Deep Generative Models: Continous Latent Variables

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https://github.com/philschulz/VITutorial

Generative Models

First Attempt: Log-linear Models

Second Attempt: Wake-Sleep

This is how we do: Variational Autoencoders

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Recap: Generative Models

Joint distribution over observed data x and latent variables Z.

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

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

Recap: Variational Inference

Objective

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

- The ELBO is a lower bound on $\log p(x)$
- Mean field assumption: $q(z) = \prod_{i=1}^{N} q(z_i)$

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Feature-rich Generative Models

Let us assume that z has internal structure (features). How can we exploit that?

First Idea

Make $p(x|z, \alpha)$ a log-linear model.

- Only discrete data
- Trainable with EM if we can efficiently enumerate $\mathcal{X}$ and $\mathcal{Z}$.

Log-linear Model

Let us treat z as observed.

$$p(x|z, \alpha = w) = \frac{\exp\left(w^\top f(x, z)\right)}{\sum_{x \in \mathcal{X}} \exp\left(w^\top f(x, z)\right)}$$

Log-linear Model

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Weight Gradient

$$\frac{d}{dw} \log p(x|z, w) = f(x, z) - \mathbb{E}\left[f(X, z)|z, w\right]$$

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Weight Gradient

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Updates need to be performed iteratively.

Log-linear model with latent variables

Now let us treat z as latent.

Log-linear model with latent variables

Now let us treat z as latent.

Model

$$p(x, z|w) = \underbrace{\frac{\exp\left(w^\top f(x,z)\right)}{\sum_{x\in\mathcal{X}} \exp\left(w^\top f(x,z)\right)}}_{p(x|z,w)} \times \underbrace{p(z)}_{\text{arbitrary}}$$

Log-linear model with latent variables

Posterior

$$p(z|x, w)$$

Log-linear model with latent variables

Posterior

$$p(z|x,w) = \frac{p(x,z|w)}{p(x|w)}$$

Log-linear model with latent variables

Posterior

$$p(z|x,w) = \frac{p(x,z|w)}{p(x|w)} = \frac{p(x,z|w)}{\sum_z p(x,z|w)} =$$

Log-linear model with latent variables

Posterior

$$p(z|x,w) = \frac{p(x,z|w)}{p(x|w)} = \frac{p(x,z|w)}{\sum_z p(x,z|w)} = \frac{\frac{\exp\left(w^\top f(x,z)\right)}{\sum_{x\in\mathcal{X}} \exp(w^\top f(x,z))} \times p(z)}{\sum_z \frac{\exp(w^\top f(x,z))}{\sum_{x\in\mathcal{X}} \exp(w^\top f(x,z))} \times p(z)}$$

Log-linear model with latent variables

Weight Gradient (treat $p(z|x, w)$ as fixed)

$$\frac{d}{dw}\mathbb{E}_{p(z|x,w)}\left[\log p(x, z|w)\right] =$$

Log-linear model with latent variables

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Log-linear model with latent variables

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$$\frac{d}{dw}\mathbb{E}_{p(z|x,w)}\left[\log p(x, z|w)\right] =$$
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$$\sum_z p(z|x, w)\frac{d}{dw}\log p(x, z|w) =$$

$$\sum_z p(z|x, w)\left(\frac{d}{dw}\log p(x|z, w) + \frac{d}{dw}p(z)\right)$$

Log-linear model with latent variables

Weight Gradient (treat $p(z|x, w)$ as fixed)

$$\frac{d}{dw}\mathbb{E}_{p(z|x,w)}\left[\log p(x, z|w)\right] =$$

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$$\sum_z p(z|x, w)\frac{d}{dw}\log p(x, z|w) =$$

$$\sum_z p(z|x, w)\left(\overbrace{\frac{d}{dw}\log p(x|z, w)}^{\text{We've already solved this!}} + \overbrace{\frac{d}{dw}p(z)}^{0}\right)$$

Log-linear model with latent variables

Weight Gradient (treat $p(z|x, w)$ as fixed)

$$\frac{d}{dw}\mathbb{E}_{p(z|x,w)}\left[\log p(x, z|w)\right] =$$
$$\mathbb{E}_{p(z|x,w)}\left[f(x, Z)|x, w\right] - \mathbb{E}_{p(z|x,w)}\left[\mathbb{E}\left[(f(X, Z)|Z, w\right]\right]$$

Log-linear model with latent variables

Weight Gradient (treat $p(z|x, w)$ as fixed)

$$\frac{d}{dw}\mathbb{E}_{p(z|x,w)}\left[\log p(x, z|w)\right] =$$
$$\mathbb{E}_{p(z|x,w)}\left[f(x, Z)|x, w\right] - \mathbb{E}_{p(z|x,w)}\left[\mathbb{E}\left[(f(X, Z)|Z, w\right]\right]$$

Procedurally

E_count$(f(x, z))$ - { E_count$(f(x, z))$ $\times\mathbb{E}\left[f(X, z)|z, w\right]$ }

EM

E-step $p(z|x,w) = \frac{p(x,z|w)}{\sum_z p(x,z|w)}$ in $\mathcal{O}(|\mathcal{X}| \times |\mathcal{Z}|)$

M-step Iteratively optimise w to match E_count(x,z) with E_count$(x,z) \times \mathbb{E}[X|z,w]$

Restrictions

- Only log-linear models
- Scales badly

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

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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

