Variational Auto-encoders

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Outline

The Basic Problem

The marginal likelihood

$$p(x) = \int p(x, z)\mathrm{d}z$$

is generally **intractable**, which prevents us from computing quantities that depend on the posterior $p(z|x)$

- e.g. gradients in MLE
- e.g. predictive distribution in Bayesian modelling

Strategy

Accept that $p(z|x)$ is not computable.

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- approximate it by an auxiliary distribution $q(z|x)$ that is computable
- choose $q(z|x)$ as close as possible to $p(z|x)$ to obtain a faithful approximation

Evidence lowerbound

$$\log p(x) = \log \int p(x, z) \mathrm{d}z$$

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

Evidence lowerbound

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

Evidence lowerbound

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

Evidence lowerbound

$$
\begin{aligned}
\log p(x) &= \log \int p(x,z)\mathrm{d}z \\
&= \log \int q(z|x)\frac{p(x,z)}{q(z|x)}\mathrm{d}z \\
&= \log \left(\mathbb{E}_{q(z|x)}\left[\frac{p(x,z)}{q(z|x)}\right]\right) \\
&\geq \underbrace{\mathbb{E}_{q(z|x)}\left[\log \frac{p(x,z)}{q(z|x)}\right]}_{\text{ELBO}} \\
&= \mathbb{E}_{q(z|x)}\left[\log p(x,z)\right] - \mathbb{E}_{q(z|x)}\left[\log q(z)\right]
\end{aligned}
$$

Evidence lowerbound

$$\begin{aligned}
\log p(x) &= \log \int p(x,z)\mathrm{d}z \\
&= \log \int {\color{red} q(z|x)} \frac{p(x,z)}{\color{red} q(z|x)} \mathrm{d}z \\
&= \log \left(\mathbb{E}_{q(z|x)} \left[\frac{p(x,z)}{q(z|x)} \right] \right) \\
&\geq \underbrace{\mathbb{E}_{q(z|x)} \left[\log \frac{p(x,z)}{q(z|x)} \right]}_{\text{ELBO}} \\
&= \mathbb{E}_{q(z|x)} \left[\log p(x,z) \right] - \mathbb{E}_{q(z|x)} \left[\log q(z) \right] \\
&= \mathbb{E}_{q(z|x)} \left[\log p(x,z) \right] + \mathbb{H} \left(q(z|x) \right)
\end{aligned}$$

An approximate posterior

$$\log p(x) \geq \underbrace{\mathbb{E}_{q(z|x)}\left[\log \frac{p(x,z)}{q(z|x)}\right]}_{\text{ELBO}}$$

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$$= \mathbb{E}_{q(z|x)}\left[\log \frac{p(z|x)}{q(z|x)}\right] + \underbrace{\log p(x)}_{\text{constant}}$$

$$= \underbrace{-\mathbb{E}_{q(z|x)}\left[\log \frac{q(z|x)}{p(z|x)}\right]}_{\text{KL}(q(z|x)||p(z|x))} + \log p(x)$$

An approximate posterior

$$\begin{aligned}
\log p(x) &\geq \underbrace{\mathbb{E}_{q(z|x)}\left[\log \frac{p(x,z)}{q(z|x)}\right]}_{\text{ELBO}} \\
&= \mathbb{E}_{q(z|x)}\left[\log \frac{p(z|x)p(x)}{q(z|x)}\right] \\
&= \mathbb{E}_{q(z|x)}\left[\log \frac{p(z|x)}{q(z|x)}\right] + \underbrace{\log p(x)}_{\text{constant}} \\
&= -\underbrace{\mathbb{E}_{q(z|x)}\left[\log \frac{q(z|x)}{p(z|x)}\right]}_{\text{KL}(q(z|x)||p(z|x))} + \log p(x)
\end{aligned}$$

We have derived a lower bound on the log-evidence whose gap is exactly $\text{KL}\left(q(z|x) \mid\mid p(z|x)\right)$.

