Deep Generative Models: Discrete Latent Variables

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https://vitutorial.github.io
https://github.com/vitutorial/VITutorial

Deep Generative Models

First Attempt: Wake-Sleep

Revisiting the Inference Gradient

Control Variates and Baselines

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**

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

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Marginal likelihood

$$p(x|\theta) = \int p(x, z|\theta)\,\mathrm{d}z = \int p(z) \underbrace{p(x|z,\theta)}_{\text{highly nonlinear!}} \,\mathrm{d}z$$

intractable in general

Goals

We want

- richer probabilistic models

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We need approximate inference techniques!

Wake-sleep Algorithm

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

Wake-sleep Architecture

2 Neural Networks:

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

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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
- Training is performed in a “hard EM” fashion

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 liklelihood of data given latent state $p(x|z, \theta)$

Wake-sleep Training

Wake Phase

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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

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

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

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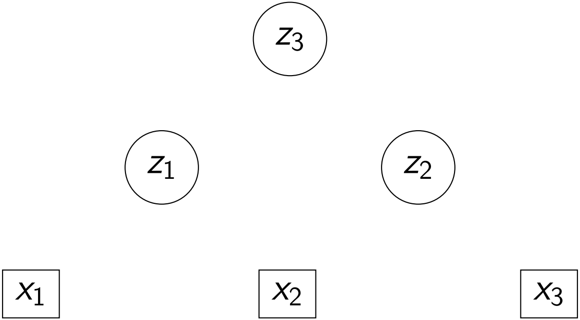
This is simply supervised learning with imputed latent data!

Wake Phase Sampling



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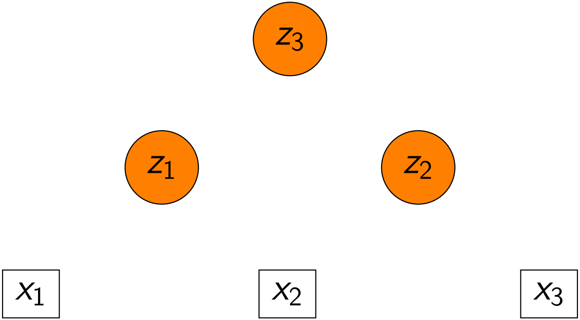

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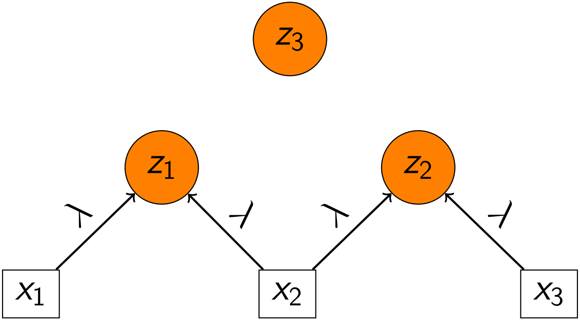

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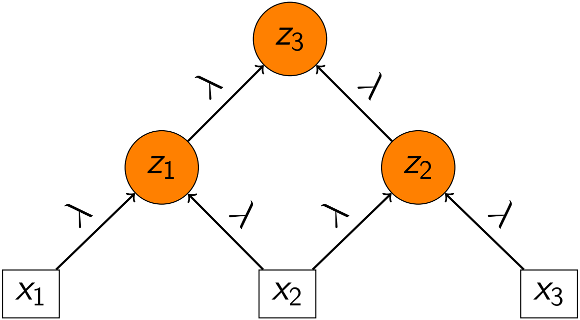
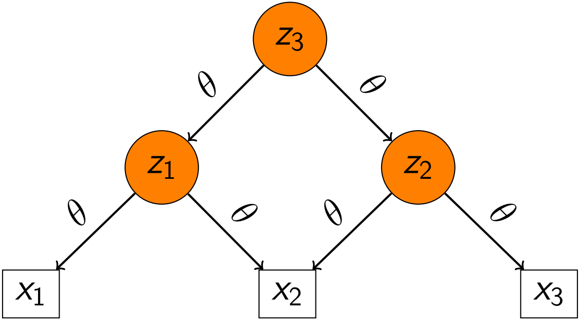


Wake Phase Update



Sleep Phase Objective

Needed to find alternative objective because

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

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is not an expectation!

