mathbb{E}_{z\sim q_x(z)}\left[\log q_x(z) - \log p(z|x)\right] \\
&= \mathbb{E}_{z\sim q_x(z)}\left[\log q_x(z) - \log \frac{p(z,x)}{p(x)}\right] \\
&= \mathbb{E}_{z\sim q_x(z)}\left[\log q_x(z) - \log p(z) - \log p(x|z) + \log p(x)\right] \\
&= \underbrace{\mathbb{E}_{z\sim q_x(z)}\left[\log q_x(z) - \log p(z) - \log p(x|z)\right]}_{\text{Only this part depends on } z} + \log p(x)
\end{aligned}
$$

$$
\log p(x) = \mathbb{E}_{z\sim q_x(z)}\left[-\log q_x(z) + \log p(z) + \log p(x \mid z)\right] + D_{KL}\left[q_x(z) \| p(z \mid x)\right]
$$

Same as with Jensen's, but now we know the gap = KL

Variational Lower Bound (VLB)

- We now have an objective amenable to stochastic optimization

$$D_{\mathrm{KL}}\left[q_x(z) \parallel p(z|x)\right] = \mathbb{E}_{z\sim q_x(z)}\left[\log q_x(z) - \log p(z) - \log p(x|z)\right] + \log p(x)$$

- Turns out we can get more out of this exercise

$$\begin{aligned}\log p(x) &= -\mathbb{E}_{z\sim q_x(z)}\left[\log q_x(z) - \log p(z) - \log p(x|z)\right] + D_{\mathrm{KL}}\left[q_x(z) \parallel p(z|x)\right] \\ &= \underbrace{\mathbb{E}_{z\sim q_x(z)}\left[\log p(z) + \log p(x|z) - \log q_x(z)\right]}_{\text{Variational Lower Bound}} + \underbrace{D_{\mathrm{KL}}\left[q_x(z) \parallel p(z|x)\right]}_{\geq 0}\end{aligned}$$

  - note: the optimal $q_x(z)$ of VLB is $p(z|x)$, at which point VLB is tight (= $\log p(x)$)

VLB Maximization

- Given a data distribution $x \sim p_{data}$, we can train the generative model by maximizing the VLB under data distribution

$$\mathbb{E}_{\mathbf{x}\sim p_{\text{data}}}\left[\mathbb{E}_{\mathbf{z}\sim q_x(\mathbf{z})}\left[\log p(\mathbf{z}) + \log p(\mathbf{x}|\mathbf{z}) - \log q_x(\mathbf{z})\right]\right] \leq \mathbb{E}_{\mathbf{x}\sim p_{\text{data}}}\left[\log p(\mathbf{x})\right]$$

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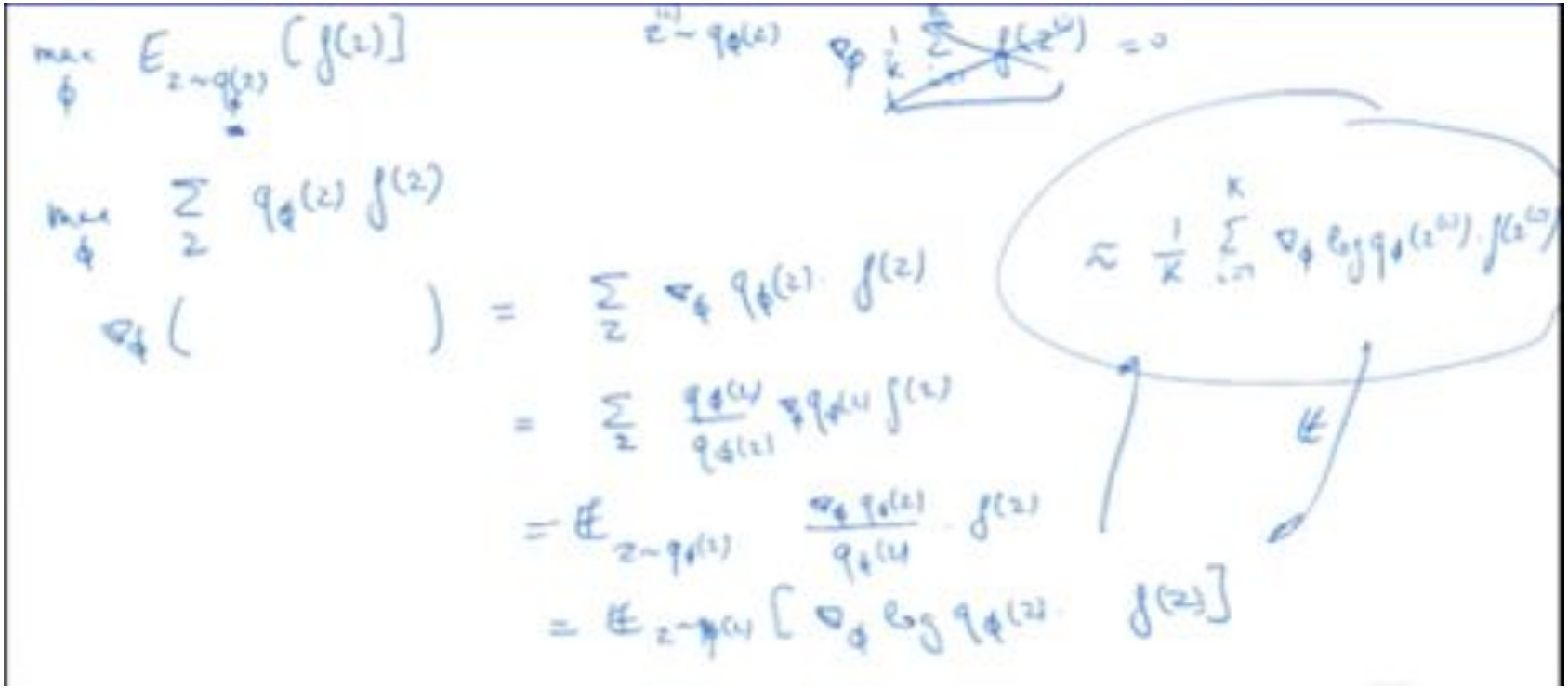
Likelihood Ratio Gradient

[live derivation -- for general case; for Gaussian on next slide]

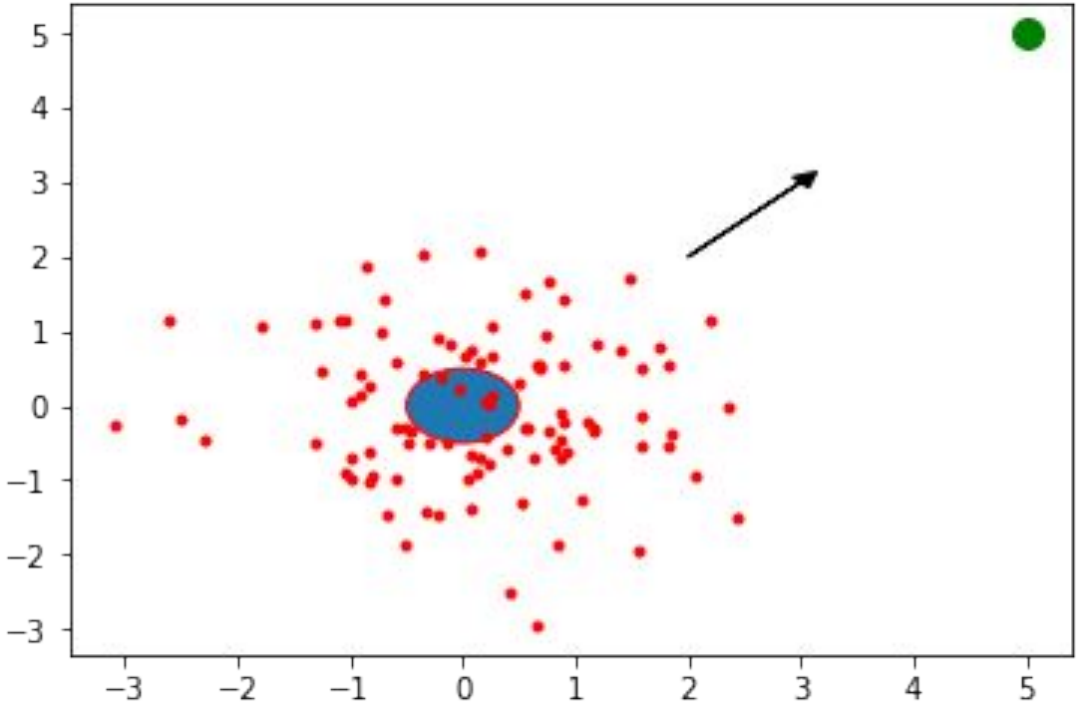
Likelihood Ratio Gradient



Likelihood Ratio Gradient - Toy Problem

Learn $\mu \in \mathbb{R}^2$ to minimize the objective below to reach the green point

$$\mathcal{L} = \mathbb{E}_{x \sim N(\mu, I)} \left\| x - \begin{bmatrix} 5 \\ 5 \end{bmatrix} \right\|_2^2$$



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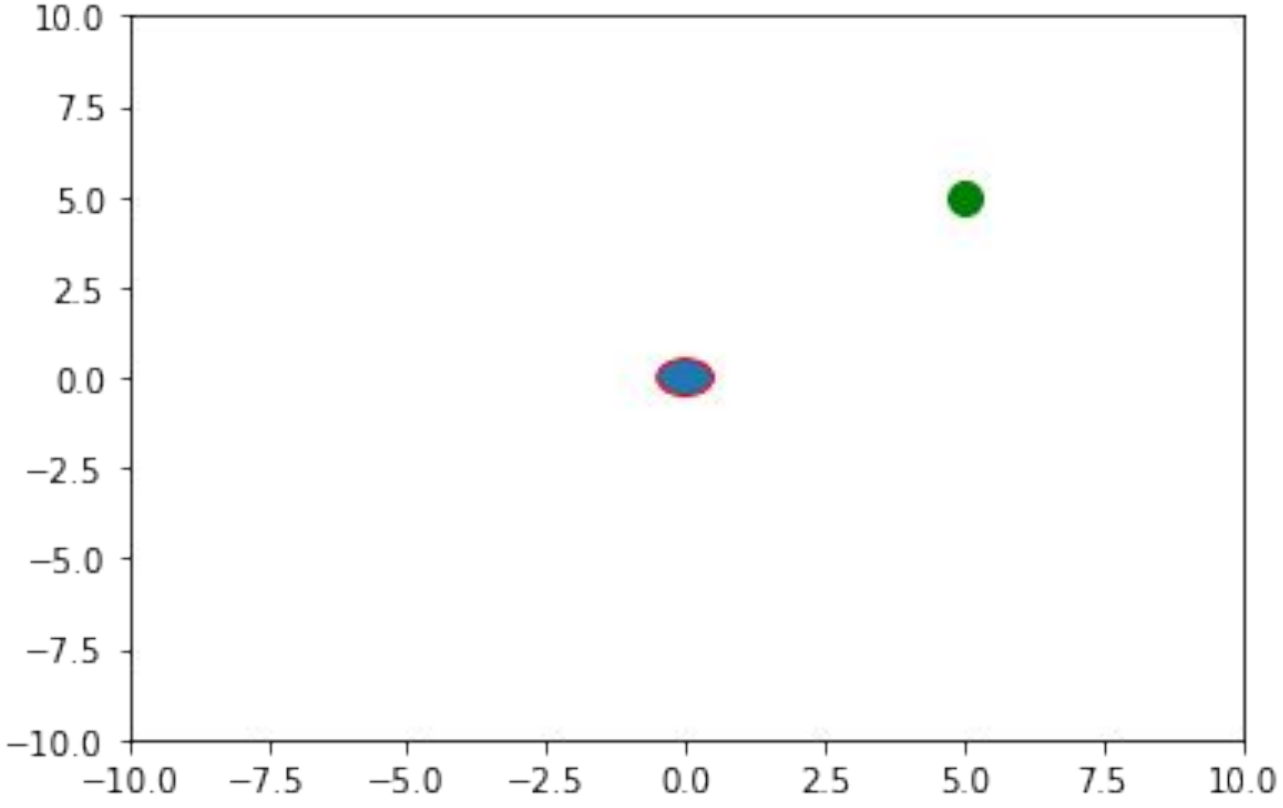