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 $p(x|z, \theta)$

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- 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 $p(x|z, \theta)$

Sleep Phase

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

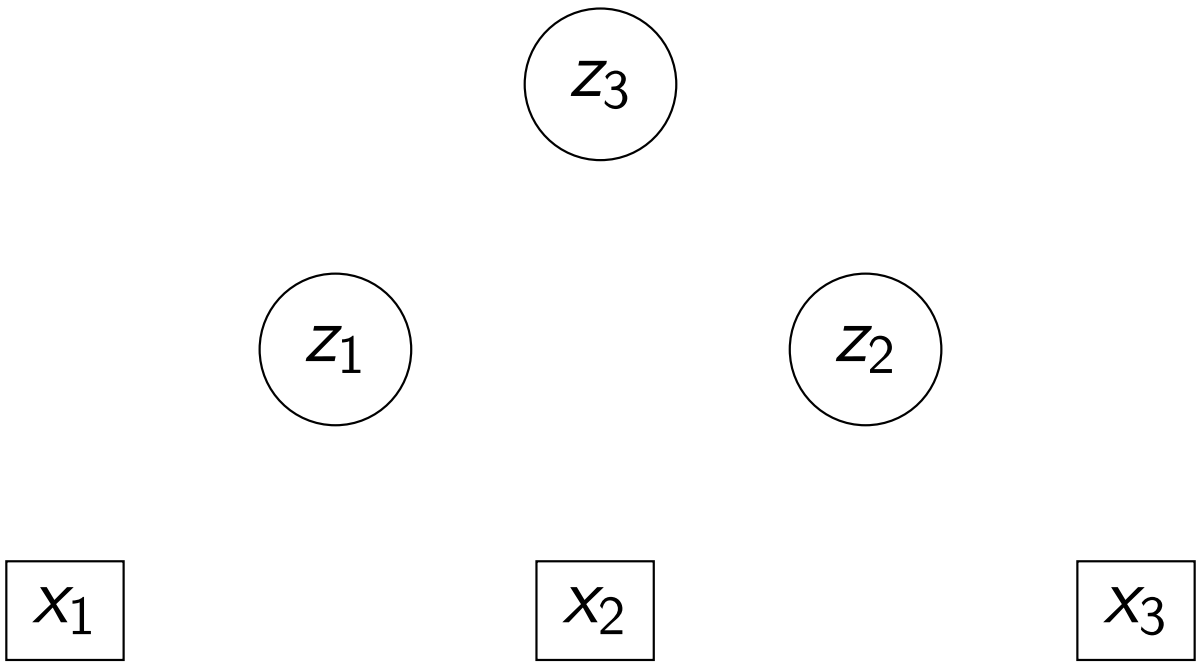
Wake Phase Objective

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

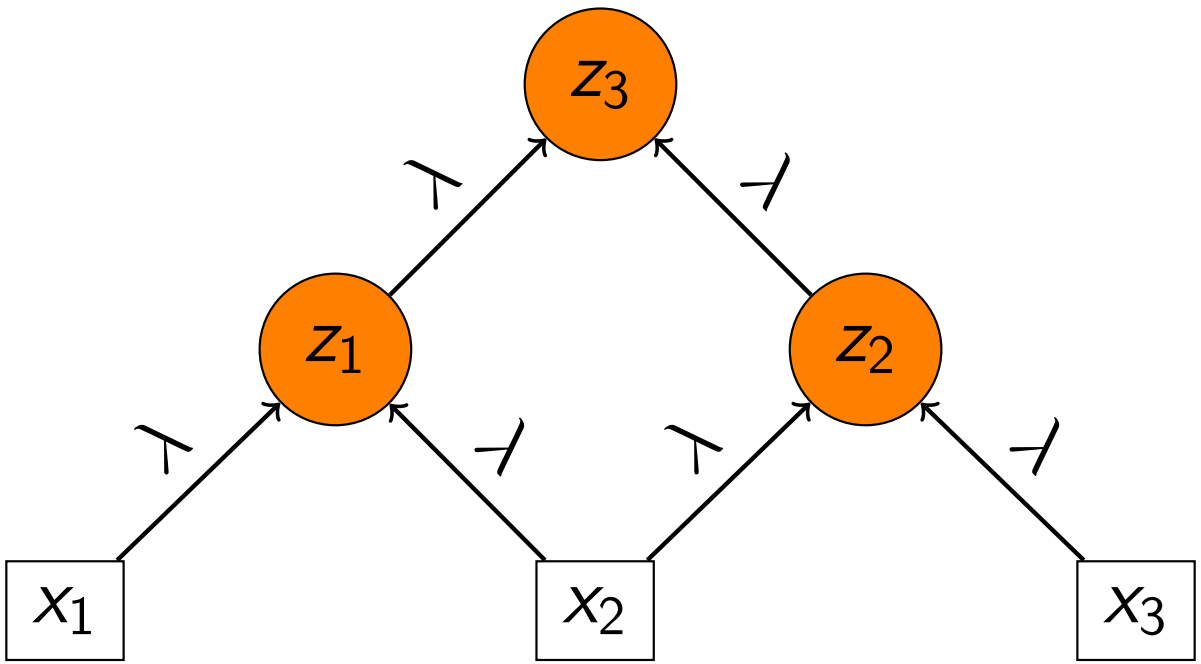
$$\max_{\theta} \ \log p(x|z, \theta)$$

This is simply supervised learning with imputed latent data!

