

Deep Generative Models: Discrete Latent Variables

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VI Tutorial @ DTU-DIKU 2019 Summer School
vitutorial.github.io/tour/dtudiku2019

- 1 First Attempt: Wake-Sleep
- 2 Neural Variational Inference
- 3 Score function estimator
- 4 Variance reduction

Generative Models

Joint distribution over observed data x and latent variables z .

$$p(x, z|\theta) = \underbrace{p(z)}_{\text{prior}} \underbrace{p(x|z, \theta)}_{\text{likelihood}}$$

The likelihood and prior are often standard distributions (Gaussian, Bernoulli) with simple dependence on conditioning information.

Deep generative models

Joint distribution with **deep observation model**

$$p(x, z|\theta) = \underbrace{p(z)}_{\text{prior}} \underbrace{p(x|z, \theta)}_{\text{likelihood}}$$

mapping from z to $p(x|z, \theta)$ is a NN with parameters θ

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Marginal likelihood

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

intractable in general

Goals

We want

- richer probabilistic models

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- complex observation models parameterised by NNs

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We need **approximate inference** techniques!

ELBO recap

And we've developed the ELBO

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And we've developed the ELBO

$$\begin{aligned} \log p(x) &= \log \int p(z, x) dz = \log \int q(z|x) \frac{p(z, x)}{q(z|x)} dz \\ &\stackrel{\text{JI}}{\geq} \underbrace{\mathbb{E}_{q(z|x)} \left[\log \frac{p(z, x)}{q(z|x)} \right]}_{\text{ELBO}} \end{aligned}$$

ELBO recap

And we've developed the ELBO

$$\log p(x) = \log \int p(z, x) dz = \log \int q(z|x) \frac{p(z, x)}{q(z|x)} dz$$

$$\stackrel{\text{JL}}{\geq} \underbrace{\mathbb{E}_{q(z|x)} \left[\log \frac{p(z, x)}{q(z|x)} \right]}_{\text{ELBO}}$$

$$\begin{aligned} \text{ELBO} &= \mathbb{E}_{q(z|x)} \left[\log \frac{p(z|x)p(x)}{q(z|x)} \right] \\ &= - \underbrace{\text{KL} (q(z|x) \parallel p(z|x))}_{\text{gap}} + \log p(x) \end{aligned}$$

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Wake-sleep Algorithm

- Generalise latent variables to Neural Networks
- Train generative neural model
- Use variational inference! (kind of)

Wake-sleep Architecture

2 Neural Networks:

Wake-sleep Architecture

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- A generation network to model the data (the one we want to optimise) – parameters: θ

Wake-sleep Architecture

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Wake-sleep Architecture

2 Neural Networks:

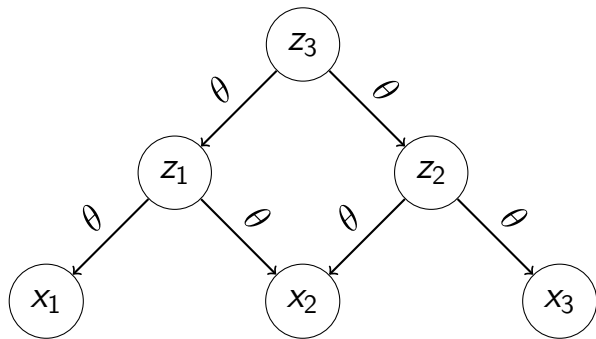
- A generation network to model the data (the one we want to optimise) – parameters: θ
- An inference (recognition) network (to model the latent variable) – parameters: λ
- Original setting: binary hidden units

