Deep Generative Models: Continuous Latent Variables

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

Score Function Estimator

Integration by substitution

Variational Autoencoders

Semisupervised Learning

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Score Function Estimator

- Stochastic Gradient Estimator
- $\frac{\partial}{\partial \lambda} \mathbb{E}_{q(z|\lambda)} [\log p(x|z,\theta)] = \mathbb{E}_{q(z|\lambda)} \left[\frac{\partial}{\partial \lambda} \log q(z|\lambda) \log p(x|z,\theta)\right]$
- Very general
- High variance

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- Very general
- High variance
- Can we do better?

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Basic Proof

We can express an integral over x in terms of an integral over y.
Let f be continuous and $h(x) = y$ be invertible s.t $h^{-1}(y) = x$.

$$\int_a^b f(x)\mathrm{d}x$$

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$$= F\left(\underbrace{h^{-1}(y)}_{x}\right)\Big|_{h(a)}^{h(b)} = \int_{h(a)}^{h(b)} f\left(h^{-1}(y)\right) \underbrace{\frac{\mathrm{d}h^{-1}(y)}{\mathrm{d}y}}_{\frac{\mathrm{d}x}{\mathrm{d}y}} \mathrm{d}y$$

Observations

$$\int_a^b f(x)\mathrm{d}x = \int_{h(a)}^{h(b)} f\left(h^{-1}(y)\right) \frac{\mathrm{d}h^{-1}(y)}{\mathrm{d}y}\mathrm{d}y$$

- h^{-1} increasing $\implies \frac{\mathrm{d}h^{-1}(y)}{\mathrm{d}y} > 0$

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- h^{-1} increasing $\implies \frac{\mathrm{d}h^{-1}(y)}{\mathrm{d}y} > 0$
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- h^{-1} decreasing $\implies \frac{\mathrm{d}h^{-1}(y)}{\mathrm{d}y} < 0$ and $h(a) \geq h(b)$
  - $\frac{\mathrm{d}h^{-1}(y)}{\mathrm{d}y}$ corrects for the bounds of integration

$$\int f(x)\mathrm{d}x = \int f\left(h^{-1}(y)\right) \left|\frac{\mathrm{d}h^{-1}(y)}{\mathrm{d}y}\right| \mathrm{d}y$$

Observations

$$\int f\left(h^{-1}(y)\right)\left|\frac{\mathrm{d}h^{-1}(y)}{\mathrm{d}y}\right|\mathrm{d}y$$

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- $\left|\frac{\mathrm{d}h^{-1}(y)}{\mathrm{d}y}\right| > 1 \implies h^{-1}$ locally expands area around y

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- $\left|\frac{\mathrm{d}h^{-1}(y)}{\mathrm{d}y}\right| > 1 \implies h^{-1}$ locally expands area around y
- $\left|\frac{\mathrm{d}h^{-1}(y)}{\mathrm{d}y}\right| < 1 \implies h^{-1}$ locally shrinks area around y

Probability Densities

Fact

As before $h(x) = y$ and $h^{-1}(y) = x$. Let X and Y be random variables with densities f_x and f_y. Then

$$F(x) = F(y = h(x)) \text{ or } 1 - F(y = h(x))$$

where

$$F(x) = \int^x p_x(x)\mathrm{d}x \ .$$

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Fact

$$\frac{\mathrm{d}h(x)}{\mathrm{d}x} = \frac{\mathrm{d}y}{\mathrm{d}x} = \frac{\mathrm{d}y}{\mathrm{d}h^{-1}(y)} = \left(\frac{\mathrm{d}h^{-1}(y)}{\mathrm{d}y} \right)^{-1}$$

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The Original Problem

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

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The first term again requires approximation by sampling

Inference Network Gradient

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

Inference Network Gradient

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

Inference Network Gradient

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\begin{aligned}
&\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 expectation!

Possible Solutions

- We could just use the score function gradient estimator
- Or we could use what we have learned about variable substitution . . .