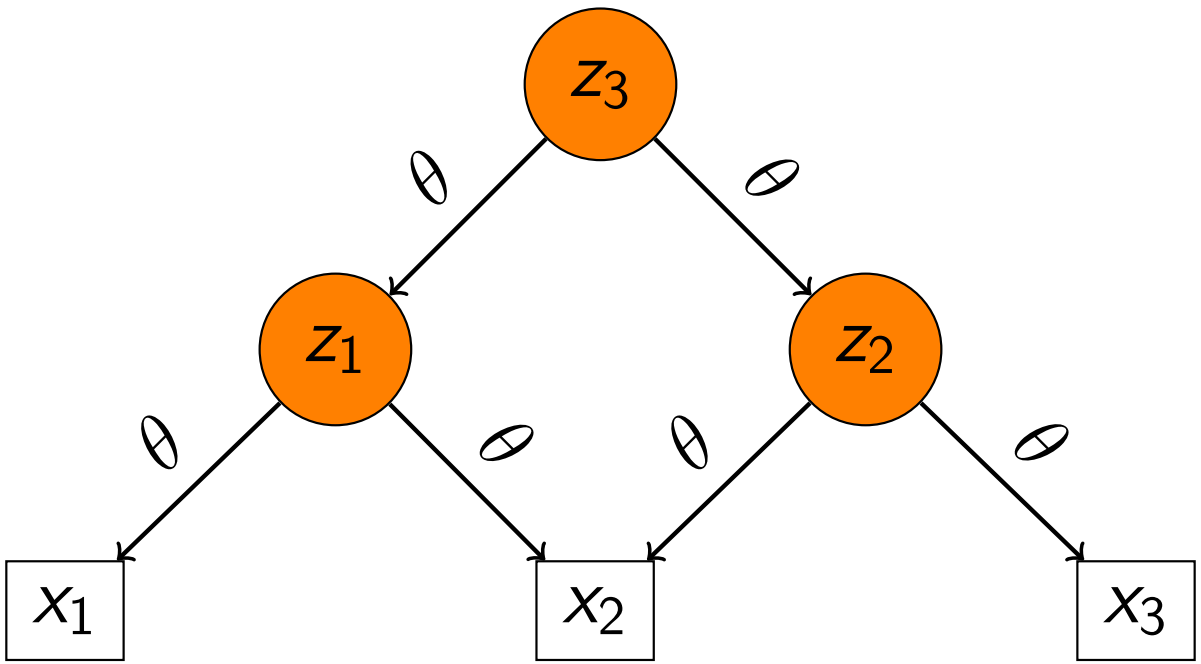
Wake Phase Sampling



Wake Phase Sampling



Wake Phase Update

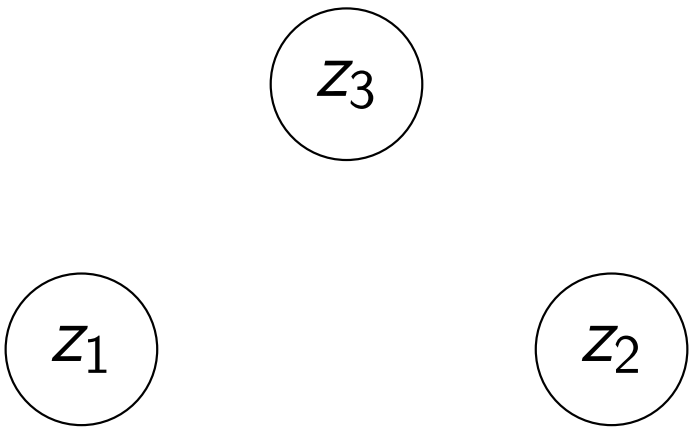


Sleep Phase Objective

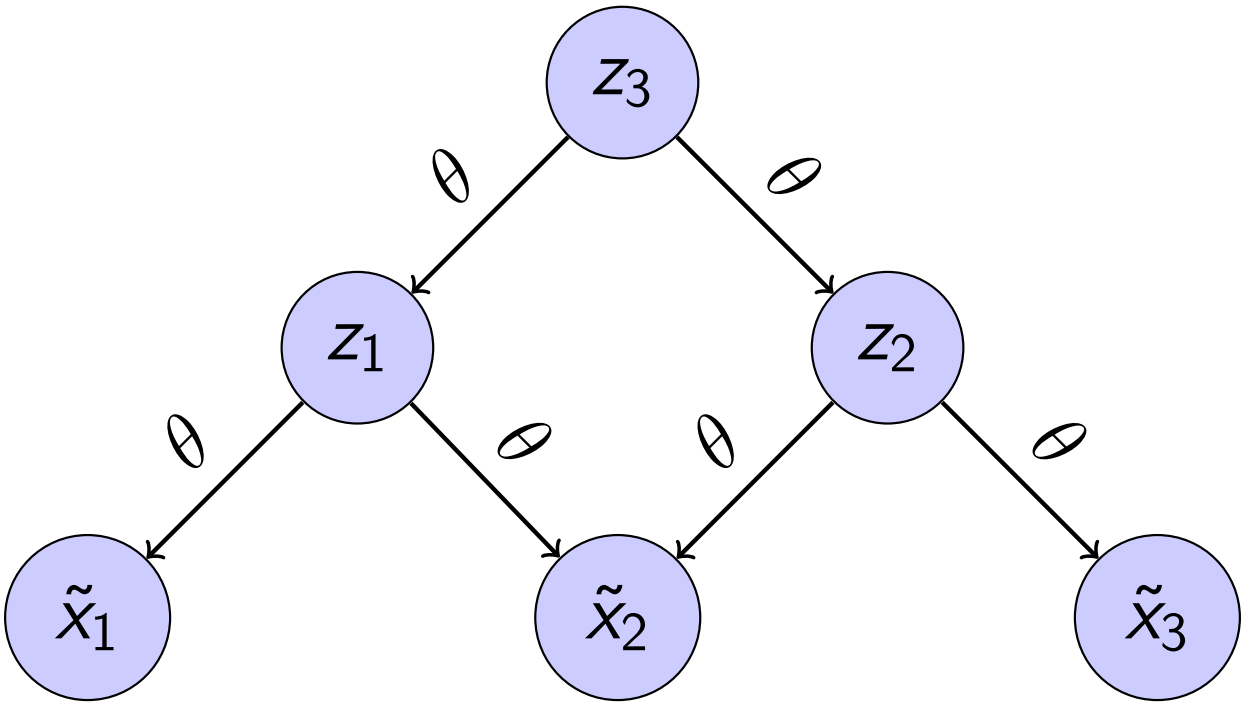
Assumes fake data $\tilde{x}$ and latent variables z to be fixed random draw from $p(x, z|\theta)$.

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

