Deep Generative Models: Discrete Latente Variables

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https://github.com/philschulz/VITutorial

First Attempt: Wake-Sleep

Neural Variational Inference

Score function estimator

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

Deep generative models

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

Marginal likelihood

$$p(x|\theta) = \int p(x, z|\theta)\,\mathrm{d}z = \int p(z)p(x|z, \theta)\,\mathrm{d}z$$

intractable in general

Goals

We want

- richer probabilistic models

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- complex observation models parameterised by NNs

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but we can't perform gradient-based MLE

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but we can't perform gradient-based MLE

We need approximate inference techniques!

First Attempt: Wake-Sleep

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Variance reduction

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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- An inference (recognition) network (to model the latent variable) – parameters: λ

Wake-sleep Architecture

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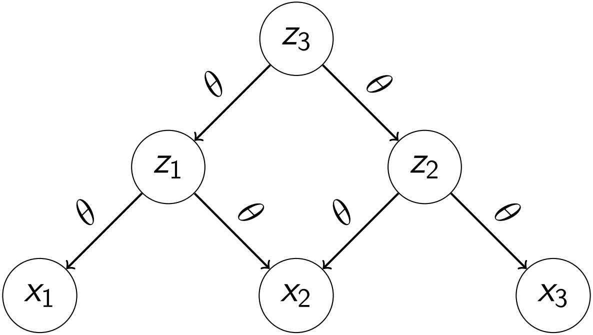
- An inference (recognition) network (to model the latent variable) – parameters: λ
- Original setting: binary hidden units

Wake-sleep Architecture

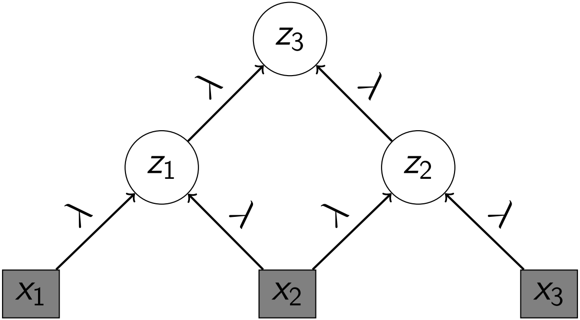
2 Neural Networks:

- 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 join log-liklelihood 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 join log-liklelihood 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

$$\arg\min_{\theta} \mathrm{KL}\left(q(z|x,\lambda) \;||\; p(z|x,\theta)\right)$$

Wake Phase Objective

Objective

$$\begin{aligned}
&\arg\min_{\theta} \mathrm{KL}\left(q(z|x,\lambda) \;||\; p(z|x,\theta)\right) \\
&= \arg\max_{\theta} \; \underbrace{\mathbb{E}_{q(z|x,\lambda)}\left[\log p(z,x|\theta)\right] + \mathbb{H}[q(z|x,\lambda)]}_{\mathcal{G}(\theta)}
\end{aligned}$$

Wake Phase Objective

Objective

$$\arg\min_{\theta} \mathrm{KL}\left(q(z|x,\lambda) \;||\; p(z|x,\theta)\right)$$
$$= \arg\max_{\theta} \; \underbrace{\mathbb{E}_{q(z|x,\lambda)}\left[\log p(z,x|\theta)\right] + \mathbb{H}[q(z|x,\lambda)]}_{\mathcal{G}(\theta)}$$

Gradient estimate

$$\boldsymbol{\nabla}_{\theta}\mathcal{G}(\theta) = \boldsymbol{\nabla}_{\theta}\mathbb{E}_{q(z|x,\lambda)}\left[\log p(z,x|\theta)\right] + \boldsymbol{\nabla}_{\theta}\mathbb{H}[q(z|x,\lambda)]$$

