Deep Generative Models: Discrete Latent Variables

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https://vitutorial.github.io/tour/ua2020

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gourmet

Discrete Latent Variables

- Language is an inherently discrete structure.

Discrete Latent Variables

- Language is an inherently discrete structure.
- Many structures used to describe language are discrete, e.g. trees, graphs, tags, etc.

1. First Attempt: Wake-Sleep
2. Neural Variational Inference and Learning
3. Score Function Estimator

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 neural network 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
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We need approximate inference techniques!

ELBO recap

And we've developed the ELBO

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

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

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

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

Wake-Sleep Algorithm

- Generalise latent variables to neural networks.
- Train generative neural model.
- Use variational inference! (kind of)
- Hinton et al. (1995)

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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2 neural networks:

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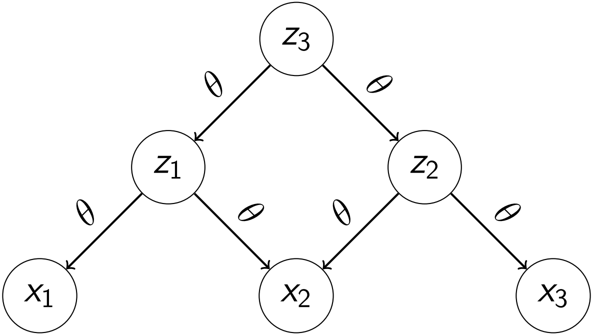
- Original setting: binary hidden units

Wake-Sleep Architecture

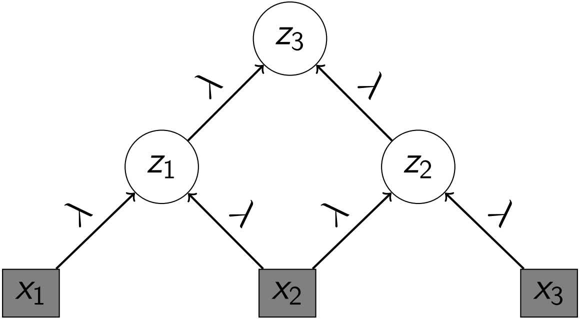
2 neural networks:

- 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-likelihood of data and latents $p(x, z|\theta)$

Wake-sleep Training

Wake Phase

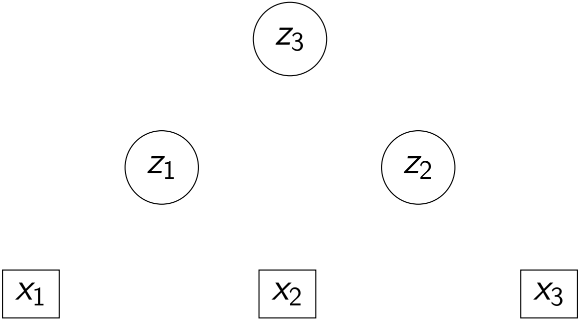
- Use inference network to sample hidden unit setting z from $q(z|x, \lambda)$
- Update generation parameters θ to maximize joint log-likelihood of data and latents $p(x, z|\theta)$

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 Sampling

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



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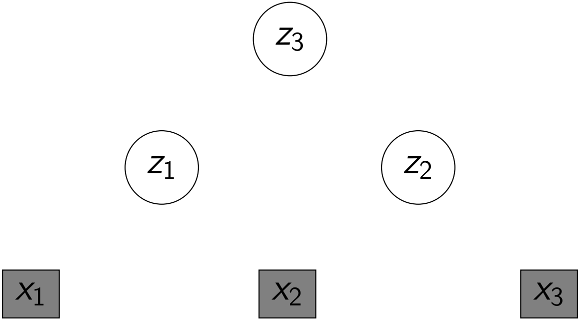

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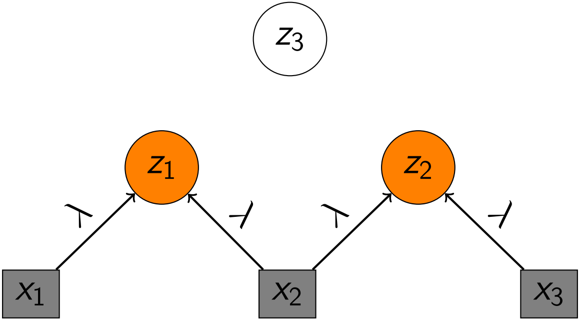

