Deep Generative Models: Continuous Latent Variables

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https://github.com/philschulz/VITutorial

Deep Generative Models

First Attempt: Wake-Sleep

This is how we do: Variational Autoencoders

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

Deep generative models

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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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We need approximate inference techniques!

Deep Generative Models

First Attempt: Wake-Sleep

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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

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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 $q(z|x, \lambda)$.

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

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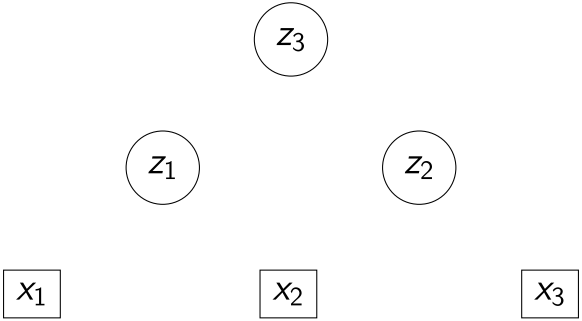
This is simply supervised learning with imputed latent data!

Wake Phase Sampling



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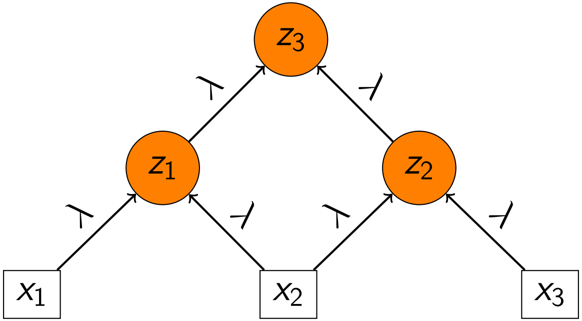
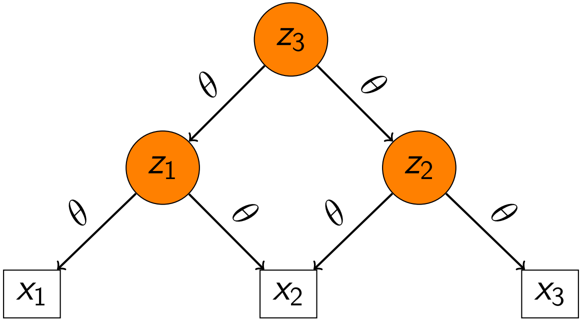


Wake Phase Update



Sleep Phase Objective

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

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

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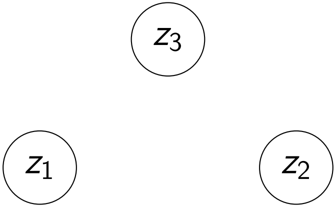
Sleep Phase Sampling



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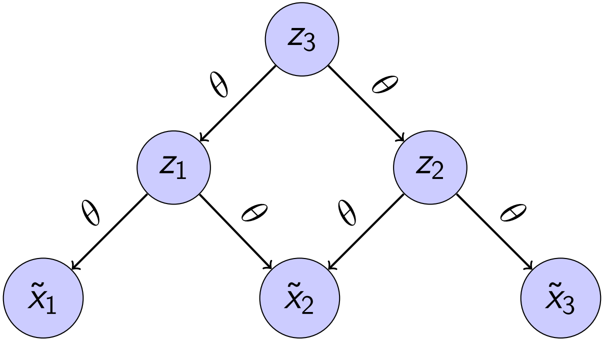

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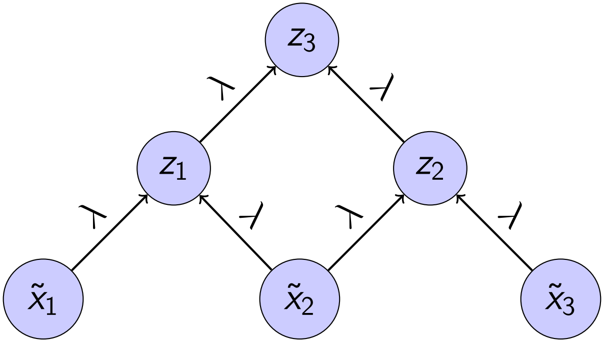

Wake-sleep Algorithm

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.)