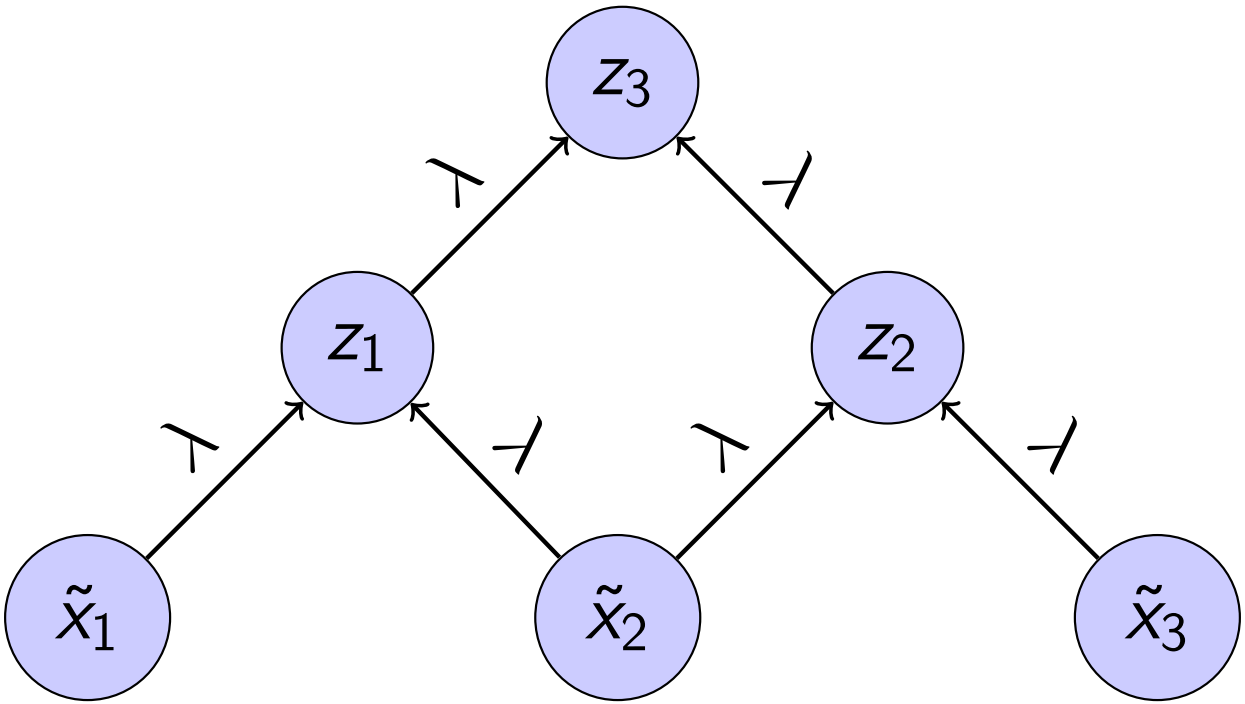
Sleep Phase Sampling



Sleep Phase Sampling



Sleep Phase Update



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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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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$p(x) = \int p(x|z, \theta)p(z)\mathrm{d}z$ is hard to compute.