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Gradient estimate

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

Wake Phase Objective

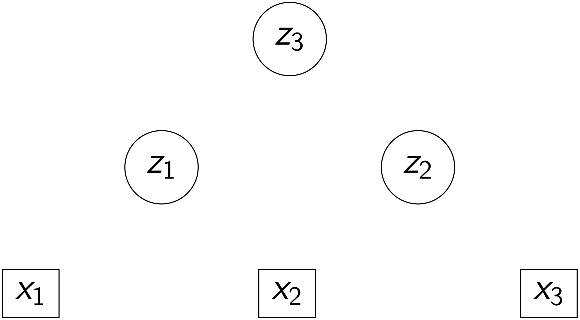
Assumes latent state z to be fixed random draws from $q(z|x, \lambda)$.

$$\arg\min_{\theta} \mathrm{KL}\left(q(z|x, \lambda) \;||\; p(z|x, \theta)\right)$$
$$\overset{\mathrm{MC}}{\approx} \arg\max_{\theta} \log p(z, x|\theta)$$

This is simply supervised learning with imputed latent data!

Wake Phase Sampling

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



Wake Phase Sampling

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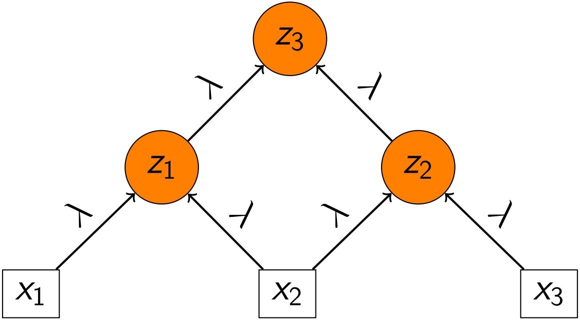
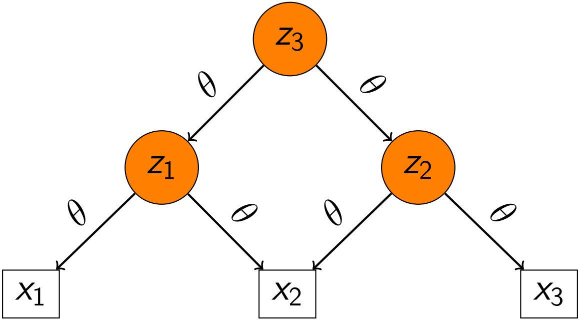


Wake Phase Update

Update θ



Sleep Phase Objective

Objective

$$\arg\min_{\lambda} \mathrm{KL}\left(q(z|x,\lambda) \mid\mid p(z|x,\theta)\right)$$

Sleep Phase Objective

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$$\begin{aligned}
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$$\boldsymbol{\nabla}_{\lambda}\mathcal{R}(\lambda) = \boldsymbol{\nabla}_{\lambda}\mathbb{E}_{q(z|x,\lambda)}\left[\log p(z,x|\theta)\right] + \boldsymbol{\nabla}_{\lambda}\mathbb{H}[q(z|x,\lambda)]$$

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Let's change the objective!

Sleep Phase (Convenient) Objective

Flip the direction of the KL

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

Sleep Phase (Convenient) Objective

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Sleep Phase (Convenient) Objective

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Gradient

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\end{aligned}
$$

Sleep Phase (Convenient) Objective

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

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

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$$
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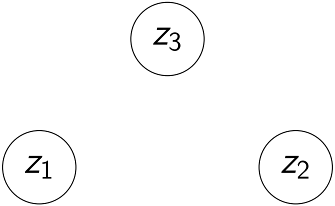
& \arg\max_{\lambda} \; \mathbb{E}_{p(x,z|\theta)} [\log q(z|x, \lambda)] \\
\overset{\text{MC}}{\approx} \; & \arg\max_{\lambda} \; \log q(z|\tilde{x}, \lambda)
\end{aligned}
$$

where $z \sim p(z)$ and $\tilde{x} \sim p(x|z)$ (fake data!)

