


Machine Learning for Graphs and Sequential Data

Deep Generative Models - Variational Autoencoders

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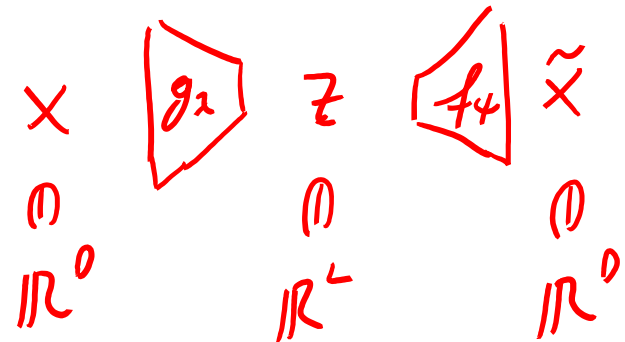
Summer Term 2020

Data Analytics and
Machine Learning 

Roadmap

■ Chapter: Deep Generative Models

1. Introduction
2. Normalizing Flows
3. **Variational Inference**
 - Latent variable models
 - Maximization using lower bounds
 - Optimizing the ELBO
 - **Variational Autoencoders**
4. Generative Adversarial Networks
5. Summary



Recap: Latent Variable Models

- We define a generative model with latent variables

$$p_{\theta}(\mathbf{x}) = \int p_{\theta}(\mathbf{x}, \mathbf{z}) d\mathbf{z} = \int p_{\theta}(\mathbf{x}|\mathbf{z}) p_{\theta}(\mathbf{z}) d\mathbf{z}$$

- This latent structure allows us to define a complex distribution $p_{\theta}(\mathbf{x})$, even though $p_{\theta}(\mathbf{z})$ and $p_{\theta}(\mathbf{x}|\mathbf{z})$ are “relatively simple”
- Since the log-likelihood is intractable, we maximize the ELBO instead
$$\log p_{\theta}(\mathbf{x}) \geq \mathbb{E}_{\mathbf{z} \sim q_{\phi}(\mathbf{z})} [\log p_{\theta}(\mathbf{x}, \mathbf{z}) - \log q_{\phi}(\mathbf{z})] =: \mathcal{L}(\theta, \phi)$$
- How do we actually define and learn such models in practice?

Designing an LVM

- In variational inference, our optimization problem is

$$\max_{\theta, \phi} \mathbb{E}_{\mathbf{z} \sim q_{\phi}(\mathbf{z})} [\log p_{\theta}(\mathbf{x}|\mathbf{z}) + \log p_{\theta}(\mathbf{z}) - \log q_{\phi}(\mathbf{z})]$$

- To define a latent variable model, we need to answer several questions
 1. What are our latent variables \mathbf{z} ?
 2. What is the data \mathbf{x} ?
 3. What is the prior $p_{\theta}(\mathbf{z})$ on the latent variables?
 4. What is the conditional likelihood $p_{\theta}(\mathbf{x}|\mathbf{z})$ of the data given the latent variables?
 5. What is the variational distribution $q_{\phi}(\mathbf{z})$?
- These choices (especially 3, 4, 5) are to some degree arbitrary – different choices will produce different models
- We will learn about the most popular models used in practice – but many other choices are also possible!

Choosing $p_{\theta}(\mathbf{z})$

- We usually choose \mathbf{z} to be continuous

$$\mathbf{z} \in \mathbb{R}^L$$

- The main advantage of making \mathbf{z} continuous is that it's easier to sample with reparametrization from continuous distributions (i.e. $q(\mathbf{z})$)

- We pick the simplest possible prior on \mathbf{z} – standard normal distribution

$$p(\mathbf{z}) = \mathcal{N}(\mathbf{z}|\mathbf{0}, \mathbf{I})$$

- Note that we don't write $p_{\theta}(\mathbf{z})$ anymore since there are no learnable parameters θ
- We will introduce complexity to our model when designing $p_{\theta}(\mathbf{x}|\mathbf{z})$
- Picking a simple prior will significantly simplify some calculations later

Representing the Data

$$p_e(x|z)$$

- The data x depends on our application, e.g. color images are often represented as real-valued vectors

$$x \in \mathbb{R}^D$$

- Black-and-white images can be represented as binary vectors

$$x \in \{0,1\}^D$$

- Most examples in this week's lecture (and online) deal with images because
 - It's a popular topic – well-studied, we know what works well, code available
 - We can show pretty pictures of the results
- However, we can apply these methods across many domains – music, text, graphs, time series, data from the Large Hadron Collider, ...