Generative Model with NN Likelihood

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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.

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

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

- assume $\mathrm{KL}\left(q(z|x,\lambda) \,||\, p(z)\right)$ analytical
  true for exponential families

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$$

- assume $\mathrm{KL}\left(q(z|x,\lambda)\,||\,p(z)\right)$ 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

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

Generator Network Gradient

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

Generator Network Gradient

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

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

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

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

Inference Network Gradient

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

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The first term again requires approximation by sampling

Inference Network Gradient

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

Not an expected gradient!

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

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- $h(z, \lambda)$ 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

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

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Gaussian transformation

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

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

Inference Network Gradient

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

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Derivatives of Gaussian transformation

Recall:

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

We get two gradient paths!

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- one is deterministic
$\frac{\partial h^{-1}(\epsilon,\lambda)}{\partial\mu(\phi,\lambda)} = \frac{\partial}{\partial\mu(\phi,\lambda)}[\mu(\phi, \lambda) + \sigma(\phi, \lambda) \odot \epsilon] = 1$

Derivatives of Gaussian transformation

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

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- the other is stochastic
  $\frac{\partial h^{-1}(\epsilon,\lambda)}{\partial \sigma(\phi,\lambda)} = \frac{\partial}{\partial \sigma(\phi,\lambda)}[\mu(\phi, \lambda) + \sigma(\phi, \lambda) \odot \epsilon] = \epsilon$

Gaussian KL

ELBO

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

Gaussian KL

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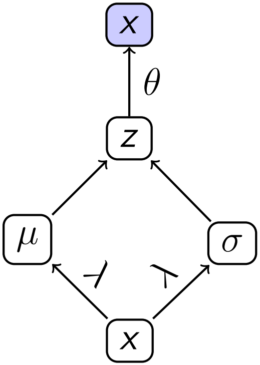
$$\mathbb{E}_{q(z|x,\lambda)}\left[\log p(x|z,\theta)\right] - \mathrm{KL}\left(q(z|x,\lambda) \;||\; p(z)\right)$$

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

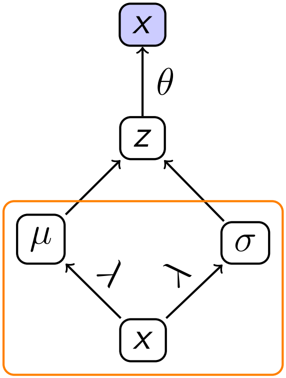


$$\begin{tikzcd}
 & x & \\
 & z \arrow[u, "\theta"'] & \\
\mu \arrow[ur] & & \sigma \arrow[ul] \\
 & x \arrow[ul, "\lambda"'] \arrow[ur, "\lambda"] &
\end{tikzcd}$$

Computation Graph

inference model

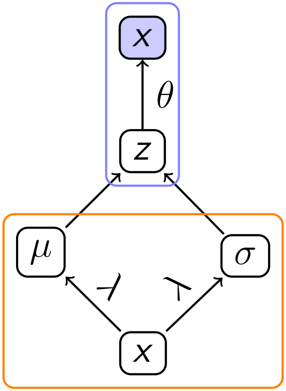
$$\begin{tikzcd} & x & \\ & z \arrow[u, "\theta"'] & \\ \mu \arrow[ur] & & \sigma \arrow[ul] \\ & x \arrow[ul, "\lambda"'] \arrow[ur, "\lambda"] & \end{tikzcd}$$



Computation Graph

generation model

inference model



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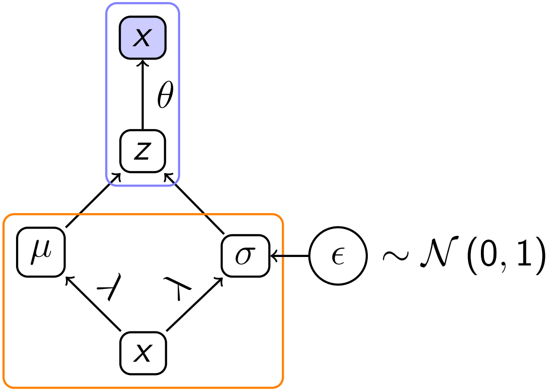

