

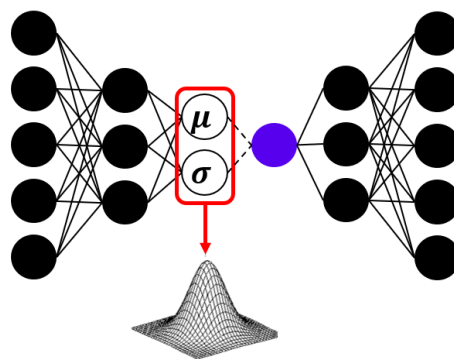
An Introduction to Variational Inference

杨帆

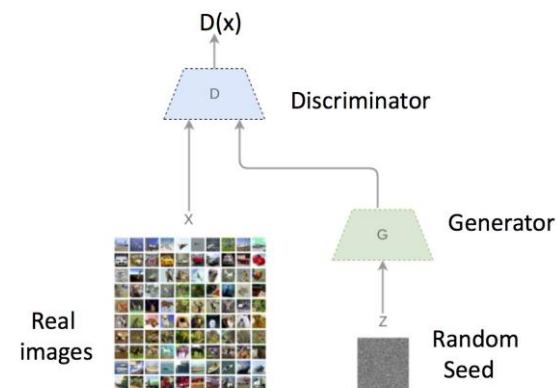
2018年6月4日

Motivations For This Talk

- Some trends in machine learning: make ML to be
 - Robust to uncertain and adversarial inputs
 - Unsupervised, semi-supervised or self-supervised
 - Interpretable
 - Nonparametric and automatic
- Probabilistic generative models are promising tools for these goals
 - E.g., two popular probabilistic generative models: VAE and GAN



Variational Autoencoders



Generative Adversarial Networks

This Talk

- Gives a high-level impression of how probabilistic model works
 - Introduces the variational inference method
 - which is the basis of VAE
 - Helps us understand the VAE
-
- NOTE: there will be some math and statistics, please interrupt me if you do not understand them.

Outline

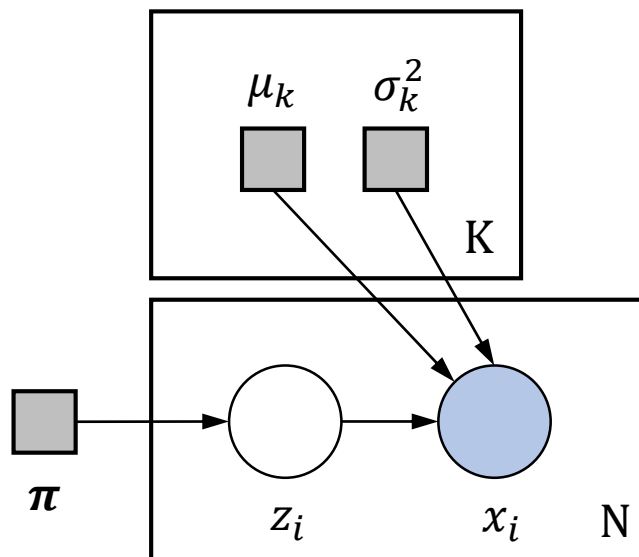
- Probabilistic Generative Models
- Variational Inference
- Variational Autoencoder

Outline

- **Probabilistic Generative Models**
- Variational Inference
- Variational Autoencoder

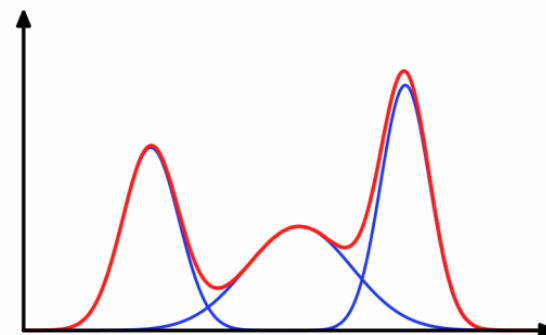
Probabilistic Generative Models

- Example: Gaussian Mixture Models



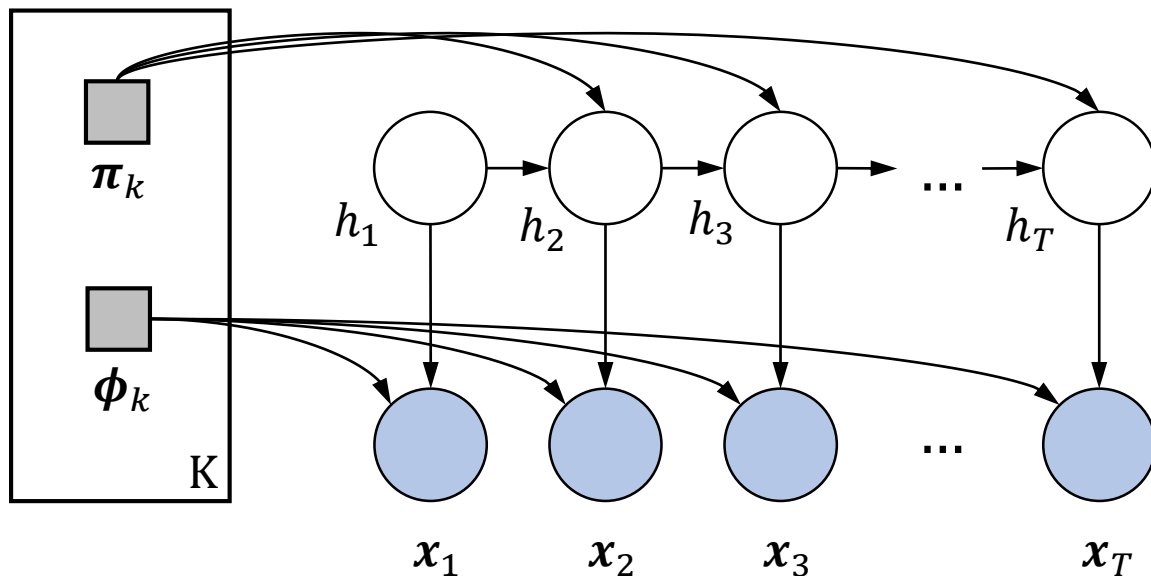
$$z_i \sim \text{categorical}(\pi_1, \dots, \pi_K), \quad i = 1, \dots, N,$$

