

Deep Generative Models

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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

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

- ▶ 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.

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

Log-linear Model

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Weight Gradient

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

Log-linear Model

Let us treat z as observed.

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

Weight Gradient

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

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

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

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

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

Log-linear model with latent variables

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

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

Log-linear model with latent variables

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

$$\begin{aligned}\frac{d}{dw} \mathbb{E}_{p(z|x, w)} [\log p(x, z|w)] &= \\ \frac{d}{dw} \sum_z p(z|x, w) \log p(x, z|w) &= \end{aligned}$$

Log-linear model with latent variables

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Log-linear model with latent variables

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

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Log-linear model with latent variables

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

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

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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)

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

Log-linear model with latent variables

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

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

$$\mathbb{E}_{p(z|x, w)} [f(x, Z)|x, w] - \mathbb{E}_{p(z|x, w)} [\mathbb{E} [(f(X, Z)|Z, w)]]$$

Procedurally

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

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 $\text{E_count}(x, z)$
with $\text{E_count}(x, z) \times \mathbb{E}[X|z, w]$

Restrictions

- ▶ Only log-linear models
- ▶ Scales badly

Generative Models

First Attempt: Log-linear Models

Second Attempt: Wake-Sleep

This is how we do: Variational Autoencoders

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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- ▶ 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 likelihood 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 $q(z|\tilde{x}, \lambda)$

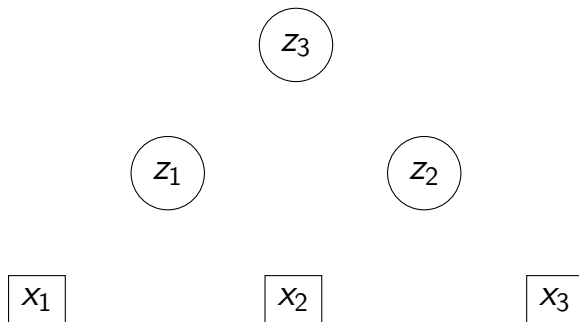
Wake Phase Objective

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

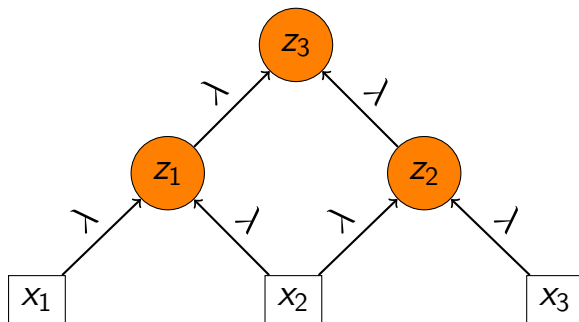
$$\max_{\theta} \log p(x|z, \theta)$$

This is simply supervised learning with imputed latent data!

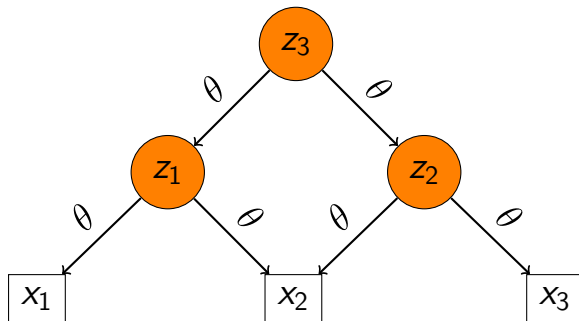
Wake Phase Sampling



Wake Phase Sampling



Wake Phase Update

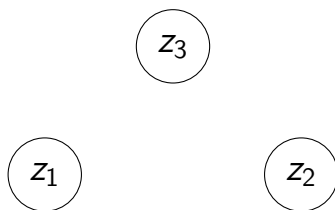


Sleep Phase Objective

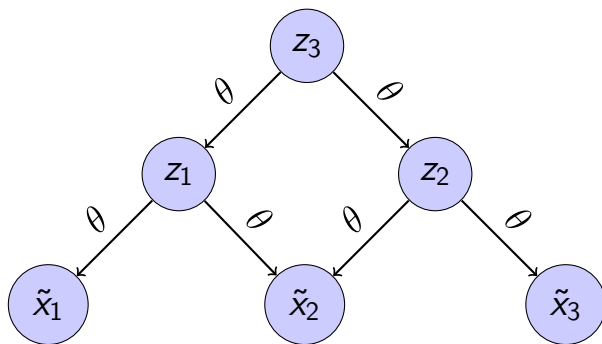
Assumes fake data \tilde{x} and latent variables z to be fixed random draw from $p(x, z|\theta)$.