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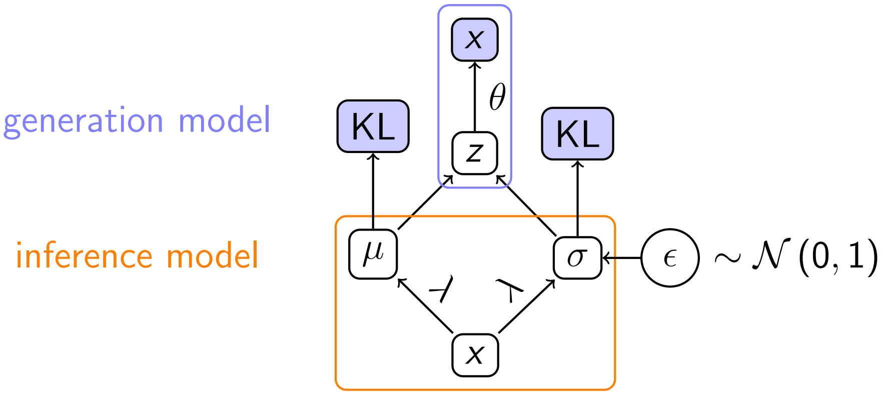
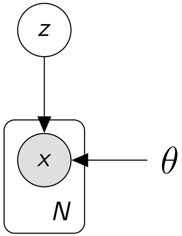


Example: Unigram Document Model



Generative story

- Draw a document embedding
  $Z \sim \mathcal{N}(0, I)$
- Draw N words
  $X_i | z \sim \mathrm{Cat}(f(z, \theta))$

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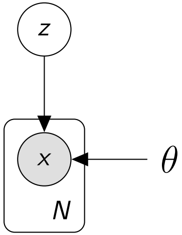

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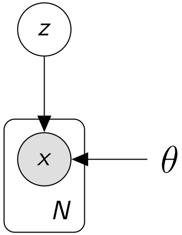
- Draw N words $X_i | z \sim \mathrm{Cat}(f(z, \theta))$

Designing $f(z, \theta)$

Example: Unigram Document Model



Generative story

- Draw a document embedding
  $Z \sim \mathcal{N}(0, I)$
- Draw N words
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Designing $f(z, \theta)$

$$h = \text{relu}(W_1 z + b_1)$$

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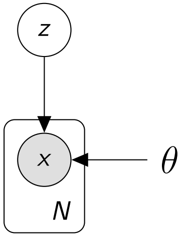

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Designing $f(z, \theta)$

$$h = \text{relu}(W_1 z + b_1)$$
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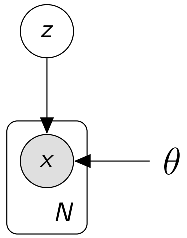

Generative story

- Draw a document embedding $Z \sim \mathcal{N}(0, I)$
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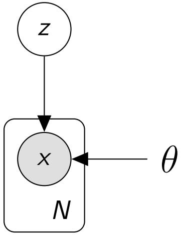
Designing $f(z, \theta)$

$$\begin{aligned} h &= \text{relu}(W_1 z + b_1) \\ f(z, \theta) &= \text{softmax}(W_2 h + b_2) \\ \theta &= \{W_1, b_1, W_2, b_2\} \end{aligned}$$

Example: Unigram Document Model



Likelihood

Generative story

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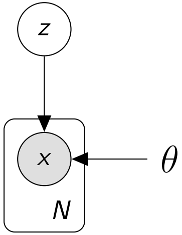

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- Draw a document embedding
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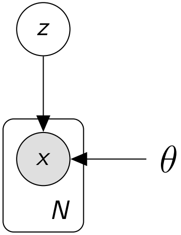
Likelihood

$$p(x_1^N | z, \theta) = \prod_{i=1}^{N} p(x_i | z, \theta)$$

Example: Unigram Document Model



Generative story

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Likelihood

$$p(x_1^N | z, \theta) = \prod_{i=1}^{N} p(x_i | z, \theta) = \prod_{i=1}^{N} \text{Cat}(x_i | \underbrace{f(z, \theta)}_{=\psi})$$

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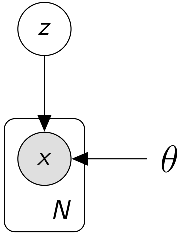