Variational Inference

Objective

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

- The ELBO is a lower bound on $\log p(x)$

Blei et al. (2016)

Mean field assumption

Suppose we have N latent variables

- assume the posterior factorises as N independent terms
- each with an independent set of parameters

$$q(z_1, \ldots, z_N) = \underbrace{\prod_{i=1}^{N} q_{\lambda_i}(z_i)}_{\text{mean field}}$$

Amortised variational inference

Amortise the cost of inference using NNs

$$q(z_1, \ldots, z_N | x_1, \ldots, x_N) = \prod_{i=1}^{N} q_\lambda(z_i | x_i)$$

with a shared set of parameters

- e.g. $Z|x \sim \mathcal{N}(\underbrace{\mu_\lambda(x), \sigma_\lambda(x)^2}_{\text{inference network}})$

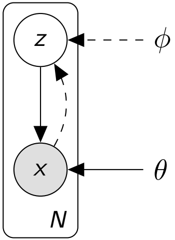
Outline

1. Variational inference

2. Variational auto-encoder
   - Semi supervised VAE
   - Beyond mean field

Variational auto-encoder

Generative model with NN likelihood



- complex (non-linear) observation model $p_\theta(x|z)$
- complex (non-linear) mapping from data to latent variables $q_\phi(z|x)$

Jointly optimise generative model $p_\theta(x|z)$ and inference model $q_\phi(z|x)$ under the same objective (ELBO)

Kingma and Welling (2013)

Objective

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

Objective

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

Objective

$$
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&= \mathbb{E}_{q_\phi(z|x)}\left[\log p_\theta(x|z) + \log p(z)\right] + \mathbb{H}\left(q_\phi(z|x)\right) \\
&= \mathbb{E}_{q_\phi(z|x)}\left[\log p_\theta(x|z)\right] - \mathrm{KL}\left(q_\phi(z|x) \,||\, p(z)\right)
\end{aligned}
$$

Objective

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

Parameter estimation

$$
\arg\max_{\theta,\phi} \; \mathbb{E}_{q_\phi(z|x)}\left[\log p_\theta(x|z)\right] - \mathrm{KL}\left(q_\phi(z|x) \,||\, p(z)\right)
$$

Objective

$$\log p_\theta(x) \geq \overbrace{\mathbb{E}_{q_\phi(z|x)}\left[\log p_\theta(x, z)\right] + \mathbb{H}\left(q_\phi(z|x)\right)}^{\text{ELBO}}$$
$$= \mathbb{E}_{q_\phi(z|x)}\left[\log p_\theta(x|z) + \log p(z)\right] + \mathbb{H}\left(q_\phi(z|x)\right)$$
$$= \mathbb{E}_{q_\phi(z|x)}\left[\log p_\theta(x|z)\right] - \mathrm{KL}\left(q_\phi(z|x) \,||\, p(z)\right)$$

Parameter estimation

$$\arg\max_{\theta,\phi} \; \mathbb{E}_{q_\phi(z|x)}\left[\log p_\theta(x|z)\right] - \mathrm{KL}\left(q_\phi(z|x) \,||\, p(z)\right)$$

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

Objective

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

$$\arg\max_{\theta,\phi} \; \mathbb{E}_{q_\phi(z|x)}\left[\log p_\theta(x|z)\right] - \mathrm{KL}\left(q_\phi(z|x) \,||\, p(z)\right)$$

- assume $\mathrm{KL}\left(q_\phi(z|x) \,||\, p(z)\right)$ analytical
  true for exponential families
- approximate $\mathbb{E}_{q_\phi(z|x)}\left[\log p_\theta(x|z)\right]$ by sampling
  true because we design $q_\phi(z|x)$ to be simple

Generative Network Gradient

$$\frac{\partial}{\partial \theta}\left(\mathbb{E}_{q_\phi(z|x)}\left[\log p_\theta(x|z)\right] - \overbrace{\mathrm{KL}\left(q_\phi(z|x) \mid\mid p(z)\right)}^{\text{constant wrt } \theta}\right)$$

Generative Network Gradient

$$\frac{\partial}{\partial \theta}\left(\mathbb{E}_{q_\phi(z|x)}\left[\log p_\theta(x|z)\right] - \overbrace{\mathrm{KL}\left(q_\phi(z|x) \,||\, p(z)\right)}^{\text{constant wrt } \theta}\right)$$

$$= \underbrace{\mathbb{E}_{q_\phi(z|x)}\left[\frac{\partial}{\partial \theta}\log p_\theta(x|z)\right]}_{\text{expected gradient :)}}$$