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Problem

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

Generative Model with NN Likelihood

Solution: VI

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

Generative Model with NN Likelihood

Solution: VI

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

Generative Model with NN Likelihood

Solution: VI

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

Generative Model with NN Likelihood

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$$= \mathbb{E}_{q(z|x,\lambda)}\left[\log p(x|z,\theta)\right] - \underbrace{\mathrm{KL}\left(q(z|x,\lambda) \,||\, p(z)\right)}_{\substack{\text{assume analytical} \\ \text{(true for exponential families)}}}$$

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$$= \mathbb{E}_{q(z|x,\lambda)}\left[\log p(x|z,\theta) + \log p(z)\right] + \mathbb{H}\left(q(z|x,\lambda)\right)$$
$$= \underbrace{\mathbb{E}_{q(z|x,\lambda)}\left[\log p(x|z,\theta)\right]}_{\text{approximate by sampling}} - \underbrace{\mathrm{KL}\left(q(z|x,\lambda) \,||\, p(z)\right)}_{\substack{\text{assume analytical} \\ \text{(true for exponential families)}}}$$

Generator Network Gradient

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

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

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

Generator Network Gradient

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

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

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

Inference Network Gradient

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

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The first term again requires approximation by sampling

Inference Network Gradient

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

Inference Network Gradient

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MC estimator non-differentiable

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MC estimator non-differentiable

- Sampling z neglects $\frac{d}{d\lambda}q(z|x,\lambda)$

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MC estimator non-differentiable

- Sampling z neglects $\frac{d}{d\lambda}q(z|x,\lambda)$
- Differentiating $q(z|x,\lambda)$ breaks the expectation

Inference Network Gradient

Reparametrisation trick

Find a transformation $h : z \mapsto \epsilon$ such that ϵ does not depend on λ.

- $h(z, \lambda)$ needs to be invertible
- $h(z, \lambda)$ needs to be differentiable

Inference Network Gradient

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Find a transformation $h : z \mapsto \epsilon$ such that ϵ does not depend on λ.

- $h(z, \lambda)$ needs to be invertible
- $h(z, \lambda)$ needs to be differentiable
- $h(z, \lambda) = \epsilon$
- $h^{-1}(\epsilon, \lambda) = z$

Gaussian Transformation

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Affine property

$$Ax + b \sim \mathcal{N}\left(\mu + b, A\Sigma A^T\right) \text{ for } x \sim \mathcal{N}\left(\mu, \Sigma\right)$$

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$$Ax + b \sim \mathcal{N}\left(b, AA^T\right) \text{ for } x \sim \mathcal{N}\left(0, \mathrm{I}\right)$$

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Gaussian transformation

$$h(z, \lambda) = \frac{z - \mu(x, \lambda)}{\sigma(x, \lambda)} = \epsilon \sim \mathcal{N}\left(0, \mathrm{I}\right)$$

$$h^{-1}(\epsilon, \lambda) = \mu(x, \lambda) + \sigma(x, \lambda) \odot \epsilon \quad \epsilon \sim \mathcal{N}\left(0, \mathrm{I}\right)$$

Inference Network Gradient

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

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$$= \frac{d}{d\lambda} \int q(\epsilon) \log \left(p(x| \overbrace{h^{-1}(\epsilon,\lambda)}^{=z}, \theta) \right) \mathrm{d}\epsilon$$

Inference Network Gradient

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$$= \int q(\epsilon) \frac{d}{d\lambda} \left[\log p(x| \overbrace{h^{-1}(\epsilon,\lambda)}^{=z}, \theta) \right] \mathrm{d}\epsilon$$

Inference Network Gradient

$$= \int q(\epsilon) \frac{d}{dz} \log p(x| \overbrace{h^{-1}(\epsilon, \lambda)}^{=z}, \theta) \times \frac{d}{d\lambda} h^{-1}(\epsilon, \lambda) \mathrm{d}\epsilon$$

Inference Network Gradient

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$$= \mathbb{E}_{q(\epsilon)} \left[\frac{d}{dz} \log p(x| \overbrace{h^{-1}(\epsilon, \lambda)}^{=z}, \theta) \times \frac{d}{d\lambda} h^{-1}(\epsilon, \lambda) \right]$$

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$$\overset{\text{MC}}{\approx} \frac{1}{S} \sum_{i=1}^{S} \frac{d}{dz} \log p(x| \overbrace{h^{-1}(\epsilon, \lambda)}^{=z}, \theta) \times \frac{d}{d\lambda} h^{-1}(\epsilon, \lambda)$$

Derivatives of Gaussian transformation

Recall:

$$h^{-1}(\epsilon, \lambda) = \mu(x, \lambda) + \sigma(x, \lambda) \odot \epsilon \ .$$

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This gives us 2 gradient paths.

$$\frac{dh^{-1}(\epsilon, \lambda)}{d\mu(x, \lambda)} = \frac{d}{d\mu(x, \lambda)} \left[\mu(x, \lambda) + \sigma(x, \lambda) \odot \epsilon\right] = 1$$

$$\frac{dh^{-1}(\epsilon, \lambda)}{d\sigma(x, \lambda)} = \frac{d}{d\sigma(x, \lambda)} \left[\mu(x, \lambda) + \sigma(x, \lambda) \odot \epsilon\right] = \epsilon$$