Choosing $p_{\theta}(x|z)$

 $\mu(z)$

- The choice of $p_{\theta}(x|z)$ depends on what data x we are modeling
- For every $z \in \mathbb{R}^L$, we need to obtain a probability distribution over x

 $\psi = \{w, b\}$

- Idea: Pick a parametric distribution $p_{\theta}(x|z)$ whose parameters are produced by some function f_{ψ} that takes z as input

 $x \in \mathbb{R}^2$
 $z \in \mathbb{R}$

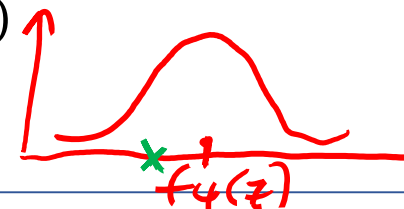
- For example, for $x \in \mathbb{R}^D$ we could choose

$$p_{\theta}(x|z) = \mathcal{N}(x | \underline{\mu} = f_{\psi}(z), I)$$

 $f_{\psi}(z) = w \cdot z + b$
 $\uparrow = \mu$
 $\in \mathbb{R}^{2 \times 1}$

where $f_{\psi} : \mathbb{R}^L \rightarrow \mathbb{R}^D$ is some nonlinear function (a neural network)

and $\theta = \mu \in \mathbb{R}^D$ are the parameters of $p_{\theta}(x|z)$

 $f_{\psi}(z)$


Choosing $p_{\theta}(\mathbf{x}|\mathbf{z})$

$\mathcal{N}_e(\mathbf{x})$

- Choice of $p_{\theta}(\mathbf{x}|\mathbf{z})$ involves a trade-off between expressiveness and efficiency

$$p_{\theta}(\mathbf{x}|\mathbf{z}) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu} = f_{\psi}(\mathbf{z}), \mathbf{I}) = \prod_{j=1}^D \mathcal{N}(x_j|\mu = f_{\psi}(\mathbf{z})_j, 1)$$

- Each pixel x_j is conditionally independent of the others given \mathbf{z} (but they become dependent if we marginalize out \mathbf{z})
- We could have a more expressive $p_{\theta}(\mathbf{x}|\mathbf{z})$ (e.g. full covariance, normalizing flow) but that would make the evaluation less efficient

- Different data types require different likelihoods.

- E.g., for a binary $\mathbf{x} \in \{0,1\}^D$ we could use

$\mathcal{N}_e(\mathbf{x}|\mathbf{z}) =$

$\mathcal{N}(\mathbf{x}|\boldsymbol{\mu} = f_{\psi}(\mathbf{z}),$

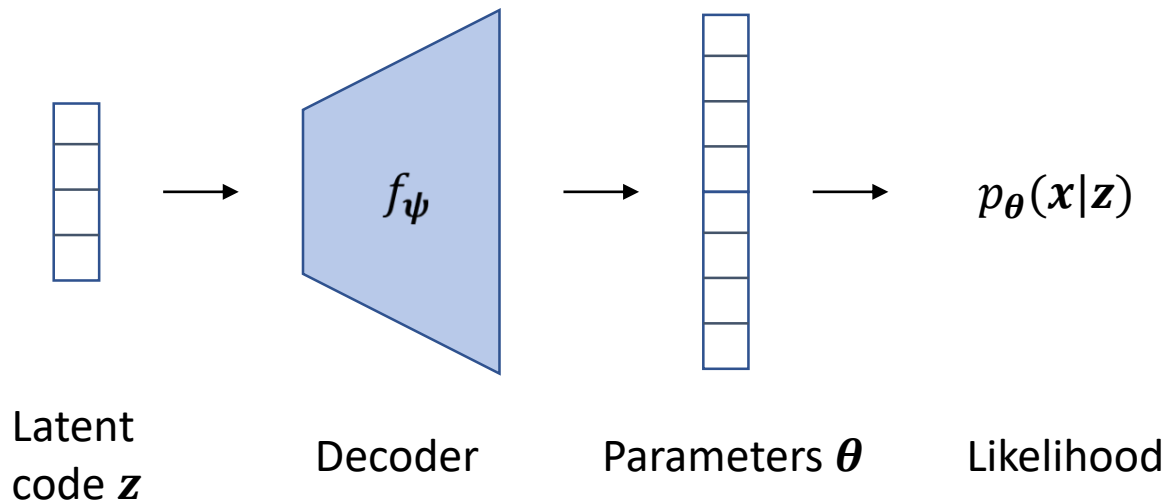
$\Sigma = \text{DIAG}(f'_{\psi}(\mathbf{z}))$

$$p_{\theta}(\mathbf{x}|\mathbf{z}) = \prod_{j=1}^D \text{Bernoulli}(x_j|\underbrace{\sigma(f_{\psi}(\mathbf{z})_j)}_{\theta})$$

$g_{\omega}(y) = x$
 $\omega = f_{\psi}(\mathbf{z})$
 $p_{\theta}(y)$ \mathbb{R}^D

The Decoder f_ψ

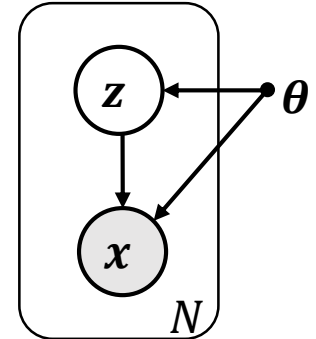
- The neural network f_ψ is often called “the decoder”, since it converts the latent variable \mathbf{z} (a.k.a. the latent code) into the parameters $\boldsymbol{\theta}$ of $p_\theta(\mathbf{x}|\mathbf{z})$