$$x_i | z_i \sim \mathcal{N}(\mu_{z_i}, \sigma_{z_i}^2) \quad i = 1, \dots, N.$$



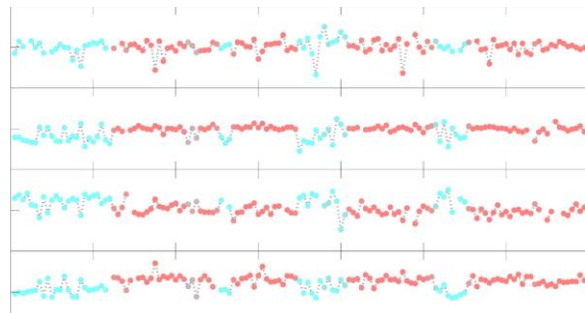
Probabilistic Generative Models

- Example: Hidden Markov Models



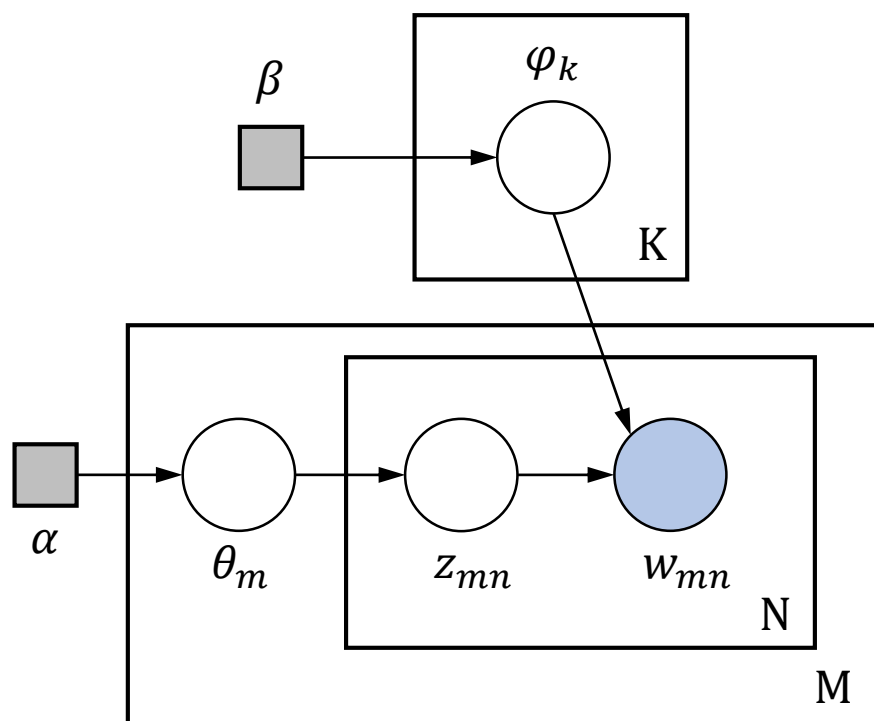
$$h_t \sim \text{categorical}(\boldsymbol{\pi}_{h_{t-1}})$$

$$x_t | h_t \sim F(\boldsymbol{\phi}_{h_t})$$



Probabilistic Generative Models

- Example: Latent Dirichlet Allocation

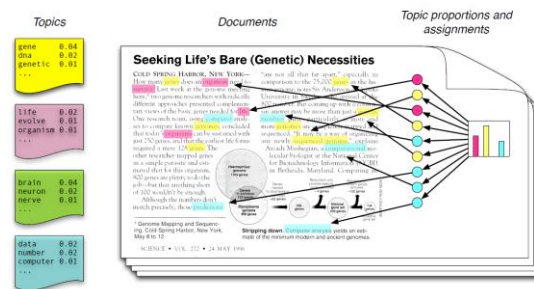


$$\varphi_k \sim \text{Dir}(\beta), \quad k = 1, \dots, K,$$

$$\theta_m \sim \text{Dir}(\alpha), \quad m = 1, \dots, M,$$

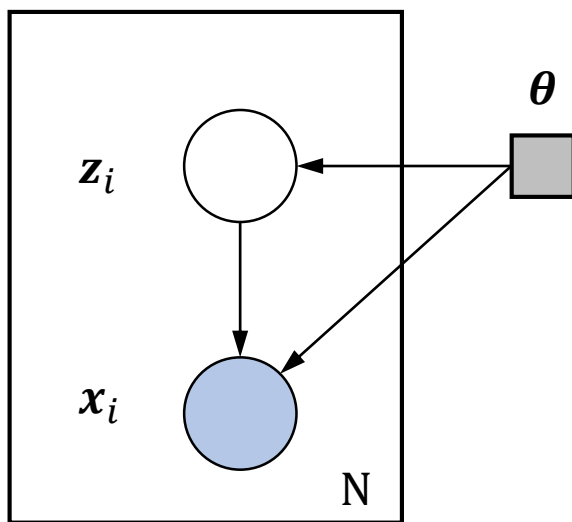
$$z_{mn} | \theta_m \sim \text{categorical}(\theta_m),$$

$$w_{mn} | \varphi, z_{mn} \sim \text{categorical}(\varphi_{z_{mn}})$$



Probabilistic Generative Models

- Example: Deep Latent Gaussian Models



$$\mathbf{z}_i \sim \mathcal{N}(\mathbf{0}, \mathbb{I}), \quad i = 1, \dots, N,$$