Wake-sleep Architecture

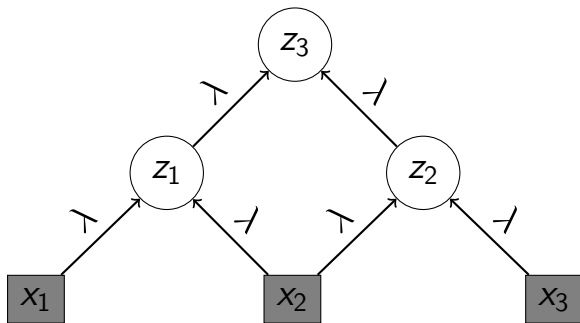
2 Neural Networks:

- A generation network to model the data (the one we want to optimise) – parameters: θ
- An inference (recognition) network (to model the latent variable) – parameters: λ
- Original setting: binary hidden units
- Training is performed in a “hard EM” fashion

Generator



Inference Network



Wake-sleep Training

Wake Phase

- Use inference network to sample hidden unit setting z from $q(z|x, \lambda)$
- Update generation parameters θ to maximize joint log-likelihood of data and latents $p(x, z|\theta)$

Wake-sleep Training

Wake Phase

- Use inference network to sample hidden unit setting z from $q(z|x, \lambda)$
- Update generation parameters θ to maximize joint log-likelihood of data and latents $p(x, z|\theta)$

Sleep Phase

- Produce dream sample \tilde{x} from random hidden unit z
- Update inference parameters λ to maximize probability of latent state $q(z|\tilde{x}, \lambda)$

Wake Phase Objective

Objective

$$\begin{aligned} \arg \max_{\theta} \mathbb{E}_{p(x)} [\text{ELBO}(\theta, \lambda|x)] \\ = \arg \max_{\theta} \mathbb{E}_{p(x)} [\mathbb{E}_{q(z|x, \lambda)} [\log p(z, x|\theta)] + \mathbb{H}[q(z|x, \lambda)]] \end{aligned}$$

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Gradient wrt θ for $x \sim p(x)$

$$\nabla_{\theta} \mathbb{E}_{q(z|x, \lambda)} [\log p(z, x|\theta)] + \nabla_{\theta} \mathbb{H}[q(z|x, \lambda)]$$

Wake Phase Objective

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Wake Phase Objective

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Gradient wrt θ for $x \sim p(x)$

$$\begin{aligned} \nabla_{\theta} \mathbb{E}_{q(z|x, \lambda)} [\log p(z, x|\theta)] + \nabla_{\theta} \mathbb{H}[q(z|x, \lambda)] \\ = \mathbb{E}_{q(z|x, \lambda)} [\nabla_{\theta} \log p(z, x|\theta)] \\ \stackrel{\text{MC}}{\approx} \nabla_{\theta} \log p(z, x|\theta) \quad \text{where } z \sim q(z|x, \lambda) \end{aligned}$$

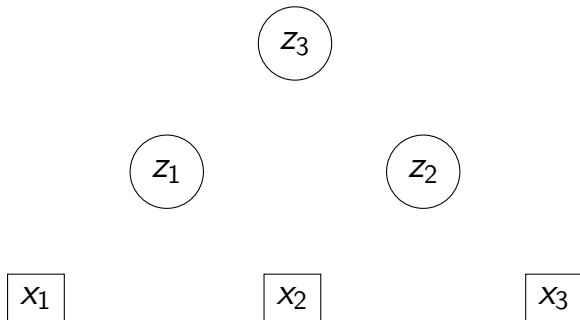
Wake Phase Objective

Assumes z to be fixed random draw from $q(z|x, \lambda)$
and maximises $\log p(z, x|\theta)$.

This is simply supervised learning with imputed latent data!