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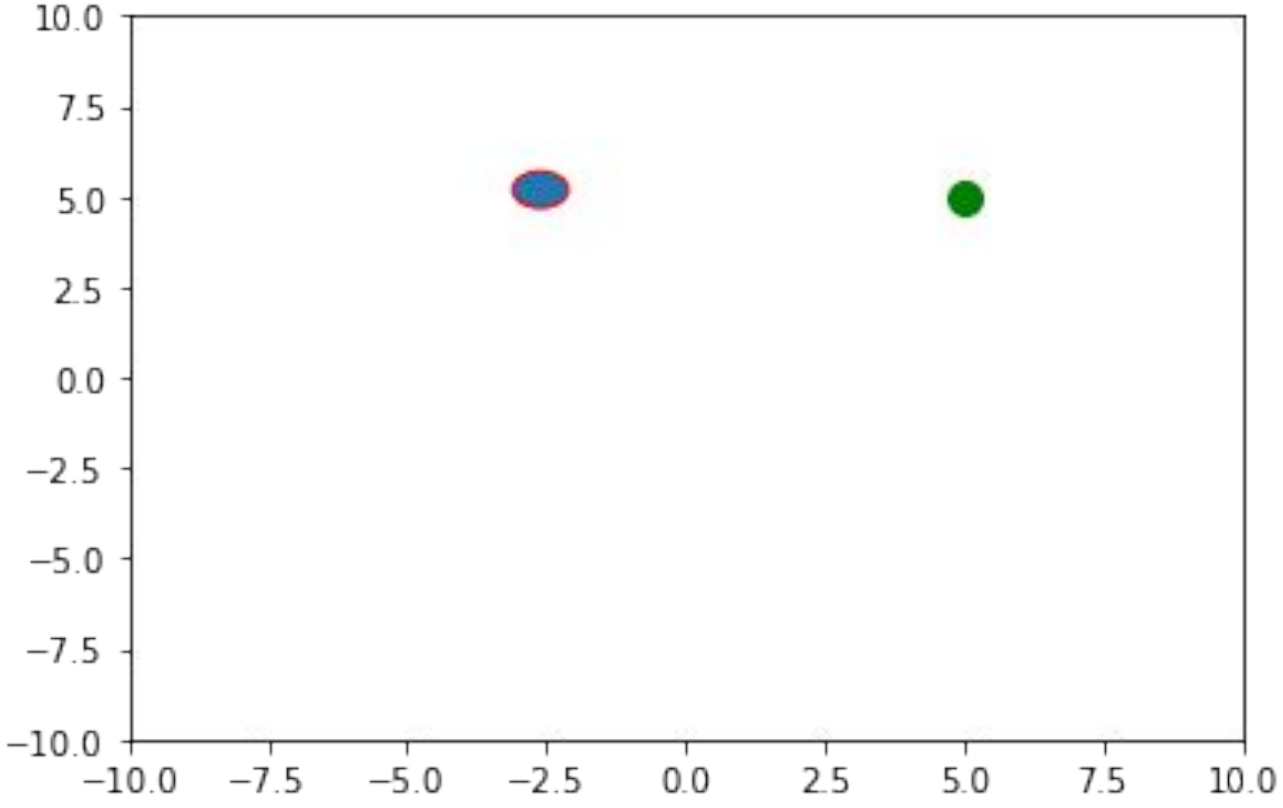
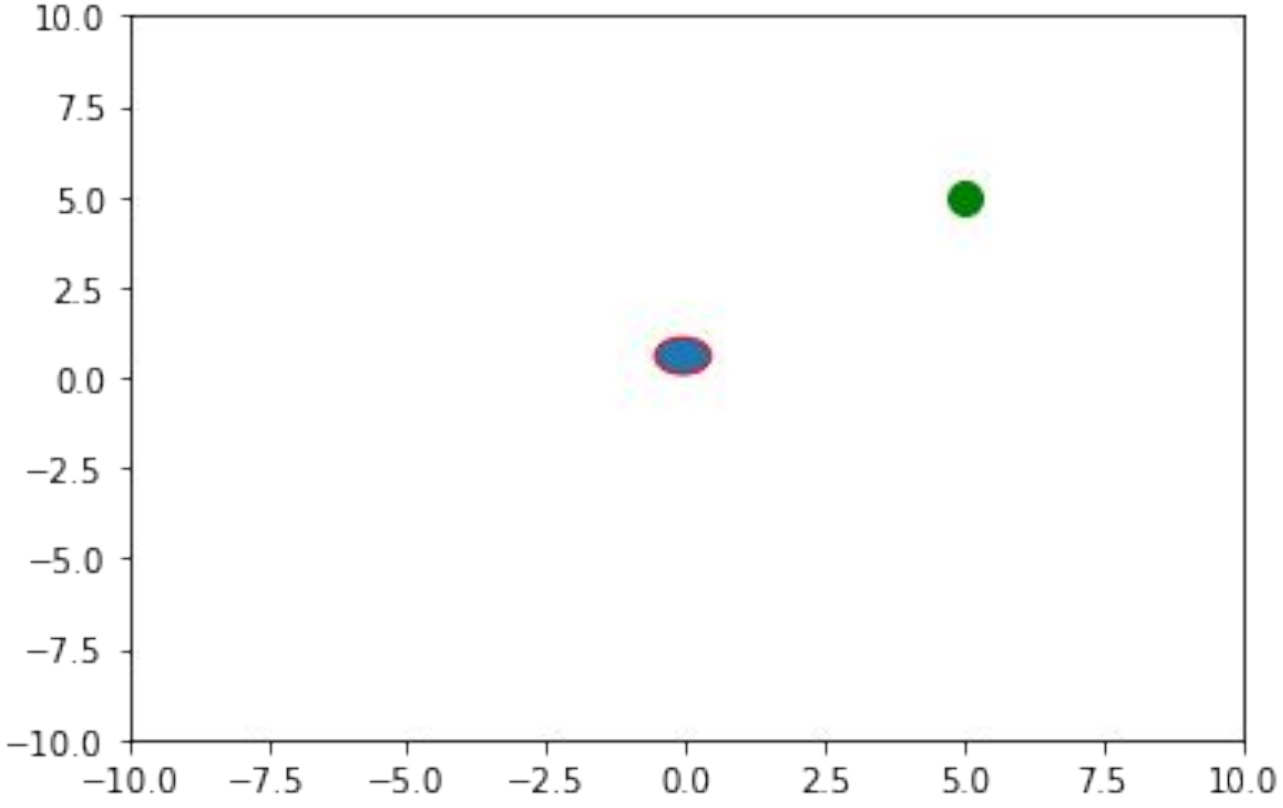
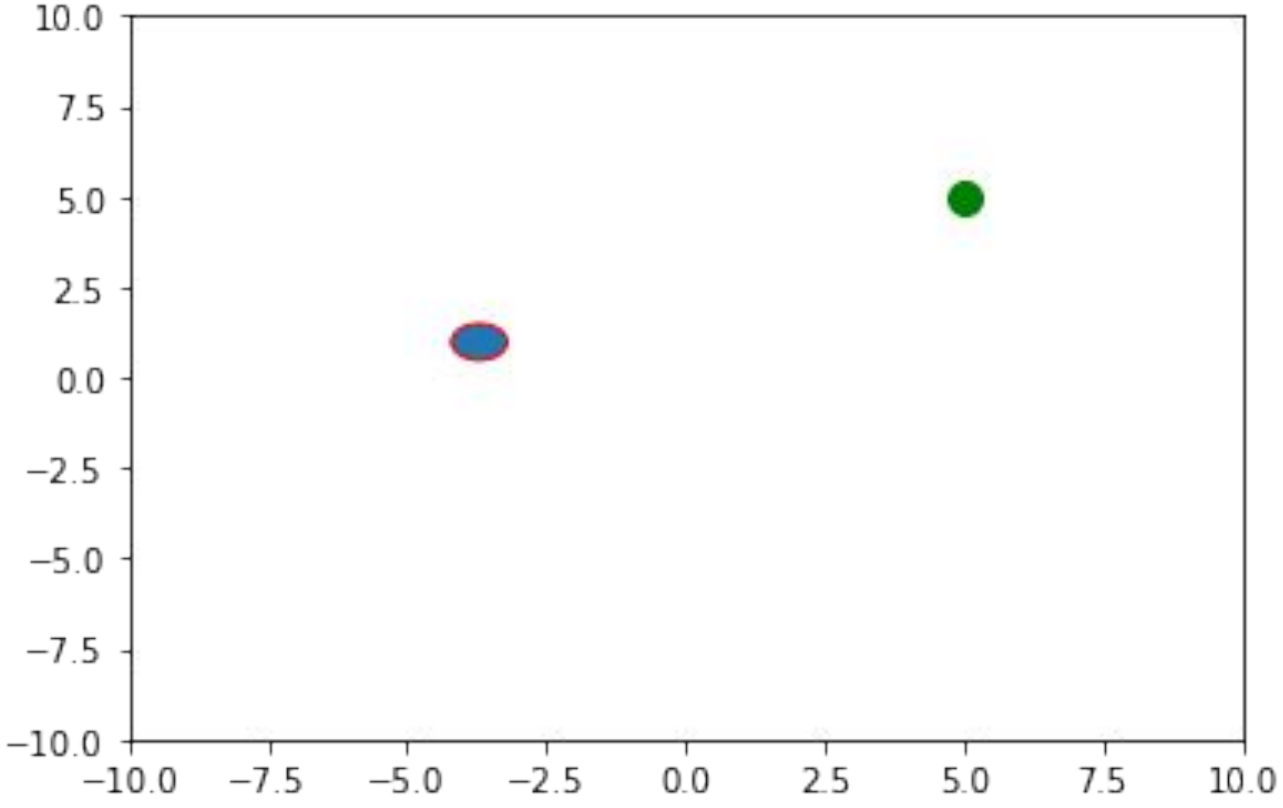


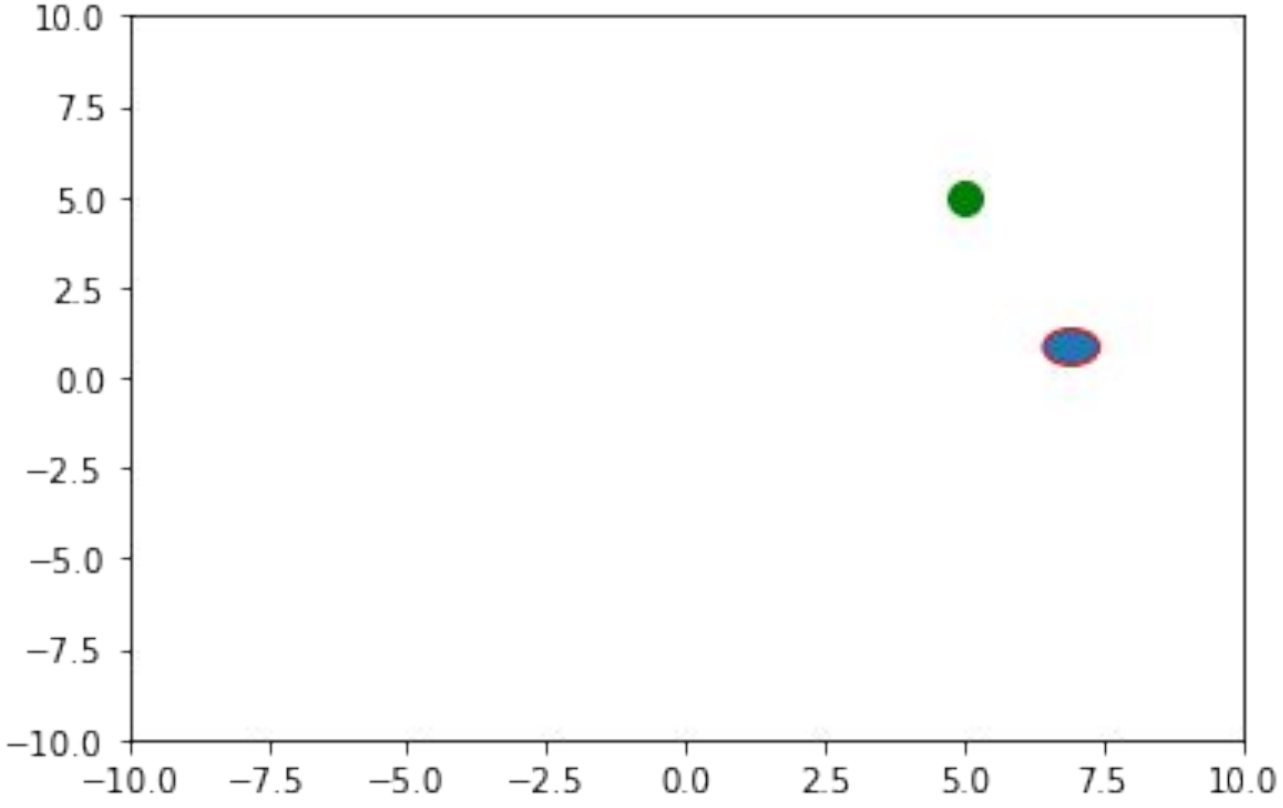
Likelihood Ratio Gradient - Toy Problem



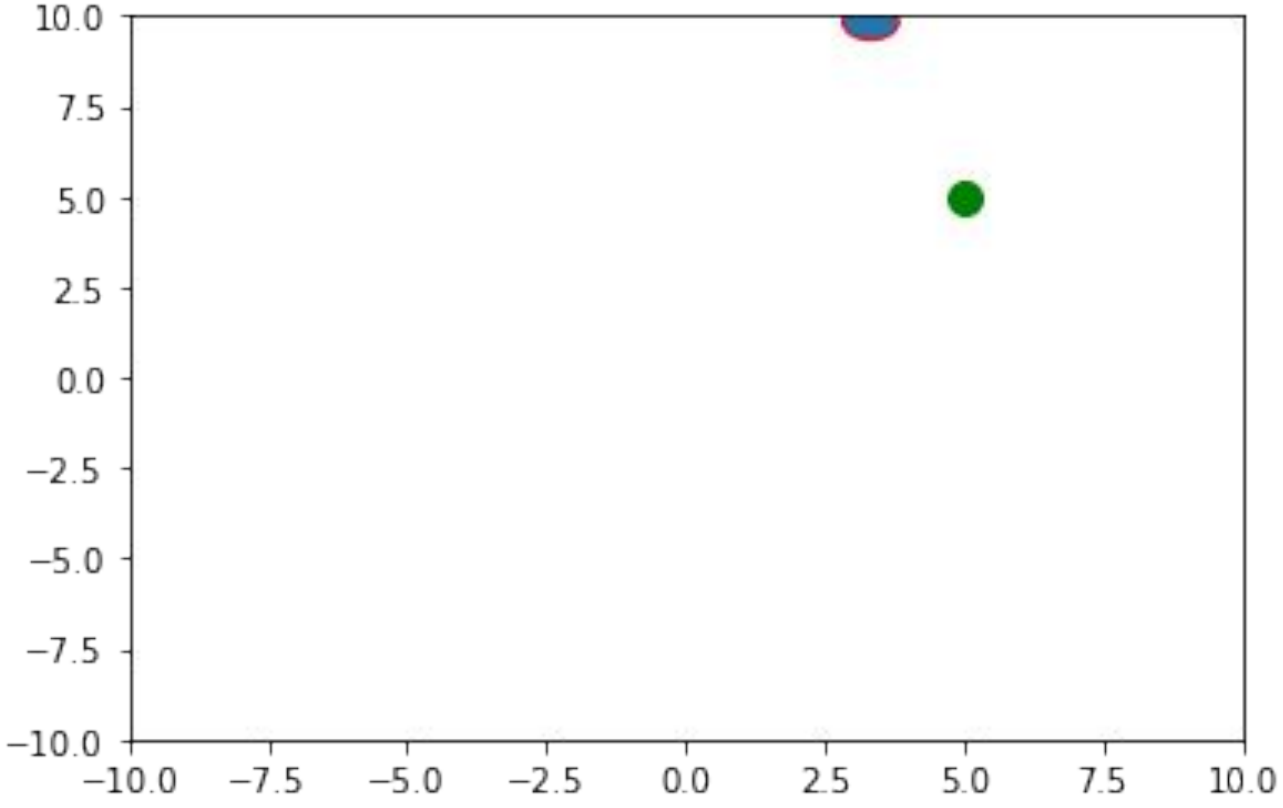
Likelihood Ratio Gradient - Toy Problem



Likelihood Ratio Gradient - Toy Problem



Likelihood Ratio Gradient - Toy Problem



Pathwise Derivative aka Reparameterization Trick

[live derivation -- for general case; for Gaussian of next slide]

