Deep Generative Models: Discrete Latent Variables

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

Who am I

I'm an assistant professor at the University of Amsterdam

probabll.github.io

Stuff I typically work on

- machine learning
  VAEs, NFs, gradient estimation for discrete variables
- probabilistic models
  Bayesian models, deep latent variable models
- natural language processing
  translation, parsing, text classification, question answering

Why discrete latent variable models

Discreteness is everywhere!

- Natural languages (text)
- Programming languages
- DNA sequences and molecules
- Knowledge graphs
- Social networks

Classic discrete latent variable models

- Mixture models: MoG
- State space models: Hidden Markov Model (HMM)
- Hierarchical models: Latent Dirichlet Allocation (LDA), Factorical HMMs
- Feature models: Indian Buffet Process (IBP)

Classic discrete latent variable models

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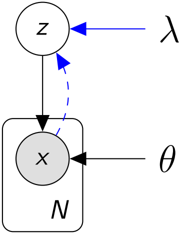
Discreteness can be use to encode inductive biases

- e.g. discrete sources of variation

Building block



- z can be a category, a binary feature vector, a sequence, a tree, a graph
- we pick a convenient likelihood function for $X|z$ depending on the nature of the data (e.g. Bernoulli, Categorical, Gaussian, Product of independent or correlated Bernoullis/Categoricals/Gaussians).

Key: distributions are parameterised by NNs

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

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

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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- richer probabilistic models
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We need approximate inference techniques!

ELBO recap

And we've developed the ELBO

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

ELBO recap

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ELBO recap

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

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

ELBO recap

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

$$\text{ELBO} = \mathbb{E}_{q(z|x)}\left[\log \frac{p(z|x)p(x)}{q(z|x)}\right]$$

$$= -\underbrace{\mathrm{KL}\left(q(z|x) \mid\mid p(z|x)\right)}_{\text{gap}} + \log p(x)$$

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

2 Neural Networks:

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

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Wake-sleep Architecture

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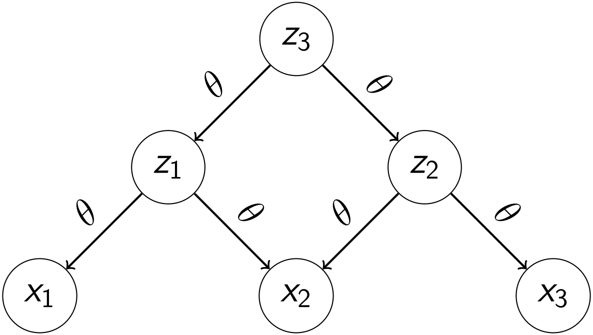
- Original setting: binary hidden units

Wake-sleep Architecture

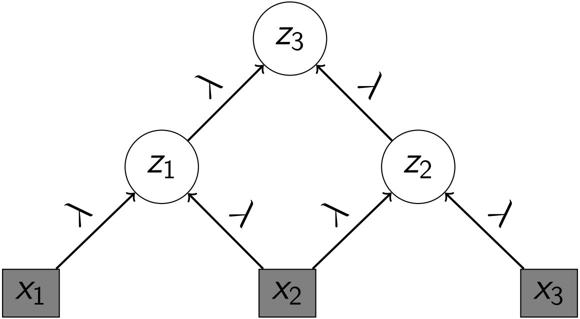
2 Neural Networks:

- 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-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 joint 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

$$\arg\max_{\theta} \; \mathbb{E}_{p(x)} \left[\mathrm{ELBO}(\theta, \lambda | x)\right]$$

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

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Gradient wrt θ for $x \sim p(x)$

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

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$$= \mathbb{E}_{q(z|x,\lambda)} \left[\nabla_{\theta} \log p(z, x|\theta) \right]$$
$$\overset{\text{MC}}{\approx} \nabla_{\theta} \log p(z, x|\theta) \quad \text{where } z \sim q(z|x,\lambda)$$