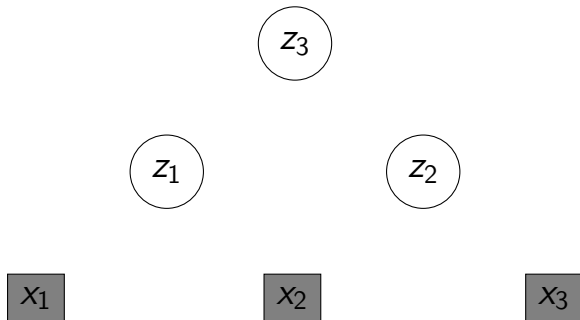
Wake Phase Sampling

Sampling $z \sim q(z|x, \lambda)$



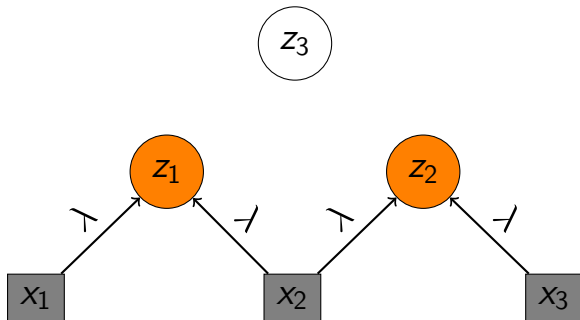
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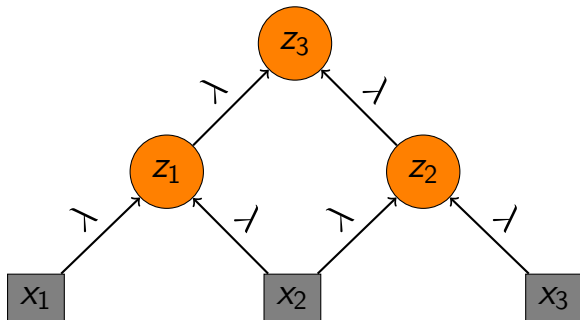
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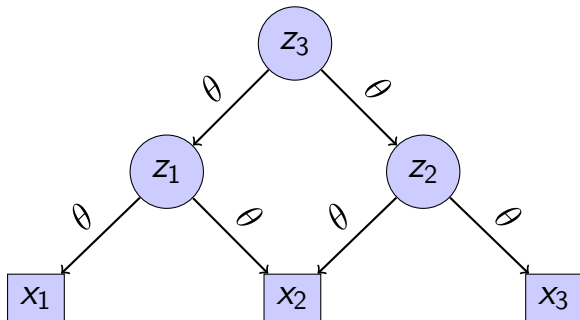
Wake Phase Sampling

Sampling $z \sim q(z|x, \lambda)$



Wake Phase Update

Compute $\log p(x, z|\theta)$ and update θ



Sleep Phase Objective

Objective

$$\begin{aligned} & \arg \max_{\theta} \mathbb{E}_{p(x)} [\text{ELBO}(\theta, \lambda|x)] \\ &= \arg \max_{\theta} \mathbb{E}_{p(x)} [\mathbb{E}_{q(z|x, \lambda)} [\log p(z, x|\theta)] + \mathbb{H}[q(z|x, \lambda)]] \end{aligned}$$

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Gradient wrt λ for $x \sim p(x)$

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Let's change the objective!

Sleep Phase (Convenient) Objective

Flip the direction of the KL

$$\arg \min_{\lambda} \mathbb{E}_{p(x)} [\text{KL} (p(z|x, \theta) || q(z|x, \lambda))]$$

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Sleep Phase (Convenient) Objective

Flip the direction of the KL

$$\begin{aligned}
 & \arg \min_{\lambda} \mathbb{E}_{p(x)} [\text{KL} (p(z|x, \theta) \parallel q(z|x, \lambda))] \\
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Gradient wrt λ

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 &= \mathbb{E}_{p(z|\theta)p(x|z, \theta)} [\nabla_{\lambda} \log q(z|x, \lambda)]
 \end{aligned}$$

Sleep Phase (Convenient) Objective

Assumes **fake data** \tilde{x} and latent variables z to be fixed random draws from $p(x, z|\theta)$ via

$$z \sim p(z|\theta)$$

$$\tilde{x} \sim p(x|z, \theta)$$

and maximises $\log q(z|\tilde{x}, \lambda)$.