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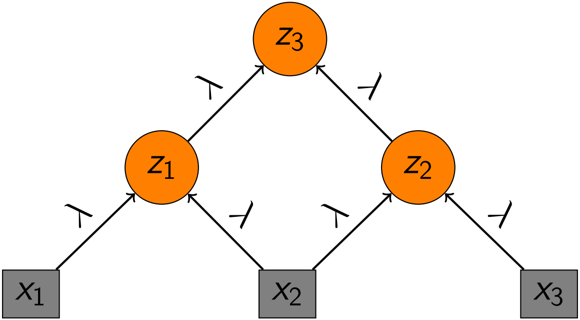
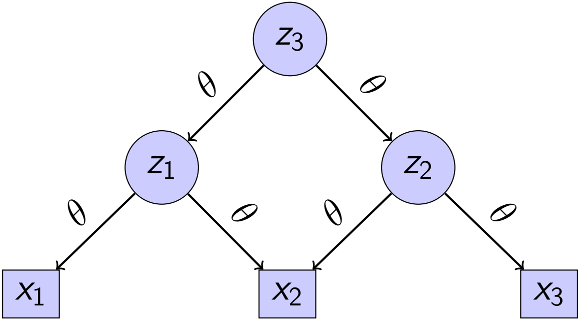


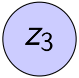
Wake Phase Update

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



Sleep Phase Sampling

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



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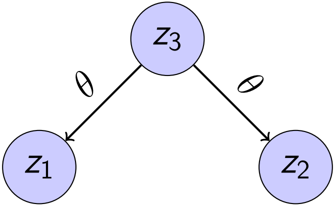

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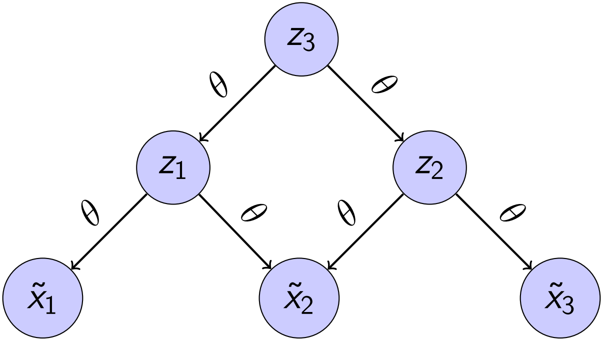
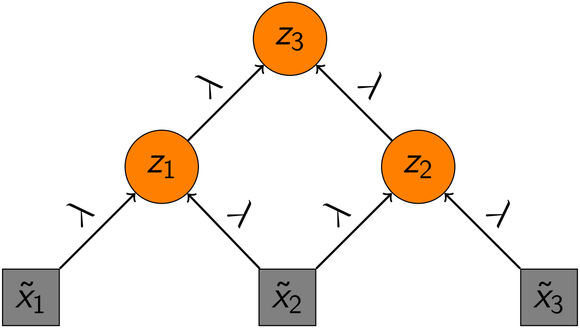


Sleep Phase Update

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



Wake Phase Objective

Objective

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

Wake Phase Objective

Objective

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

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

Wake Phase Objective

Objective

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

Approximation: optimize the lower-bound alone.

Wake Phase Objective

Objective

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

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

Wake Phase Objective

Objective

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

Gradient wrt θ for $x \sim p(x)$

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

Wake Phase Objective

Objective

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

Wake Phase Objective

Objective

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

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

Gradient wrt θ for $x \sim p(x)$

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

Wake Phase Objective

Assumes 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!

Sleep Phase Objective

Objective

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

Sleep Phase Objective

Objective

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

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Gradient wrt λ for $x \sim p(x)$

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

Sleep Phase Objective

Objective

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

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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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&\stackrel{\text{asm}}{=} \arg\max_{\lambda} \mathbb{E}_{p(x,z|\theta)} \left[\log q(z|x,\lambda) \right] - \underbrace{\mathbb{E}_{p(x,z|\theta)} \left[\log p(z|x,\theta) \right]}_{\text{constant}}
\end{aligned}
$$

Sleep Phase (Convenient) Objective

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\end{aligned}
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Gradient wrt λ

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

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Gradient wrt λ

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Gradient wrt λ

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

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

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

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

Sleep Phase (Convenient) Objective

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

$$
\begin{aligned}
z &\sim p(z|\theta) \\
\tilde{x} &\sim p(x|z, \theta)
\end{aligned}
$$

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

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:

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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.

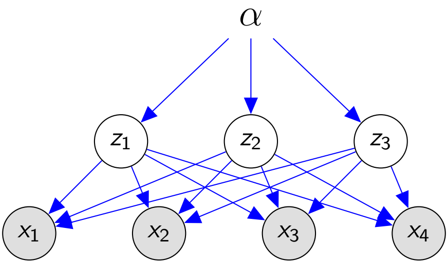
Latent factor model

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

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.