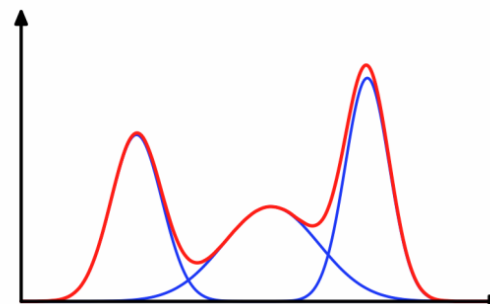
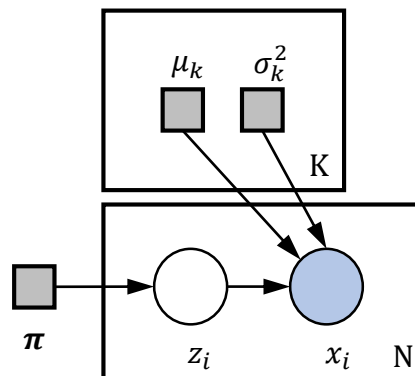
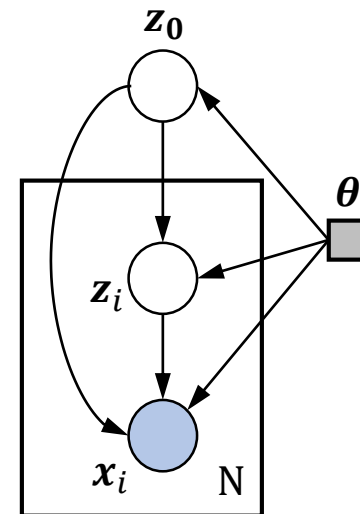
$$\mathbf{x}_i | \mathbf{z}_i \sim \mathcal{N}(\boldsymbol{\mu}(\mathbf{z}_i), \boldsymbol{\sigma}^2(\mathbf{z}_i) \mathbb{I}), \quad i = 1, \dots, N.$$

where $\boldsymbol{\mu}(\cdot)$ and $\boldsymbol{\sigma}(\cdot)$ are neural networks,
 $\boldsymbol{\theta} = \{\text{parameters of } \boldsymbol{\mu} \text{ and } \boldsymbol{\sigma}\}$

Probabilistic Generative Models: Basic Tasks

- Parameter Learning: fit the model to the dataset
 - Maximum likelihood estimation for the parameters θ
- Inference: compute unknown probability distributions
 - **Posterior** distribution of latent variable z
 - **Marginal** distribution of observations x

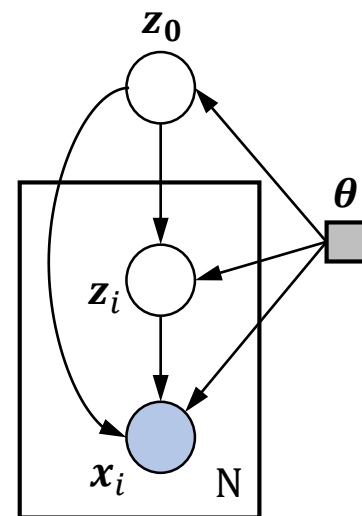
$$p(z|x) = \frac{p(x, z)}{p(x)}$$



The Need for **Approximate** Inference

- **Posterior** distribution of latent variables $\mathbf{z} = \{\mathbf{z}_i\}, i = 1 \dots M$
- **Marginal** distribution of observations $\mathbf{x} = \{\mathbf{x}_i\}, i = 1 \dots N$

$$p(\mathbf{z}|\mathbf{x}) = \frac{p(\mathbf{x}, \mathbf{z})}{p(\mathbf{x})} = \frac{\overbrace{p(\mathbf{x}|\mathbf{z}) p(\mathbf{z})}^{\text{likelihood prior}}}{\underbrace{\int p(\mathbf{x}, \mathbf{z}) d\mathbf{z}}_{\text{marginal/evidence}}}$$



For many models, the integral (or sum) is **intractable**:

- Unavailable in closed form, or
- Requires exponential time to compute.