Pathwise Derivative aka Reparameterization Trick

$$\mathbb{E}_{z \sim q_\phi(z)}[f(z)]$$

$$= \mathbb{E}_{\varepsilon \sim N(0,1)}[f(\mu + \varepsilon\sigma)]$$

no ϕ

$$\approx \frac{1}{K}\sum_{i=1}^{K} f(\mu + \varepsilon^{(i)}\sigma)$$

$$\nabla_{\mu,\sigma}\left(\right)$$

$q_\phi(z) = N(\mu, \sigma^2)$

$z = \mu + \varepsilon \cdot \sigma \qquad \varepsilon \sim N(0,1)$

$$\nabla_\mu f(\mu + \varepsilon^{(i)} \cdot \sigma)$$

$$\| \mu + \varepsilon^{(i)} \cdot \sigma - \left(\begin{smallmatrix} \cdot \\ \cdot \end{smallmatrix}\right) \|^2$$

Pathwise Derivative (PD)

- Stochastic gradient possible if z is continuous now (more technical condition?)
  - Common choice: \eps ~ Normal, f(\eps) = \mu + \sigma \eps
  - Any flow that you just learned!
- Also known as reparameterization trick
- Can work with only 1~2 samples

Pathwise Derivative (PD)

One other way to optimize this objective when z is continuous is to cast z as a function of a simple fixed noise such as standard gaussian.

$$z = g(\epsilon, \phi), \epsilon \sim \mathcal{N}(0, I)$$

$$\mathbb{E}_{z \sim q_\phi(\cdot|x)} [f(z)] = \mathbb{E}_{\epsilon \sim \mathcal{N}(0,I)} [f(g(\epsilon, \phi))]$$

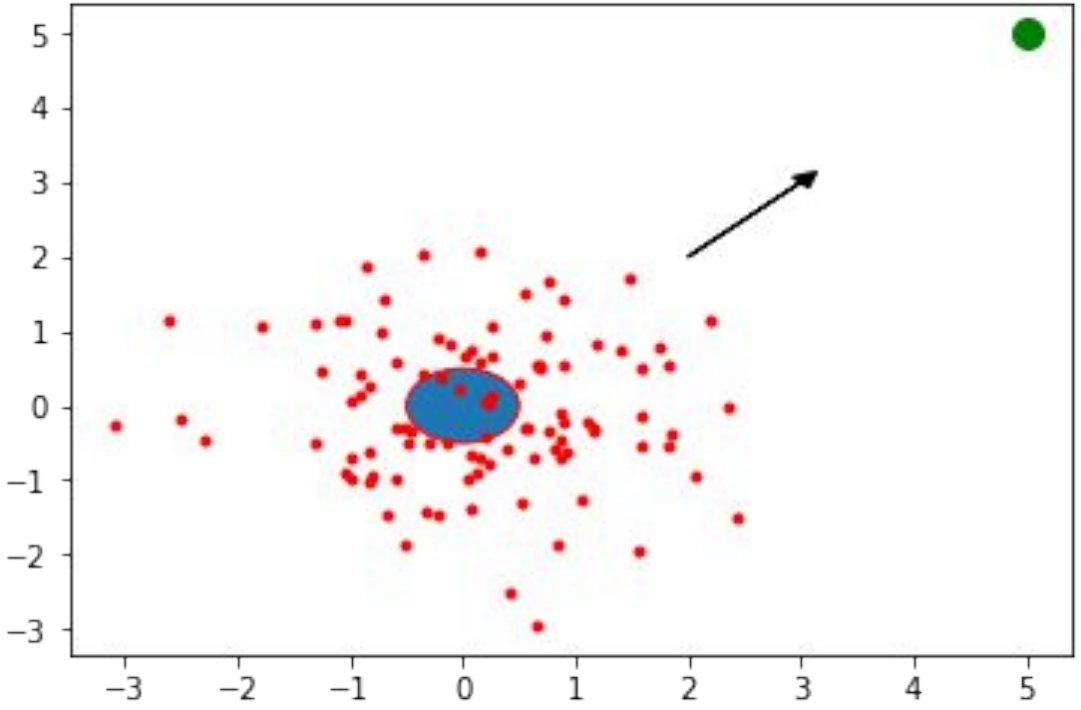
When f is differentiable,

$$\nabla_\phi \mathbb{E}_{z \sim q_\phi(\cdot|x)} [f(z)] = \mathbb{E}_{\epsilon \sim \mathcal{N}(0,I)} [\nabla_\phi f(g(\epsilon, \phi))]$$

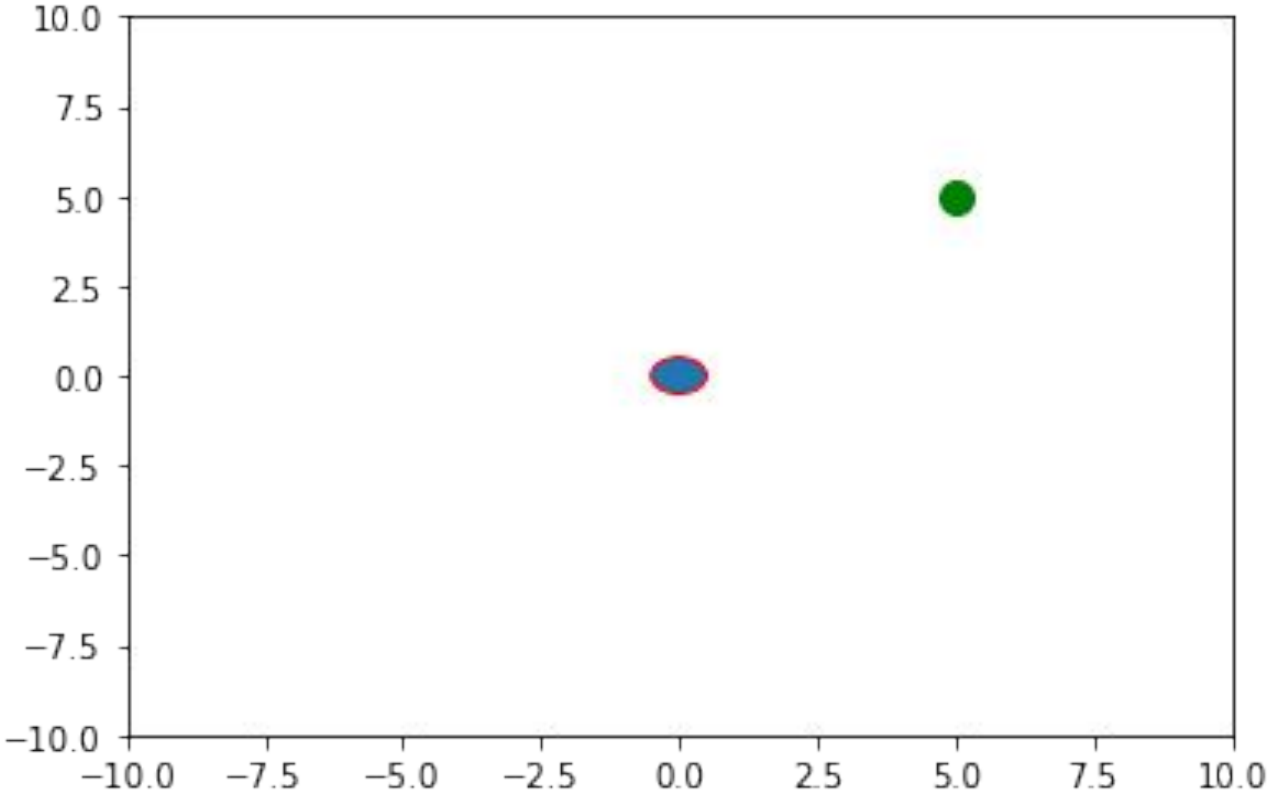
Pathwise Derivative - Toy Problem

Learn $\mu \in \mathbb{R}^2$ to minimize the objective below to reach the green point

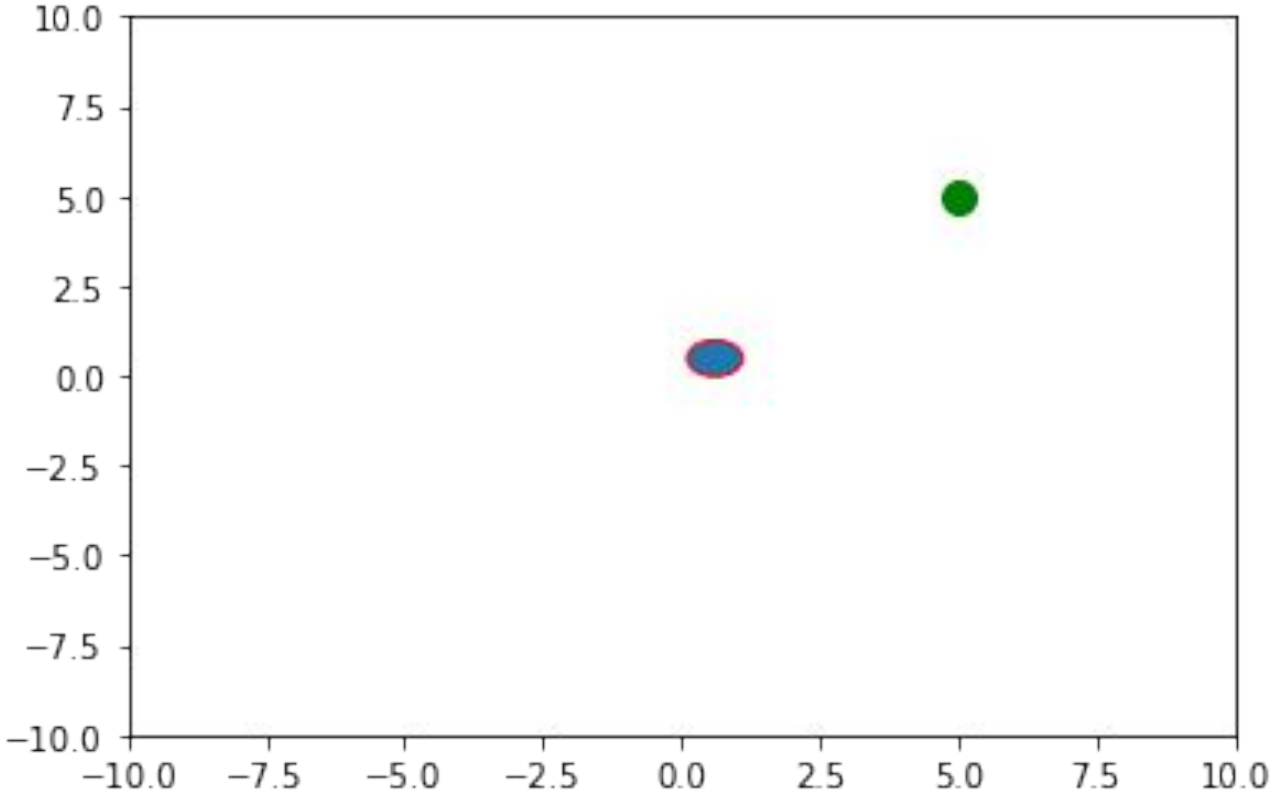
$$\mathcal{L} = \mathbb{E}_{x \sim N(\mu, I)} \left\| x - \begin{bmatrix} 5 \\ 5 \end{bmatrix} \right\|_2^2$$