Idea

Optimize q towards a sample from p.

Sleep Phase Objective

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

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

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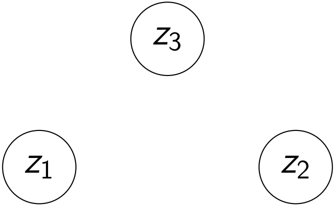

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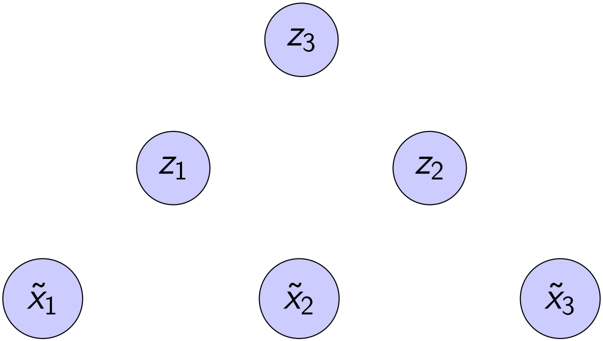

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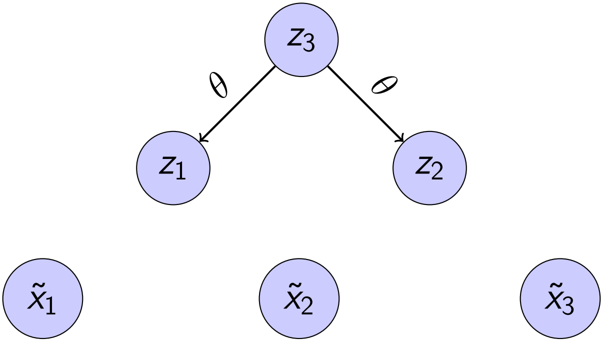

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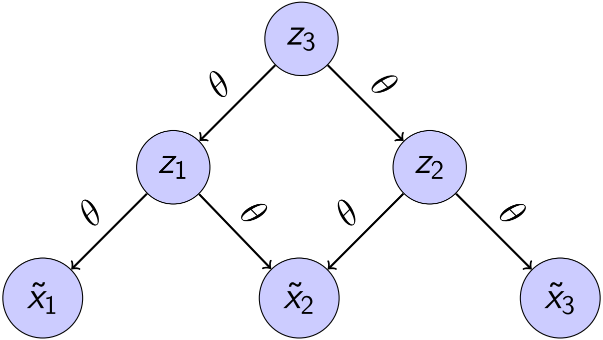

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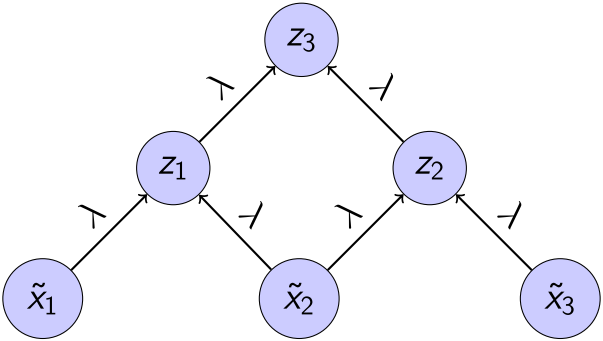

Wake-sleep Algorithm

Advantages

- Simple layer-wise updates
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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

Generative Model with NN Likelihood

Goal

Define model $p(x, z|\theta) = p(x|z, \theta)p(z)$ where the likelihood $p(x|z, \theta)$ is given by a neural network. (We fix $p(z)$ for simplicity.)

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$p(x) = \int \underbrace{p(x|z, \theta)}_{\text{highly non-linear!}} p(z)\mathrm{d}z$ is hard to compute.

Solution: Variational Inference

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

Solution: Variational Inference

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- assume $\mathrm{KL}\left(q(z|x,\lambda) \mid\mid p(z)\right)$ analytical
  true for exponential families
- approximate $\mathbb{E}_{q(z|x,\lambda)}\left[\log p(x|z,\theta)\right]$ by sampling
  feasible because $q(z|x,\lambda)$ is simple

Generator Network Gradient

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

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$$\overset{\text{MC}}{\approx} \frac{1}{S}\sum_{i=1}^{S}\frac{\partial}{\partial\theta}\log p(x|z_i,\theta)$$

where $z_i \sim q(z|x,\lambda)$

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where $z_i \sim q(z|x,\lambda)$

Note: $q(z|x,\lambda)$ does not depend on θ.