Approximate Inference of $p(\mathbf{z}|\mathbf{x})$

- Monte Carlo sampling: MCMC (Metropolis-Hasting or Gibbs sampling)
 - Approximate the posterior using samples
 - ✓ Converge to the posterior asymptotically
 - ✗ Computationally intensive
- Variational Inference: turn inference into an optimization problem
 - Set up a **family** of approximate densities \mathbb{Q} over the latent variables
 - Find the member q^* in the family \mathbb{Q} that is closest to the exact posterior

$$q^*(\mathbf{z}) = \arg \min_{q(\mathbf{z}) \in \mathbb{Q}} \text{KL}(q(\mathbf{z}) \| p(\mathbf{z}|\mathbf{x}))$$

- ✓ Tends to be faster and easier to scale to large datasets

Outline

- Probabilistic Generative Models
- **Variational Inference**
- Variational Autoencoder

Variational Inference

- Optimization problem:

$$q^*(\mathbf{z}) = \arg \min_{q(\mathbf{z}) \in \mathbb{Q}} \text{KL}(q(\mathbf{z}) \| p(\mathbf{z}|\mathbf{x}))$$

where

$$\text{KL}(q(\mathbf{z}) \| p(\mathbf{z}|\mathbf{x})) = \int q(\mathbf{z}) \log \frac{q(\mathbf{z})}{p(\mathbf{z}|\mathbf{x})} d\mathbf{z}$$

$$= \mathbb{E}_q[\log q(\mathbf{z})] - \mathbb{E}_q[\log p(\mathbf{z}|\mathbf{x})] \leftarrow \text{intractable}$$

$$= \mathbb{E}_q[\log q(\mathbf{z})] - \mathbb{E}_q[\log p(\mathbf{z}, \mathbf{x})] + \log p(\mathbf{x}) \leftarrow \begin{array}{l} \text{constant,} \\ \text{but intractable} \end{array}$$

- Because we cannot compute the KL, we optimize an alternative objective called **ELBO**:

$$\text{ELBO}(q) = \mathbb{E}_q[\log p(\mathbf{z}, \mathbf{x})] - \mathbb{E}_q[\log q(\mathbf{z})]$$

- Maximizing the ELBO is equivalent to minimizing the KL divergence

Interpretations of the ELBO

$$\text{ELBO}(q) = \mathbb{E}_q[\log p(\mathbf{z}, \mathbf{x})] - \mathbb{E}_q[\log q(\mathbf{z})]$$

- **E**vidence **L**ower **B**ound

$$\log p(\mathbf{x}) = \text{KL}(q(\mathbf{z}) \| p(\mathbf{z} | \mathbf{x})) + \text{ELBO}(q) \geq \text{ELBO}(q)$$

- Maximizing the ELBO is equivalent to minimizing the KL divergence
-

- Another perspective

$$\begin{aligned} \text{ELBO}(q) &= \mathbb{E}_q[\log p(\mathbf{z}, \mathbf{x})] - \mathbb{E}_q[\log q(\mathbf{z})] \\ &= \mathbb{E}_q[\log p(\mathbf{x} | \mathbf{z})] + \mathbb{E}_q[\log p(\mathbf{z})] - \mathbb{E}_q[\log q(\mathbf{z})] \\ &= \mathbb{E}_q[\log p(\mathbf{x} | \mathbf{z})] - \text{KL}(q(\mathbf{z}) \| p(\mathbf{z})) \end{aligned}$$

↑
encourage q to place mass on
configurations of \mathbf{z}
that explain the observed data \mathbf{x}

↖
regularization
term

Variational Inference: Maximizing the **ELBO**

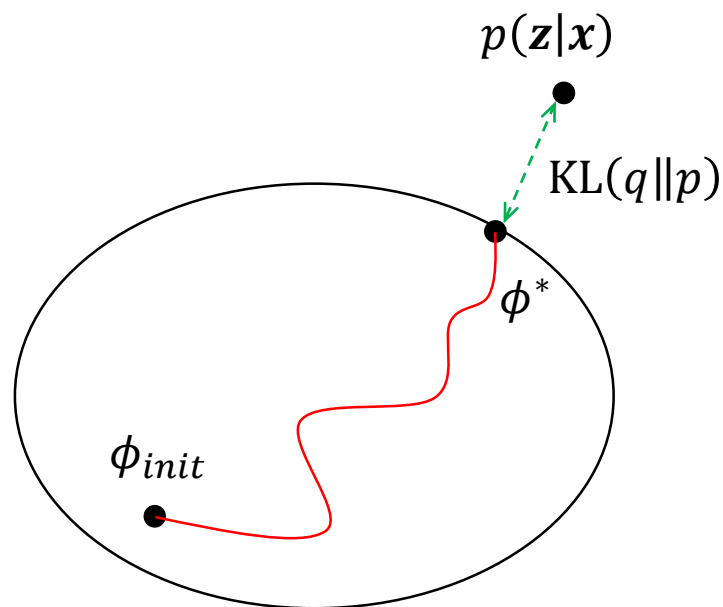
$$\text{ELBO}(q) = \mathbb{E}_q[\log p(\mathbf{z}, \mathbf{x})] - \mathbb{E}_q[\log q(\mathbf{z})]$$

- Given a family of distributions $\mathbb{Q} = \{q_\phi\}$
 - ϕ are the parameters of these distributions
 - Called **variational parameters**
 - E.g., mean and variance of gaussians
- Our task: try to find

$$q^*(\mathbf{z}) = \arg \min_{q_\phi(\mathbf{z}) \in \mathbb{Q}} \text{KL}(q_\phi(\mathbf{z}) \| p(\mathbf{z}|\mathbf{x}))$$

equivalent to find:

$$\begin{aligned} \phi^* &= \arg \min_{\phi} \text{KL}(q_\phi(\mathbf{z}) \| p(\mathbf{z}|\mathbf{x})) \\ &= \arg \max_{\phi} \text{ELBO}(q_\phi) \end{aligned}$$



