Variational Autoencoder

Assigment3 for Advanced Machine Learning

Weiwen Chen

2020.5.28

Outline

- Autoencoder
- Variational Autoencoder(VAE)
- β-VAE, CC-VAE

Autoencoders

oh

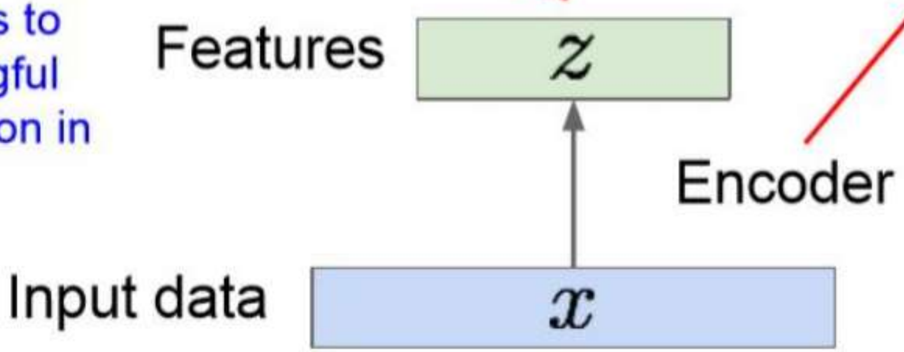
Some background first: Autoencoders

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

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

Q: Why dimensionality reduction?

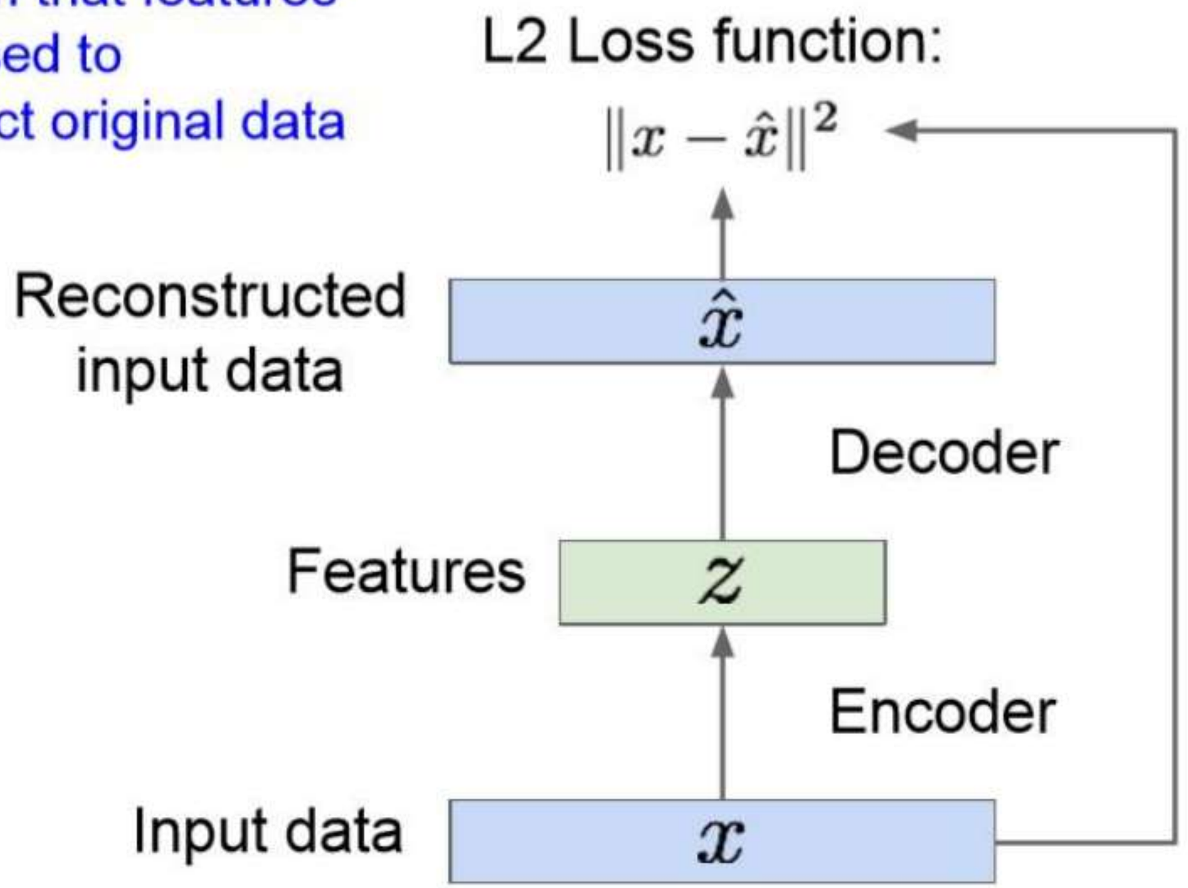
A: Want features to capture meaningful factors of variation in data