Inference Network Gradient

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

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\end{aligned}
$$

The first term again requires approximation by sampling

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Not an expectation!

Back to Basic Calculus

$$\frac{\mathrm{d}}{\mathrm{d}\lambda} \log f(\lambda)$$

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Consequence

$$\frac{\mathrm{d}}{\mathrm{d}\lambda} f(\lambda) = \frac{\mathrm{d}}{\mathrm{d}\lambda} \log f(\lambda) \times f(\lambda)$$

Score Function Estimator

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

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

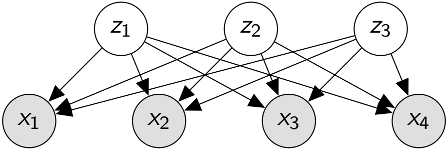
Example Model

Let us consider a latent factor model for topic modelling. Each document x consists of n i.i.d. categorical draws from that model. The categorical distribution in turn depends on the binary latent factors $z = (z_1, \ldots, z_k)$ which are also i.i.d.

$$\begin{aligned} Z_j &\sim \text{Bernoulli}(\phi) & (1 \le j \le k) \\ X_i | z &\sim \text{Categorical}(g(z)) & (1 \le i \le n) \end{aligned}$$

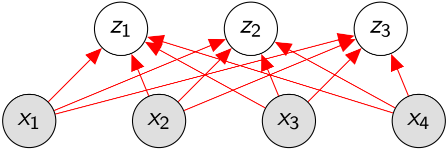
Here $g(\cdot)$ is a function computed by neural network with softmax output.

Example Model



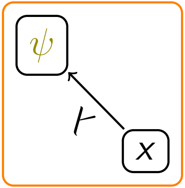
At inference time the latent variables are marginally dependent. For our variational distribution we are going to assume that they are not (recall: mean field assumption).

Inference Network



The inference network needs to predict k Bernoulli parameters ψ. Any neural network with sigmoid output will do that job.

Computation Graph



inference model

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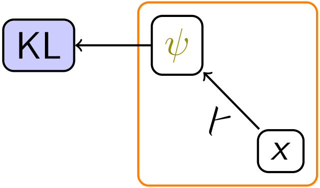

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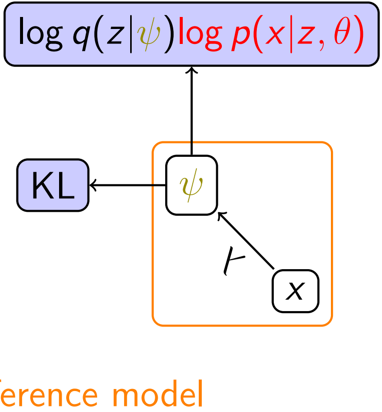

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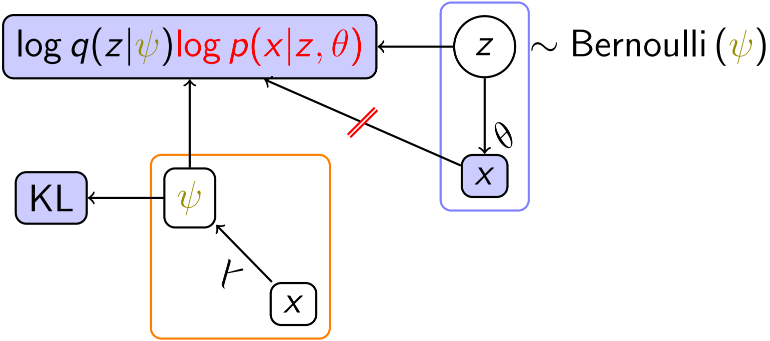

inference model

generation model

Pros and Cons

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

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- Cons
  - High Variance!

Baselines

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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

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

Baselines

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

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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.

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

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- Differentiating ELBO wrt λ does not yield an expectation.
- Use score function estimator.
- High variance.
- Always use baselines for variance reduction!

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