Deep Generative Models: Continuous Latent Variables

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https://github.com/philschulz/VITutorial

branch: yandex2019 module: modules/M3a

Deep Generative Models

Variational Autoencoders

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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.)

Example: Language Model

A deterministic language model is **one** distribution over observations:

$$p(x|\theta) = \prod_{i=1}^{n} p(x_i|x_{<i}, \theta)$$

Every sentence gets mapped from the same conditioning context, namely, the beginning of sequence symbol.

Example: Language Model (cont.)

With latent variables we can model the data as a draw from a complex marginal, which mixes conditionals from different points in space

$$p(x|\theta) = \int p(z) \prod_{i=1}^{n} p(x_i|z, x_{<i}, \theta)\mathrm{d}z$$

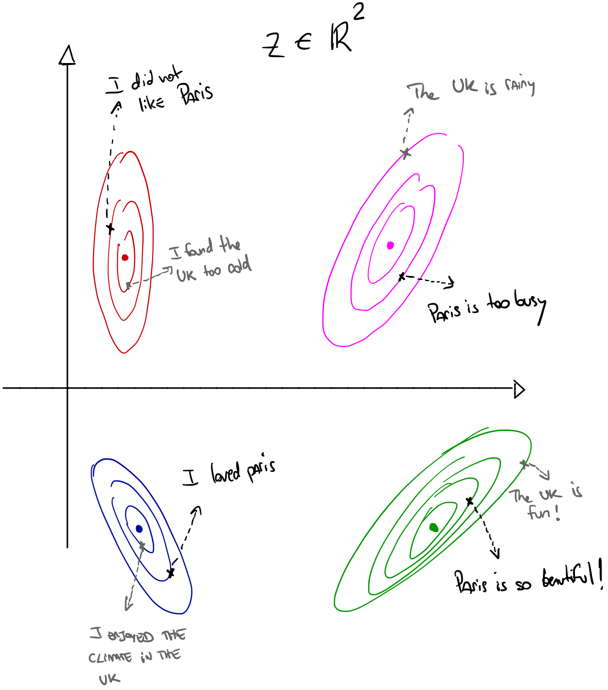
Example: Language Model (cont.)

With latent variables we can model the data as a draw from a complex marginal, which mixes conditionals from different points in space

$$p(x|\theta) = \int p(z) \prod_{i=1}^{n} p(x_i|z, x_{<i}, \theta)\mathrm{d}z$$

Good training can lead to considerable amount of structure in the posterior

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



$z \in \mathbb{R}^2$
I did not like Paris
The UK is rainy
I found the UK too cold
Paris is too busy
I loved paris
The UK is fun!
Paris is so beautiful!
I ENJOYED THE CLIMATE IN THE UK

Example: Language Model (architecture)

Generative model:

$$Z \sim \mathcal{N}(0, I)$$
$$X_i | z, x_{<i} \sim \mathrm{Cat}(f(z, x_{<i}; \theta))$$

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$$h_0 = \tanh\left(W^{(\mathrm{init})} z + b^{(\mathrm{init})}\right)$$

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$$f(z, x_{<i}) = \mathrm{softmax}(W^{(\mathrm{out})} h_i + b^{(\mathrm{out})})$$
$$\theta = \theta_{\mathrm{rnn}} \cup \{W^{(\mathrm{init})}, b^{(\mathrm{init})}, W^{(\mathrm{out})}, b^{(\mathrm{out})}\}$$

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Problem

$p(x|\theta) = \int p(z)p(x|z, \theta)\mathrm{d}z$ is intractable!

Deep Generative Models

Variational Autoencoders

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

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

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

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\end{aligned}
$$

$$
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$$

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

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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
- 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

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

Generator Network Gradient

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

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

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

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

Generator Network Gradient

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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

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

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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Inference Network Gradient

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

The first term again requires approximation by sampling

Inference Network Gradient

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

Inference Network Gradient

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

Not an expected gradient!

Score function estimator?

Can we apply the log-derivative trick?

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

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

Yes, it's a general result!

What about variance?

The learning signal can only scale the gradient:

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

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Can we do better?

Inference Network Gradient

Problem

We need to re-express the gradient, but the measure of integration depends on λ

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

Inference Network Gradient

Problem

We need to re-express the gradient, but the measure of integration depends on λ

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

What if we could re-express $q(z|x,\lambda)$ in terms of some other distribution that does not depend on λ?