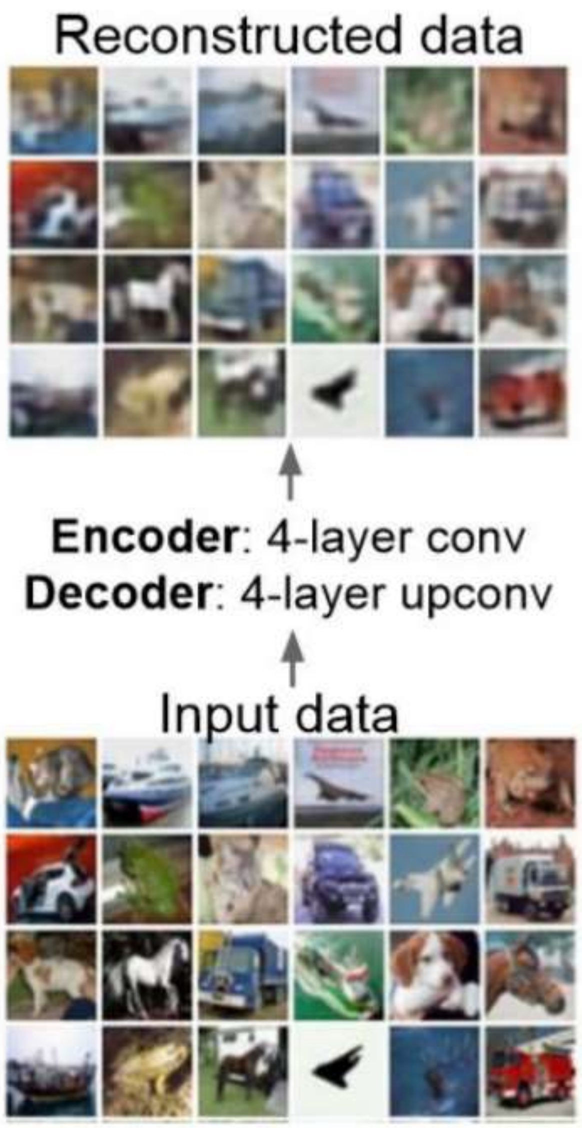


Originally: Linear + nonlinearity (sigmoid)
Later: Deep, fully-connected
Later: ReLU CNN