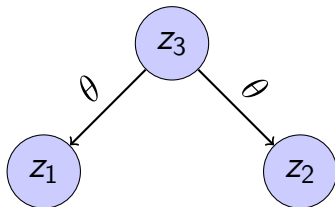
Sleep Phase Sampling

Sampling $(z, \tilde{x}) \sim p(x, z|\theta)$



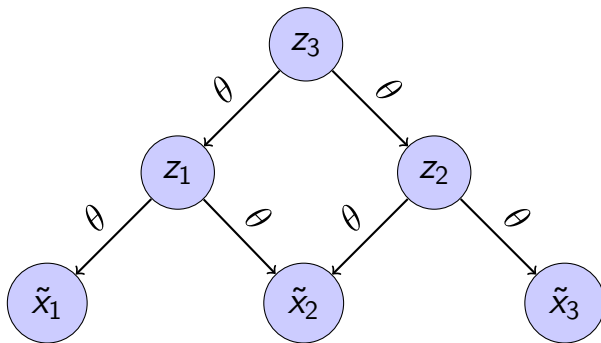
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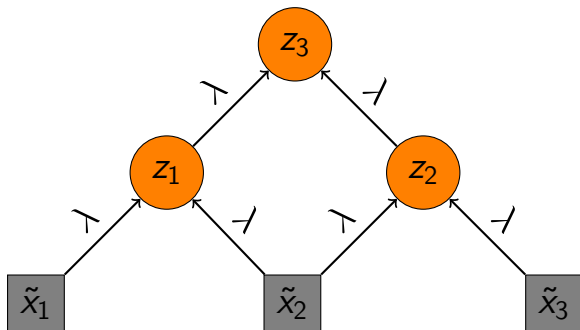
Sleep Phase Sampling

Sampling $(z, \tilde{x}) \sim p(x, z|\theta)$



Sleep Phase Update

Compute $\log q(z|\tilde{x}, \lambda)$ and update λ



Wake-sleep Algorithm

Advantages

- Simple layer-wise updates
- Amortised inference: all latent variables are inferred from the same weights λ

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Drawbacks

- Inference and generative networks are trained on different objectives
- Inference weights λ are updated on fake data \tilde{x}
- Generative weights are bad initially, giving wrong signal to the updates of λ

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Variational Inference Learning (NVIL)

Generative model with NN likelihood

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Let us consider a latent factor model for topic modelling:

Variational Inference Learning (NVIL)

Generative model with NN likelihood

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- a document $x = (x_1, \dots, x_N)$ consists of n i.i.d. categorical draws from that model

Variational Inference Learning (NVIL)

Generative model with NN likelihood

Let us consider a latent factor model for topic modelling:

- a document $x = (x_1, \dots, x_N)$ consists of n i.i.d. categorical draws from that model
- the categorical distribution in turn depends on binary latent factors $z = (z_1, \dots, z_K)$ which are also i.i.d.

Latent factor model

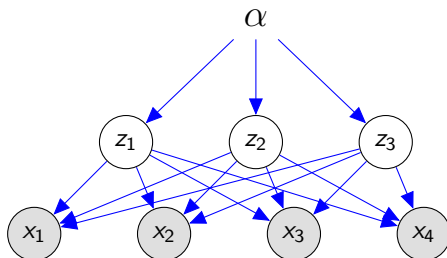
$$Z_j \sim \text{Bernoulli}(\alpha) \quad (1 \leq k \leq K)$$

$$X_i|z \sim \text{Categorical}(f(z; \theta)) \quad (1 \leq i \leq N)$$

Here $0 < \alpha < 1$ specifies a Bernoulli prior
and $f(\cdot; \theta)$ is a function computed by a
neural network with softmax output, e.g.