- We use different decoder architectures for different data types
 - E.g., a popular choice of f_ψ for images is [transposed convolution](#)

Choosing $q_{\phi}(\mathbf{z})$

- We have specified $p_{\theta}(\mathbf{x}|\mathbf{z})$ and $p(\mathbf{z})$, the last missing component is the variational distribution $q_{\phi}(\mathbf{z})$
- Our dataset consists of N (i.i.d.) samples $\mathbf{x}^{(i)} \in \mathbb{R}^D$
- Each sample $\mathbf{x}^{(i)}$ corresponds to a separate latent variable $\mathbf{z}^{(i)}$
 - Our variational distribution is over all $\mathbf{z}^{(i)}$'s: $q_{\phi}(\mathbf{z}^{(1)}, \dots, \mathbf{z}^{(N)})$
- For simplicity, we use the mean field assumption



$$q_{\phi}(\mathbf{z}^{(1)}, \dots, \mathbf{z}^{(N)}) = \prod_{i=1}^N q_{\phi^{(i)}}(\mathbf{z}^{(i)})$$

$$p_{\theta}(\mathbf{z}^{(i)} | \mathbf{x}^{(i)})$$

Choosing $q_{\phi}(\mathbf{z})$

$$\text{CAT}(0.9, 0.1) = q_{\phi^{(1)}}(\mathbf{z}^{(1)})$$

$$\mathbf{z} \sim \text{CAT}(\pi)$$

- Mean field assumption

$$q_{\phi}(\mathbf{z}^{(1)}, \dots, \mathbf{z}^{(N)}) = \prod_{i=1}^N q_{\phi^{(i)}}(\mathbf{z}^{(i)})$$

- How should we model each $q_{\phi^{(i)}}(\mathbf{z}^{(i)})$?

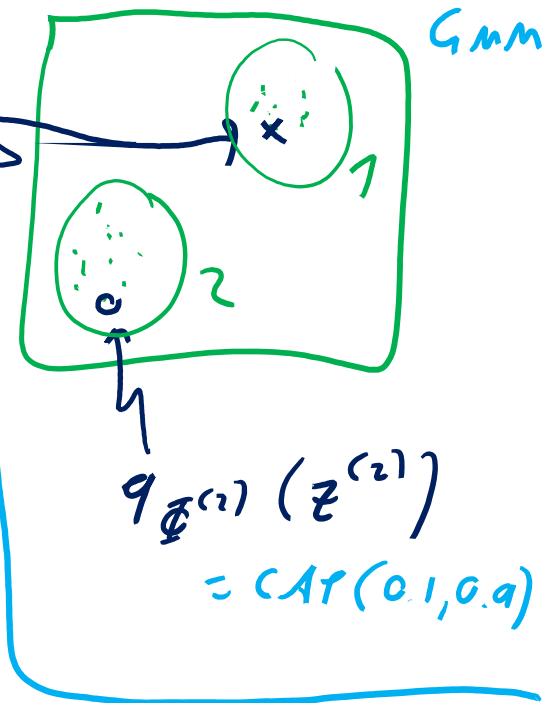
- Simple choice – multivariate normal

$$q_{\phi^{(i)}}(\mathbf{z}^{(i)}) = \mathcal{N}(\mathbf{z}^{(i)} | \boldsymbol{\mu}^{(i)}, \boldsymbol{\Sigma}^{(i)}) \quad \text{where } \boldsymbol{\phi}^{(i)} = \{\boldsymbol{\mu}^{(i)}, \boldsymbol{\Sigma}^{(i)}\}$$

- Usually $\boldsymbol{\Sigma}^{(i)}$ is diagonal

- Another popular option – normalizing flows with forward parametrization

$$\mu(\mathbf{z}) = \mathcal{N}(\mathbf{z} | 0, 1) \quad \mathbf{z} \sim \mathcal{N}(0, 1)$$



Why is Normal $q_\phi(\mathbf{z})$ a Good Choice?

$$\mathbb{E}_{\mathbf{z} \sim q_\phi(\mathbf{z})} \left[\log \frac{p_\theta(\mathbf{x}, \mathbf{z})}{q_\phi(\mathbf{z})} \right]$$

- ELBO for a single instance \mathbf{x}

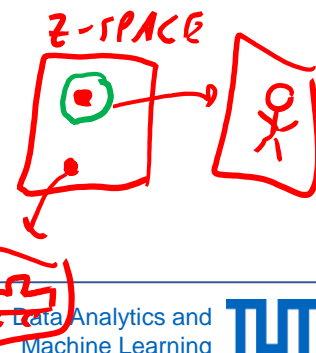
$$\begin{aligned} \mathcal{L}(\theta, \phi) &= \mathbb{E}_{\mathbf{z} \sim q_\phi(\mathbf{z})} [\log p_\theta(\mathbf{x}|\mathbf{z}) + \log p(\mathbf{z}) - \log q_\phi(\mathbf{z})] \\ &= \mathbb{E}_{\mathbf{z} \sim q_\phi(\mathbf{z})} [\log p_\theta(\mathbf{x}|\mathbf{z})] - \text{KL}(q_\phi(\mathbf{z}) || p(\mathbf{z})) \end{aligned}$$