Sleep Phase Sampling

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



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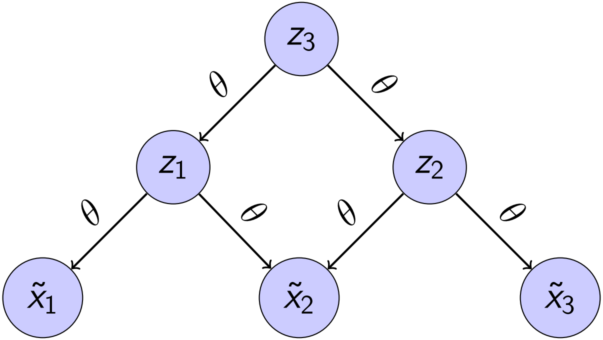
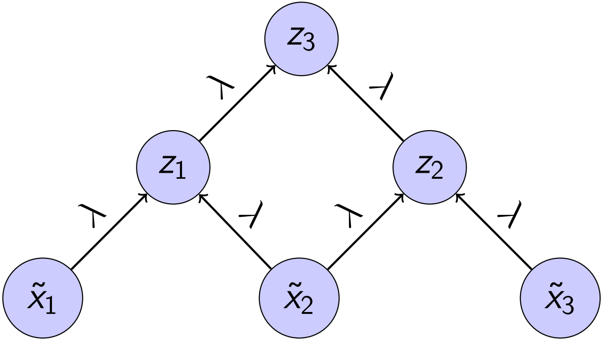


Sleep Phase Update

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

First Attempt: Wake-Sleep

Neural Variational Inference

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Variance reduction

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)

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- a document $x = (x_1, \ldots, x_N)$ 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.

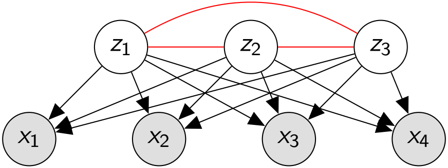
Latent factor model

$$\begin{aligned} Z_j &\sim \text{Bernoulli}(\phi) && (1 \leq k \leq K) \\ X_i | z &\sim \text{Categorical}(f(z;\theta)) && (1 \leq i \leq N) \end{aligned}$$

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

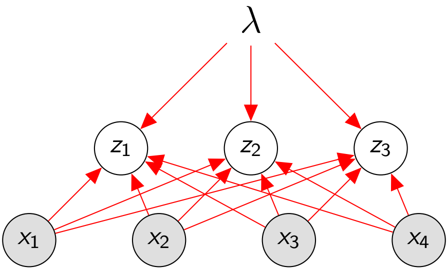
$$\begin{aligned} f(z;\theta) &= \text{softmax}(Wz + b) \\ \theta &= \{W, b\} \end{aligned}$$

Example Model



At inference time the 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

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

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

Example architecture

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

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

Objective

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

Parameter estimation

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

KL

KL between K independent Bernoulli distributions is tractable

$$\mathrm{KL}\left(q(z|x,\lambda)\ ||\ p(z|\phi)\right) = \sum_{k=1}^{K} \mathrm{KL}\left(q(z_k|x,\lambda)\ ||\ p(z_k|\phi)\right)$$

$$= \sum_{k=1}^{K} b_k \log \frac{b_k}{\phi} + (1-b_k) \log \frac{1-b_k}{1-\phi}$$

Generative Network Gradient

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

Generative Network Gradient

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

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

Generative Network Gradient

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$$\overset{\text{MC}}{\approx} \frac{1}{S}\sum_{s=1}^{S}\frac{\partial}{\partial \theta}\log p(x|z^{(s)},\theta) \quad \text{where } z^{(s)} \sim q(z|x,\lambda)$$

Inference Network Gradient

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

Inference Network Gradient

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

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

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

Inference Network Gradient

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

Inference Network Gradient

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

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

- MC estimator is non-differentiable

Inference Network Gradient

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

- 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

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

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

Score function estimator

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

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

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

Score function estimator: remarks

We can now build an MC estimator

$$\begin{aligned}
&\frac{\partial}{\partial \lambda} \mathbb{E}_{q(z|x,\lambda)} [\log p(x|z,\theta)] \\
&= \mathbb{E}_{q(z|x,\lambda)} \left[\log p(x|z,\theta) \frac{\partial}{\partial \lambda} \log q(z|x,\lambda) \right] \\
&\overset{\text{MC}}{\approx} \frac{1}{S} \sum_{s=1}^{S} \log p(x|z^{(s)},\theta) \frac{\partial}{\partial \lambda} \log q(z^{(s)}|x,\lambda)
\end{aligned}$$