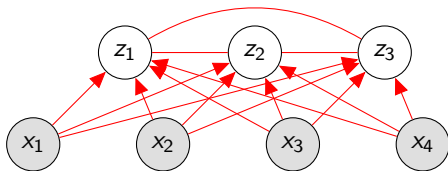
$$f(z; \theta) = \text{softmax}(Wz + b)$$
$$\theta = \{W, b\}$$

Example Model



Joint distribution: independent latent variables

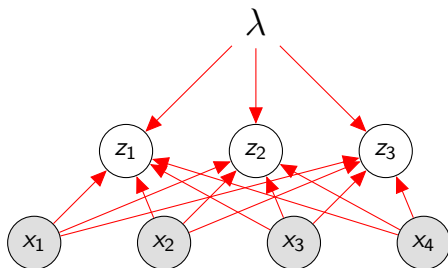
Example Model



Posterior: latent variables are marginally dependent.

For our variational distribution we are going to assume that they are not (recall: mean field assumption).

Mean Field Inference



The inference network needs to predict K Bernoulli parameters b_1^K . Any neural network with sigmoid output will do that job.

Inference Network

$$q(z|x, \lambda) = \prod_{k=1}^K \text{Bern}(z_k | b_k)$$

where $b_1^K = g(x; \lambda)$

Example architecture

$$h = \frac{1}{N} \sum_{i=1}^N E_{x_i} \quad b_1^K = \text{sigmoid}(Mh + c)$$

$$\lambda = \{E, M, c\}$$

Objective

$$\text{ELBO} = \mathbb{E}_{q(z|x, \lambda)} [\log p(x, z|\theta)] + \mathbb{H}(q(z|x, \lambda))$$

Objective

$$\begin{aligned}\text{ELBO} &= \mathbb{E}_{q(z|x, \lambda)} [\log p(x, z|\theta)] + \mathbb{H}(q(z|x, \lambda)) \\ &= \mathbb{E}_{q(z|x, \lambda)} [\log p(x|z, \theta)] - \text{KL}(q(z|x, \lambda) \parallel p(z))\end{aligned}$$

Objective

$$\begin{aligned}\text{ELBO} &= \mathbb{E}_{q(z|x, \lambda)} [\log p(x, z|\theta)] + \mathbb{H}(q(z|x, \lambda)) \\ &= \mathbb{E}_{q(z|x, \lambda)} [\log p(x|z, \theta)] - \text{KL}(q(z|x, \lambda) \parallel p(z))\end{aligned}$$

Parameter estimation

$$\arg \max_{\theta, \lambda} \mathbb{E}_{q(z|x, \lambda)} [\log p(x|z, \theta)] - \text{KL}(q(z|x, \lambda) \parallel p(z))$$

KL

KL between K independent Bernoulli distributions is tractable

$$\text{KL}(q(z|x, \lambda) \parallel p(z|\alpha)) = \sum_{k=1}^K \text{KL}(q(z_k|x, \lambda) \parallel p(z_k|\alpha))$$

KL

KL between K independent Bernoulli distributions is tractable

$$\begin{aligned}\text{KL}(q(z|x, \lambda) \parallel p(z|\alpha)) &= \sum_{k=1}^K \text{KL}(q(z_k|x, \lambda) \parallel p(z_k|\alpha)) \\ &= \sum_{k=1}^K \text{KL}(\text{Bernoulli}(b_k) \parallel \text{Bernoulli}(\alpha))\end{aligned}$$

KL

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$$\begin{aligned}\text{KL}(q(z|x, \lambda) \parallel p(z|\alpha)) &= \sum_{k=1}^K \text{KL}(q(z_k|x, \lambda) \parallel p(z_k|\alpha)) \\ &= \sum_{k=1}^K \text{KL}(\text{Bernoulli}(b_k) \parallel \text{Bernoulli}(\alpha)) \\ &= \sum_{k=1}^K b_k \log \frac{b_k}{\alpha} + (1 - b_k) \log \frac{1 - b_k}{1 - \alpha}\end{aligned}$$