Traditional Variational Inference

- Recall that $\mathbf{x} = \{\mathbf{x}_i\}, i = 1 \dots N$
- Expand the ELBO:

$$\text{ELBO}(q) = \mathbb{E}_q[\log p(\mathbf{z}, \mathbf{x})] - \mathbb{E}_q[\log q(\mathbf{z})]$$

$$= \sum_{i=1}^N \mathbb{E}_q \left[\log \frac{p(\mathbf{z}, \mathbf{x}_i)}{q(\mathbf{z})} \right]$$

$$\int q(\mathbf{z})(\dots) d\mathbf{z}$$

- Traditional VI:
 - (1) Design a class of **tractable** densities $q_\phi(\mathbf{z}) \in \mathbb{Q}$
 - (2) Derive closed-form expression of the expectation
 - (3) Derive the gradient of the closed-form expectation
 - (4) Use coordinate ascent to update ϕ

Variational Inference: Modern Challenges

$$\text{ELBO}(q) = \mathbb{E}_q[\log p(\mathbf{z}, \mathbf{x})] - \mathbb{E}_q[\log q(\mathbf{z})]$$

$$= \sum_{i=1}^N \mathbb{E}_q \left[\log \frac{p(\mathbf{z}, \mathbf{x}_i)}{q(\mathbf{z})} \right]$$

$\int q(\mathbf{z})(\dots) d\mathbf{z}$

Modern challenges

- Traditional VI:

- (1) Design a class of **tractable** densities $q_\phi(\mathbf{z}) \in \mathbb{Q}$
- (2) Derive closed-form expression of \mathbb{E}_q
- (3) Derive the gradient of the closed-form \mathbb{E}_q
- (4) Use coordinate ascent to update ϕ

- The ELBO involves the whole dataset, but dataset can be **large**
- We want a flexible family \mathbb{Q} (e.g., neural networks), but for such $q \in \mathbb{Q}$, \mathbb{E}_q is generally **intractable**
- We want to handle complex generative models

Variational Inference: Toward Modernization

- Using stochastic optimization to:
 - Scale up VI to massive data
 - Enable VI with flexible families of approximation densities
 - Enable VI on a wide class of complex/difficult models

$$\text{ELBO}(q_\phi) = \sum_{i=1}^N \mathbb{E}_q \left[\log \frac{p(\mathbf{z}, \mathbf{x}_i)}{q_\phi(\mathbf{z})} \right]$$

$\int q(\mathbf{z})(\dots) d\mathbf{z}$

Modern challenges

- ~~The ELBO involves the whole dataset, but dataset can be **large**~~ ← **mini-batch**
- We want a flexible family \mathbb{Q} (e.g., neural networks), but for such $q \in \mathbb{Q}$, \mathbb{E}_q is generally **intractable**
- We want to handle complex generative models

$$\begin{aligned} \nabla_\phi \text{ELBO}(q_\phi) &= \sum_{i=1}^N \nabla_\phi \mathbb{E}_q \left[\log \frac{p(\mathbf{z}, \mathbf{x}_i)}{q_\phi(\mathbf{z})} \right] \\ &\approx \frac{N}{S} \sum_{i=1}^S \nabla_\phi \mathbb{E}_q \left[\log \frac{p(\mathbf{z}, \mathbf{x}_i)}{q_\phi(\mathbf{z})} \right] \end{aligned}$$

???

REINFORCE Gradients

$$\nabla_{\phi} \mathbb{E}_q \left[\log \frac{p(\mathbf{z}, \mathbf{x}_i)}{q_{\phi}(\mathbf{z})} \right]$$

- Remember that \mathbb{E}_q is intractable: $\int q(\mathbf{z})(\dots) d\mathbf{z}$
- A similar problem in reinforcement learning: maximizing the expected reward f : $\mathbb{E}_p[f(\dots)]$
- REINFORCE gradients (also called *score function estimator*)

$$\nabla \mathbb{E}_p[f(\dots)] = \mathbb{E}_p[\nabla \log p(x) f(\dots)]$$

- REINFORCE gradient of the ELBO:

$$\begin{aligned} \nabla_{\phi} \mathbb{E}_q \left[\log \frac{p(\mathbf{z}, \mathbf{x}_i)}{q_{\phi}(\mathbf{z})} \right] &= \mathbb{E}_q \left[\nabla_{\phi} \log q_{\phi}(\mathbf{z}) \log \frac{p(\mathbf{z}, \mathbf{x}_i)}{q_{\phi}(\mathbf{z})} \right] \\ &\approx \frac{1}{M} \sum_{k=1}^M \nabla_{\phi} \log q_{\phi}(\mathbf{z}_k) \log \frac{p(\mathbf{z}_k, \mathbf{x}_i)}{q_{\phi}(\mathbf{z}_k)}, \quad \mathbf{z}_k \sim q_{\phi}(\mathbf{z}) \end{aligned}$$

Monte Carlo Approximation of the Gradient

- We have a gradient estimator for each *single data point* \mathbf{x}_i :

$$\nabla_{\phi} \text{ELBO}(q_{\phi}, \mathbf{x}_i) \approx \frac{1}{M} \sum_{k=1}^M \nabla_{\phi} \log q_{\phi}(\mathbf{z}_k) \log \frac{p(\mathbf{z}_k, \mathbf{x}_i)}{q_{\phi}(\mathbf{z}_k)}, \quad \mathbf{z}_k \sim q_{\phi}(\mathbf{z})$$

- This enables scalable stochastic optimization
 - We can update the variational parameters ϕ using a single data point
- This also enables more flexible families of $q_{\phi} \in \mathbb{Q}$
 - Only require that we can sample from q , rather than requiring \mathbb{E}_q is tractable
- Problem: the **variance** of this gradient estimator is high
 - There are some variance reduction techniques
- One key contribution of the VAE papers is that they proposed a new gradient estimator