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

Score function estimator: remarks

We can now build an MC estimator

$$\frac{\partial}{\partial \lambda}\mathbb{E}_{q(z|x,\lambda)}\left[\log p(x|z,\theta)\right]$$
$$= \mathbb{E}_{q(z|x,\lambda)}\left[\log p(x|z,\theta)\frac{\partial}{\partial \lambda}\log q(z|x,\lambda)\right]$$
$$\overset{\text{MC}}{\approx} \frac{1}{S}\sum_{s=1}^{S} \log p(x|z^{(s)},\theta)\frac{\partial}{\partial \lambda}\log q(z^{(s)}|x,\lambda)$$

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

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

Score function estimator: remarks

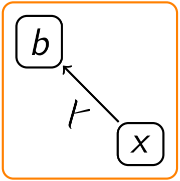
We can now build an MC estimator

$$
\begin{aligned}
&\frac{\partial}{\partial \lambda}\mathbb{E}_{q(z|x,\lambda)}\left[\log p(x|z,\theta)\right] \\
&= \mathbb{E}_{q(z|x,\lambda)}\left[\log p(x|z,\theta)\frac{\partial}{\partial \lambda}\log q(z|x,\lambda)\right] \\
&\overset{\text{MC}}{\approx} \frac{1}{S}\sum_{s=1}^{S} \log p(x|z^{(s)},\theta)\frac{\partial}{\partial \lambda}\log q(z^{(s)}|x,\lambda)
\end{aligned}
$$

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

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

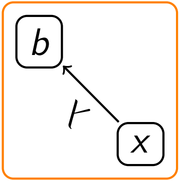
Computation Graph



inference model

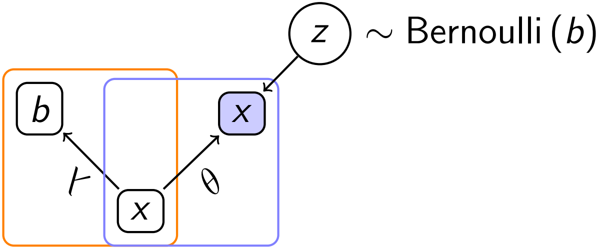
Computation Graph

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



inference model

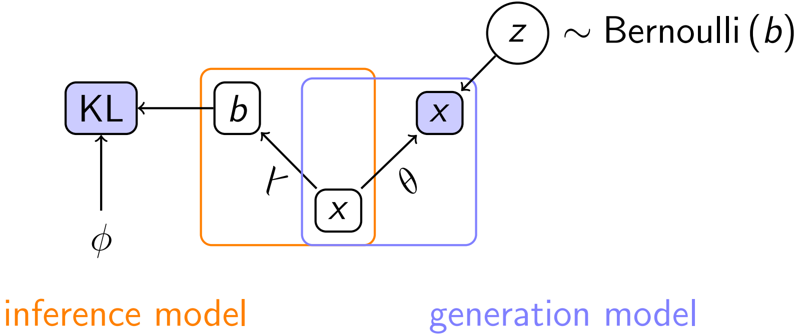
Computation Graph



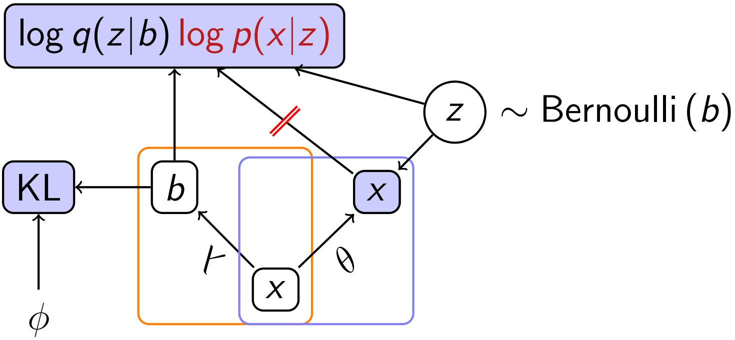
inference model

generation model

Computation Graph



Computation Graph



inference model

generation model

Pros and Cons

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

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- Pros
  - Applicable to all distributions
  - Many libraries come with samplers for common distributions
- Cons
  - High Variance!