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

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

Inference Network Gradient

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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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\overset{\text{MC}}{\approx}\frac{1}{S}\sum_{i=1}^{S}\frac{\partial}{\partial\lambda}\log p(x|\overbrace{h^{-1}(\epsilon_i,\lambda)}^{=z},\theta)
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where $\epsilon_i \sim q(\epsilon)$

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$$\overset{\text{MC}}{\approx}\frac{1}{S}\sum_{i=1}^{S}\underbrace{\frac{\partial}{\partial z}\log p(x|\overbrace{h^{-1}(\epsilon_i,\lambda)}^{=z},\theta)\times\frac{\partial}{\partial \lambda}h^{-1}(\epsilon_i,\lambda)}_{\text{chain rule}}$$

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

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Gaussian transformation

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

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

Gaussian Transformation

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

where

$$q(\epsilon)=\mathcal{N}(\epsilon;0,\mathrm{I})$$

Derivatives of Gaussian transformation

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

We get two gradient paths!

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

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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

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

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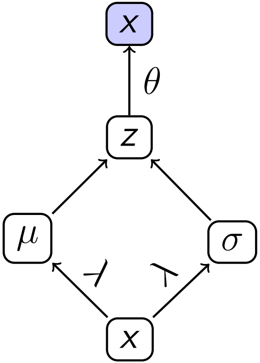
Analytical computation of $-\mathrm{KL}\left(q(z|x,\lambda) \mid\mid p(z)\right)$:

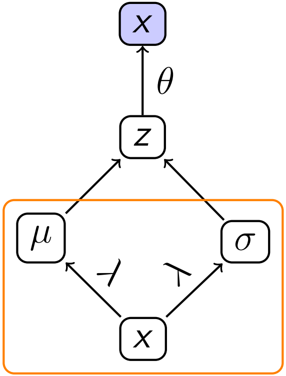
$$\frac{1}{2}\sum_{i=1}^{N}\left(1 + \log\left(\sigma_i^2\right) - \mu_i^2 - \sigma_i^2\right)$$

Computation Graph



Computation Graph

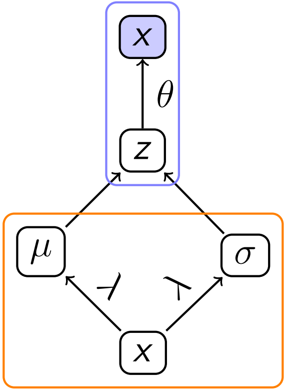
inference model



Computation Graph

generation model

inference model



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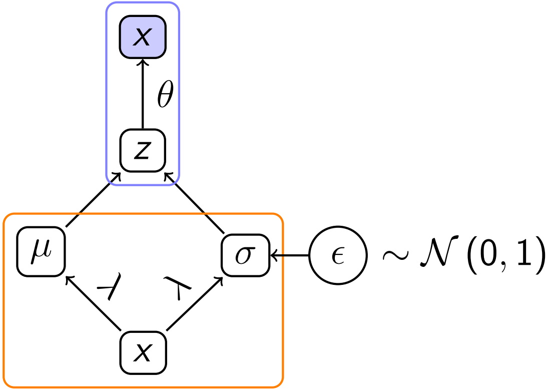

Computation Graph

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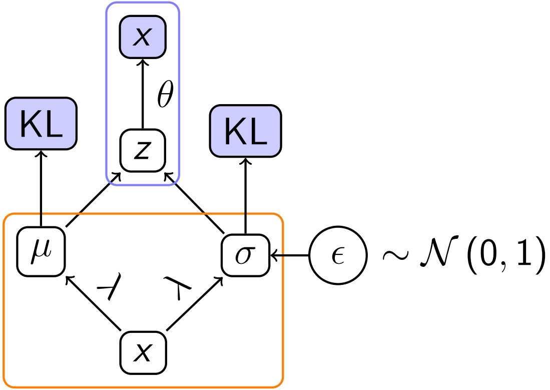

Comparison Between Estimators

- Score function gradient

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

- Reparametrisation gradient

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

Discrete Variables

Why not use reparametrization for discrete variables?

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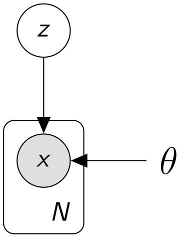
Why not use reparametrization for discrete variables?

Discrete CDF are step functions.