Outline

- Probabilistic Generative Models
- Variational Inference
- **Variational Autoencoder**

Auto-Encoding Variational Bayes.
Kingma DP, Welling M. ICLR 2014

Stochastic Backpropagation and Approximate Inference in Deep Generative Models.
Rezende DJ, Mohamed S, Wierstra D. ICML 2014

Stronger Assumptions Enable A New Estimator

- Recall the REINFORCE gradient estimator:

$$\nabla_{\phi} \text{ELBO}(q_{\phi}, \mathbf{x}_i) \approx \frac{1}{M} \sum_{k=1}^M \nabla_{\phi} \log q_{\phi}(\mathbf{z}_k) \log \frac{p(\mathbf{z}_k, \mathbf{x}_i)}{q_{\phi}(\mathbf{z}_k)}, \quad \mathbf{z}_k \sim q_{\phi}(\mathbf{z})$$

- This estimator requires:
 - Sampling from q
 - Evaluation of $\nabla_{\phi} \log q_{\phi}(\mathbf{z})$ and $\log p(\mathbf{z}, \mathbf{x})$
- The VAE papers made two further assumptions:
 - Sampling from $q_{\phi}(\mathbf{z})$ can be reparametrized to sampling from a simple distribution (e.g., standard gaussian)

$$\mathbf{z} \sim q_{\phi}(\mathbf{z}) \Leftrightarrow$$

$$\mathbf{z} = \text{transform}(\boldsymbol{\epsilon}, \phi), \quad \boldsymbol{\epsilon} \sim \text{simple}(\boldsymbol{\epsilon})$$

- $\log p(\mathbf{z}, \mathbf{x})$ and $\log q_{\phi}(\mathbf{z})$ are differentiable with respect to \mathbf{z}

The Reparameterization Trick

- Now we assume the simple distribution is standard gaussian \mathcal{N}

$$\mathbf{z} \sim q_{\phi}(\mathbf{z}) \Leftrightarrow \\ \mathbf{z} = t(\boldsymbol{\epsilon}, \phi), \quad \boldsymbol{\epsilon} \sim \mathcal{N}(\boldsymbol{\epsilon})$$

- Then

$$\begin{aligned} \nabla_{\phi} \text{ELBO}(q_{\phi}, \mathbf{x}_i) &= \nabla_{\phi} \mathbb{E}_{\mathbf{q}} \left[\log \frac{p(\mathbf{z}, \mathbf{x}_i)}{q_{\phi}(\mathbf{z})} \right] \\ &= \nabla_{\phi} \mathbb{E}_{\mathcal{N}(\boldsymbol{\epsilon})} \left[\log \frac{p(t(\boldsymbol{\epsilon}, \phi), \mathbf{x}_i)}{q_{\phi}(t(\boldsymbol{\epsilon}, \phi))} \right] && \leftarrow \text{reparameterization} \\ &= \mathbb{E}_{\mathcal{N}(\boldsymbol{\epsilon})} \left[\nabla_{\phi} \log \frac{p(t(\boldsymbol{\epsilon}, \phi), \mathbf{x}_i)}{q_{\phi}(t(\boldsymbol{\epsilon}, \phi))} \right] && \leftarrow \text{property of gaussian} \\ &= \mathbb{E}_{\mathcal{N}(\boldsymbol{\epsilon})} \left[\nabla_{\mathbf{z}} \log \frac{p(\mathbf{z}, \mathbf{x}_i)}{q_{\phi}(\mathbf{z})} \nabla_{\phi} t(\boldsymbol{\epsilon}, \phi) \right] && \leftarrow \text{chain rule of derivative} \end{aligned}$$

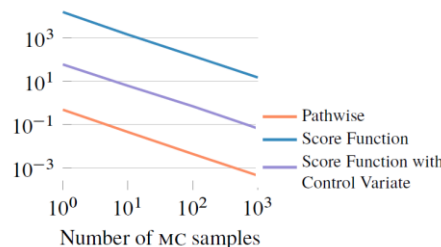
$$\approx \frac{1}{M} \sum_{k=1}^M \nabla_{\mathbf{z}} \log \frac{p(\mathbf{z}, \mathbf{x}_i)}{q_{\phi}(\mathbf{z})} \nabla_{\phi} t(\boldsymbol{\epsilon}_k, \phi), \quad \boldsymbol{\epsilon}_k \sim \mathcal{N}(\boldsymbol{\epsilon})$$

Two Gradient Estimators

- REINFORCE gradient estimator (also call *score function estimator*)

$$\nabla_{\phi} \text{ELBO}(q_{\phi}, x_i) \approx \frac{1}{M} \sum_{k=1}^M \nabla_{\phi} \log q_{\phi}(\mathbf{z}_k) \log \frac{p(\mathbf{z}_k, x_i)}{q_{\phi}(\mathbf{z}_k)}, \quad \mathbf{z}_k \sim q_{\phi}(\mathbf{z})$$

- Requires: (1) sampling from q . (2) evaluation of $\nabla_{\phi} \log q_{\phi}(\mathbf{z})$ and $\log p(\mathbf{z}, x)$
- Variance can be a big problem



- Reparameterization trick (also called *path-wise gradient estimator*)

$$\nabla_{\phi} \text{ELBO}(q_{\phi}, x_i) \approx \frac{1}{M} \sum_{k=1}^M \nabla_{\mathbf{z}} \log \frac{p(\mathbf{z}, x_i)}{q_{\phi}(\mathbf{z})} \nabla_{\phi} t(\epsilon_k, \phi), \quad \epsilon_k \sim \mathcal{N}(\epsilon)$$