Gaussian KL

ELBO

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

Gaussian KL

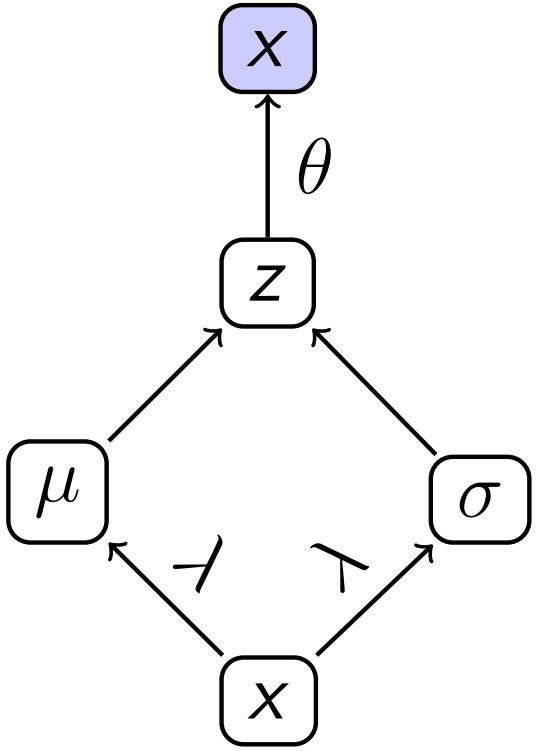
ELBO

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

Analytical computation of $-\mathrm{KL}\left(q(z|x,\lambda) \,||\, p(z)\right)$:

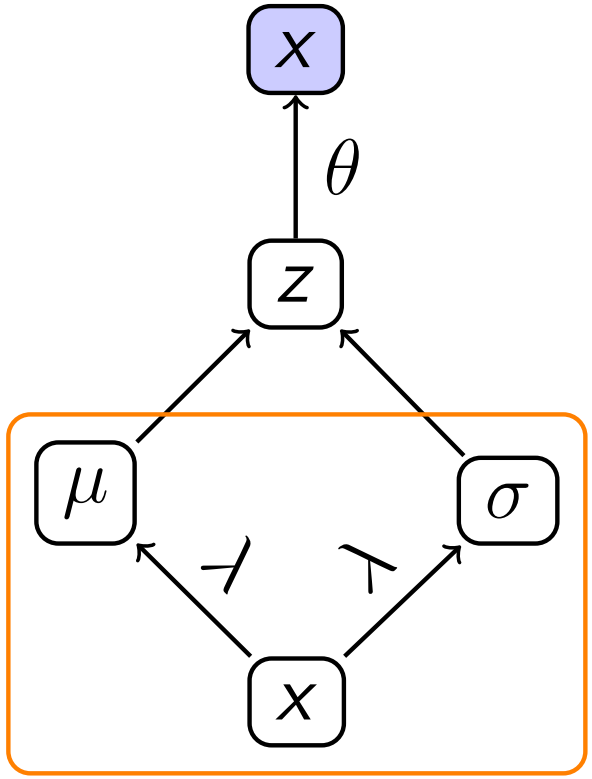
$$\frac{1}{2}\sum_{i=1}^{N}\left(1 + \log\left(\sigma_i^2\right) - \mu_i^2 - \sigma_i^2\right)$$