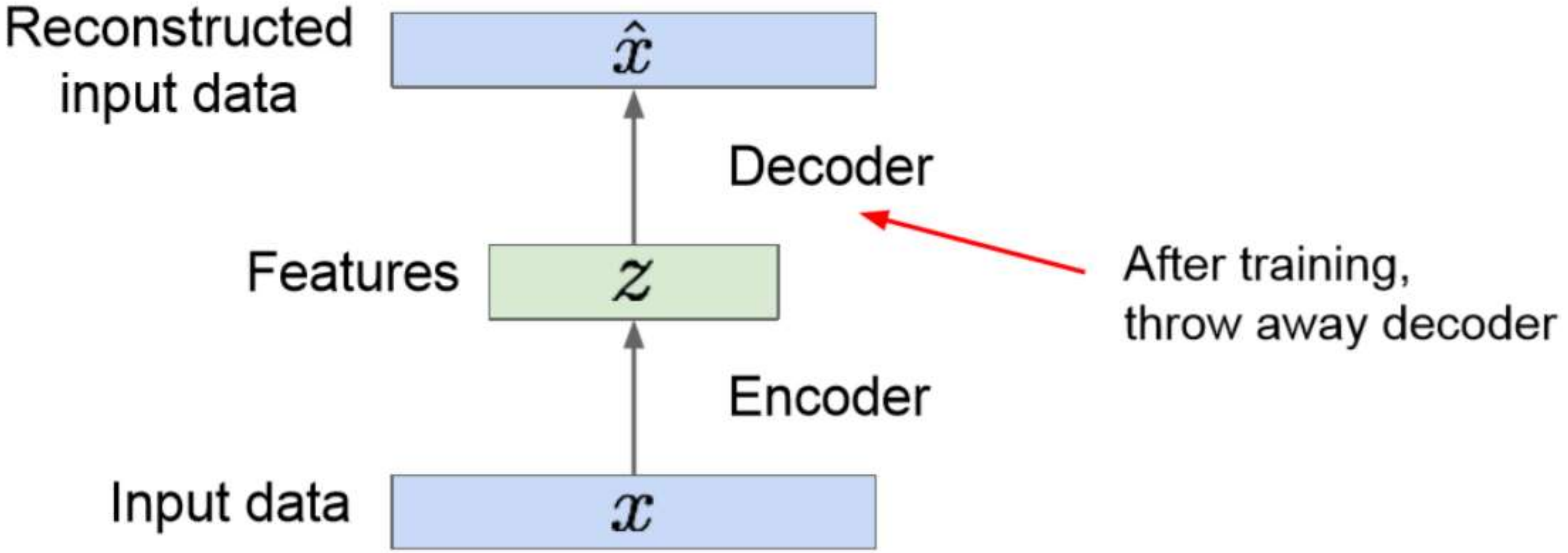
Some background first: Autoencoders

Train such that features can be used to reconstruct original data



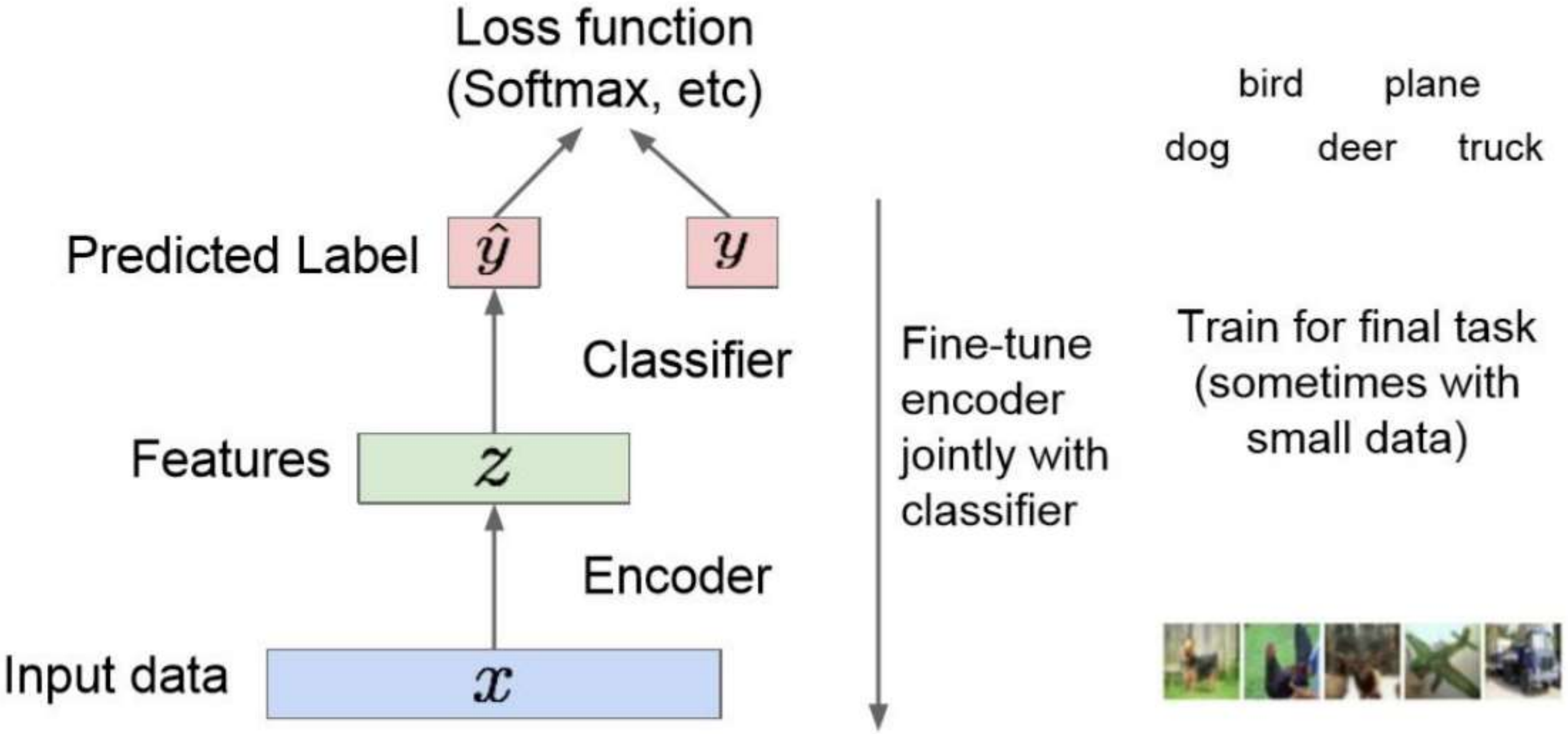


Autoencoder

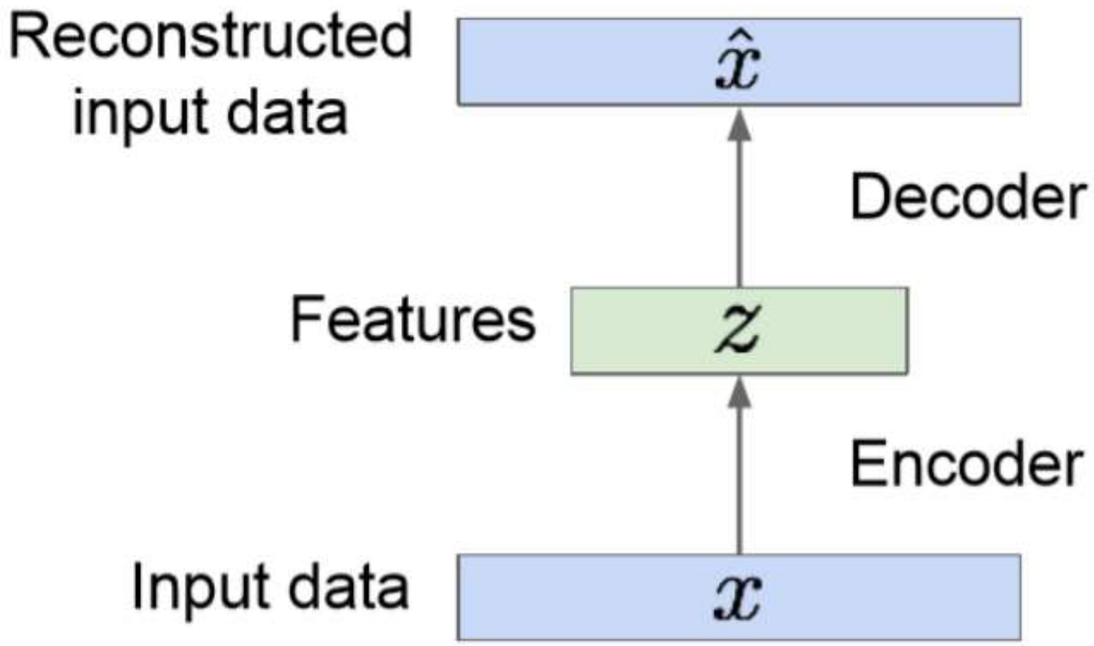


Some background first: Autoencoders

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



Some background first: Autoencoders



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

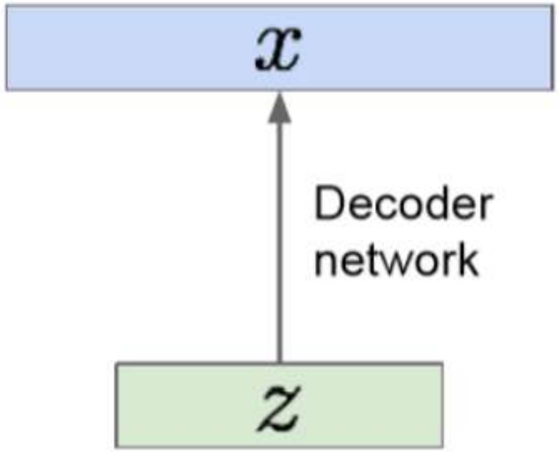
Features capture factors of variation in training data. Can we generate new images from an autoencoder?

Variational Autoencoder

Oh

Variational Autoencoders

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



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

We want to estimate the true parameters θ^* of this generative model.

How to train the model?

Remember strategy for training generative models from FVBNs. Learn model parameters to maximize likelihood of training data

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

Q: What is the problem with this?

Intractable!