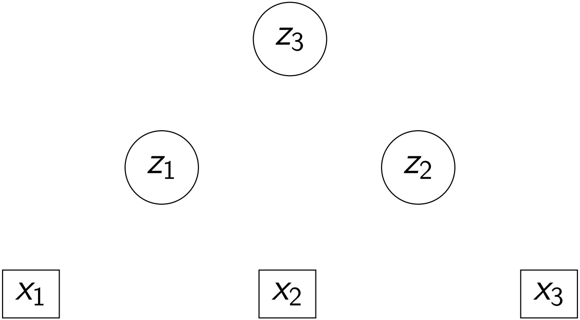
Wake Phase Objective

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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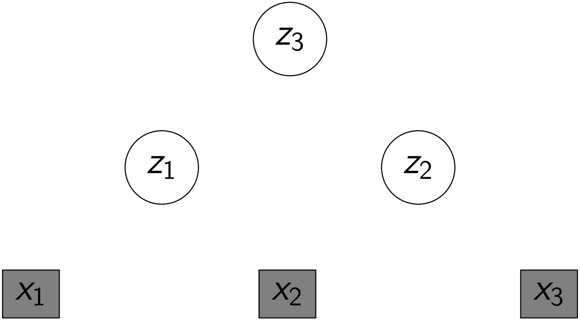

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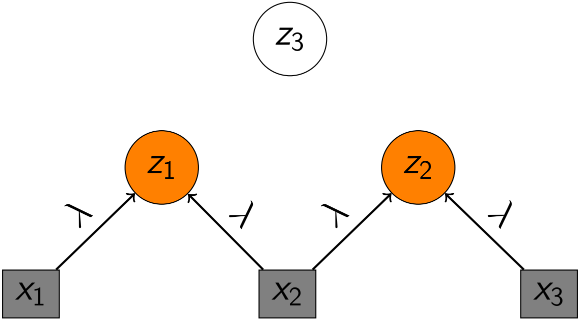

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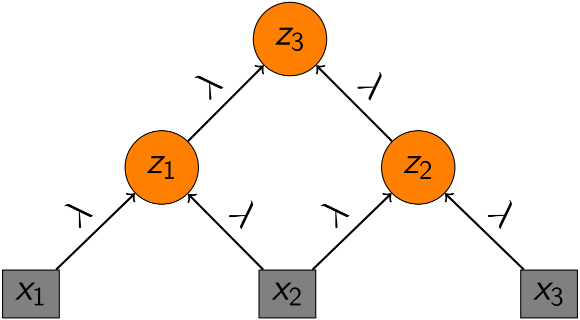
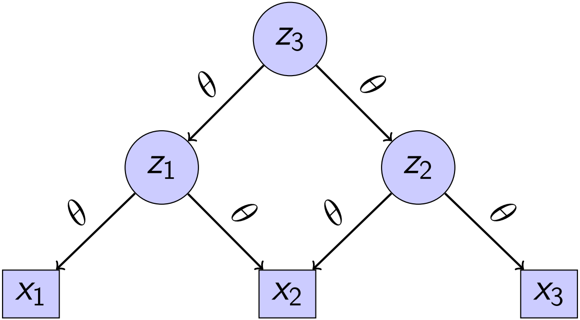


Wake Phase Update

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



Sleep Phase Objective

Objective

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

Sleep Phase Objective

Objective

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Gradient wrt λ for $x \sim p(x)$

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

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Let's change the objective!

Sleep Phase (Convenient) Objective

Flip the direction of the KL

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

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Gradient wrt λ

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$$\overset{\text{MC}}{\approx} \nabla_{\lambda} \log q(z|\tilde{x},\lambda) \quad \text{where } z \sim p(z|\theta)$$
$$\tilde{x} \sim p(x|z,\theta)$$

Sleep Phase (Convenient) Objective

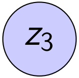
Assumes fake data $\tilde{x}$ and latent variables z to be fixed random draws from $p(x, z|\theta)$ via

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

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

Sleep Phase Sampling

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



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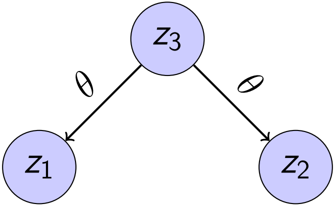