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

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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Special case

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

Gaussian Transformation

Let an inference network compute

$$u = \mu(x;\lambda) \quad s \; = \sigma(x;\lambda)$$

for a posterior $Z \sim \mathcal{N}(u, s^2)$, then we have:

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Gaussian Transformation

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$$u = \mu(x; \lambda) \quad s \; = \sigma(x; \lambda)$$

for a posterior $Z \sim \mathcal{N}(u, s^2)$, then we have:

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

and conversely, for $\epsilon \sim \mathcal{N}(0, I)$, we have:

$$h^{-1}(\epsilon, \lambda; x) = \mu(x; \lambda) + \sigma(x; \lambda) \odot \epsilon = z \sim \mathcal{N}(u, s^2)$$

Inference Network Gradient

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

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

Inference Network Gradient

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

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Derivatives of Gaussian transformation

Recall:

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

We get two gradient paths!

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

Derivatives of Gaussian transformation

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We get two gradient paths!

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

Gaussian KL

ELBO

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

Gaussian KL

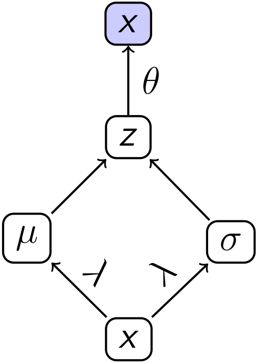
ELBO

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

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

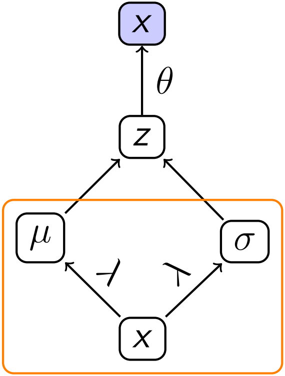
$$\frac{1}{2}\sum_{i=1}^{N}\left(1+\log\left(\sigma_i^2\right)-\mu_i^2-\sigma_i^2\right)$$

Computation Graph



Computation Graph

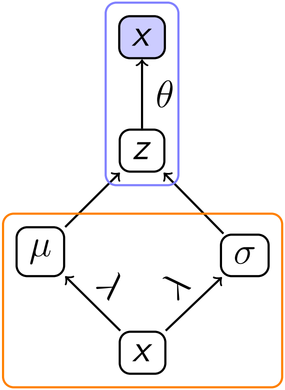
inference model



Computation Graph

generation model

inference model



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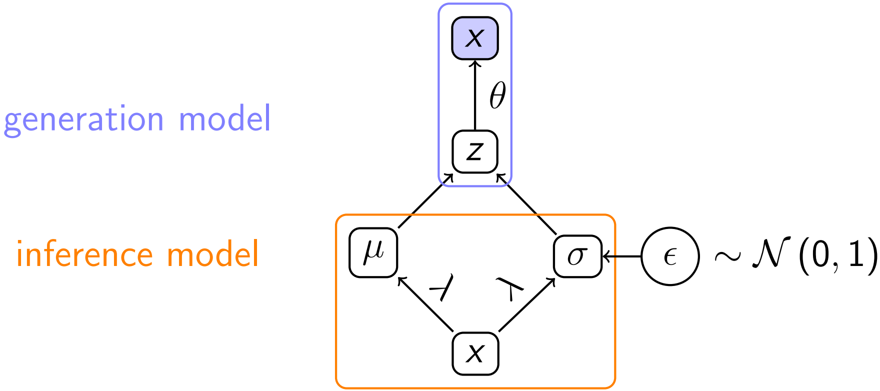

Computation Graph

generation model

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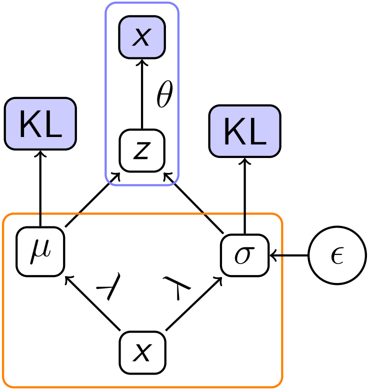
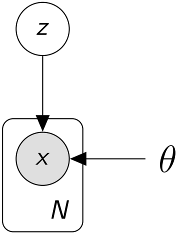


$\sim \mathcal{N}(0, 1)$

Example: Unigram Document Model



Generative story

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

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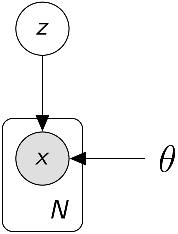

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Designing $f(z, \theta)$

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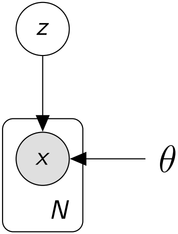