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

Variational Autoencoders: Intractability

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

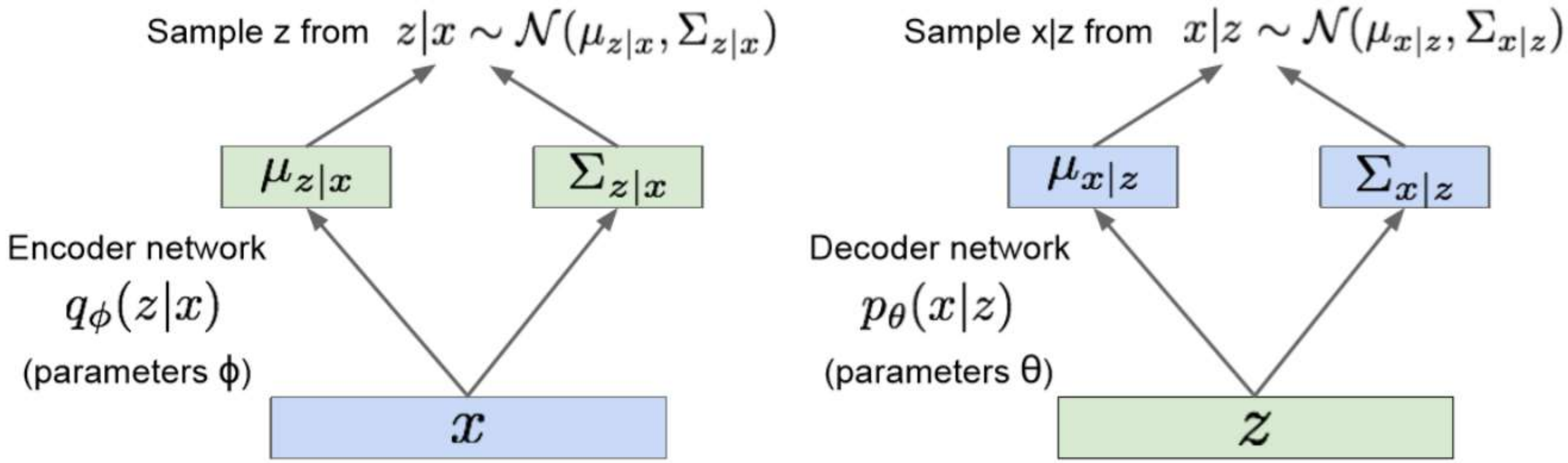
Posterior density also intractable: $p_\theta(z|x) = p_\theta(x|z) p_\theta(z) / p_\theta(x)$

Solution: In addition to decoder network modeling $p_\theta(x|z)$, define additional encoder network $q_\phi(z|x)$ that approximates $p_\theta(z|x)$

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

Variational Autoencoders

Since we're modeling probabilistic generation of data, encoder and decoder networks are probabilistic



Encoder and decoder networks also called "recognition"/"inference" and "generation" networks

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

Variational Autoencoders

Now equipped with our encoder and decoder networks, let's work out the (log) data likelihood:

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

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

Variational Autoencoders

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

Variational Autoencoders

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

Variational Autoencoders

Now equipped with our encoder and decoder networks, let's work out the (log) data likelihood:

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

Variational Autoencoders

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

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

Variational Autoencoders

Now equipped with our encoder and decoder networks, let's work out the (log) data likelihood:

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

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

We want to maximize the data likelihood

Decoder network gives $p_\theta(x|z)$, can compute estimate of this term through sampling. (Sampling differentiable through reparam. trick, see paper.)

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

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

Variational Autoencoders

Now equipped with our encoder and decoder networks, let's work out the (log) data likelihood:

$$
\begin{aligned}
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&= \mathbf{E}_z\left[\log \frac{p_\theta(x^{(i)} \mid z)p_\theta(z)}{p_\theta(z \mid x^{(i)})}\right] \quad (\text{Bayes' Rule})\\
&= \mathbf{E}_z\left[\log \frac{p_\theta(x^{(i)} \mid z)p_\theta(z)}{p_\theta(z \mid x^{(i)})}\frac{q_\phi(z \mid x^{(i)})}{q_\phi(z \mid x^{(i)})}\right] \quad (\text{Multiply by constant})\\
&= \mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right] - \mathbf{E}_z\left[\log \frac{q_\phi(z \mid x^{(i)})}{p_\theta(z)}\right] + \mathbf{E}_z\left[\log \frac{q_\phi(z \mid x^{(i)})}{p_\theta(z \mid x^{(i)})}\right] \quad (\text{Logarithms})\\
&= \boxed{\underbrace{\mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right] - D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z))}_{\mathcal{L}(x^{(i)},\theta,\phi)}} + \underbrace{D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z \mid x^{(i)}))}_{\boxed{\geq 0}}
\end{aligned}
$$

We want to maximize the data likelihood

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

Variational Autoencoders

Now equipped with our encoder and decoder networks, let's work out the (log) data likelihood:

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

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

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We want to maximize the data likelihood

$$\log p_\theta(x^{(i)}) \geq \mathcal{L}(x^{(i)},\theta,\phi)$$

Variational lower bound ("ELBO")

$$\theta^*, \phi^* = \arg\max_{\theta,\phi} \sum_{i=1}^{N} \mathcal{L}(x^{(i)},\theta,\phi)$$

Training: Maximize lower bound

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Variational Autoencoders

Now equipped with our encoder and decoder networks, let's work out the (log) data likelihood:

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

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

Make approximate posterior distribution close to prior

Reconstruct the input data

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

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

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$$\log p_\theta(x^{(i)}) \geq \mathcal{L}(x^{(i)},\theta,\phi)$$

Variational lower bound ("ELBO")

$$\theta^*, \phi^* = \arg\max_{\theta,\phi} \sum_{i=1}^{N} \mathcal{L}(x^{(i)},\theta,\phi)$$