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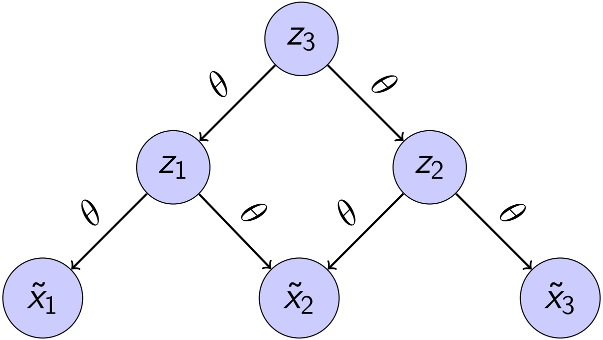
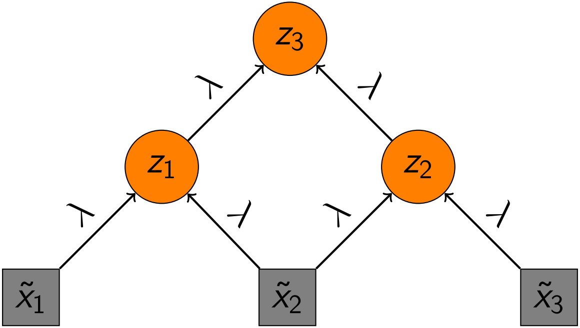


Sleep Phase Update

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

Variational Inference Learning (NVIL)

Generative model with NN likelihood

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Generative model with NN likelihood

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

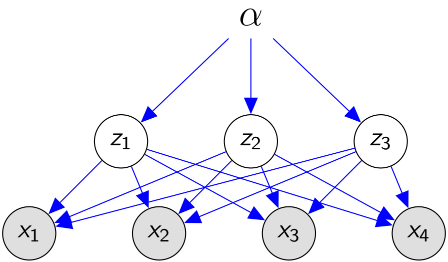
Latent factor model

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

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.

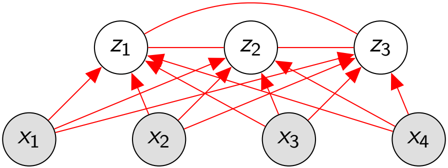
$$
\begin{aligned}
f(z;\theta) &= \text{softmax}(Wz + b) \\
\theta &= \{W, b\}
\end{aligned}
$$

Example Model



Joint distribution: independent latent variables

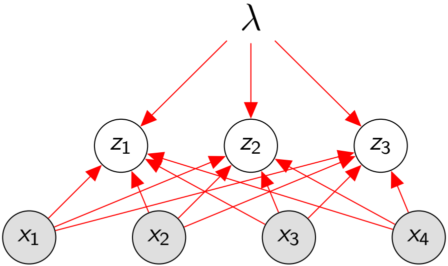
Example Model



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

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

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

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

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

Objective

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

Objective

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

Parameter estimation

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

KL

KL between K independent Bernoulli distributions is tractable

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

KL

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$$= \sum_{k=1}^{K} \mathrm{KL}\left(\mathrm{Bernoulli}\left(b_k\right)\right) \mid\mid \mathrm{Bernoulli}\left(\alpha\right))$$

KL

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$$= \sum_{k=1}^{K} \mathrm{KL}\left(\mathrm{Bernoulli}\left(b_k\right)\right) \mid\mid \mathrm{Bernoulli}\left(\alpha\right))$$

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

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

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

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

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

Inference Network Gradient

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

Inference Network Gradient

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

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

Inference Network Gradient

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

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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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&= \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

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\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

$$
\begin{aligned}
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\end{aligned}$$

Score function estimator: remarks

We can now build an MC estimator

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

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

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

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

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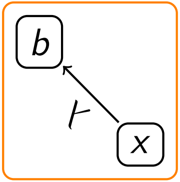
- magnitude of $\log p(x|z,\theta)$ varies widely
- model likelihood does not contribute to direction of gradient