Generative Network Gradient

$$\frac{\partial}{\partial \theta} \left(\mathbb{E}_{q(z|x, \lambda)} [\log p(x|z, \theta)] - \overbrace{\text{KL}(q(z|x, \lambda) || p(z))}^{\text{constant wrt } \theta} \right)$$

Generative Network Gradient

$$\begin{aligned}
 & \frac{\partial}{\partial \theta} \left(\mathbb{E}_{q(z|x, \lambda)} [\log p(x|z, \theta)] - \overbrace{\text{KL}(q(z|x, \lambda) || p(z))}^{\text{constant wrt } \theta} \right) \\
 &= \underbrace{\mathbb{E}_{q(z|x, \lambda)} \left[\frac{\partial}{\partial \theta} \log p(x|z, \theta) \right]}_{\text{expected gradient :)}}
 \end{aligned}$$

Generative Network Gradient

$$\begin{aligned}
 & \frac{\partial}{\partial \theta} \left(\mathbb{E}_{q(z|x, \lambda)} [\log p(x|z, \theta)] - \overbrace{\text{KL}(q(z|x, \lambda) || p(z))}^{\text{constant wrt } \theta} \right) \\
 &= \underbrace{\mathbb{E}_{q(z|x, \lambda)} \left[\frac{\partial}{\partial \theta} \log p(x|z, \theta) \right]}_{\text{expected gradient :)}} \\
 &\stackrel{\text{MC}}{\approx} \frac{1}{S} \sum_{s=1}^S \frac{\partial}{\partial \theta} \log p(x|z^{(s)}, \theta) \quad \text{where } z^{(s)} \sim q(z|x, \lambda)
 \end{aligned}$$

Inference Network Gradient

$$\frac{\partial}{\partial \lambda} \left(\mathbb{E}_{q(z|x, \lambda)} [\log p(x|z, \theta)] - \overbrace{\text{KL} (q(z|x, \lambda) || p(z))}^{\text{analytical}} \right)$$

Inference Network Gradient

$$\begin{aligned}
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 &= \frac{\partial}{\partial \lambda} \mathbb{E}_{q(z|x, \lambda)} [\log p(x|z, \theta)] - \underbrace{\frac{\partial}{\partial \lambda} \text{KL}(q(z|x, \lambda) \parallel p(z))}_{\text{analytical computation}}
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 \end{aligned}$$

The first term again requires approximation by sampling, but there is a problem

Inference Network Gradient

$$\frac{\partial}{\partial \lambda} \mathbb{E}_{q_{\lambda}(z|x)} [\log p_{\theta}(x|z)]$$

Inference Network Gradient

$$\begin{aligned} & \frac{\partial}{\partial \lambda} \mathbb{E}_{q_{\lambda}(z|x)} [\log p_{\theta}(x|z)] \\ &= \frac{\partial}{\partial \lambda} \sum_z q(z|x, \lambda) \log p(x|z, \theta) \end{aligned}$$

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 &= \frac{\partial}{\partial \lambda} \sum_z q(z|x, \lambda) \log p(x|z, \theta) \\
 &= \underbrace{\sum_z \frac{\partial}{\partial \lambda} (q(z|x, \lambda)) \log p(x|z, \theta)}_{\text{not an expectation}}
 \end{aligned}$$

Inference Network Gradient

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- MC estimator is non-differentiable

Inference Network Gradient

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 & \frac{\partial}{\partial \lambda} \mathbb{E}_{q_{\lambda}(z|x)} [\log p_{\theta}(x|z)] \\
 &= \frac{\partial}{\partial \lambda} \sum_z q(z|x, \lambda) \log p(x|z, \theta) \\
 &= \underbrace{\sum_z \frac{\partial}{\partial \lambda} (q(z|x, \lambda)) \log p(x|z, \theta)}_{\text{not an expectation}}
 \end{aligned}$$