Training: Maximize lower bound

Variational Autoencoders

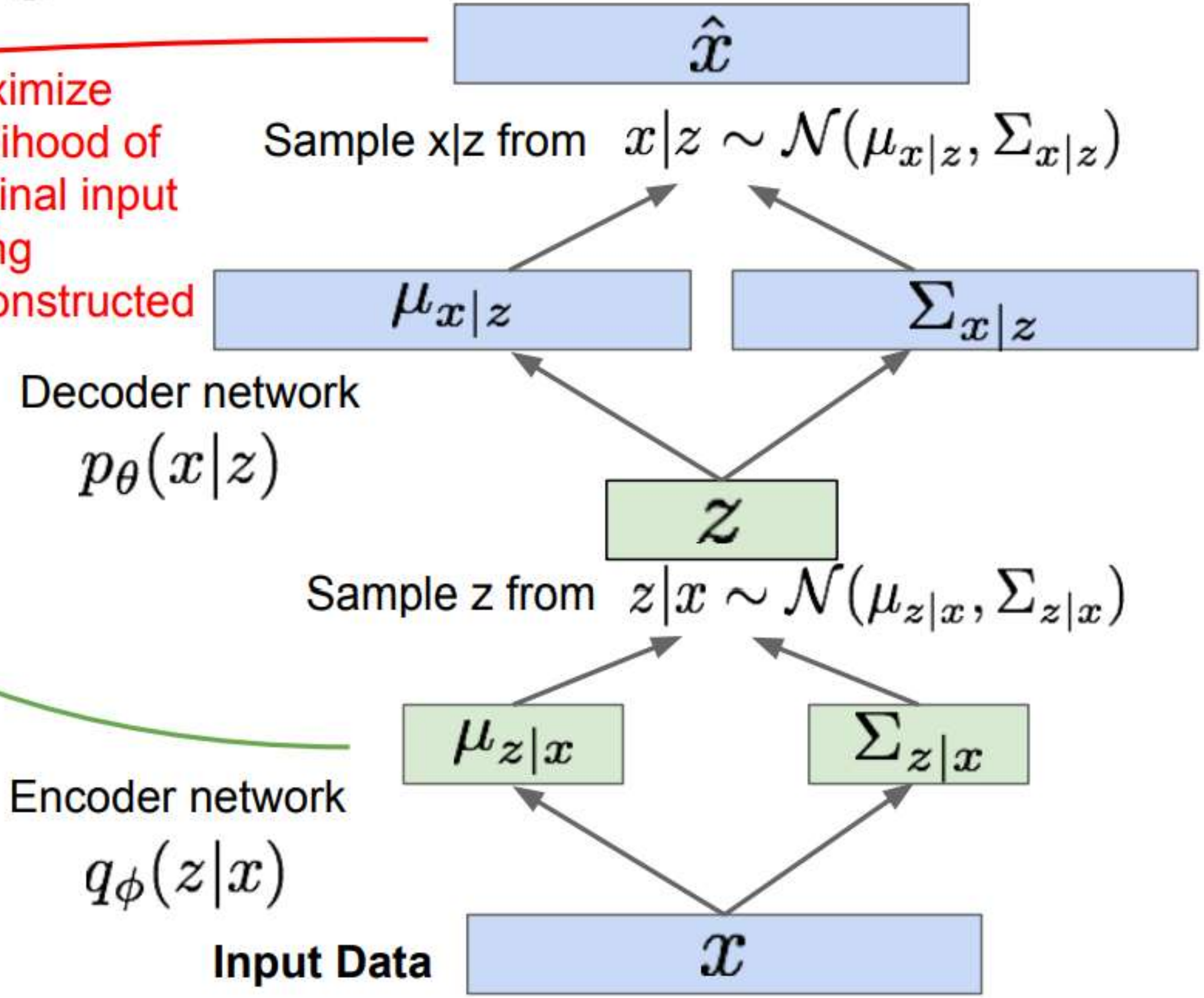
Putting it all together: maximizing the likelihood lower bound

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

Maximize likelihood of original input being reconstructed

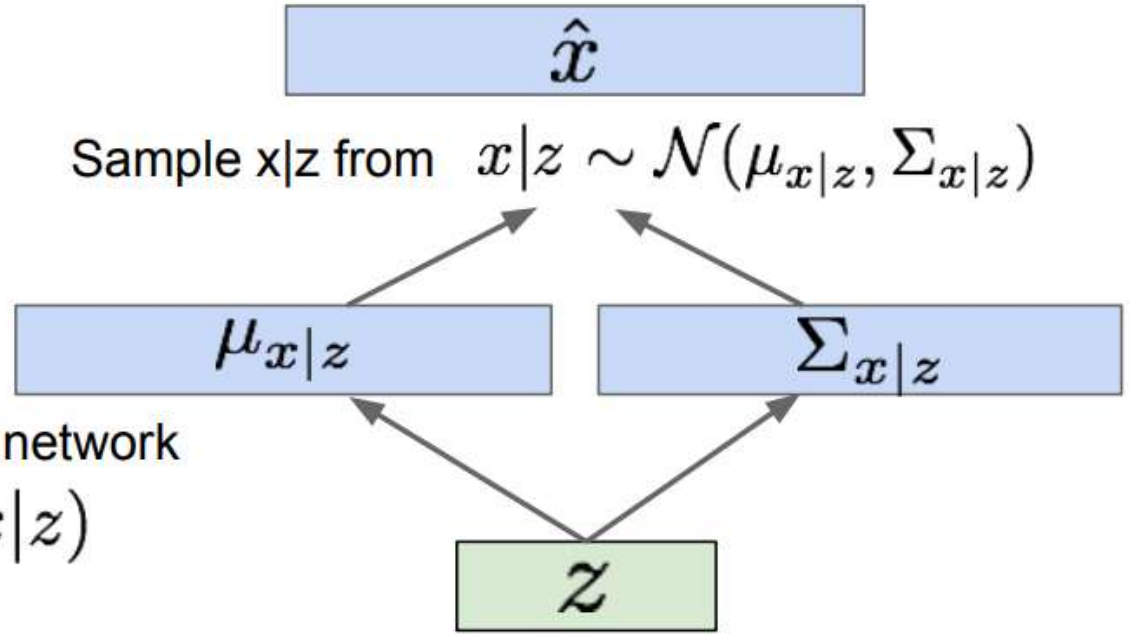
Make approximate posterior distribution close to prior

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



Variational Autoencoders: Generating Data!

Use decoder network. Now sample z from prior!