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$$= \prod_{i=1}^{N} \psi_{x_i}$$

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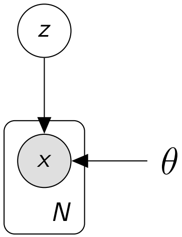

Marginal

Generative story

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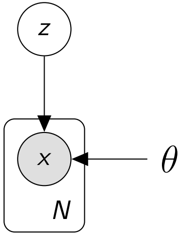
Example: Unigram Document Model



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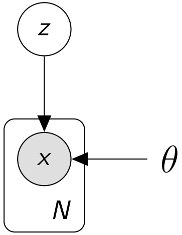
Marginal

$$p(x_1^N | \theta) = \int p(z) \prod_{i=1}^{N} p(x_i | z, \theta) \, \mathrm{d}z$$

Example: Unigram Document Model



Generative story

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Marginal

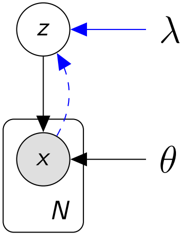
$$p(x_1^N|\theta) = \int p(z) \prod_{i=1}^{N} p(x_i|z, \theta)\, \mathrm{d}z$$

$$= \int \mathcal{N}(z|0, I) \prod_{i=1}^{N} \mathrm{Cat}(x_i|f(z, \theta))\, \mathrm{d}z$$

Example: Unigram Document Model

Inference model

- $Z|x_1^N \sim \mathcal{N}(\mu(x_1^N, \lambda), \sigma(x_1^n, \lambda)^2)$



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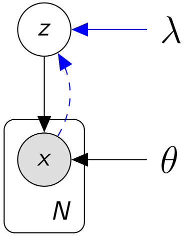
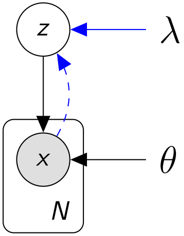
- $Z|x_1^N \sim \mathcal{N}(\mu(x_1^N, \lambda), \sigma(x_1^n, \lambda)^2)$

Designing the *inference network*



Example: Unigram Document Model



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Designing the *inference network*

$$s = \sum_{i=1}^{N} E_{x_i}$$

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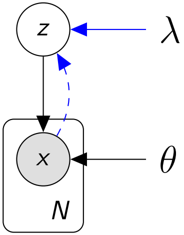

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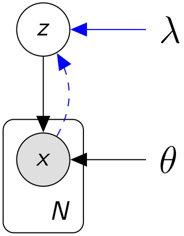

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Designing the *inference network*

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$$\mu(x_1^N, \lambda) = M_2 h + c_2$$

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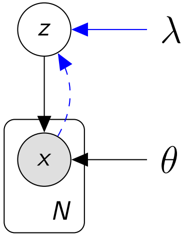

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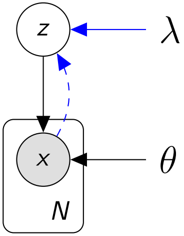

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$$\lambda = \{E, M_1^3, c_1^3\}$$

Example: Unigram Document Model

Generative Model

- Prior: $Z \sim \mathcal{N}(0, I)$
- Likelihood: $X_i | z \sim \text{Cat}(f(z, \theta))$

Inference Model

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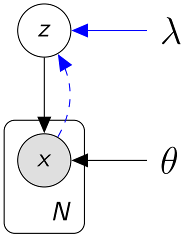

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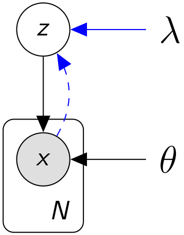

ELBO

$$\log p(x_1^N | \theta) \geq \mathbb{E}_{\frac{z-u}{s} \sim \mathcal{N}(0,I)} \left[\sum_{i=1}^{N} \log \psi_{x_i} \right] - \text{KL}\left(\mathcal{N}(z | u, s^2) \,||\, \mathcal{N}(z | 0, I) \right)$$

where $u = \mu(x_1^N, \lambda)$, $s = \sigma(x_1^N, \lambda)$, and $\psi = f(z, \theta)$

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.

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

where $\beta \to 1$.

Variational Autoencoder

Advantages

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

Drawbacks

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

Summary

- 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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