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

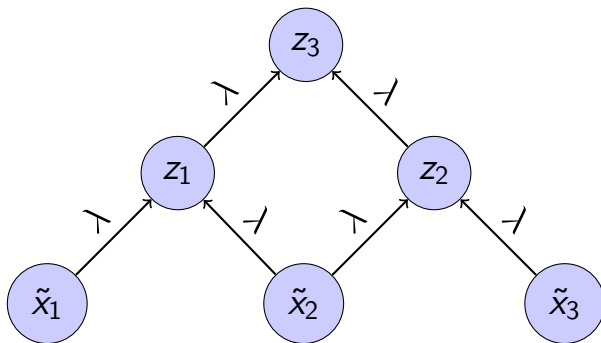
Sleep Phase Sampling



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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Problem

$p(x) = \int p(x|z, \theta)p(z)dz$ is hard to compute.

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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.)

Problem

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

Generative Model with NN Likelihood

Solution: VI

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

Generative Model with NN Likelihood

Solution: VI

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

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Generative Model with NN Likelihood

Solution: VI

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 \log p(x) &\geq \overbrace{\mathbb{E}_{q(z|x, \lambda)} [\log p(x, z|\theta)] + \mathbb{H}(q(z|x, \lambda))}^{\text{ELBO}} \\
 &= \mathbb{E}_{q(z|x, \lambda)} [\log p(x|z, \theta) + \log p(z)] + \mathbb{H}(q(z|x, \lambda)) \\
 &= \mathbb{E}_{q(z|x, \lambda)} [\log p(x|z, \theta)] - \underbrace{\text{KL}(q(z|x, \lambda) || p(z))}_{\substack{\text{assume analytical} \\ \text{(true for exponential families)}}}
 \end{aligned}$$

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

Generation Network Gradient

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

Generation Network Gradient

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Generation Network Gradient

$$\begin{aligned}
 & \frac{d}{d\theta} \mathbb{E}_{q(z|x, \lambda)} [\log p(x|z, \theta)] - \overbrace{\text{KL}(q(z|x, \lambda) || p(z))}^{\text{constant}} \\
 &= \mathbb{E}_{q(z|x, \lambda)} \left[\frac{d}{d\theta} \log p(x|z, \theta) \right] \\
 &\approx^{\text{MC}} \frac{1}{S} \sum_{i=1}^S \frac{d}{d\theta} \log p(x|z_i, \theta)
 \end{aligned}$$

Generation Network Gradient

$$\begin{aligned}
 & \frac{d}{d\theta} \mathbb{E}_{q(z|x, \lambda)} [\log p(x|z, \theta)] - \overbrace{\text{KL}(q(z|x, \lambda) || p(z))}^{\text{constant}} \\
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 &\approx \frac{1}{S} \sum_{i=1}^S \frac{d}{d\theta} \log p(x|z_i, \theta)
 \end{aligned}$$

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

Inference Network Gradient

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

Inference Network Gradient

$$\begin{aligned} & \frac{d}{d\lambda} \left[\mathbb{E}_{q(z|x, \lambda)} [\log p(x|z, \theta)] - \text{KL} (q(z|x, \lambda) \parallel p(z)) \right] \\ &= \frac{d}{d\lambda} \mathbb{E}_{q(z|x, \lambda)} [\log p(x|z, \theta)] - \underbrace{\frac{d}{d\lambda} \text{KL} (q(z|x, \lambda) \parallel p(z))}_{\text{analytical computation}} \end{aligned}$$

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The first term again requires approximation by sampling

Inference Network Gradient

$$\begin{aligned} & \frac{d}{d\lambda} \mathbb{E}_{q(z|x, \lambda)} [\log p(x|z, \theta)] \\ &= \frac{d}{d\lambda} \int q(z|x, \lambda) \log p(x|z, \theta) dz \end{aligned}$$

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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

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
- ▶ $h(z, \lambda) = \epsilon$
- ▶ $h^{-1}(\epsilon, \lambda) = z$

Gaussian Transformation

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Affine property

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

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

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Gaussian transformation

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

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

Inference Network Gradient

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

Inference Network Gradient

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

Inference Network Gradient

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

Inference Network Gradient

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

Inference Network Gradient

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 &= \mathbb{E}_{p(\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]
 \end{aligned}$$

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 &= \mathbb{E}_{p(\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] \\
 &\stackrel{\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)
 \end{aligned}$$

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.