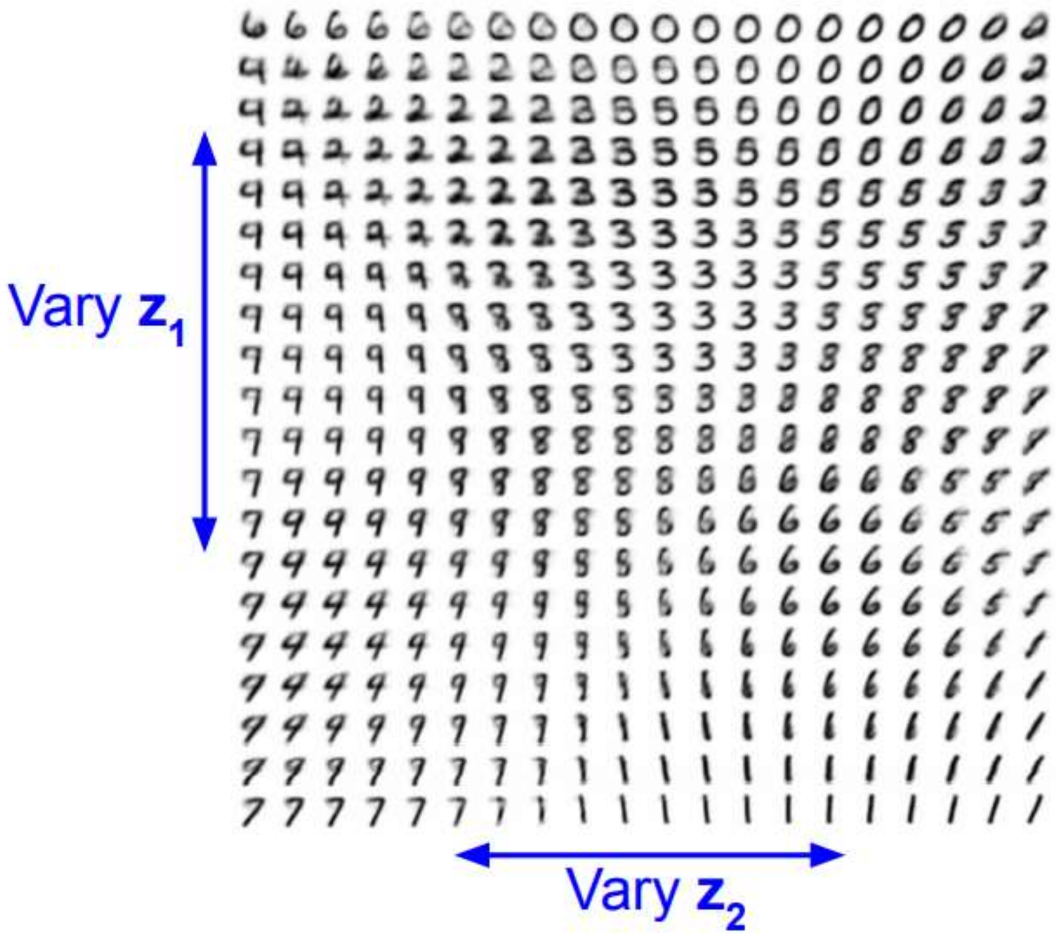


Decoder network

$p_\theta(x|z)$

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

Data manifold for 2-d **z**



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

Variational Autoencoders: Generating Data!

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

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

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

Degree of smile

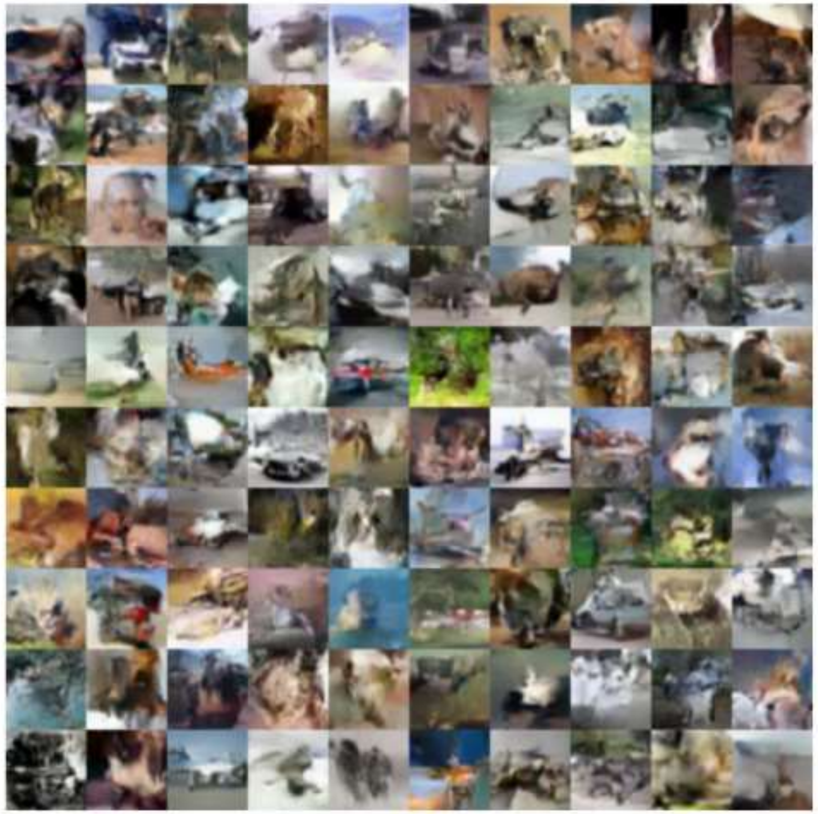
Vary $\mathbf{z}_1$

Vary $\mathbf{z}_2$

Head pose

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

Variational Autoencoders: Generating Data!