Computation Graph



Computation Graph

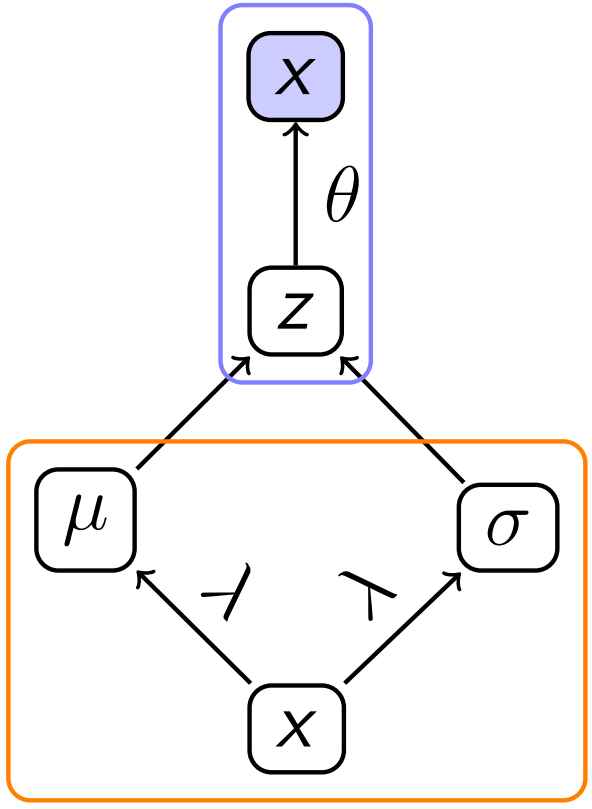
inference model



Computation Graph

generation model

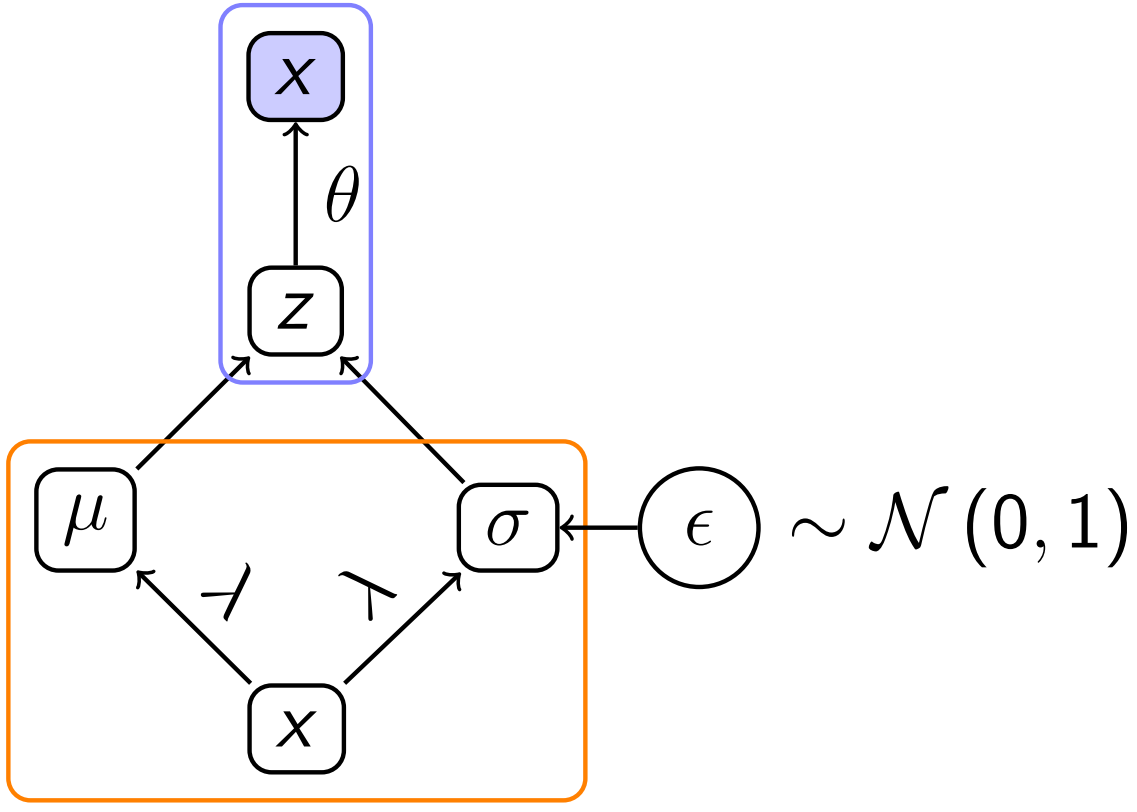
inference model



Computation Graph

generation model

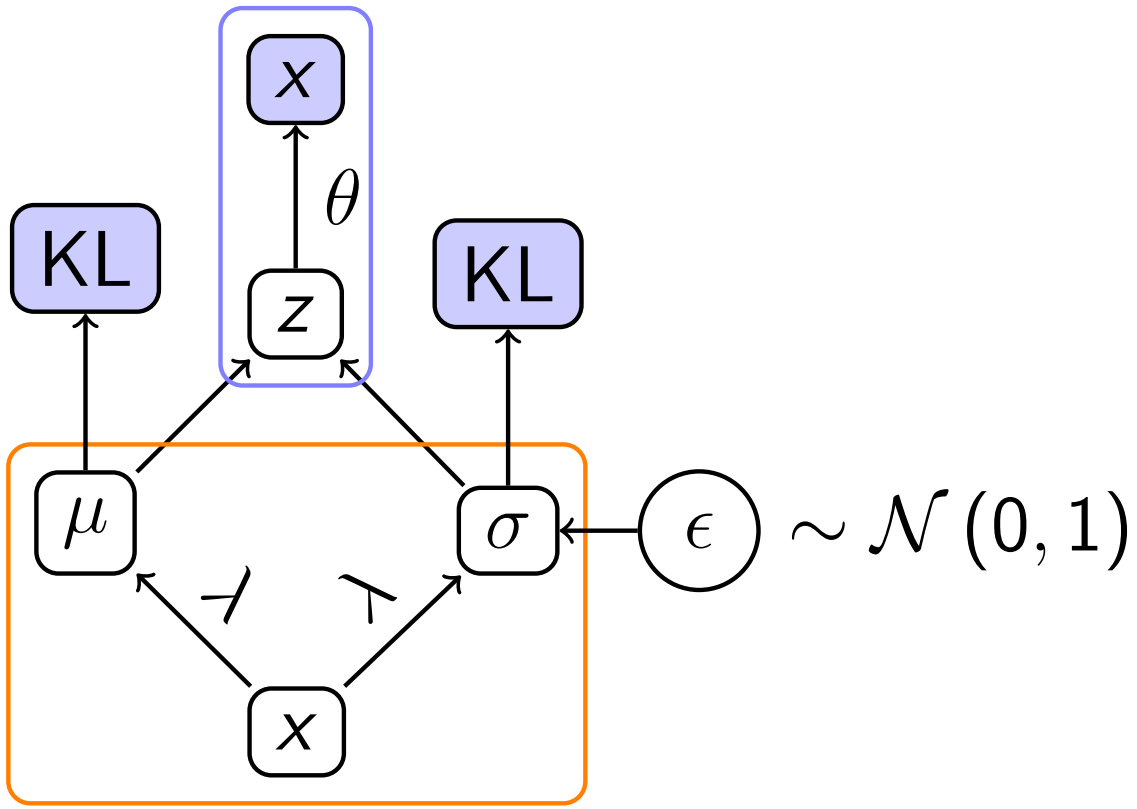
inference model



Computation Graph

generation model

inference model



Example

- Data: binary mnist
- Likelihood: product of Bernoullis
  - Let $\phi = \sigma(\mathrm{NN}(z))$
  - $\prod_{i=1}^{N} p(x_i|\phi) = \prod_{i=1}^{N} \phi^{x_i} \times (1-\phi)^{1-x_i}$
- Prior over z: $\mathcal{N}(0,1)$
- $q(z|x,\lambda) = \mathcal{N}\left(\mu(x,\lambda), \sigma(x,\lambda)^2\right)$
- $\mu(x,\lambda) = \mathrm{NN}_\mu(x;\lambda)$
- $\sigma(x,\lambda) = \mathrm{NN}_\sigma(x;\lambda)$