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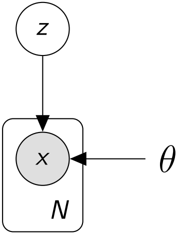
Designing $f(z, \theta)$

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

Example: Unigram Document Model



Generative story

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

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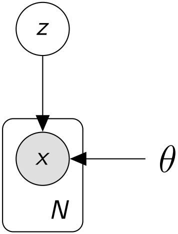

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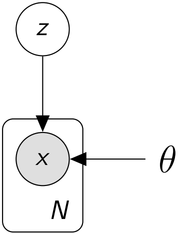

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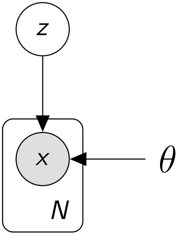

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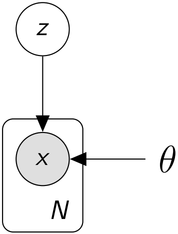

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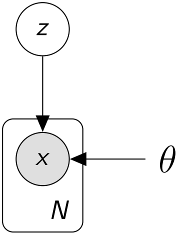

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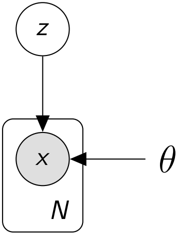

Marginal

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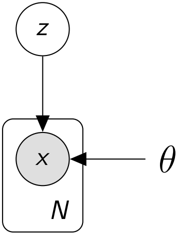

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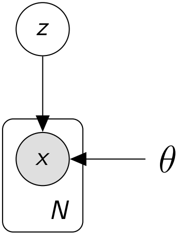

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$$
\begin{aligned}
p(x|\theta) &= \int p(z) \prod_{i=1}^{N} p(x_i|z,\theta)\,\mathrm{d}z \\
&= \int \mathcal{N}(z|0, I) \prod_{i=1}^{N} \mathrm{Cat}(x_i|f(z;\theta))\,\mathrm{d}z
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$$

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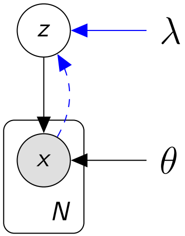

Inference model

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

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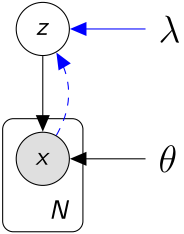

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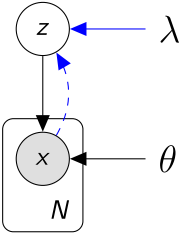

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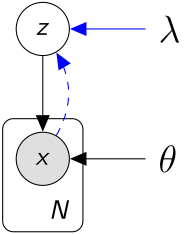

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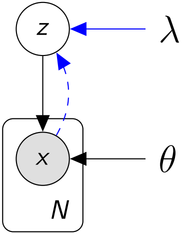

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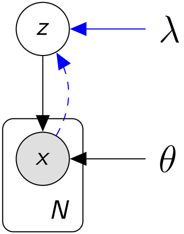

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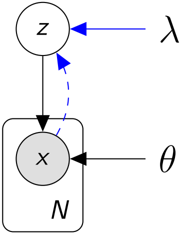

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$$\lambda = \{E, M_1^3, c_1^3\}$$

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Inference Model

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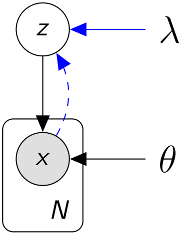

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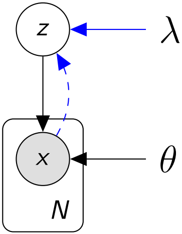

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ELBO

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

where $u = \mu(x; \lambda)$, $s = \sigma(x; \lambda)$, and $\psi = f(z = u + \epsilon \odot s, \theta)$

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.

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

where $\beta \to 1$.

Aside

Another strategy is to promote the posterior to deviate a bit from the prior by not penalising for the first few nats of information:

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

where $R \geq 0$ is known as "free bits"

Aside

But note that if we scale down the KL term permanently, or allow too many free bits, then the conditional $p(x|z, \theta)$ will over-specialise to samples from the approximate posterior $q(z|x, \lambda)$. This can lead to bad generalisation and/or poor samples when generating from the prior.

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Advantages

- Backprop training
- Easy to implement
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- Amortised inference

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Drawbacks

- Discrete latent variables are not possible
- 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

Implementation

Try one of our notebooks, e.g.

- Original VAE: MNIST
  https://github.com/philschulz/VITutorial/blob/master/code/vae_notebook_pytorch.ipynb
- SentenceVAE
  https://github.com/probabll/dgm4nlp/blob/master/notebooks/sentencevae/

Literature I

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