32x32 CIFAR-10

Labeled Faces in the Wild

Summary

- Encoder transforms input image into parameters of the Gaussian distributed latent space **Mean** and **Covariance** – Force it to be unit norm distribution KL divergence

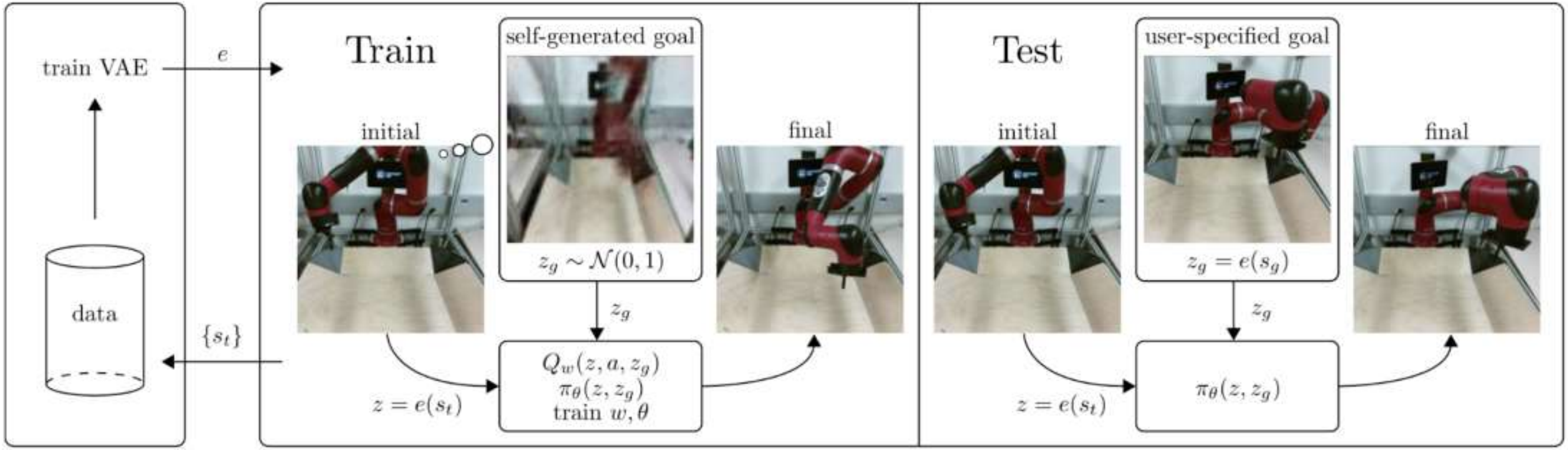
- Decoder transforms latent space sample into **original input** sample Reconstruction loss

- Random sample a point from the latent distribution that is assumed to generate the input image

One Application on Robotic

RIG (Reinforcement learning with Imagined Goals)
Context-Conditioned VAE

RIG (RL with Imagined Goals)



Ashvin Nair, et al. “Visual reinforcement learning with imagined goals” NeuriPS. 2018.

RIG (RL with Imagined Goals)

Let's say a β-VAE has an encoder q_ϕ mapping input states to latent variable z which i
a Gaussian distribution and a decoder p_ψ mapping z back to the states. The state en
is set to be the mean of β-VAE encoder.

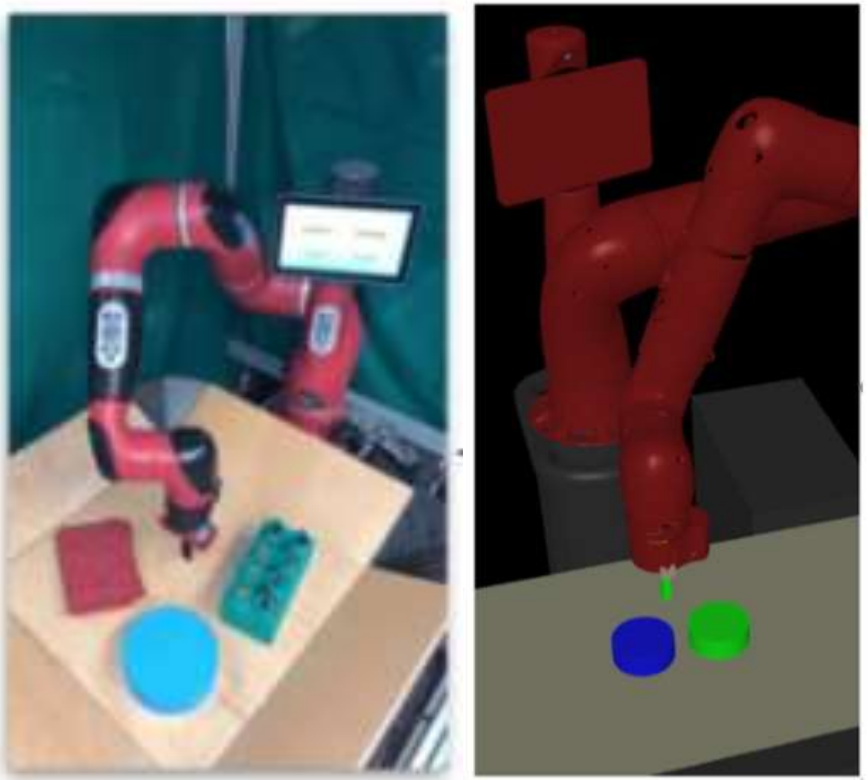
$$
\begin{aligned}
z &\sim q_\phi(z|s) = \mathcal{N}(z; \mu_\phi(s), \sigma^2_\phi(s)) \\
\mathcal{L}_{\beta\text{-VAE}} &= -\mathbb{E}_{z\sim q_\phi(z|s)}[\log p_\psi(s|z)] + \beta D_{\text{KL}}(q_\phi(z|s) \| p_\psi(s)) \\
e(s) &\triangleq \mu_\phi(s)
\end{aligned}
$$

$$r(s, g) = -\|e(s) - e(g)\|$$

Ashvin Nair, et al. "Visual reinforcement learning with imagined goals" NeuriPS. 2018.