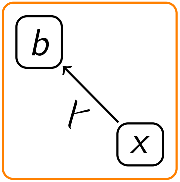
Computation Graph



inference model

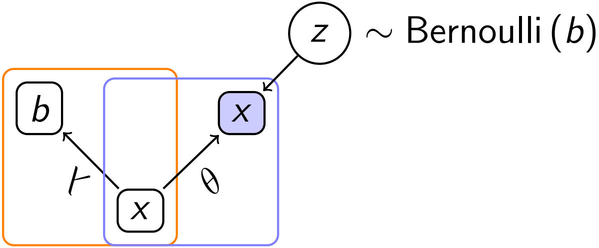
Computation Graph

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



inference model

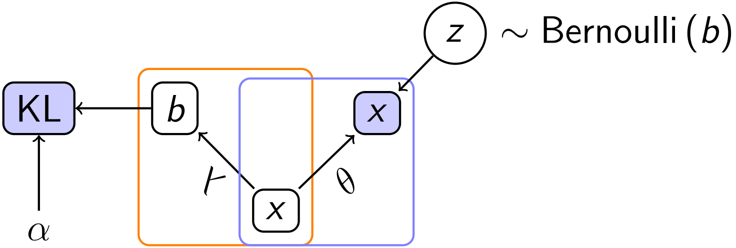
Computation Graph



inference model

generation model

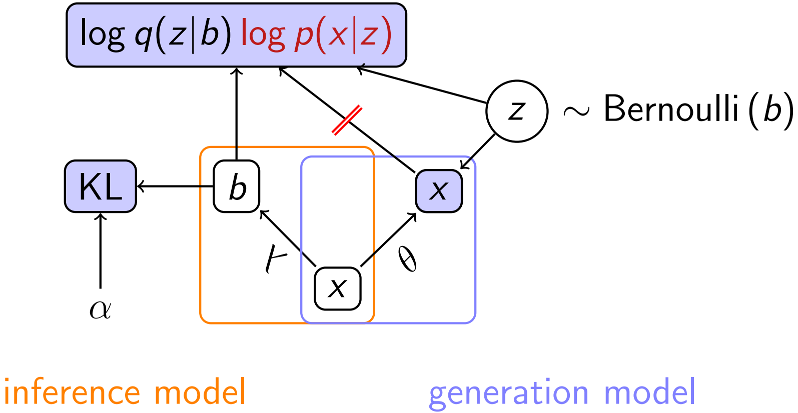
Computation Graph



inference model

generation model

Computation Graph



Pros and Cons

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

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  - Many libraries come with samplers for common distributions
- Cons
  - High Variance!

When variance is high we can

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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 $\mathrm{Var}(f) > \mathrm{Var}(\hat{f})$.

Equivalent expectations

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

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- say we know $\bar{c} = \mathbb{E}[c(z)]$
- then for $\hat{f}(z) \triangleq f(z) - b(c(z) - \mathbb{E}[c(z)])$
  it holds that $\mathbb{E}[\hat{f}(z)] = \mathbb{E}[f(z)]$
- and $\mathrm{Var}(\hat{f}) = \mathrm{Var}(f) - 2b\,\mathrm{Cov}(f, c) + b^2\,\mathrm{Var}(c)$

Choosing the control variate

1. $\hat{f}(z) \triangleq f(z) - b(c(z) - \mathbb{E}[c(z)])$
2. $\mathrm{Var}(\hat{f}) = \mathrm{Var}(f) - 2b\,\mathrm{Cov}(f, c) + b^2\,\mathrm{Var}(c)$

How do we choose b and $c(z)$?

Choosing the control variate

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Of course, $\mathbb{E}[c(z)]$ must be known!

MC

We then use the estimate

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

MC

We then use the estimate

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

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.

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

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$$
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&= \int \frac{\partial}{\partial\lambda} q(z|x,\lambda)\mathrm{d}z \\
&= \frac{\partial}{\partial\lambda}\int q(z|x,\lambda)\mathrm{d}z \\
&= \frac{\partial}{\partial\lambda} 1 = 0
\end{aligned}
$$

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

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

and

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

we have

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

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

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

b is known as *baseline* in RL literature.

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

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- A neural network prediction based on x e.g. $b(x; \omega)$

Examples of baselines

- 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. $b(x) = \log p(x|z^\star, \theta)$ where $z^\star = \arg\max_z q(z|x, \lambda)$

Trainable baselines

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

The model is trained using an L_2-loss.

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

Summary

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

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- NVIL: a single objective (ELBO) for both models

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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
  github.com/vitutorial/exercises/tree/master/SST

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