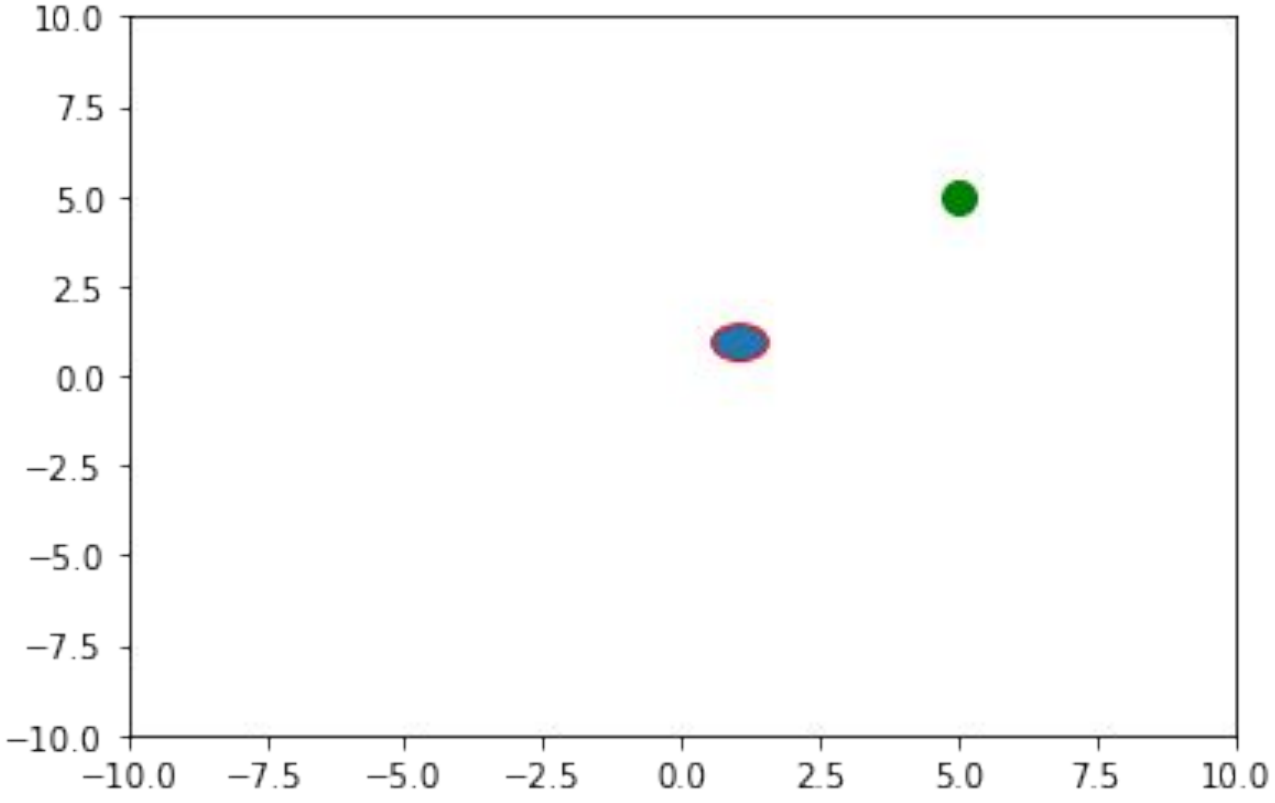
Pathwise Derivative - Toy Problem



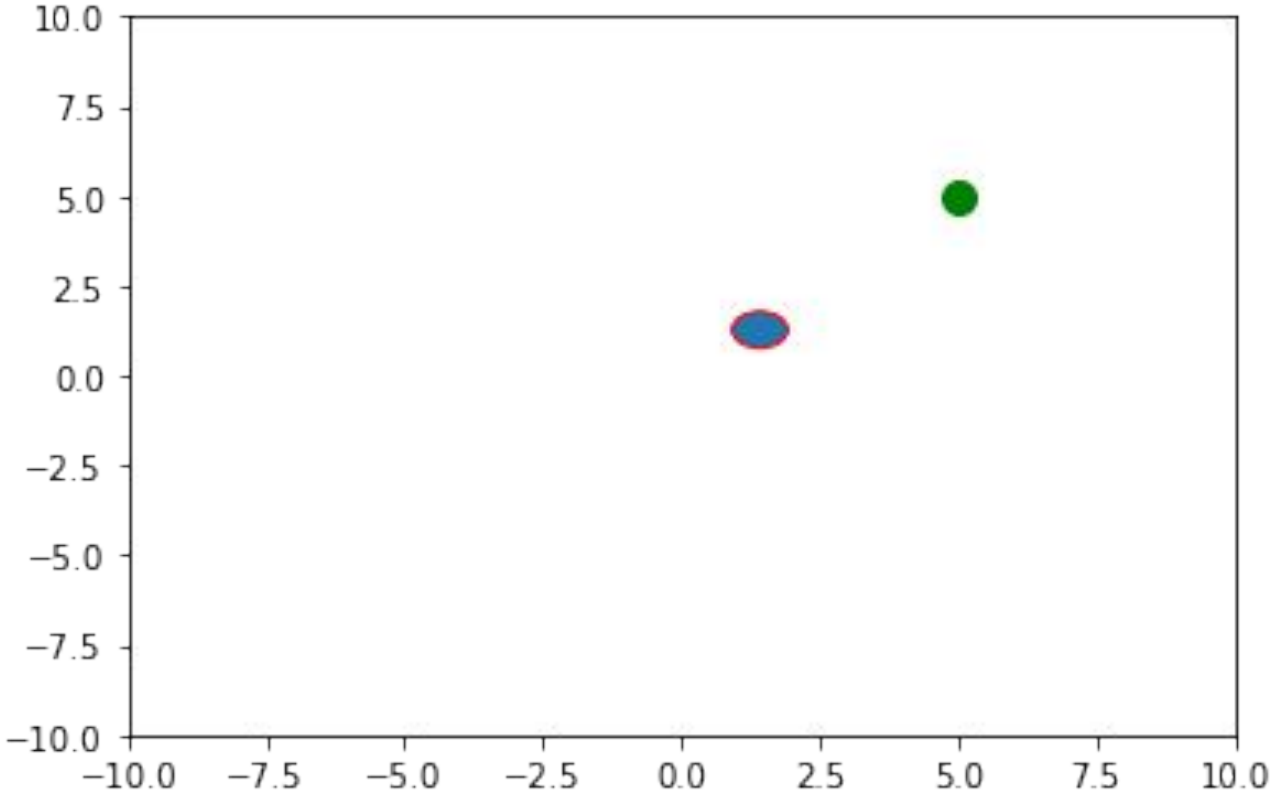
Pathwise Derivative - Toy Problem



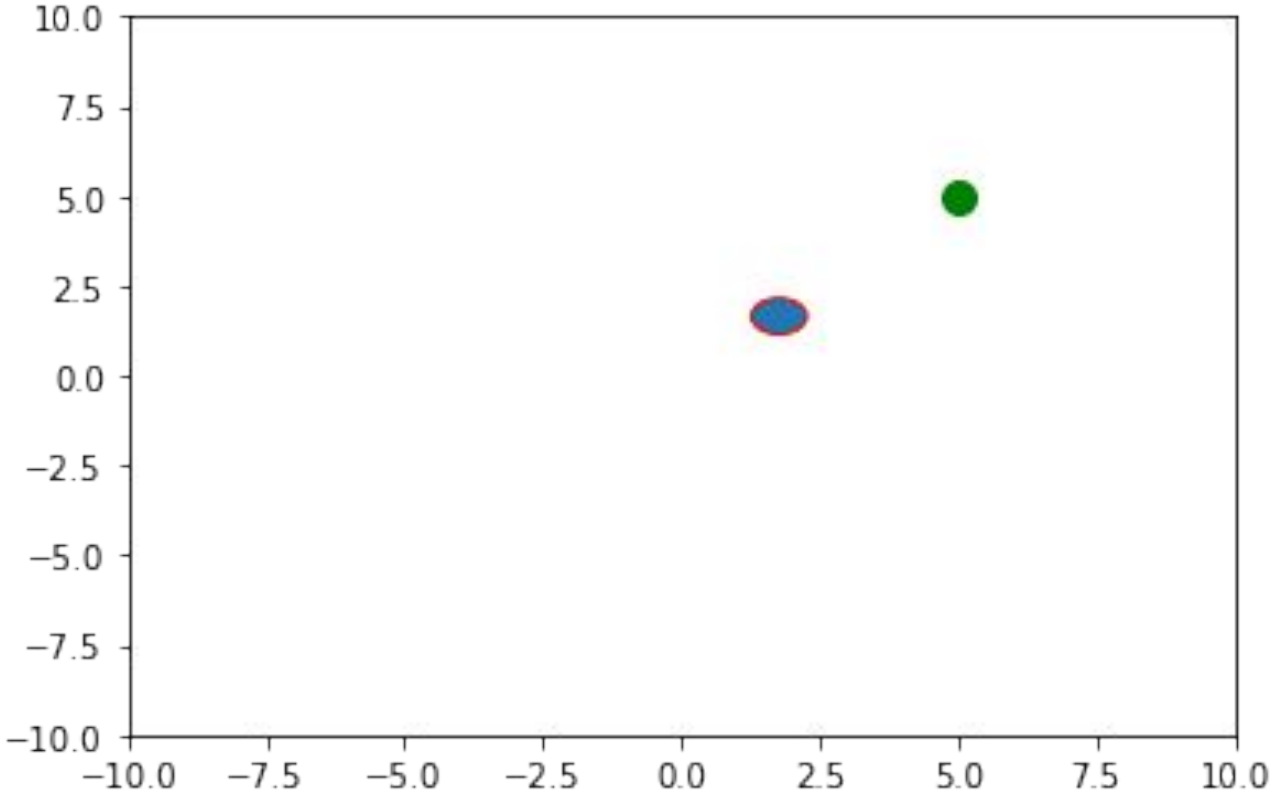
Pathwise Derivative - Toy Problem



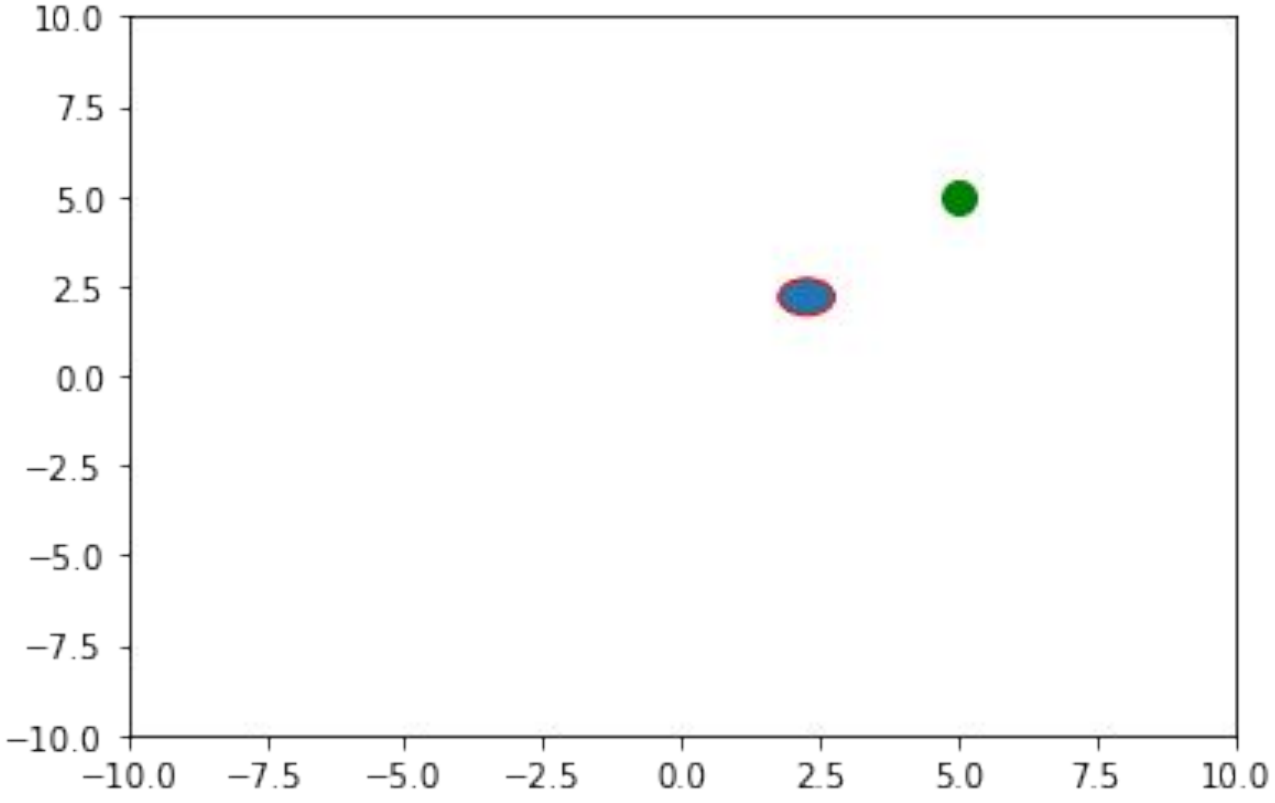
Pathwise Derivative - Toy Problem



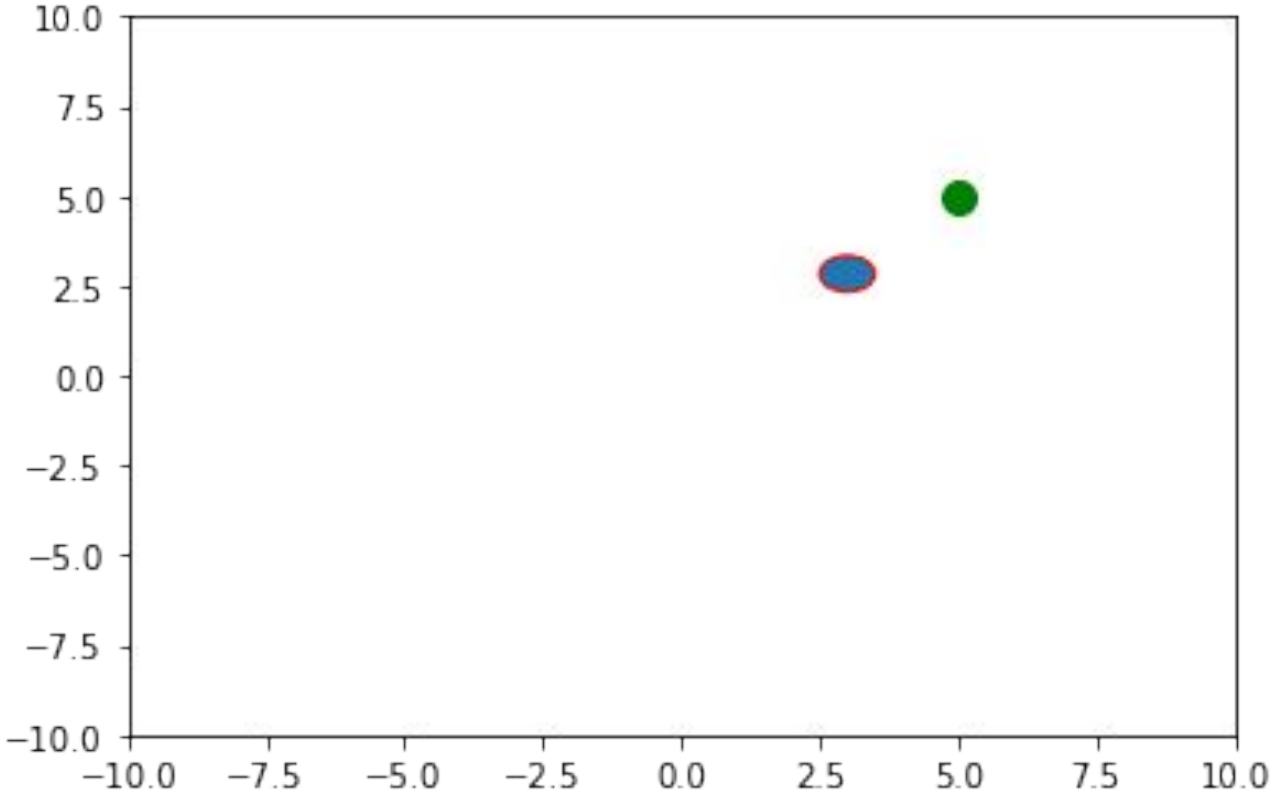
Pathwise Derivative - Toy Problem



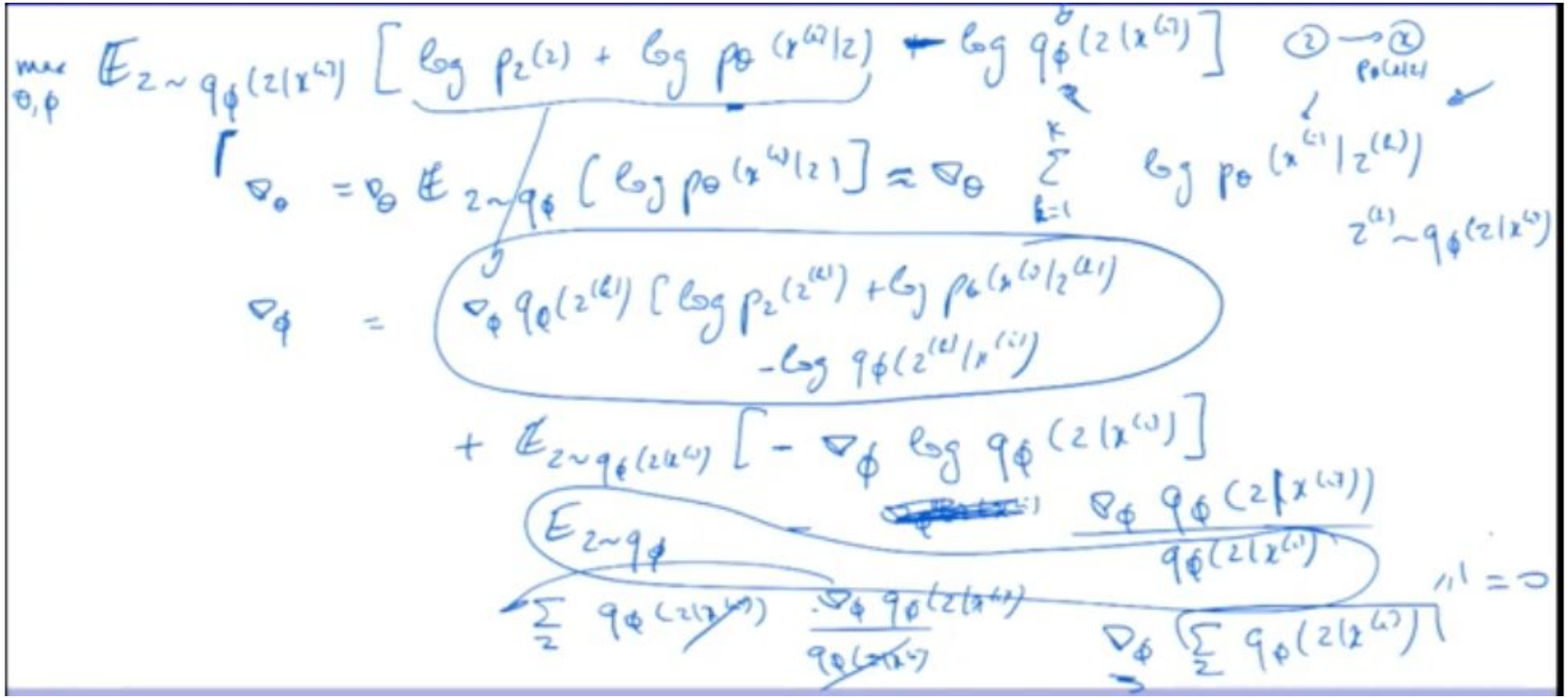
Pathwise Derivative - Toy Problem



Pathwise Derivative - Toy Problem



VAE and Likelihood Ratio Gradient



Likelihood Ratio Estimator

We are interested in $\text{argmax}_\phi \mathbb{E}_{z\sim q_\phi(\cdot|x)}\left[f(z)\right]$

How do we compute $\nabla_\phi \mathbb{E}_{z\sim q_\phi(\cdot|x)}\left[f(z)\right]$?

$$\nabla_\phi \sum_z q_\phi(z|x) f(z) = \sum_z \nabla_\phi q_\phi(z|x) f(z) = \sum_z \underbrace{\frac{\nabla_\phi q_\phi(z|x)}{q_\phi(z|x)}} f(z) q_\phi(z|x)$$

$$\Rightarrow \nabla_\phi \mathbb{E}_{z\sim q_\phi(\cdot|x)}\left[f(z)\right] = \sum_z \left(\nabla_\phi \log q_\phi(z|x) f(z)\right) q_\phi(z|x) = \mathbb{E}_{z\sim q_\phi(\cdot|x)}\left[\nabla_\phi \log q_\phi(z|x) f(z)\right]$$

$$\phi \leftarrow \phi + \alpha \nabla_\phi \mathbb{E}_{z\sim q_\phi(\cdot|x)}\left[\nabla_\phi \log q_\phi(z|x) f(z)\right]$$

Issue: High variance gradients, needs many samples of z to form a good estimate

VAE and Pathwise Derivative [skip]

[empty slide for live derivation what's on next slide]

Stochastic optimization of VLB [skip]

$$z = (z_1, z_2, \cdots, z_K) \sim p(z; \beta) = \prod_{k=1}^{K} \beta_k^{z_k} (1 - \beta_k)^{1 - z_k}$$

$$x = (x_1, x_2, \cdots, x_L) \sim p_\theta(x|z) \Leftrightarrow \text{Bernoulli}(x_i; \text{DNN}(z))$$

$$\text{VLB} = \mathbb{E}_{z \sim q(z; \phi(x))} \left[\log p(x|z) - \log q(z; \phi(x)) + \log p(z) \right]$$

In the Bernoulli setting, this becomes:

$$\mathbb{E}_{z \sim q(z; \phi(x))} \left[\log p(x|z; \theta) - \log q(z; \phi(x)) + \log p(z; \beta) \right]$$

Core problem: how to optimize the expectation from which z is drawn

Directly optimizing VLB [skip]

- Wake-Sleep not effective, especially when p_{model} is far away from p_{data}
- Can we directly optimize VLB?

Recall, we want

$$\phi, \theta \leftarrow \text{argmax}_{\theta,\phi} \left(\mathbb{E}_{z \sim q_\phi(\cdot|x)} \left[\log p_\theta(x|z) - \log q_\phi(z|x) + \log p(z) \right] \right)$$

Optimization with respect to ϕ is of the form

$$\text{argmax}_\phi \mathbb{E}_{z \sim q_\phi} \left[f(z) \right]$$

Well studied problem in reinforcement learning where no assumption on f is made.

PD applied to VLB

Variational AutoEncoder

$q_\phi(z|x)$ is modeled as a Gaussian with parameters μ and σ a DNN encoder (parameters ϕ) of x. The DNN decoder $p_\theta(x|z)$ is differentiable.

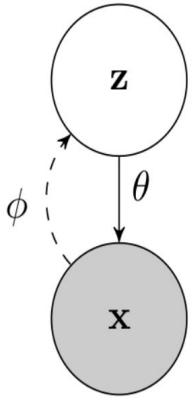
$$\text{Let } z = \Sigma^{1/2}(x;\phi)\epsilon + \mu(x;\phi)$$

$$\begin{aligned}\text{VLB} &= \mathbb{E}_{\epsilon\sim\mathcal{N}(0,I)}\left[\log p_\theta(x|z) - \log q_\phi(z|x) + \log p(z)\right] \\ &= \mathbb{E}_{\epsilon\sim\mathcal{N}(0,I)}\left[\log p_\theta(x|z)\right] - KL(q_\phi(z|x)||p(z))\end{aligned}$$

$\nabla_\theta\,[\text{VLB}]$ and $\nabla_\phi\,[\text{VLB}]$ can now be efficiently computed with SGD.

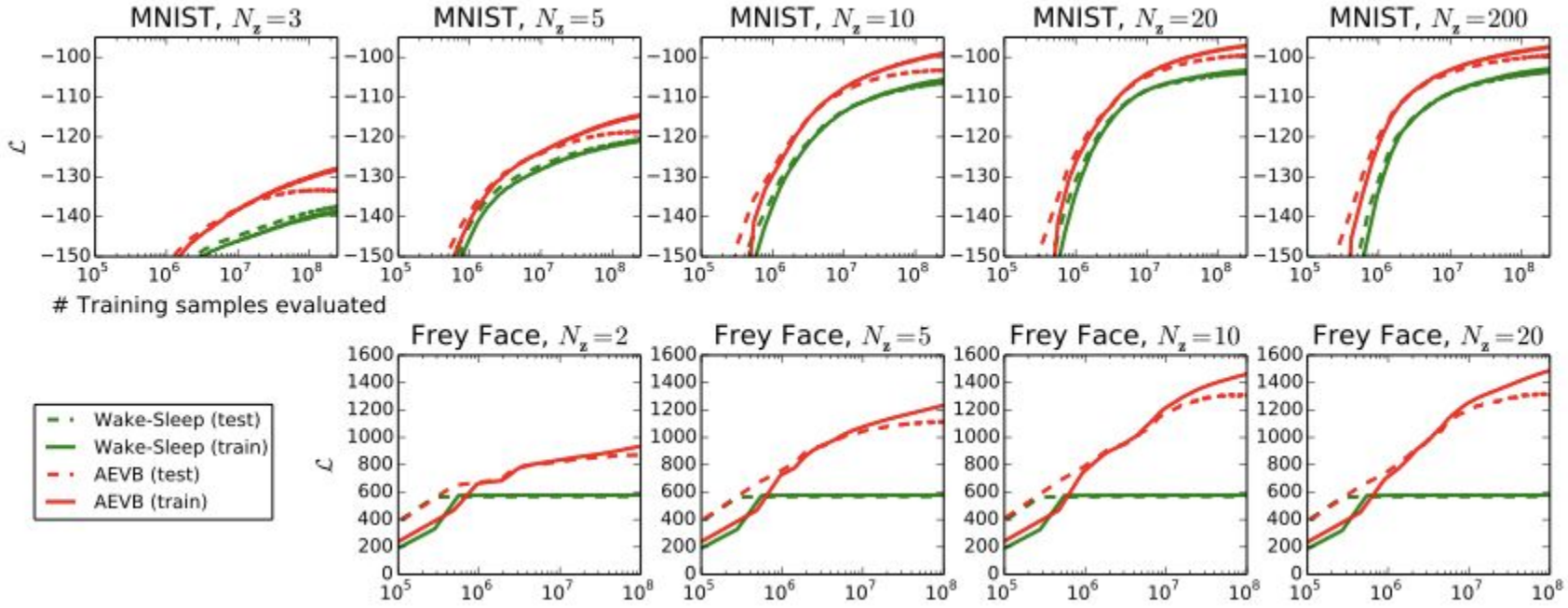
VAE

$$q_\phi(z|x) = \mathcal{N}(\mu_\phi(x), \sigma_\phi(x))$$

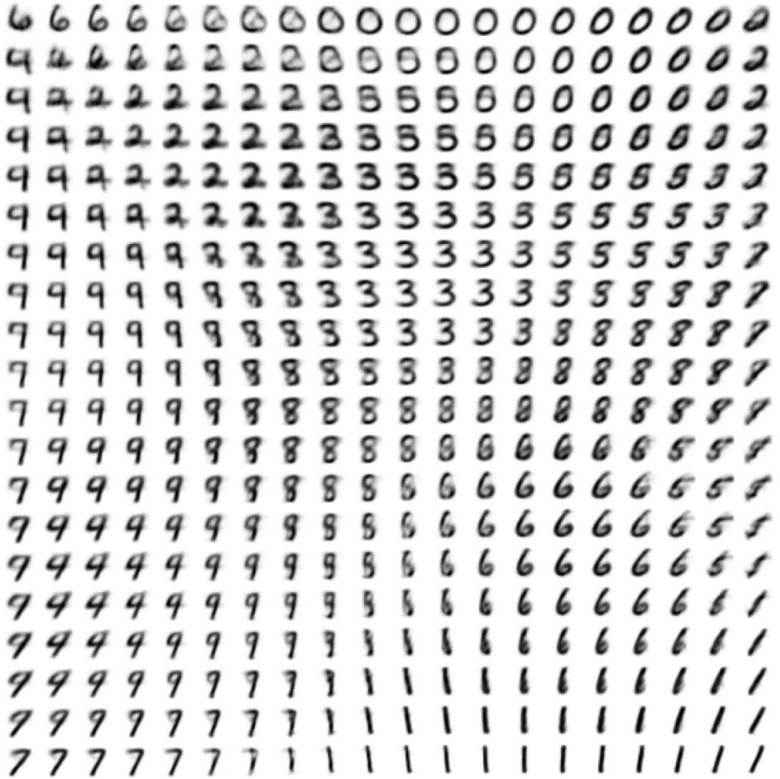


$$p_\theta(x|z) = \mathcal{N}(\mu_\theta(z), \sigma_\theta(z))$$

VAE

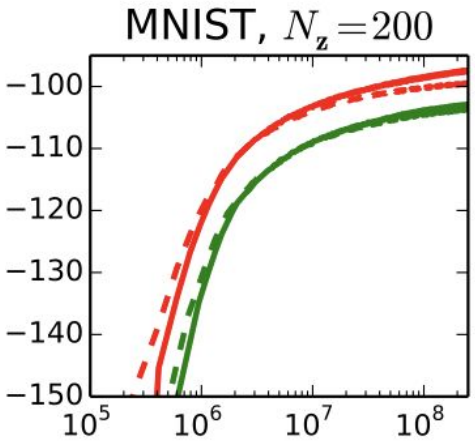

MNIST, $N_z = 3$
MNIST, $N_z = 5$
MNIST, $N_z = 10$
MNIST, $N_z = 20$
MNIST, $N_z = 200$
$\mathcal{L}$
Training samples evaluated
Frey Face, $N_z = 2$
Frey Face, $N_z = 5$
Frey Face, $N_z = 10$
Frey Face, $N_z = 20$
Wake-Sleep (test)
Wake-Sleep (train)
AEVB (test)
AEVB (train)