- Recall that $p(\mathbf{z}) = \mathcal{N}(\mathbf{z}|\mathbf{0}, \mathbf{I})$ and $q_\phi(\mathbf{z}) = \mathcal{N}(\mathbf{z}|\boldsymbol{\mu}, \boldsymbol{\Sigma})$
- We can compute the KL divergence between two multivariate normal distributions in closed form

$$\text{KL}(q_\phi(\mathbf{z}) || p(\mathbf{z})) = \frac{1}{2} (\text{tr}(\boldsymbol{\Sigma}) + \boldsymbol{\mu}^T \boldsymbol{\mu} - \log(\det(\boldsymbol{\Sigma})) - L)$$

- Even simpler for diagonal covariance $\boldsymbol{\Sigma} = \text{diag}(\boldsymbol{\sigma}^2)$ (where $\boldsymbol{\sigma}^2 \in \mathbb{R}_+^L$)

$$\text{KL}(q_\phi(\mathbf{z}) || p(\mathbf{z})) = \frac{1}{2} \left(\sum_{j=1}^L (\sigma_j^2 + \mu_j^2 - \log \sigma_j^2 - 1) \right)$$



$$\log p_\theta(\mathbf{x}) = \mathcal{ELBO} + \text{KL}(q_\phi(\mathbf{z}) || p(\mathbf{z}|\mathbf{x}))$$

ELBO for Multiple Samples

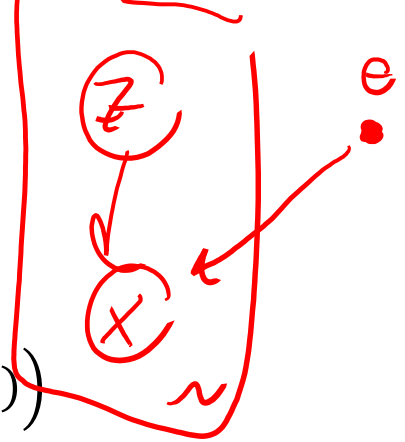
- ELBO for a single instance \mathbf{x}

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

- ELBO for the entire dataset $\{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(N)}\}$

$$\begin{aligned} \mathcal{L}(\boldsymbol{\theta}, \boldsymbol{\phi}) &= \frac{1}{N} \sum_i^N \mathcal{L}_i(\boldsymbol{\theta}, \boldsymbol{\phi}^{(i)}) \\ &= \frac{1}{N} \sum_{i=1}^N \left[\mathbb{E}_{\mathbf{z}^{(i)} \sim q_{\boldsymbol{\phi}^{(i)}}(\mathbf{z}^{(i)})} [\log p_{\boldsymbol{\theta}}(\mathbf{x}^{(i)}|\mathbf{z}^{(i)})] - \mathbb{KL} \left(q_{\boldsymbol{\phi}^{(i)}}(\mathbf{z}^{(i)}) || p(\mathbf{z}) \right) \right] \end{aligned}$$

- We have to learn a separate parameter $\boldsymbol{\phi}^{(i)}$ for each instance i
 - If the number of samples N is large, this is extremely expensive
- What if we are interested in the latent features of a new sample \mathbf{x}^{new} ?
 - We will need to learn $\boldsymbol{\phi}^{\text{new}}$ from scratch
- Can we do better than this?



Amortized Inference

- We need to find the optimal parameter $\phi_{\text{optimal}}^{(i)}$ for every sample $x^{(i)}$
- Standard approach: Solve the optimization problem for each $i = 1, \dots, N$

$$\phi_{\text{optimal}}^{(i)} = \operatorname{argmax}_{\phi^{(i)}} \mathcal{L}_i(\theta, \phi^{(i)})$$

- Better idea: Train a neural network g_λ that tries to map every $x^{(i)}$ in the training set to its optimal parameters $\phi_{\text{optimal}}^{(i)}$