First Attempt: Wake-Sleep

Neural Variational Inference

Score function estimator

Variance reduction

When variance is high we can

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- sample more

When variance is high we can

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

Control variates

Suppose we want to estimate $\mathbb{E}[f(Z)]$

$$\hat{f} \overset{\text{MC}}{\approx} \frac{1}{S}\sum_{s=1}^{S} f(z^{(s)})$$

and we know the expected value of another function $\psi(z)$ on the same support.

Control variates

Suppose we want to estimate $\mathbb{E}[f(Z)]$

$$\hat{f} \overset{\text{MC}}{\approx} \frac{1}{S}\sum_{s=1}^{S} f(z^{(s)})$$

and we know the expected value of another function $\psi(z)$ on the same support.

It holds that

$$\mathbb{E}[f(Z)] = \mathbb{E}[f(Z) - \psi(Z)] + \mathbb{E}[\psi(Z)]$$

Variance reduction

$$\hat{d} = \frac{1}{S}\left(\sum_{s=1}^{S} f(z^{(s)}) - \psi(z^{(s)})\right) + \underbrace{\mathbb{E}[\psi(Z)]}_{\mu_\psi}$$

In general

$$\mathrm{Var}(f - \psi) = \mathrm{Var}(f) - 2\,\mathrm{Cov}(f, \psi) + \mathrm{Var}(\psi)$$

If f and ψ are strongly correlated, then we improve on the original estimation problem:
if $\mathrm{Cov}(f, \psi) > \frac{\mathrm{Var}(\psi)}{2}$

Baselines

Fact

The Expectation of the score function is 0.

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$$\mathbb{E}_{q(z|x,\lambda)}\left[\frac{\partial}{\partial\lambda}\log q(z|x,\lambda)\right] = 0$$

Baselines

We attempt to centre the gradient estimate. To do this we learn a quantity C that we subtract from the reconstruction loss.

$$\mathbb{E}_{q(z|\lambda)}\left[\log q(z|\lambda)\left(\log p(x|z,\theta) - C\right)\right]$$

We call C a baseline. It does not change the expected gradient (Williams, 1992).

Baselines

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

Baselines

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

$$\underbrace{\mathbb{E}_{q(z|\lambda)}\left[\frac{\partial}{\partial\lambda}\log q(z|\lambda)\log p(x|z,\theta)\right]}_{\text{score function gradient}} -$$

Baselines

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

$$\underbrace{\mathbb{E}_{q(z|\lambda)}\left[\frac{\partial}{\partial\lambda}\log q(z|\lambda)\log p(x|z,\theta)\right]}_{\text{score function gradient}}-$$

$$\underbrace{\mathbb{E}_{q(z|\lambda)}\left[\frac{\partial}{\partial\lambda}\log q(z|\lambda)\right]}_{0}C$$

Baselines

We can make baselines input-dependent to make them more flexible.

$$\log q(z|\lambda) \left(\log p(x|z, \theta) - C(x; \omega)\right)$$

Baselines

We can make baselines input-dependent to make them more flexible.

$$\log q(z|\lambda) \left(\log p(x|z, \theta) - C(x; \omega)\right)$$

However, baselines may not depend on the random value z! Quantities that may depend on the random value ($C(z)$) are called **control variates**.

See Blei et al. (2012); Ranganath et al. (2014); Gregor et al. (2014).

Baselines

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

The model is trained using an L_2-loss.

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

Summary

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

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Summary

- 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 https://github.com/probabll/dgm4nlp/tree/master/notebooks/sst

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