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

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

Gaussian KL

ELBO

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

Gaussian KL

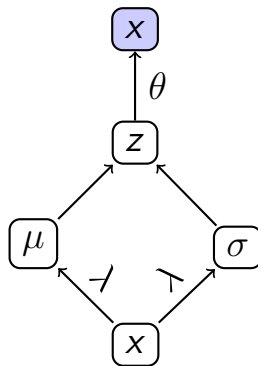
ELBO

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

Analytical computation of $-\text{KL} (q(z|x, \lambda) \parallel p(z))$:

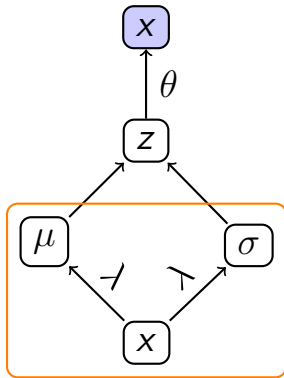
$$\frac{1}{2} \sum_{i=1}^N (1 + \log (\sigma_i^2) - \mu_i^2 - \sigma_i^2)$$

Computation Graph



Computation Graph

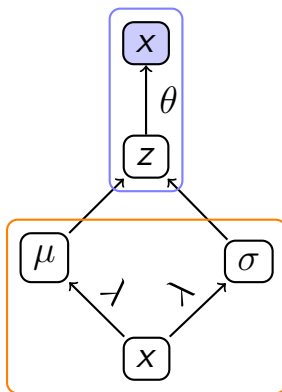
inference model



Computation Graph

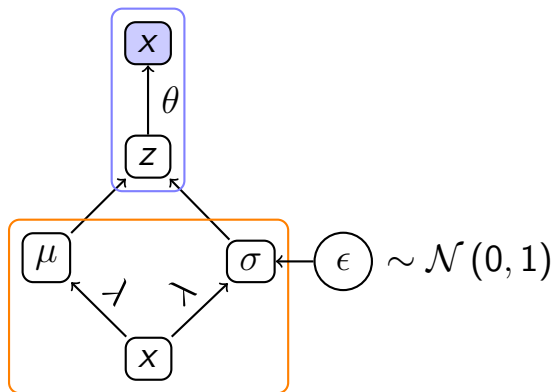
generation model

inference model



generation model

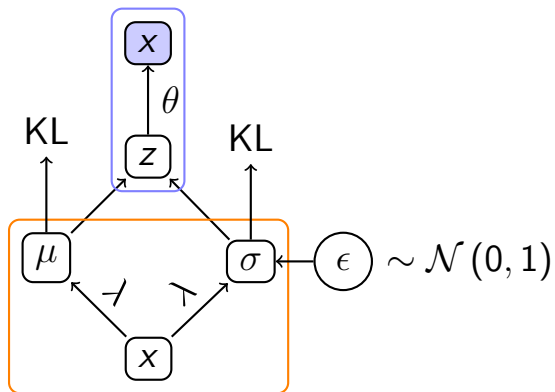
inference model



Computation Graph

generation model

inference model



Example

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

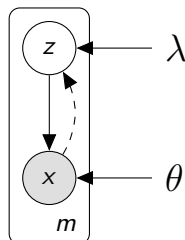
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Mean Field assumption

Variational approximation factorises over latent dimensions.

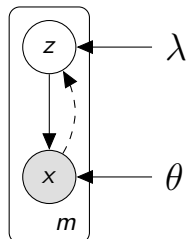
Graphical Model



- approximate posterior

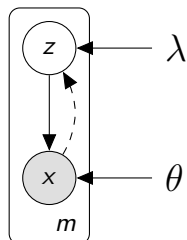
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Graphical Model



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- ▶ where
 - ▶ $\mu(x, \lambda) = \text{NN}_{\mu}(x; \lambda)$
 e.g. $\mu(x, \lambda) = W^{(u)}x + b^{(u)}$

Graphical Model



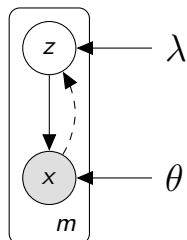
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e.g. $\sigma(x, \lambda) = \log(1 + \exp(W^{(v)}x + b^{(v)}))$

Graphical Model



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- ▶ $\lambda = (W^{(u)}, W^{(v)}, b^{(u)}, b^{(v)})$

Variational Autoencoder

Advantages

- ▶ Backprop training
- ▶ Easy to implement
- ▶ Posterior inference possible
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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

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