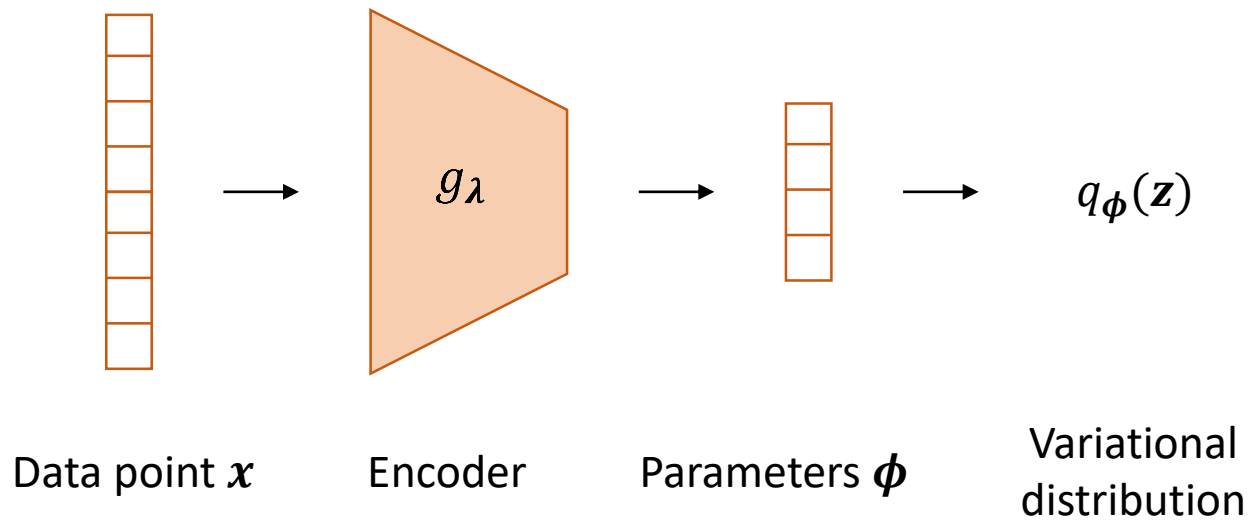
$$\max_{\lambda} \frac{1}{N} \sum_i \mathcal{L}_i(\theta, g_\lambda(x^{(i)}))$$

$\underbrace{g_\lambda(x^{(i)})}_{\approx \phi_{\text{optimal}}^{(i)}}$

- We use the same g_λ for every sample $x^{(i)}$, and can even use for new samples that we haven't seen during training

The Encoder g_λ

- We call the NN g_λ “the encoder”, since it converts a data point x into the parameters ϕ that define the distribution $q_\phi(z)$ over the latent code z



- We use different encoder architectures for different data types
 - E.g., a popular choice of g_λ for images are convolutional NNs

Putting Everything Together

- ELBO for a single sample

$$\mathcal{L}(\boldsymbol{\psi}, \boldsymbol{\lambda}) := \mathbb{E}_{\mathbf{z} \sim q_{\boldsymbol{\phi}}(\mathbf{z})} [\log p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z})] - \mathbb{KL}(q_{\boldsymbol{\phi}}(\mathbf{z}) || p(\mathbf{z}))$$

where $\boldsymbol{\theta} = f_{\boldsymbol{\psi}}(\mathbf{z})$ and $\boldsymbol{\phi} = g_{\boldsymbol{\lambda}}(\mathbf{x})$

- Recipe for optimizing the ELBO

1. Compute $\boldsymbol{\phi} = g_{\boldsymbol{\lambda}}(\mathbf{x})$
2. Compute an MC estimate of ELBO; often done using a single sample, i.e.
 - a) Draw $\mathbf{z}' \sim q_{\boldsymbol{\phi}}(\mathbf{z})$ with reparametrization
 - b) Compute $\boldsymbol{\theta} = f_{\boldsymbol{\psi}}(\mathbf{z}')$
 - c) ELBO: $\mathcal{L}(\boldsymbol{\psi}, \boldsymbol{\lambda}) \approx \log p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z}') - \mathbb{KL}(q_{\boldsymbol{\phi}}(\mathbf{z}) || p(\mathbf{z}))$
3. Backpropagate (compute $\nabla_{\boldsymbol{\psi}} \mathcal{L}(\boldsymbol{\psi}, \boldsymbol{\lambda})$ and $\nabla_{\boldsymbol{\lambda}} \mathcal{L}(\boldsymbol{\psi}, \boldsymbol{\lambda})$)
4. Update the NN weights $\boldsymbol{\psi}$ and $\boldsymbol{\lambda}$ using gradient ascent

Recall: Reparametrization Trick

- Our expectation depends on the parameters that we are optimizing

$$\mathcal{L}(\boldsymbol{\psi}, \boldsymbol{\lambda}) := \mathbb{E}_{\mathbf{z} \sim q_{\boldsymbol{\phi}}(\mathbf{z})} [\log p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z})] - \mathbb{KL}(q_{\boldsymbol{\phi}}(\mathbf{z}) || p(\mathbf{z}))$$

where $\boldsymbol{\theta} = f_{\boldsymbol{\psi}}(\mathbf{z})$ and $\boldsymbol{\phi} = g_{\boldsymbol{\lambda}}(\mathbf{x})$

- This means that we need to sample from $q_{\boldsymbol{\phi}}(\mathbf{z})$ with reparametrization

- $\boldsymbol{\epsilon} \sim b(\boldsymbol{\epsilon})$
- $\mathbf{z}' = T(\boldsymbol{\epsilon}, \boldsymbol{\phi})$

- E.g., for $q_{\boldsymbol{\phi}}(\mathbf{z})$ multivariate normal with diagonal covariance (Slide 98)

$$q_{\boldsymbol{\phi}}(\mathbf{z}) = \mathcal{N}(\mathbf{z} | \boldsymbol{\mu}, \text{diag}(\boldsymbol{\sigma}^2))$$