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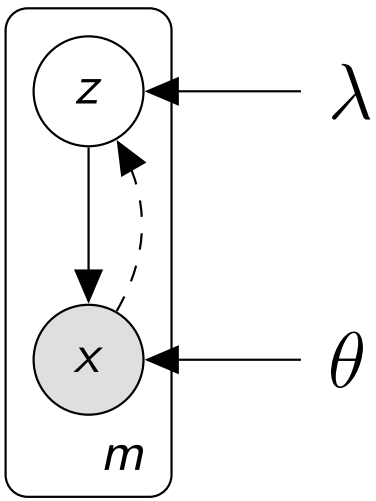
Mean Field assumption

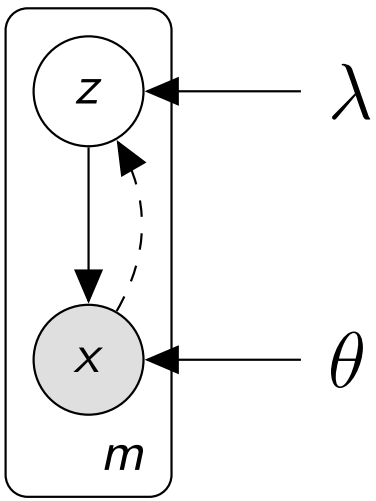
Variational approximation factorises over latent dimensions.

Graphical Model



- approximate posterior
  $q(z|x, \lambda) = \mathcal{N}\left(\mu(x, \lambda), \sigma(x, \lambda)^2\right)$

Graphical Model



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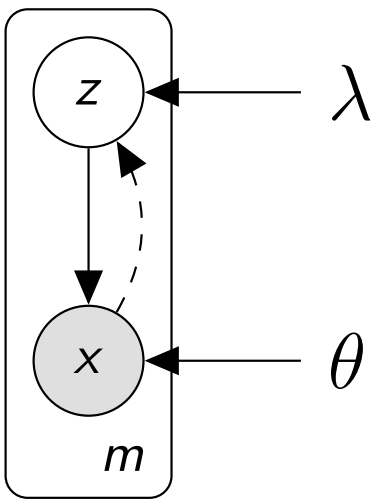
    e.g. $\mu(x, \lambda) = W^{(u)}x + b^{(u)}$

Graphical Model



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  - $\sigma(x,\lambda) = \exp(\mathrm{NN}_\sigma(x;\lambda))$
    e.g. $\sigma(x,\lambda) =$
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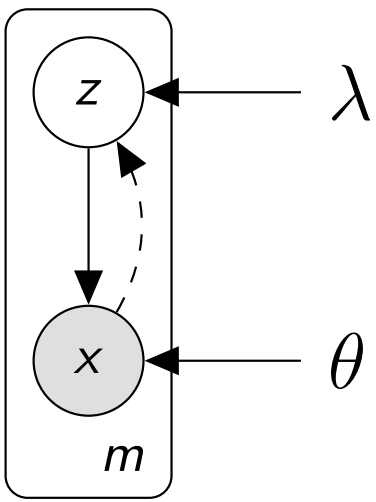
Graphical Model



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    e.g. $\sigma(x,\lambda) =$
    $\log\left(1 + \exp\left(W^{(v)}x + b^{(v)}\right)\right)$
  - $\lambda = \left(W^{(u)}, W^{(v)}, b^{(u)}, b^{(v)}\right)$

Aside

If your likelihood model is able to express dependencies between the output variables (e.g. an RNN), the model may simply ignore the latent code. In that case one often scales the KL term. The scale factor is increased gradually.

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

where $\beta \to 1$.

Variational Autoencoder

Advantages

- Backprop training
- Easy to implement
- Posterior inference possible
- One objective for both NNs

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Drawbacks

- Discrete latent variables are difficult
- Optimisation may be difficult with several latent variables

Summary

- When $|\mathcal{X}|$ and $|\mathcal{Z}|$ are not too large, we can do EM with features
- Otherwise use VI with simple approximation
- Wake-Sleep: train inference and generation networks with separate objectives
- VAE: train both networks with same objective
- Reparametrisation
  - Transform parameter-free variable ϵ into latent value z
  - Update parameters with stochastic gradient estimates

Literature I

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G. E. Hinton, P. Dayan, B. J. Frey, and R. M. Neal. The wake-sleep algorithm for unsupervised neural networks. *Science*, 268:1158–1161, 1995. URL http://www.gatsby.ucl.ac.uk/~dayan/papers/hdfn95.pdf.

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Diederik P. Kingma and Max Welling. Auto-Encoding Variational Bayes. 2013. URL http://arxiv.org/abs/1312.6114.

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Danilo J. Rezende, Shakir Mohamed, and Daan Wierstra. Stochastic backpropagation and approximate inference in deep generative models. In *ICML*, pages 1278–1286, 2014. URL http://jmlr.org/proceedings/papers/v32/rezende14.pdf.

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http://jmlr.org/proceedings/papers/v32/titsias14.pdf.