VAE



Compared to AR [skip]

- We now have a family of trainable latent variable models!
- But performance is lacking



Model	NLL Test
DBM 2hl [1]:	≈ 84.62
DBN 2hl [2]:	≈ 84.55
NADE [3]:	88.33
EoNADE 2hl (128 orderings) [3]:	85.10
EoNADE-5 2hl (128 orderings) [4]:	84.68
DLGM [5]:	≈ 86.60
DLGM 8 leapfrog steps [6]:	≈ 85.51
DARN 1hl [7]:	≈ 84.13
MADE 2hl (32 masks) [8]:	86.64
DRAW [9]:	≤ 80.97
PixelCNN:	81.30

Why is it called an autoencoder?

- We have seen that a variational autoencoder is a latent variable model with Gaussian prior p(z) and approximate posterior q(z|x).
  - Why is it called an “autoencoder”?

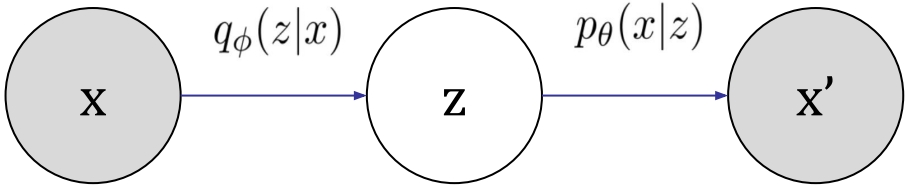
$$\log p_\theta(x) \geq \underbrace{\underbrace{\left(E_{z\sim q_x(z)} \log p_\theta(x|z)\right)}_{\text{Reconstruction loss}} - \underbrace{KL(q_\phi(z|x)||p(z))}_{\text{Regularization}}}_{L(\theta,\phi)\text{ - VAE objective}}$$

Outline

- Motivation
- Training Latent Variable Models (including VAE and IWAE)
  - Objective
    - Exact
    - Prior Sampling
    - Importance Sampling
    - Variational Lower Bound (VLB) / Evidence Lower BOund (ELBO)
  - Optimization
    - Likelihood Ratio Gradients vs. Reparameterization Trick Gradients
    - Optimizing the VLB/ELBO
- **Variations*:***
  - Different priors p(z)
  - SOTA: VQ-VAE, VQ-VAE 2.0
  - Connection to other generative models
- Related ideas:
  - Mutual Information Estimation

Parts of the VAE

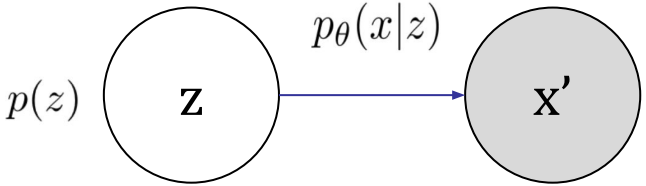
Training:



$$\underbrace{\left(E_{z\sim q_x(z)} \log p_\theta(x|z)\right)}_{\text{Reconstruction loss}}$$

$$\underbrace{KL(q_\phi(z|x)||p(z))}_{\text{Regularization}}$$

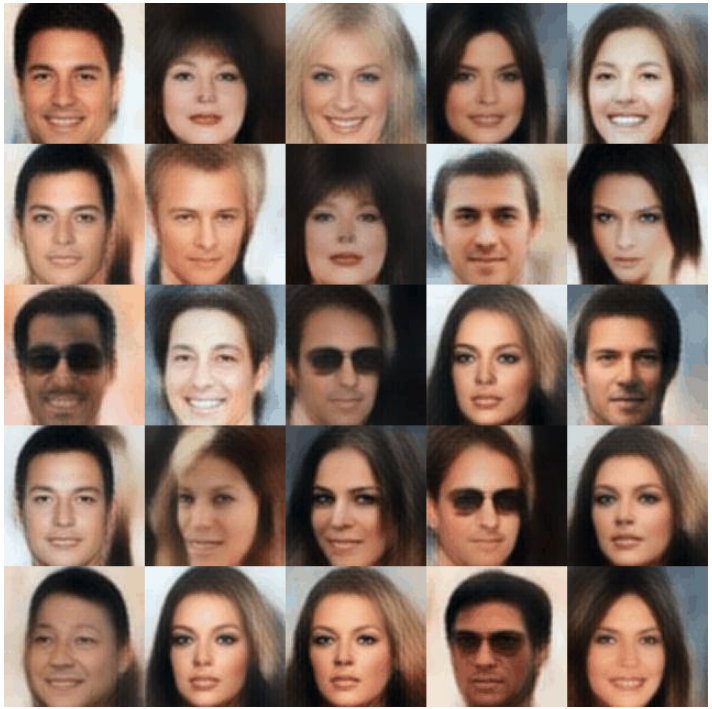
Sampling:



VAE = Generative Model

https://github.com/houxianxu/DFC-VAE

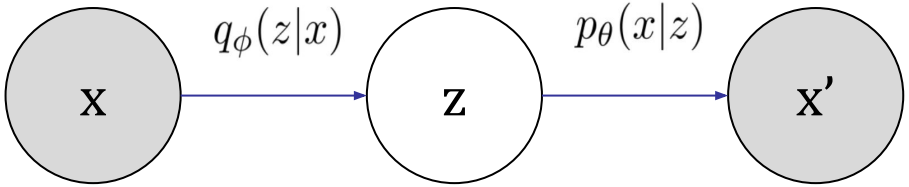
Latent Interpolation



https://github.com/houxianxu/DFC-VAE

Varieties on p(z)

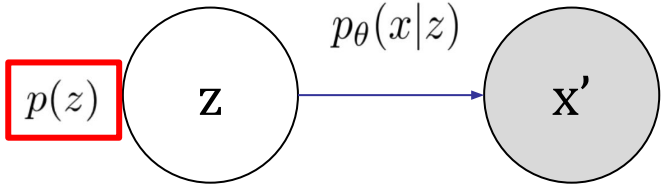
Training:



$$\underbrace{(E_{z\sim q_x(z)} \log p_\theta(x|z))}_{\text{Reconstruction loss}}$$

$$\underbrace{KL(q_\phi(z|x)||p(z))}_{\text{Regularization}}$$

Sampling:



p(z) is a prior design choice.

Varieties on p(z)

- p(z) = Unit Normal
  - Nice analytic form. Can compute KL(q(z|x) || p(z)) easily.
  - Can linearly interpolate, since approx. closed under convex combos.
  - All dimensions are independent -- a limiting assumption!

Varieties on p(z)

- p(z) = Unit Normal
  - Nice analytic form. Can compute KL(q(z|x) || p(z)) easily.
  - Can linearly interpolate, since approx. closed under convex combos.
  - All dimensions are independent -- a limiting assumption!

- p(z) = p(z_i | z_{i-1})
  - q(z_i | z_{i-1}, x)
  - i.e., sample z autoregressively. Learn both p(z) and q(z|x).
  - How to handle KL between two learned distributions?

NVAE: A Deep Hierarchical Variational Autoencoder (Vahdat and Kautz, 2020)

Residual Normal

- **Insight:** Define q(z|x) as a residual over p(z).

$$p(z_l^i|\boldsymbol{z}_{<l}) := \mathcal{N}\left(\mu_i(\boldsymbol{z}_{<l}), \sigma_i(\boldsymbol{z}_{<l})\right)$$
$$q(z_l^i|\boldsymbol{z}_{<l}, \boldsymbol{x}) := \mathcal{N}\left(\mu_i(\boldsymbol{z}_{<l}) + \Delta\mu_i(\boldsymbol{z}_{<l}, \boldsymbol{x}), \sigma_i(\boldsymbol{z}_{<l}) \cdot \Delta\sigma_i(\boldsymbol{z}_{<l}, \boldsymbol{x})\right)$$

- We get a nice analytic KL again!

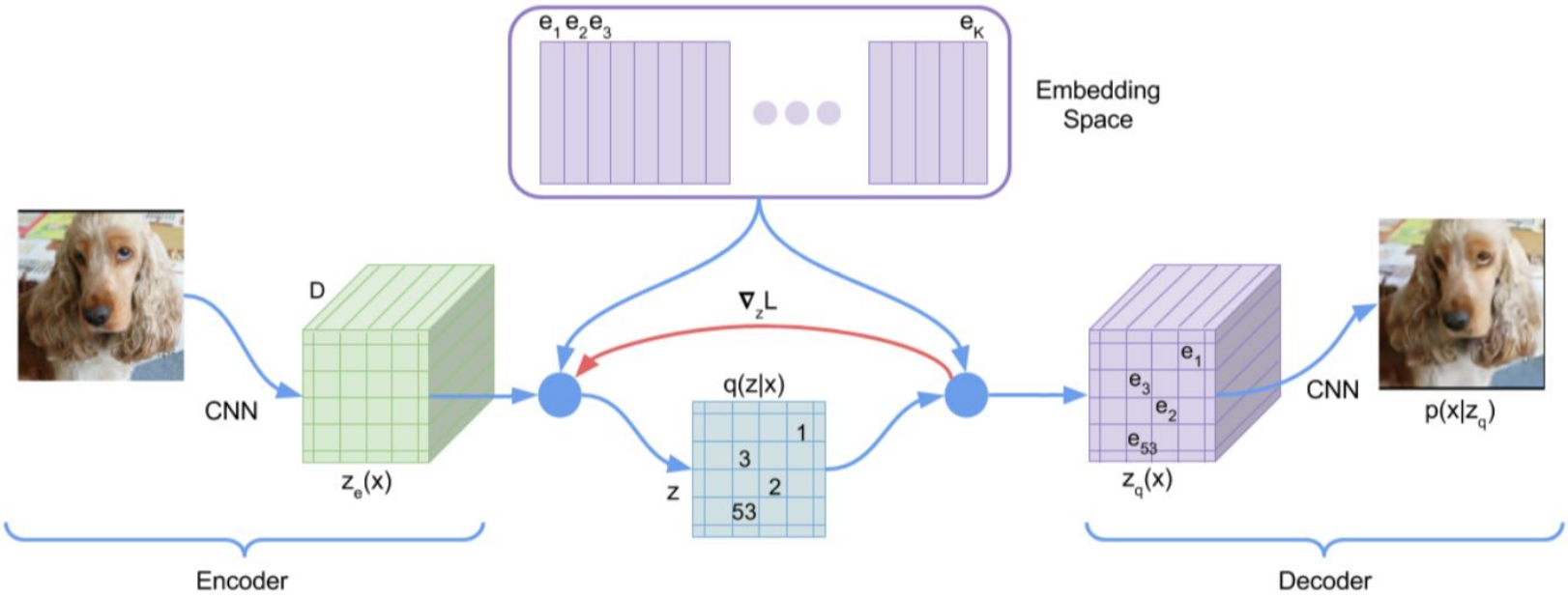
$$\mathrm{KL}\left(q(z^i|\boldsymbol{x})||p(z^i)\right) = \frac{1}{2}\left(\frac{\Delta\mu_i^2}{\sigma_i^2} + \Delta\sigma_i^2 - \log\Delta\sigma_i^2 - 1\right)$$

NVAE: A Deep Hierarchical Variational Autoencoder (Vahdat and Kautz, 2020)

Varieties on p(z)

- What if the space of z is discrete?
  - The channel capacity of z is bounded.
  - It's simple to define expressive categoricals p(z)

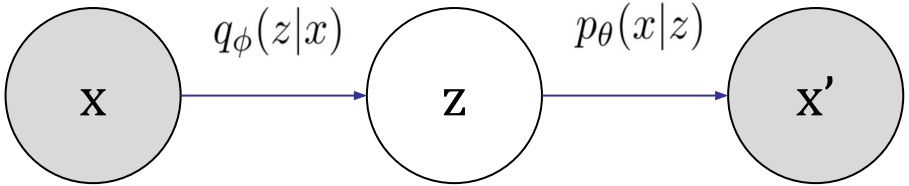
VQ-VAE



Neural Discrete Representation Learning (van den Oord et al, 2018)

Parts of the VAE

Training:



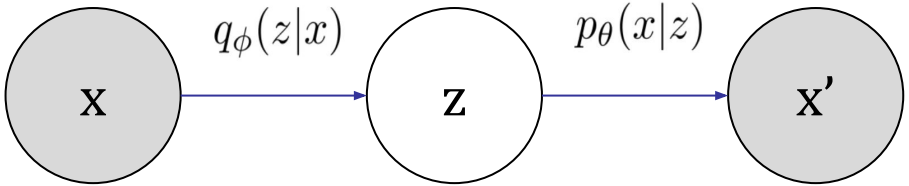
$$\underbrace{\left(E_{z\sim q_x(z)} \log p_\theta(x|z)\right)}_{\text{Reconstruction loss}}$$

$$\underbrace{KL(q_\phi(z|x)||p(z))}_{\text{Regularization}}$$

Parts of the VAE

Training:

Deterministic distribution of nearest token.



$$\underbrace{\left(E_{z\sim q_x(z)} \log p_\theta(x|z)\right)}_{\text{Reconstruction loss}}$$

$$\underbrace{KL(q_\phi(z|x)||p(z))}_{\text{Regularization}}$$

= log K

Z = Set of tokens.