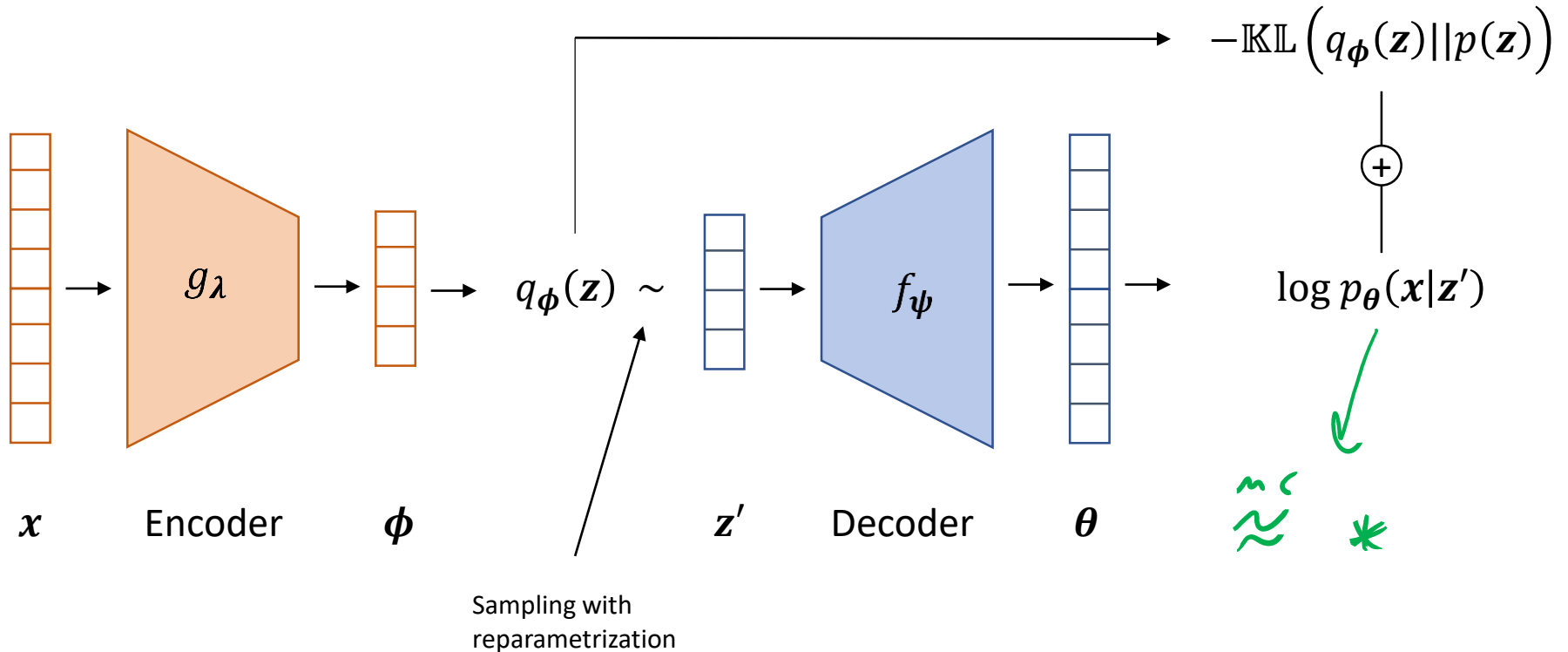
- $\boldsymbol{\epsilon} \sim \mathcal{N}(\boldsymbol{\epsilon} | \mathbf{0}, \mathbf{I})$
- $\mathbf{z}' = \boldsymbol{\sigma} \odot \boldsymbol{\epsilon} + \boldsymbol{\mu}$

$\boldsymbol{\phi} = g_{\boldsymbol{\lambda}}(\mathbf{x})$

Variational Autoencoder (VAE)