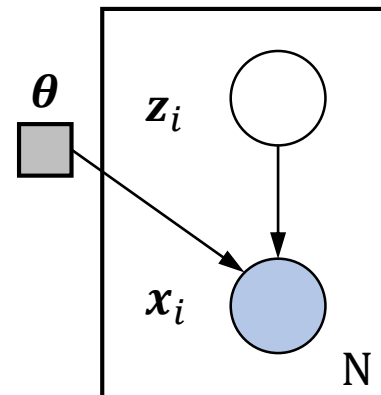
- Requires: (1) \mathbf{z} is parameterizable. (2) $\log p(\mathbf{z}, x)$ & $\log q_{\phi}(\mathbf{z})$ are differentiable
- Variance is generally much smaller

Variational Autoencoders

- Assume a deep latent gaussian generative model

$$\mathbf{z}_i \sim \mathcal{N}(\mathbf{0}, \mathbb{I}), \quad i = 1, \dots, N,$$

$$\mathbf{x}_i | \mathbf{z}_i \sim \mathcal{N}(\boldsymbol{\mu}_{\boldsymbol{\theta}}(\mathbf{z}_i), \boldsymbol{\sigma}_{\boldsymbol{\theta}}^2(\mathbf{z}_i) \mathbb{I}), \quad i = 1, \dots, N.$$



- where $\boldsymbol{\mu}_{\boldsymbol{\theta}}(\cdot)$ and $\boldsymbol{\sigma}_{\boldsymbol{\theta}}(\cdot)$ are neural networks

- Make q dependent on \mathbf{x} : $q_{\phi}(\mathbf{z}) \rightarrow q_{\phi}(\mathbf{z} | \mathbf{x}) = \prod_{i=1}^N q_{\phi}(\mathbf{z}_i | \mathbf{x}_i)$
 - Model the dependence as a neural network (i.e., the *inference network*)

$$\mathbf{z}_i | \mathbf{x}_i \sim q_{\phi}(\mathbf{z}_i | \mathbf{x}_i) = \mathcal{N}(\boldsymbol{\mu}_{\phi}(\mathbf{x}_i), \boldsymbol{\sigma}_{\phi}^2(\mathbf{x}_i) \mathbb{I})$$

where $\boldsymbol{\mu}_{\phi}(\cdot)$ and $\boldsymbol{\sigma}_{\phi}(\cdot)$ are neural networks

- Train the generative parameters $\boldsymbol{\theta}$ and the variational parameters ϕ together

Recall the Two Basic Tasks

- Parameter Learning: fit the model to the dataset
 - Maximum likelihood estimation for the parameters θ
- Inference: compute unknown probability distributions

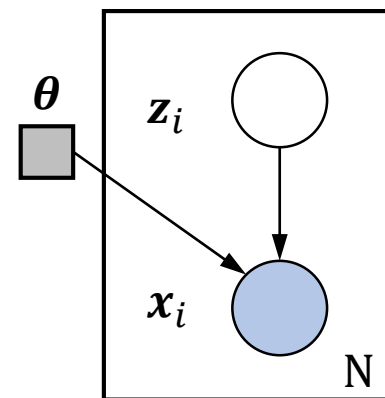
- **Posterior** distribution of latent variable z
- **Marginal** distribution of observations x

$$p(z|x) = \frac{p(x, z)}{p(x)}$$

-
- Generative parameters θ enable us to generate new data
 - Variational parameters ϕ give an approximation of the posterior

$$p(z_i|x_i) \approx q_\phi(z_i|x_i)$$

- Useful for representation learning
 - z_i is the “code” of x_i



Co-training of Generative and Variational Parameters

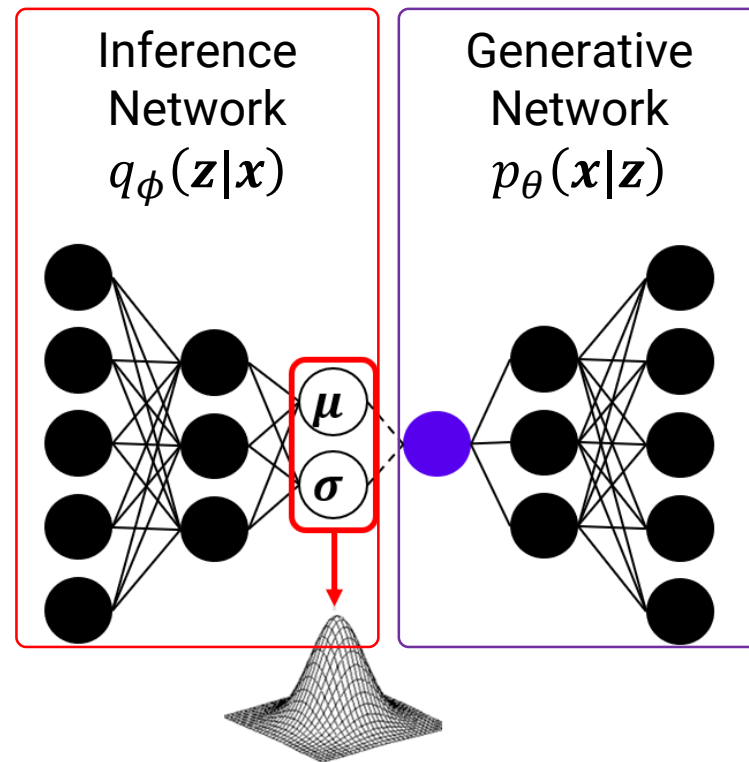
- Recall the ELBO is the Evidence Lower Bound

$$\text{ELBO}(q_\phi) = \mathbb{E}_{q_\phi} [\log p_\theta(\mathbf{z}, \mathbf{x})] - \mathbb{E}_{q_\phi} [\log q_\phi(\mathbf{z}|\mathbf{x})]$$