- MC estimator is non-differentiable
- Differentiating the expression does not yield an expectation: cannot approximate via MC

Score function estimator

We can again use the log identity for derivatives

$$\begin{aligned} & \frac{\partial}{\partial \lambda} \mathbb{E}_{q_{\lambda}(z|x)} [\log p_{\theta}(x|z)] \\ &= \sum_z \frac{\partial}{\partial \lambda} (q(z|x, \lambda)) \log p(x|z, \theta) \end{aligned}$$

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 &= \underbrace{\mathbb{E}_{q(z|x, \lambda)} \left[\log p(x|z, \theta) \frac{\partial}{\partial \lambda} \log q(z|x, \lambda) \right]}_{\text{expected gradient :)}}
 \end{aligned}$$

Score function estimator: remarks

We can now build an MC estimator

$$\begin{aligned} & \frac{\partial}{\partial \lambda} \mathbb{E}_{q(z|x, \lambda)} [\log p(x|z, \theta)] \\ &= \mathbb{E}_{q(z|x, \lambda)} \left[\log p(x|z, \theta) \frac{\partial}{\partial \lambda} \log q(z|x, \lambda) \right] \end{aligned}$$

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where $z^{(s)} \sim q(z|x, \lambda)$

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- magnitude of $\log p(x|z, \theta)$ varies widely

Score function estimator: remarks

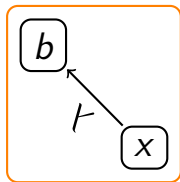
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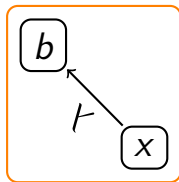
- magnitude of $\log p(x|z, \theta)$ varies widely
- model likelihood does not contribute to direction of gradient

Computation Graph



inference model

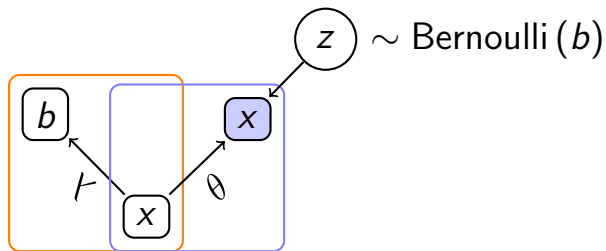
Computation Graph



$$z \sim \text{Bernoulli}(b)$$

inference model

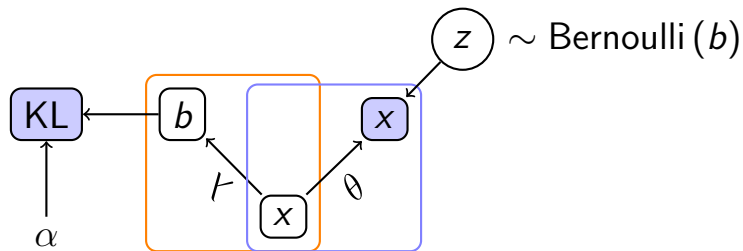
Computation Graph



inference model

generation model

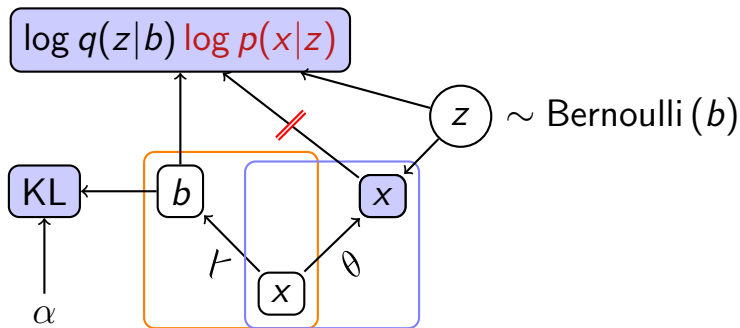
Computation Graph



inference model

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Computation Graph



inference model

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Pros and Cons

- Pros
 - Applicable to all distributions
 - Many libraries come with samplers for common distributions