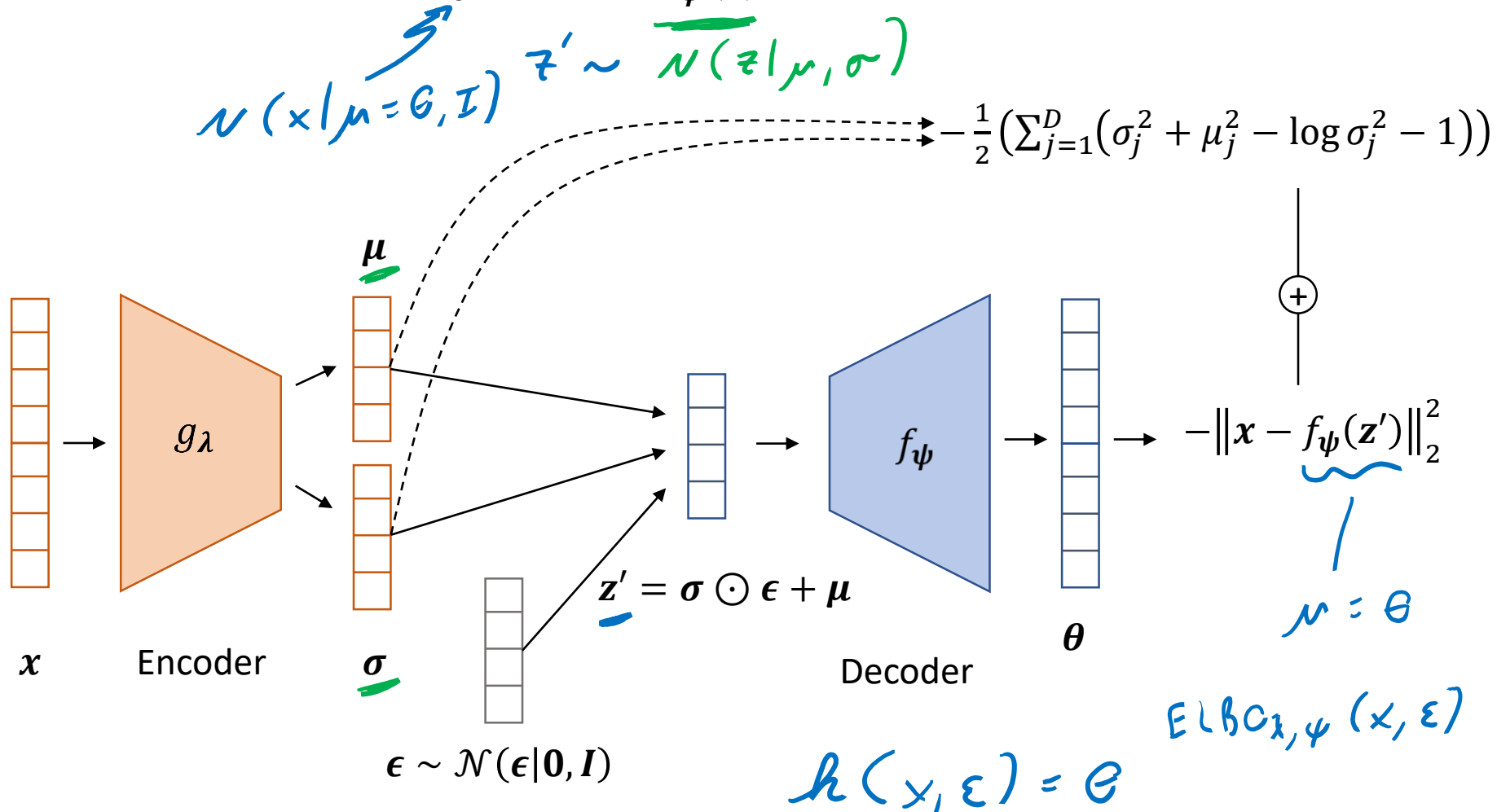
$$\mathcal{L}(\boldsymbol{\psi}, \boldsymbol{\lambda}) := \mathbb{E}_{\mathbf{z} \sim q_{\boldsymbol{\phi}}(\mathbf{z})} [\log p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z})] - \text{KL}(q_{\boldsymbol{\phi}}(\mathbf{z}) || p(\mathbf{z}))$$

where $\boldsymbol{\phi} = g_{\boldsymbol{\lambda}}(\mathbf{x})$ and $\boldsymbol{\theta} = f_{\boldsymbol{\psi}}(\mathbf{z})$