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

↑
not a constant
any more

optimizing ϕ makes q
approximate
the true posterior



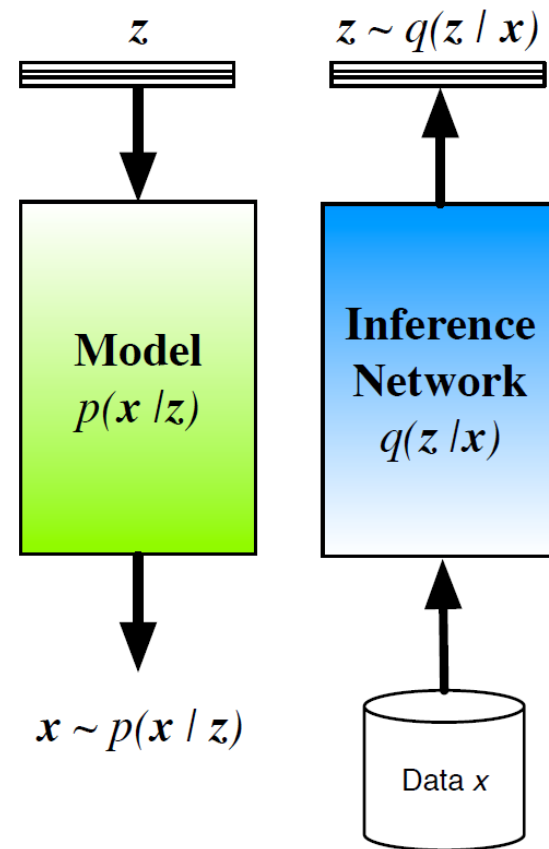
optimizing θ makes
the generative model
fit the data

Optimization of VAE

- Reformulation of the ELBO:

$$\mathbb{E}_{q_{\phi}}[\log p_{\theta}(\mathbf{x}_i | \mathbf{z}_i)] - \text{KL}(q_{\phi}(\mathbf{z}_i | \mathbf{x}_i) \| p(\mathbf{z}_i))$$

- **First term**: use the reparameterization trick to estimate the gradient
- **Second term**: solve the KL in closed-form
 - To reduce the variance of gradient estimator
- Stochastic gradient ascent on both θ and ϕ



Contributions of VAE

- Proposed the reparameterization tricks, which yield a low-variance gradient estimator
- Introduced the inference network
- Co-training of variational parameters and generative parameters

Recent Developments of VAE

- Divergences beyond KL, rethinking of ELBO
 - E.g., **W**asserstein **A**uto-**E**ncoders [ICLR 2018 Oral]
- More powerful and flexible families of approximation densities
 - E.g., Normalizing Flows
- Variance reduction of gradient estimators
 - E.g., Reducing Reparameterization Gradient Variance [NIPS 2017]
- Better ELBOs for structured models, such as sequential models
 - E.g., Auto-Encoding Sequential Monte Carlo [ICLR 2018]
- Combinations of VAE and GAN
- ...

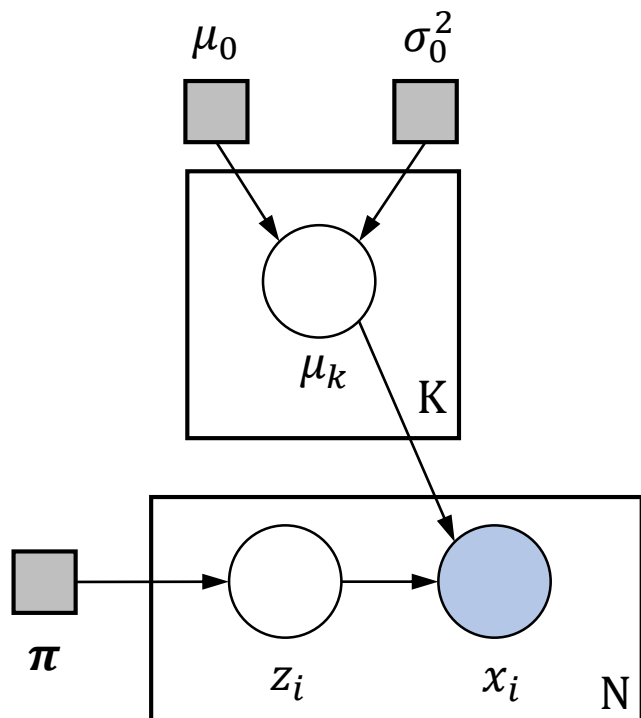
The End

Questions?

Backup Slides

Probabilistic Generative Models

- Example: Mixture of unit-variance univariate Gaussians



$$\mu_k \sim \mathcal{N}(\mu_0, \sigma_0^2), \quad k = 1, \dots, K,$$

$$z_i \sim \text{categorical}(\pi_1, \dots, \pi_K), \quad i = 1, \dots, N,$$

$$x_i | z_i, \boldsymbol{\mu} \sim \mathcal{N}(\mu_{z_i}, 1) \quad i = 1, \dots, N.$$