How to optimize?

- Use the *straight-through* optimizer.
  - I.e., pass the gradient of p(x|z) through into z_q(x).
  - Embedding Loss: move embedding vectors closer to z_q(x).
  - Commitment Loss: enforce z_q(x) to not fluctuate.

$$L = \log p(x|z_q(x)) + \|\text{sg}[z_e(x)] - e\|_2^2 + \beta\|z_e(x) - \text{sg}[e]\|_2^2$$

Recreation Loss. Embedding Loss. Commitment Loss.

Learning p(z)

- During training, p(z) is assumed to be uniform.
- After training, we want p(z) to match q(z|x).
  - We can use our favorite generative models here.
    - In the paper: PixelCNN
    - These days, it's a transformer -- model p(z) autoregressively.
    - Can also be a diffusion model! More on this in later lectures.

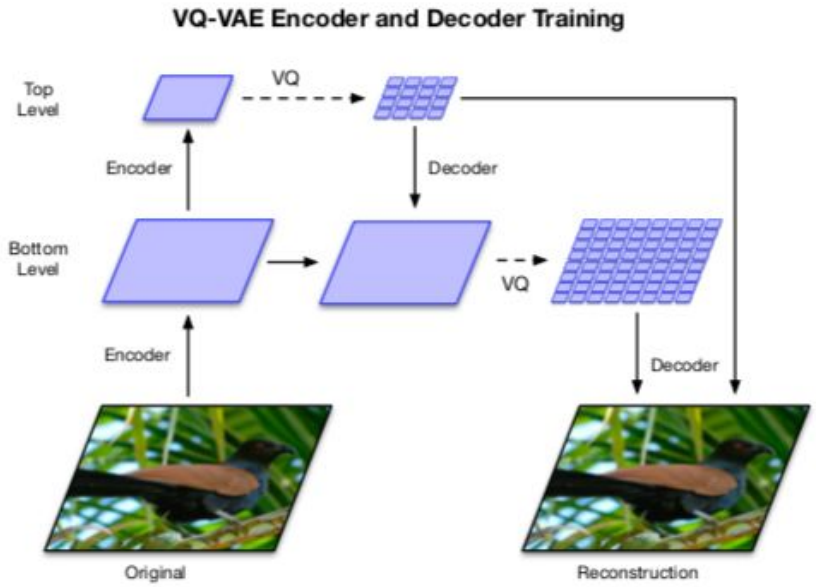
VQ-VAE -- Experiments

Figure 2: Left: ImageNet 128x128x3 images, right: reconstructions from a VQ-VAE with a 32x32x1 latent space, with K=512.

VQ-VAE -- Experiments

Figure 3: Samples (128x128) from a VQ-VAE with a PixelCNN prior trained on ImageNet images. From left to right: kit fox, gray whale, brown bear, admiral (butterfly), coral reef, alp, microwave, pickup.

VQ-VAE 2.0


VQ-VAE Encoder and Decoder Training
Top Level
VQ
Encoder
Decoder
Bottom Level
VQ
Encoder
Decoder
Original
Reconstruction

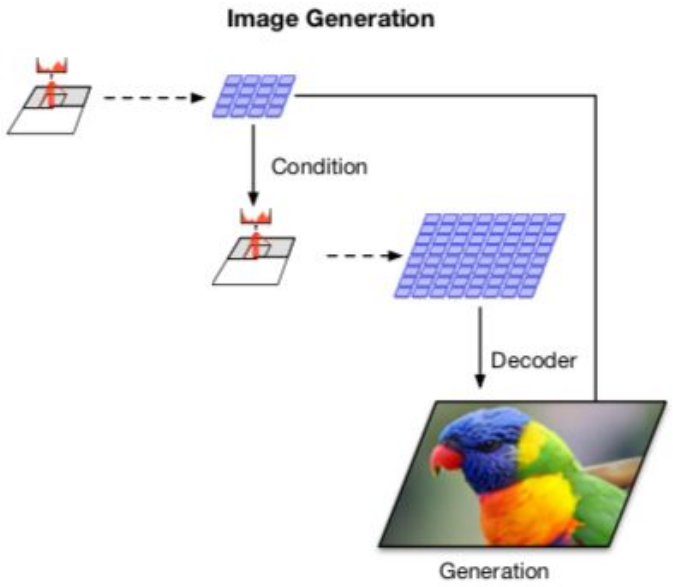


Image Generation
Condition
Decoder
Generation

VQ-VAE 2.0 -- Experiments

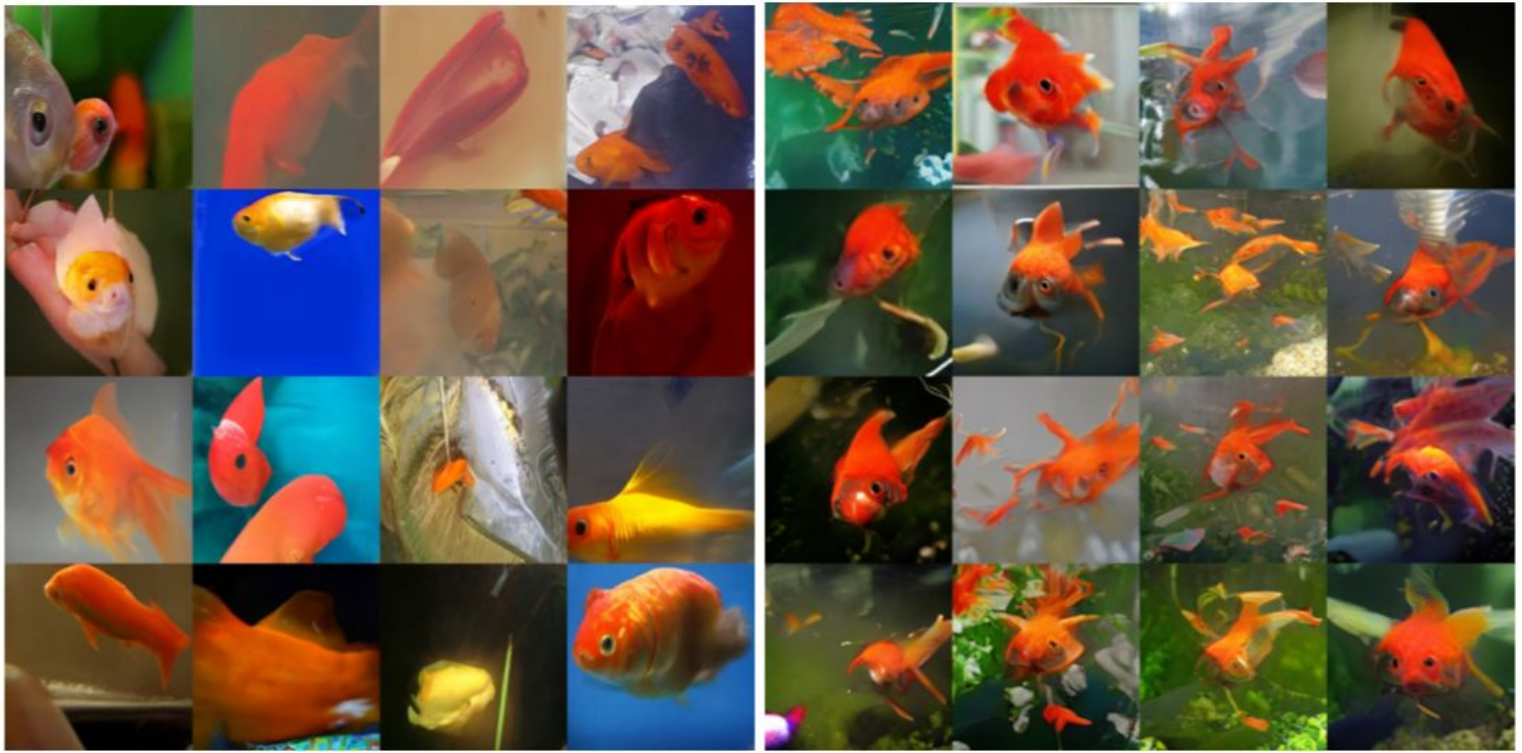
Figure 4: Class conditional random samples. Classes from the top row are: 108 sea anemone, 109 brain coral, 114 slug, 11 goldfinch, 130 flamingo, 141 redshank, 154 Pekinese, 157 papillon, 97 drake, and 28 spotted salamander.

VQ-VAE 2.0 -- Coverage

BigGAN Deep

VQ-VAE 2.0 -- Coverage

Big(



VQ-VAE 2.0

VQ-VAE 2.0 -- Coverage

BigG

VQ-VAE 2.0

VAEs as a building block.

- VAE high-level outline:
  - Learn a representation z st. p(z|x), q(x|z) exists.
  - If we can model p(z), we get p(x) = q(x|z)p(z).

- SOTA image generation methods depend on VAE backbones.
  - VQGAN -- extension of VQVAE (will be covered next lecture)
  - Stable Diffusion
  - CogView (Text-to-Image Transformer)

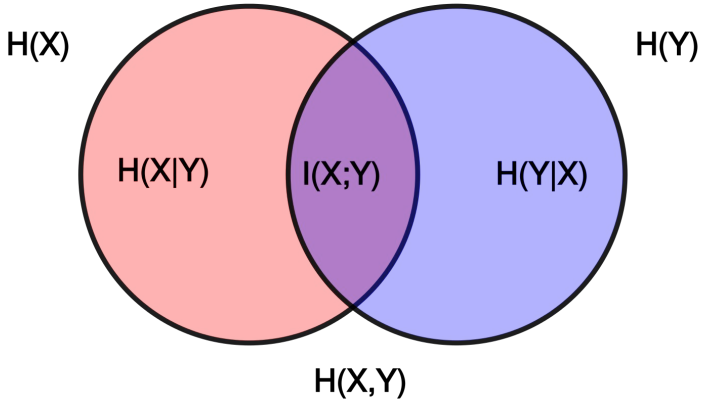
Outline

- Motivation
- Training Latent Variable Models (including VAE and IWAE)
  - Objective
    - Exact
    - Prior Sampling
    - Importance Sampling
    - Variational Lower Bound (VLB) / Evidence Lower BOund (ELBO)
  - Optimization
    - Likelihood Ratio Gradients vs. Reparameterization Trick Gradients
    - Optimizing the VLB/ELBO
- Variations*:*
  - Different priors p(z)
  - SOTA: VQ-VAE, VQ-VAE 2.0
  - Connection to other generative models
- Related ideas:
  - **Mutual Information Estimation**

Mutual Information

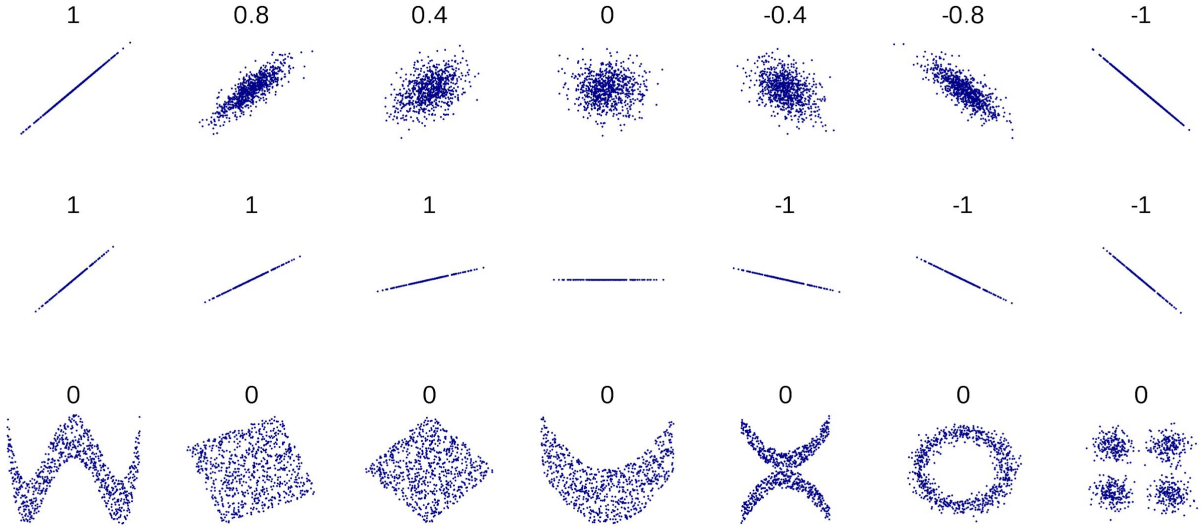
- Mutual information between two random variables X, Y: I(X; Y) is defined as

$$I(X;Y) = H(X) - H(X|Y) = H(Y) - H(Y|X)$$



Mutual Information

- Mutual Information is a general way to measure dependency between two random variables
  - Unlike the more commonly used covariance



Mutual Information

- Useful in a lot of settings where one wants to maximize dependency between two variables or estimate their dependencies:
  - Variational Information Maximisation for Intrinsically Motivated Reinforcement Learning
  - InfoGAN
  - CPC
  - ...