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- 1 First Attempt: Wake-Sleep
- 2 Neural Variational Inference
- 3 Score function estimator
- 4 Variance reduction**

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When variance is high we can

- sample more
- use variance reduction techniques (e.g. baselines and control variates)

Control variates

Intuition

To estimate $\mathbb{E}[f(z)]$ via Monte Carlo we compute the empirical average of $\hat{f}(z)$ where $\hat{f}(z)$ is chosen so that $\mathbb{E}[\hat{f}(z)] = \mathbb{E}[f(z)]$ and $\text{Var}(f) > \text{Var}(\hat{f})$.

Equivalent expectations

Let $\bar{f} = \mathbb{E}[f(z)]$ be an expectation of interest

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it holds that $\mathbb{E}[\hat{f}(z)] = \mathbb{E}[f(z)]$
- and $\text{Var}(\hat{f}) = \text{Var}(f) - 2b \text{Cov}(f, c) + b^2 \text{Var}(c)$

Choosing the control variate

- 1 $\hat{f}(z) \triangleq f(z) - b(c(z) - \mathbb{E}[c(z)])$
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Of course, $\mathbb{E}[c(z)]$ must be known!

MC

We then use the estimate

$$\bar{f} \stackrel{\text{MC}}{\approx} \frac{1}{S} \left(\sum_{s=1}^S f(z^{(s)}) - bc(z^{(s)}) \right) + b\bar{c}$$

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And recall that for us

$$f(z) = \log p(x|z, \theta) \frac{\partial}{\partial \lambda} \log q(z|x, \lambda)$$

and $z^{(s)} \sim q(z|x, \lambda)$

Expected score

The Expectation of the score function is 0.

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Baselines

With

$$f(z) = \log p(x|z, \theta) \frac{\partial}{\partial \lambda} \log q(z|x, \lambda)$$

and

$$c(z) = \frac{\partial}{\partial \lambda} \log q(z|x, \lambda)$$

we have

$$\hat{f}(z) =$$

Baselines

With

$$f(z) = \log p(x|z, \theta) \frac{\partial}{\partial \lambda} \log q(z|x, \lambda)$$

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we have

$$\hat{f}(z) = (\log p(x|z, \theta) - b) \frac{\partial}{\partial \lambda} \log q(z|x, \lambda)$$

Baselines

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$$f(z) = \log p(x|z, \theta) \frac{\partial}{\partial \lambda} \log q(z|x, \lambda)$$

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$$c(z) = \frac{\partial}{\partial \lambda} \log q(z|x, \lambda)$$

we have

$$\hat{f}(z) = (\log p(x|z, \theta) - b) \frac{\partial}{\partial \lambda} \log q(z|x, \lambda)$$

b is known as *baseline* ([Williams, 1992](#)).

Examples of baselines

- Moving average of $\log p(x|z, \theta)$
based on previous batches

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- Moving average of $\log p(x|z, \theta)$ based on previous batches
- A trainable constant b
- A neural network prediction based on x e.g. $b(x; \omega)$
- The likelihood assessed at a deterministic point, e.g. $b(x) = \log p(x|z^*, \theta)$ where $z^* = \arg \max_z q(z|x, \lambda)$

Trainable baselines

Baselines are predicted by a regression model (e.g. a neural net).

The model is trained using an L_2 -loss.

$$\min_{\omega} (b(x; \omega) - \log p(x|z, \theta))^2$$

Summary

- Wake-Sleep: train inference and generation networks with separate objectives

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- Wake-Sleep: train inference and generation networks with separate objectives
- NVIL: a single objective (ELBO) for both models
- Use score function estimator
- Always use baselines for variance reduction!

Implementation

Check one of our notebooks, e.g.

- inducing rationales for sentiment classification
github.com/vitutorial/exercises/tree/master/SST

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