Generative Network Gradient

$$\frac{\partial}{\partial\theta}\left(\mathbb{E}_{q_\phi(z|x)}\left[\log p_\theta(x|z)\right] - \overbrace{\mathrm{KL}\left(q_\phi(z|x)\;||\;p(z)\right)}^{\text{constant wrt }\theta}\right)$$

$$= \underbrace{\mathbb{E}_{q_\phi(z|x)}\left[\frac{\partial}{\partial\theta}\log p_\theta(x|z)\right]}_{\text{expected gradient :)}}$$

$$\overset{\text{MC}}{\approx} \frac{1}{K}\sum_{k=1}^{K}\frac{\partial}{\partial\theta}\log p_\theta(x|z^{(k)})$$

$$z^{(k)} \sim q_\phi(z|x)$$

Generative Network Gradient

$$\frac{\partial}{\partial\theta}\left(\mathbb{E}_{q_\phi(z|x)}\left[\log p_\theta(x|z)\right] - \overbrace{\mathrm{KL}\left(q_\phi(z|x)\,||\,p(z)\right)}^{\text{constant wrt }\theta}\right)$$

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$$\overset{\text{MC}}{\approx} \frac{1}{K}\sum_{k=1}^{K}\frac{\partial}{\partial\theta}\log p_\theta(x|z^{(k)})$$

$$z^{(k)} \sim q_\phi(z|x)$$

Note: $q_\phi(z|x)$ does not depend on θ.

Inference Network Gradient

$$\frac{\partial}{\partial \phi}\left(\mathbb{E}_{q_\phi(z|x)}\left[\log p_\theta(x|z)\right] - \overbrace{\mathrm{KL}\left(q_\phi(z|x) \mid\mid p(z)\right)}^{\text{analytical}}\right)$$

Inference Network Gradient

$$\frac{\partial}{\partial \phi}\left(\mathbb{E}_{q_\phi(z|x)}\left[\log p_\theta(x|z)\right] - \overbrace{\mathrm{KL}\left(q_\phi(z|x) \mid\mid p(z)\right)}^{\text{analytical}}\right)$$

$$= \frac{\partial}{\partial \phi}\mathbb{E}_{q_\phi(z|x)}\left[\log p_\theta(x|z)\right] - \underbrace{\frac{\partial}{\partial \phi}\mathrm{KL}\left(q_\phi(z|x) \mid\mid p(z)\right)}_{\text{analytical computation}}$$

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$$\frac{\partial}{\partial \phi}\left(\mathbb{E}_{q_\phi(z|x)}\left[\log p_\theta(x|z)\right] - \overbrace{\mathrm{KL}\left(q_\phi(z|x) \mid\mid p(z)\right)}^{\text{analytical}}\right)$$

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The first term again requires approximation by sampling, but there is a problem

Inference Network Gradient

$$\frac{\partial}{\partial \phi} \mathbb{E}_{q_\phi(z|x)} \left[\log p_\theta(x|z) \right]$$

Inference Network Gradient

$$
\begin{aligned}
&\frac{\partial}{\partial \phi} \mathbb{E}_{q_\phi(z|x)} [\log p_\theta(x|z)] \\
&= \frac{\partial}{\partial \phi} \int q_\phi(z|x) \log p_\theta(x|z) \mathrm{d}z
\end{aligned}
$$

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$$\frac{\partial}{\partial \phi} \mathbb{E}_{q_\phi(z|x)} [\log p_\theta(x|z)]$$
$$= \frac{\partial}{\partial \phi} \int q_\phi(z|x) \log p_\theta(x|z) \mathrm{d}z$$
$$= \underbrace{\int \frac{\partial}{\partial \phi} (q_\phi(z|x)) \log p_\theta(x|z) \, \mathrm{d}z}_{\text{not an expectation}}$$

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\end{aligned}
$$

- MC estimator is non-differentiable: cannot sample first

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- MC estimator is non-differentiable: cannot sample first
- Differentiating the expression does not yield an expectation: cannot approximate via MC

Score function estimator

We can again use the log identity for derivatives

$$
\begin{aligned}
&\frac{\partial}{\partial \phi}\mathbb{E}_{q_\phi(z|x)}\left[\log p_\theta(x|z)\right] \\
&= \frac{\partial}{\partial \phi}\int q_\phi(z|x)\log p_\theta(x|z)\mathrm{d}z \\
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&= \int q_\phi(z|x) \frac{\partial}{\partial \phi} (\log q_\phi(z|x)) \log p_\theta(x|z) \, \mathrm{d}z
\end{aligned}
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Score function estimator