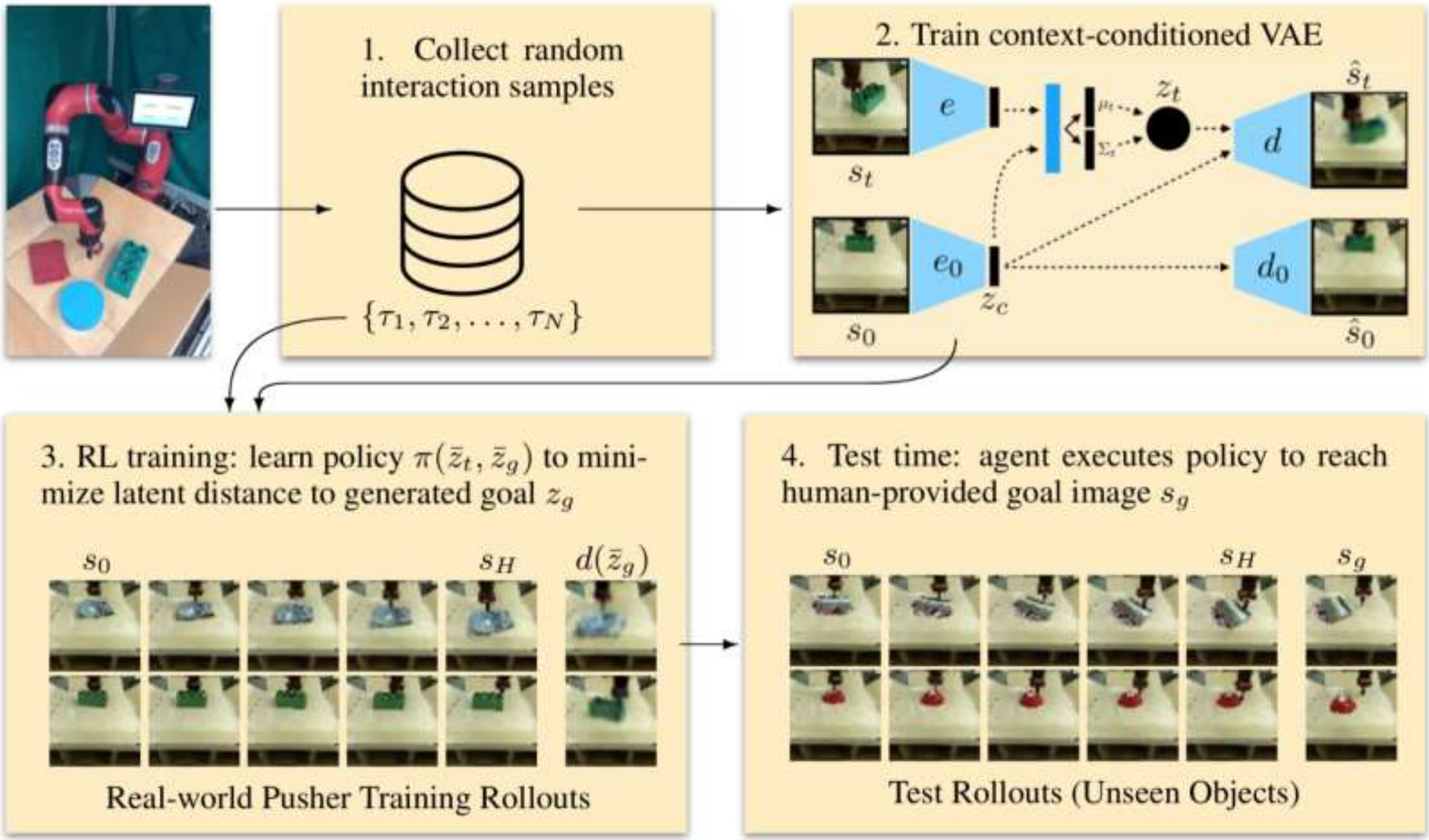
CC-VAE (Context-Conditioned VAE)

- The problem with RIG is a **lack of object variations** in the imagined goal pictures. If β-VAE is only trained with **a black puck**,
- it would not be able to create a goal with other objects like **blocks of different shapes and colors**. A follow-up improvement replaces β-VAE with a **CC-VAE**



Ashvin Nair, et al. “Contextual imagined goals for self-supervised robotic learning” CoRL. 2019.

CC-VAE (Context-Conditioned VAE)



Ashvin Nair, et al. “Contextual imagined goals for self-supervised robotic learning” CoRL. 2019.

CC-VAE (Context-Conditioned VAE)

encoder and decoder parameters ϕ and ψ, we jointly optimize both objectives when minimizing the negative evidence lower bound:

$$\mathcal{L}_{\text{VAE}} = -\mathbb{E}_{q_\phi(z|s)}[\log p(s|z)] + \beta D_{KL}(q_\phi(z|s)||p(z)). \tag{2}$$

3.3 Conditional Variational Auto-Encoders

Instead of a generative model that learns to generate the dataset distribution, one might instead desire a more structured generative model that can generate samples based on structured input. One example of this is a conditional variational auto-encoder (CVAE) that conditions the output on some input variable c and samples from $p(x|c)$ [40]. For example, to train a model that generates images of digits given the desired digit, the input variable c might be a one-hot encoded vector of the desired digit.

A CVAE trains $q_\phi(z|s, c)$ and $q_\psi(s|z, c)$, where both the encoder and decoder has access to the input variable c. The CVAE then minimizes:

$$\mathcal{L}_{\text{CVAE}} = -\mathbb{E}_{q_\phi(z|s,c)}[\log p(s|z, c)] + \beta D_{KL}(q_\phi(z|s, c)||p(z)). \tag{3}$$

Samples are generated by first sampling a latent $z \sim p(z)$. Based on c, we can then decode z with $q_\psi(s|z, c)$ and visualize the output, which is in our case an image. In our framework $c = s_0$.

Ashvin Nair, et al. “Contextual imagined goals for self-supervised robotic learning” CoRL. 2019.

CC-VAE (Context-Conditioned VAE)

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Other than the state encoder $e(s) \triangleq \mu_\phi(s)$, CC-VAE trains a second convolutional encoder $e_0(.)$ to translate the starting state s_0 into a compact context representation $c = e_0(s_0)$. Two encoders, $e(.)$ and $e_0(.)$, are intentionally different without shared weights, as they are expected to encode different factors of image variation. In addition to the loss function of CVAE, CC-VAE adds an extra term to learn to reconstruct c back to s_0, $\hat{s}_0 = d_0(c)$.

$$\mathcal{L}_{\text{CC-VAE}} = \mathcal{L}_{\text{CVAE}} + \log p(s_0|c)$$

Ashvin Nair, et al. “Contextual imagined goals for self-supervised robotic learning” CoRL. 2019.

Thank you

- End