Estimating Mutual Information

- We can try to estimate the mutual information between z and x in a latent variable model

$$
\begin{aligned}
I(z;x) &= H(z) - H(z|x) \\
&= H(z) - \mathbb{E}_{(z,x)\sim p(z,x)}[-\log p(z|x)] \\
&= H(z) + \mathbb{E}_{(z,x)\sim p(z,x)}[\log p(z|x) - \log q(z|x) + \log q(z|x)] \\
&\geq H(z) + \mathbb{E}_{(z,x)\sim p(z,x)}[\log q(z|x)]
\end{aligned}
$$

- Has intractable posterior p(z|x) but we can estimate by introducing a variational distribution q(z|x)

Decoder distribution

- So far all models use simple distribution for $p(x|z)$

- Due to lack of expressivity itself, all entropy is pushed to z and z needs to convey a lot of information

Powerful decoder

- What's the maximum VLB?

$$\begin{aligned}\mathbb{E}_{x\sim p_{\text{data}}(x)}\left[VLB\right] \leq & \mathbb{E}_{x\sim p_{\text{data}}(x)}\left[\log p_\theta(x)\right] \\ \leq & \mathbb{E}_{x\sim p_{\text{data}}(x)}\left[\log p_{\text{data}}(x)\right]\end{aligned}$$

- What if $p(x|z) = p_{\text{data}}(x)$?

$$\begin{aligned}\mathbb{E}_{x\sim p_{\text{data}}(x)}\left[VLB\right] =& \mathbb{E}_{x\sim p_{\text{data}}(x), z\sim q(z|x)}\left[\log p(x|z) + \log p(z) - \log q(z|x)\right] \\ =& \mathbb{E}_{x\sim p_{\text{data}}(x)}\left[\log p_{\text{data}}(x) + \mathbb{E}_{x\sim p_{\text{data}}(x)}\left[\log p(z) - \log q(z|x)\right]\right]\end{aligned}$$

  - q(z|x) would be set to p(z) -> z has no information

Powerful decoder

- Having information in z incurs vlb penalty of KL(q ‖ p) which is usually non-zero
- “Ignoring latent code” problems well documented in literature
  - (Fabius & van Amersfoort,2014; Chung et al., 2015; Bowman et al., 2015; Serban et al., 2016; Fraccaro et al., 2016; Xu &Sun, 2016)
  - Many proposed solutions

Weakening models

- Adding dropout in autoregressive conditioning (Bowman et al., 2015)
- PixelCNN with limited receptive field (Chen et al., 2016)
- Constant bit rate $D_{KL}(q_\varphi(z|x) \Vert p_\theta(z)) = c$ (Guu et al., 2017), (Xu & Durrett, 2018), (Davidson et al., 2018)
- Minimum bit rate $D_{KL}(q_\varphi(z|x) \Vert p_\theta(z)) \geq \delta$ (Razavi et al., 2019)

Changing training dynamics

- $D_{KL}(q_\varphi(z|x) \Vert p_\theta(z))$ warmup (Bowman et al., 2015); (Yang et al., 2017); (Kim et al., 2018); (Gulrajani et al., 2016)
- “Free-bits” (Kingma et al., 2016); (Chen et al., 2016)
- More training updates to q(z|x) (He et al., 2019)

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- ***Variations:***
  - SOTA: VQ-VAE, VQ-VAE 2.0
  - AR + VAE: Variational Lossy AutoEncoder, PixelVAE
  - ***Disentanglement: Beta VAE***
- Related ideas:
  - Variational Dequantization (flow++)
  - Mutual Information Estimation

Beta VAE

The Beta-VAE objective is identical to the VAE objective when beta = 1

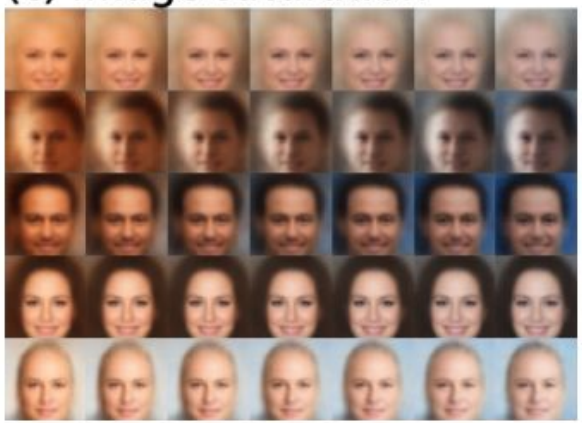
$$\mathcal{L} = \mathbb{E}_{q_\phi(z|x)}[\log p_\theta(x|z)] - \beta D_{KL}(q_\phi(z|x)||p(z))$$

Beta VAE -- Experiments

(a) Skin colour

(b) Age/gender

(c) Image saturation



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Recap: Uniform Dequantization

- **Uniform Dequantization**. Add noise to data.
  - $\mathbf{x} \in \{0, 1, 2, \ldots, 255\}$
  - We draw noise u uniformly from $[0, 1)^D$

$$\begin{aligned}
\mathbb{E}_{\mathbf{y} \sim p_{\text{data}}} \left[\log p_{\text{model}}(\mathbf{y}) \right] &= \sum_{\mathbf{x}} P_{\text{data}}(\mathbf{x}) \int_{[0,1)^D} \log p_{\text{model}}(\mathbf{x} + \mathbf{u}) \, d\mathbf{u} \\
&\leq \sum_{\mathbf{x}} P_{\text{data}}(\mathbf{x}) \log \int_{[0,1)^D} p_{\text{model}}(\mathbf{x} + \mathbf{u}) \, d\mathbf{u} \\
&= \mathbb{E}_{\mathbf{x} \sim P_{\text{data}}} \left[\log P_{\text{model}}(\mathbf{x}) \right]
\end{aligned}$$

[Theis, Oord, Bethge, 2016]

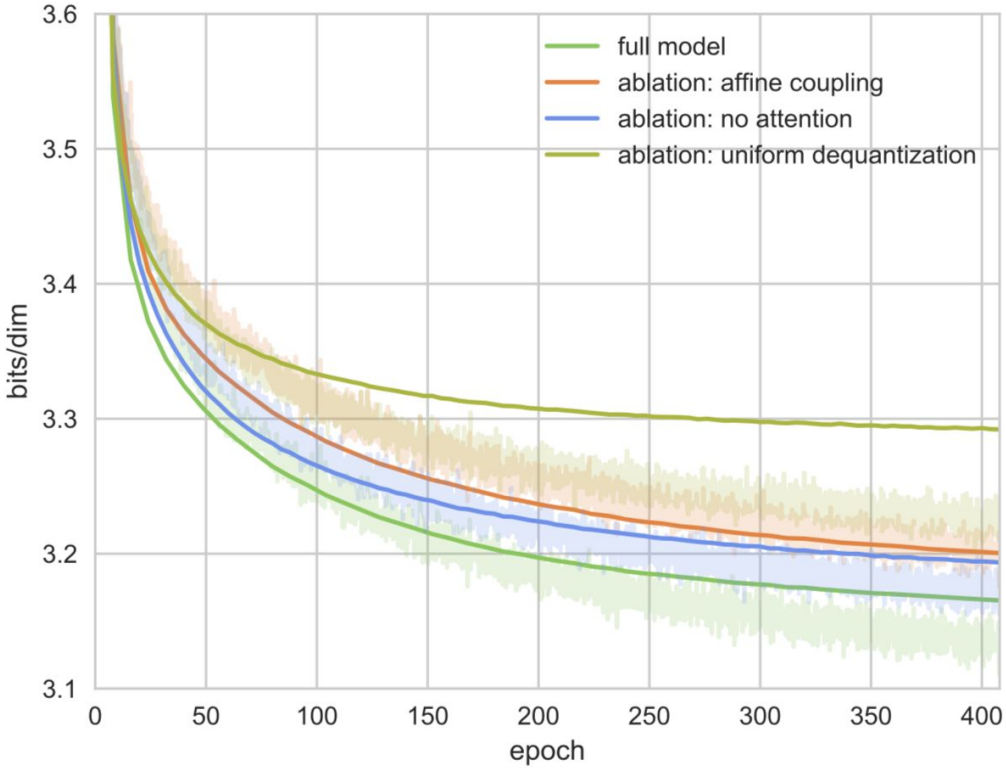
Variational Dequantization

- **Variational Dequantization**. Add a learnable noise q to data.

$$\begin{aligned}
\mathbb{E}_{\mathbf{x}\sim P_{\text{data}}}\left[\log P_{\text{model}}(\mathbf{x})\right] &= \mathbb{E}_{\mathbf{x}\sim P_{\text{data}}}\left[\log \int_{[0,1)^D} q(\mathbf{u}|\mathbf{x}) \frac{p_{\text{model}}(\mathbf{x}+\mathbf{u})}{q(\mathbf{u}|\mathbf{x})}\, d\mathbf{u}\right] \\
&\geq \mathbb{E}_{\mathbf{x}\sim P_{\text{data}}}\left[\int_{[0,1)^D} q(\mathbf{u}|\mathbf{x}) \log \frac{p_{\text{model}}(\mathbf{x}+\mathbf{u})}{q(\mathbf{u}|\mathbf{x})}\, d\mathbf{u}\right] \\
&= \mathbb{E}_{\mathbf{x}\sim P_{\text{data}}}\mathbb{E}_{\mathbf{u}\sim q(\cdot|\mathbf{x})}\left[\log \frac{p_{\text{model}}(\mathbf{x}+\mathbf{u})}{q(\mathbf{u}|\mathbf{x})}\right]
\end{aligned}$$

[Ho et al., 2019]

Variational Dequantization on CIFAR



[Ho et al., 2019]

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Extra Slides

Wake-Sleep algorithm

- Note: VLB was derived from min KL[$q_x(z)||p(z|x)$], hard to optimize because z drawn from $q_x(z)$
- What if we instead minimize KL[$p(z|x)||q_x(z)$] for any given x
  - still hard because we don't know p(z|x)
- Trick: we know z if we generate them! $\mathbf{z} \sim p_\beta(\mathbf{z}), \mathbf{x} \sim p_\theta(\mathbf{x}|\mathbf{z})$
  - caveat x ~ p_{model} instead of x ~ p_{data}
- Problem?
  - VLB is maximized with x drawn from p_{data}
  - minimizing kl(p || q) with x drawn from p_{model} doesn't guarantee the bound is tight

Wake-Sleep algorithm

Wake Phase

- Sample $x \sim p_{\text{data}}$, $z \sim q(z; \phi(x))$.
- Maximize VLB with respect to θ, β.

Sleep Phase (model *dreaming* samples)

- Sample $z \sim p(z; \beta)$, $x \sim p(x|z; \theta)$.
- Minimize $KL(p(z|x)||q(z; \phi(x)))$ with respect to ϕ now that we have samples from p_{model}.

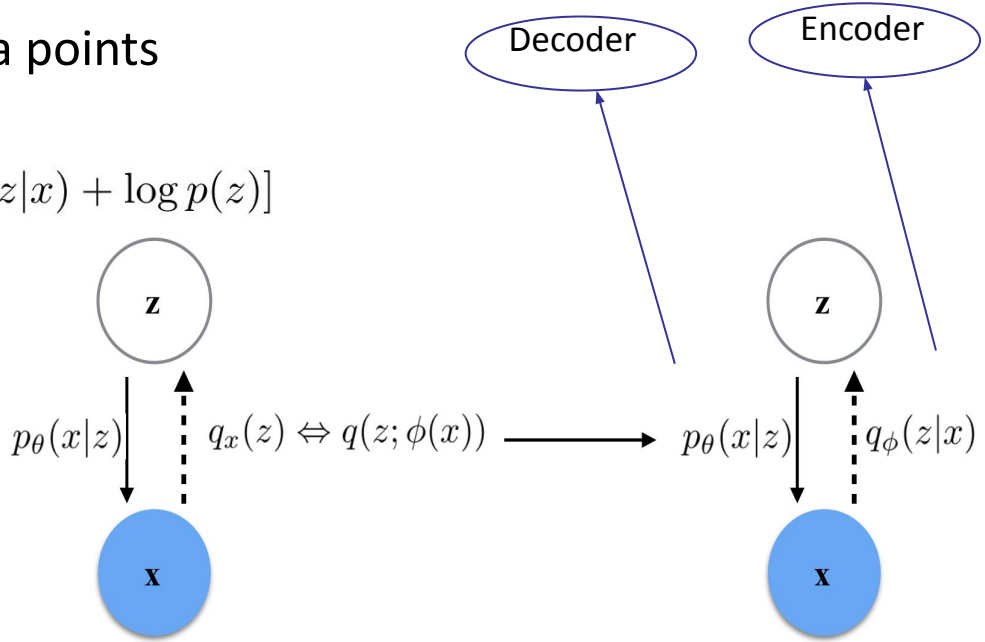
Reverse KL

$$KL(p(z|x)||q(z;\phi(x)) = E_{z\sim p(z|x)}\left[\underbrace{\log p(z|x)}_{\text{indepndent of } \phi} - \log q(z;\phi(x))\right]$$

Amortized Inference

- $q(z; \phi(x))$
  - Not scalable to large dataset
  - Expensive to evaluate new data points
- Amortized Inference

$$VLB = \mathbb{E}_{z \sim q_\phi(\cdot|x)} \left[\log p_\theta(x|z) - \log q_\phi(z|x) + \log p(z) \right]$$



Helmholtz Machine

- Helmholtz Machine [Dayan, P., Hinton, G. E.,... 1995]
  - Bernoulli latent code + observation space
  - Learned with Wake-sleep algorithm
- Did not scale to solve more complex problems due to limitations of wake-sleep