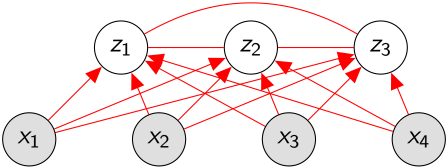
$$
\begin{aligned}
f(z;\theta) &= \text{softmax}(Wz + b) \\
\theta &= \{W, b\}
\end{aligned}
$$

Example Model



Joint distribution: independent latent variables

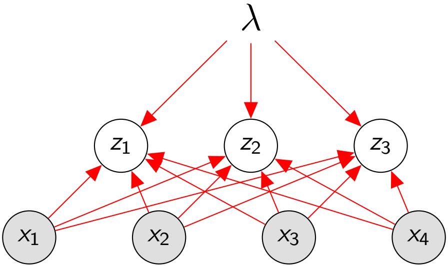
Example Model



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

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

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

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

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

KL between K independent Bernoulli distributions is tractable

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

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

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

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

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

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

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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

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

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

Inference Network Gradient

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

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\begin{aligned}
&\frac{\partial}{\partial \lambda} \mathbb{E}_{q_\lambda(z|x)} [\log p_\theta(x|z)] \\
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- MC estimator is non-differentiable

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- 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

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Score Function Estimator

We can now build an MC estimator

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Score Function Estimator

We can now build an MC estimator

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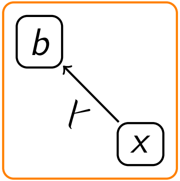
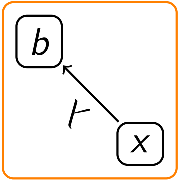
Computation Graph



inference model

Computation Graph

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



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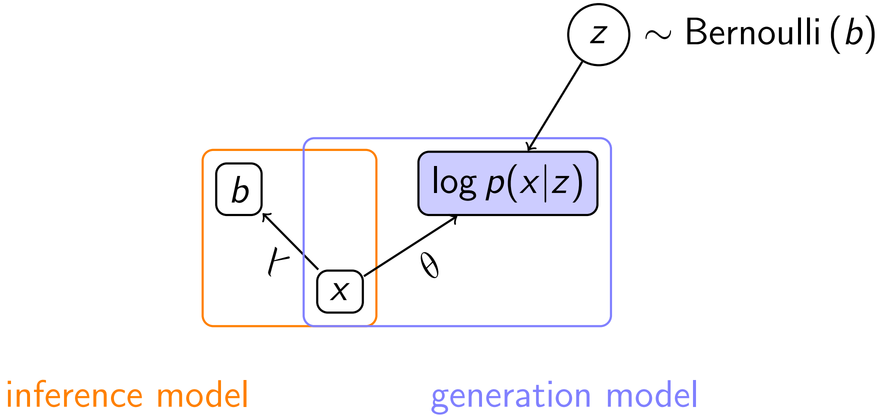
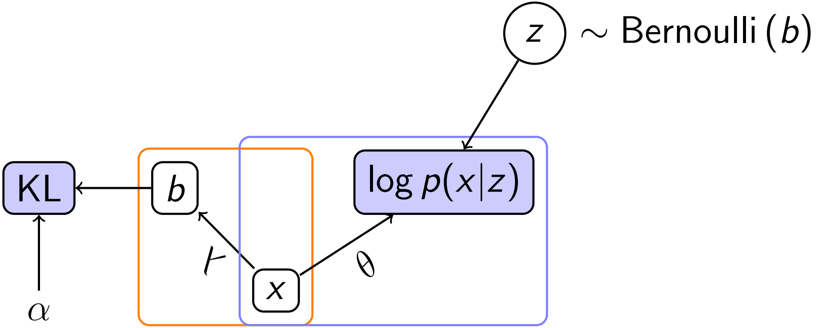


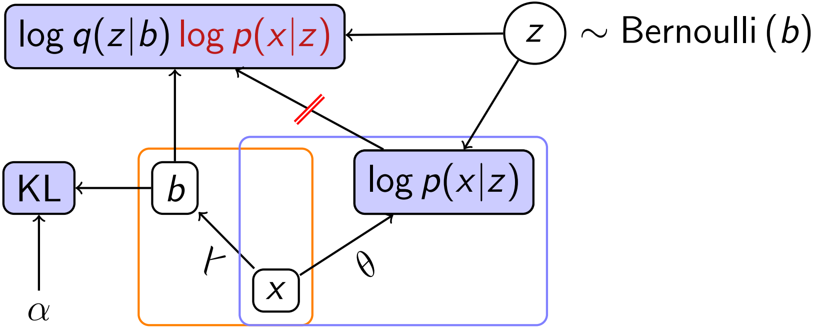
Computation Graph



inference model

generation model

Computation Graph



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Score Function Estimator: Variance

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Empirically this estimator often exhibits high variance.

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- the model likelihood does not contribute to direction of gradient

Score Function Estimator: Variance

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- sample more (better MC estimates)

Score Function Estimator: Variance

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

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- More about this tomorrow!

Pros and Cons

Pros:

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

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- High Variance!

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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`

Literature I

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