- not continuous
- derivative 0
- no invertible mappings

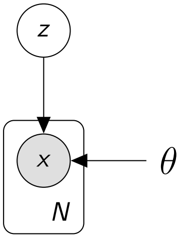
Example: Binarized MNIST



Generative story

- Draw an image embedding $Z \sim \mathcal{N}(0, I)$
- Draw N pixels
  $X_i | z \sim \text{Bernoulli}(f(z, \theta))$

Example: Binarized MNIST



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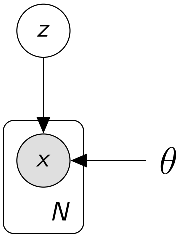

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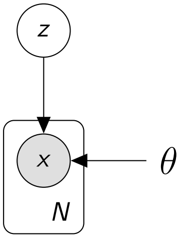

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$$h = \text{relu}(W_1 z + b_1)$$
$$f(z, \theta) = \sigma(W_2 h + b_2)$$

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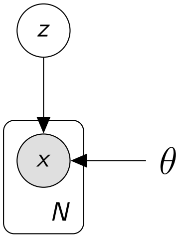

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Designing $f(z, \theta)$

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

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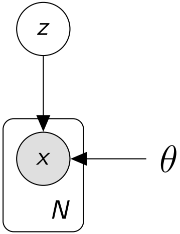

Marginal

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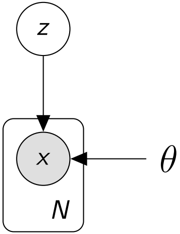

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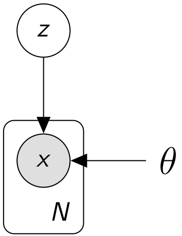

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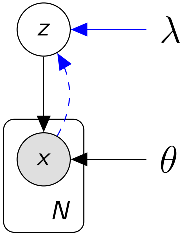

Inference model

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

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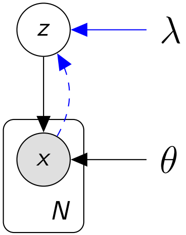

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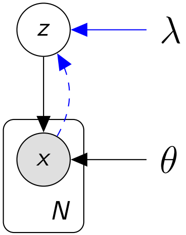
Designing the *inference network*

Example: Binarized MNIST



Inference model

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

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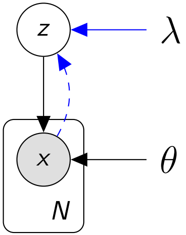

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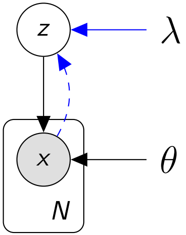

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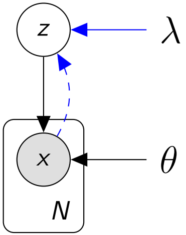

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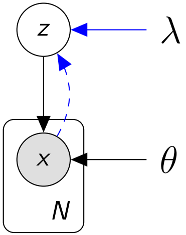

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$$\lambda = \{E, M_1^3, c_1^3\}$$

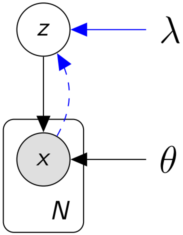
Example: Binarized MNIST

Generative Model

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

Inference Model

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



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

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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

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We now know how to handle continuous and discrete latent variables. Let us combine these two treat partially observed data.

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- walking $\rightarrow$ walks

A Simple Model (Zhou and Neubig, 2017)

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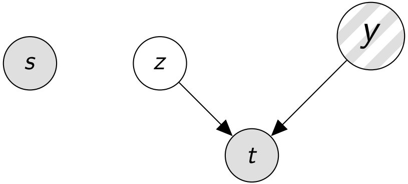
A Simple Model (Zhou and Neubig, 2017)



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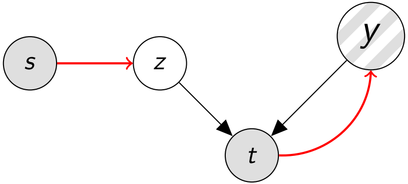

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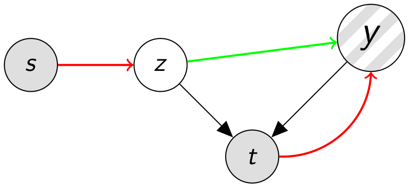

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