VAE with Gaussian $p_{\theta}(x|z)$ and $q_{\phi}(z)$

- Using our choices of $p_{\theta}(x|z)$ and $q_{\phi}(z)$ from Slides 94 & 98

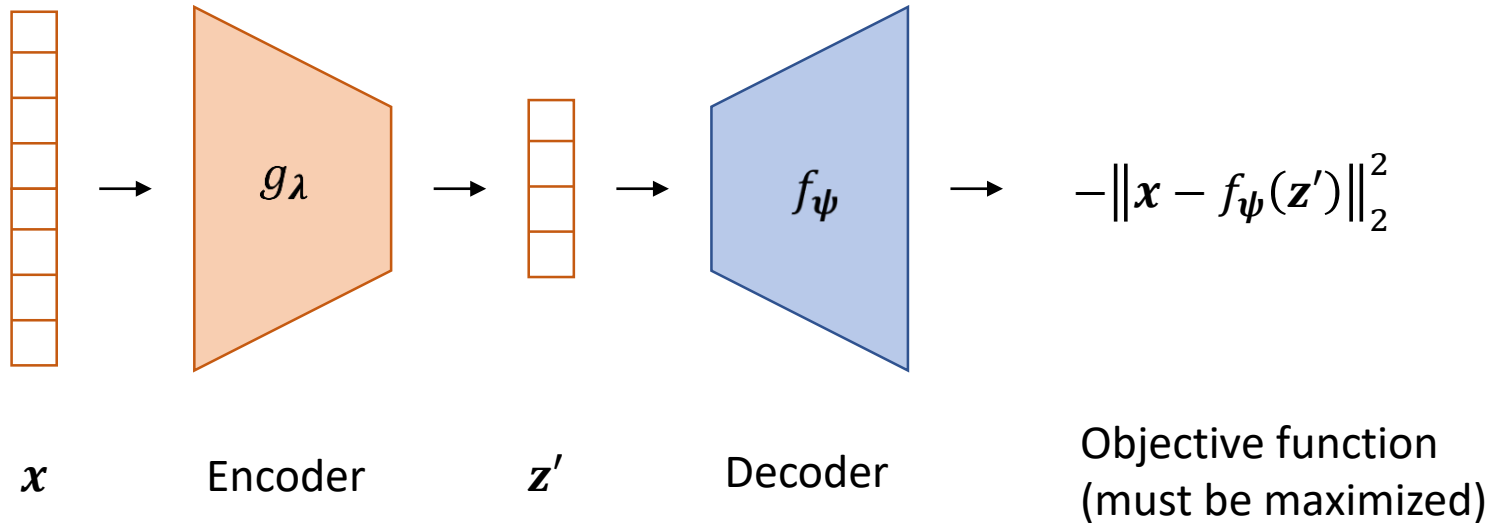


Standard Autoencoders

$$\ell(\boldsymbol{\psi}, \boldsymbol{\lambda}) = \log p_{\boldsymbol{\theta}}(\boldsymbol{x}|\boldsymbol{z}')$$

where $\boldsymbol{z}' = g_{\boldsymbol{\lambda}}(\boldsymbol{x})$ and $\boldsymbol{\theta} = f_{\boldsymbol{\psi}}(\boldsymbol{z}')$

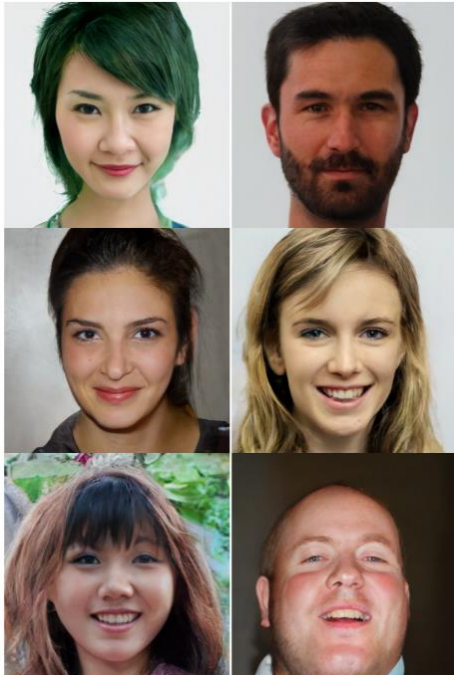
- When $\log p_{\boldsymbol{\theta}}(\boldsymbol{x}|\boldsymbol{z}')$ is Gaussian distribution, we get



- Standard AE are not generative models – they can only reconstruct the data
- Standard AE learns a single \boldsymbol{z}' for each \boldsymbol{x} , while VAE learns a distribution $q_{\boldsymbol{\phi}}(\boldsymbol{z})$

Generating Data with a VAE

- Remember: Once we have trained our generative model (i.e. we know the parameters ψ of our decoder) we can use it to generate new data
 - Sample $\mathbf{z}' \sim p(\mathbf{z}) = \mathcal{N}(\mathbf{z}|\mathbf{0}, \mathbf{I})$
 - Sample $\mathbf{x} \sim p_{\theta}(\mathbf{x}|\mathbf{z}') = \mathcal{N}(\mathbf{x}|f_{\psi}(\mathbf{z}'), \mathbf{I})$
- Note that we don't need the encoder when sampling new data



Source: Razavi et al., 2019
Generating Diverse High-Fidelity Images with VQ-VAE-2

Questions – VAE

1. Assume that each data point is represented by a vector $\mathbf{x} \in \{1, 2, \dots, C\}^D$. What distribution would you pick for $p_{\theta}(\mathbf{x}|\mathbf{z})$? How can we parametrize this distribution with a neural network?
2. Assume that each datapoint \mathbf{x} is represented by a variable-length sequence of real numbers $x_i \in \mathbb{R}^{D_i}$ (D_i might be different for different i 's). What NN architecture could we use for the encoder g_{λ} in this case?
3. Slide 94: Assume that we choose to model $p_{\theta}(\mathbf{x}|\mathbf{z})$ with a normalizing flow. Should we use forward or reverse parametrization? Why?
4. Slide 97: Assume that we choose to model $q_{\phi}(\mathbf{z})$ with a normalizing flow. Should we use forward or reverse parametrization? Why?
5. Slide 106: How can we ensure that the vector σ produced by the encoder g_{λ} is always positive?

Reading Materials

- Sections 1.2 – 1.7 and 2.1 – 2.6 of the PhD thesis of Diedrik P. Kingma cover essentially the same content as our lecture
 - <https://pure.uva.nl/ws/files/17891313/Thesis.pdf>