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&= \int q_\phi(z|x)\frac{\partial}{\partial\phi}(\log q_\phi(z|x))\log p_\theta(x|z)\,\mathrm{d}z \\
&= \underbrace{\mathbb{E}_{q_\phi(z|x)}\left[\log p_\theta(x|z)\frac{\partial}{\partial\phi}\log q_\phi(z|x)\right]}_{\text{expected gradient :)}}
\end{aligned}$$

Score function estimator: high variance

We can now build an MC estimator

$$\frac{\partial}{\partial \phi}\mathbb{E}_{q_\phi(z|x)}\left[\log p_\theta(x|z)\right]$$
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&\overset{\text{MC}}{\approx} \frac{1}{K}\sum_{k=1}^{K} \log p_\theta(x|z^{(k)})\frac{\partial}{\partial \phi}\log q_\phi(z^{(k)}|x) \\
&z^{(k)} \sim q_\phi(Z|x)
\end{aligned}
$$

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$$

but

- magnitude of $\log p_\theta(x|z)$ varies widely

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but

- magnitude of $\log p_\theta(x|z)$ varies widely
- model likelihood does not contribute to direction of gradient

Score function estimator: high variance

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$$\overset{\text{MC}}{\approx} \frac{1}{K} \sum_{k=1}^{K} \log p_\theta(x|z^{(k)}) \frac{\partial}{\partial \phi} \log q_\phi(z^{(k)}|x)$$

$$z^{(k)} \sim q_\phi(Z|x)$$

but

- magnitude of $\log p_\theta(x|z)$ varies widely
- model likelihood does not contribute to direction of gradient
- too much variance to be useful

When variance is high we can

- sample more

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When variance is high we can

- sample more
  won't scale
- use variance reduction techniques (e.g. baselines and control variates)
- stare at this $\frac{\partial}{\partial \phi} \mathbb{E}_{q_\phi(z|x)} \left[\log p_\theta(x|z)\right]$
  until we find a way to rewrite the expectation in terms of a density that **does not depend on** ϕ

Reparametrisation

Find a transformation $h : z \mapsto \epsilon$ that expresses z through a random variable ϵ such that $q(\epsilon)$ does not depend on ϕ

(Kingma and Welling, 2013; Rezende et al., 2014; Titsias and Lázaro-Gredilla, 2014)

Reparametrisation

Find a transformation $h : z \mapsto \epsilon$ that expresses z through a random variable ϵ such that $q(\epsilon)$ does not depend on ϕ

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

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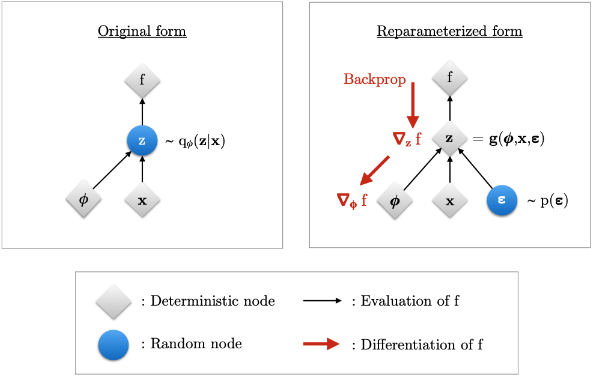
Invertibility implies

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

(Kingma and Welling, 2013; Rezende et al., 2014; Titsias and Lázaro-Gredilla, 2014)

Reparametrisation



(Kingma and Welling, 2013)

Gaussian Transformation

If $Z \sim \mathcal{N}(\mu_\phi(x), \sigma_\phi(x)^2)$ then

$$h(z, \phi) = \frac{z - \mu_\phi(x)}{\sigma_\phi(x)} = \epsilon \sim \mathcal{N}(0, \mathrm{I})$$

$$h^{-1}(\epsilon, \phi) = \mu_\phi(x) + \sigma_\phi(x) \odot \epsilon \quad \epsilon \sim \mathcal{N}(0, \mathrm{I})$$

Inference Network – Reparametrised Gradient

$$= \frac{\partial}{\partial \phi} \int q_\phi(z|x) \log p_\theta(x|z) \, \mathrm{d}z$$

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$$= \frac{\partial}{\partial \phi} \int q_\phi(z|x) \log p_\theta(x|z) \, \mathrm{d}z$$

$$= \frac{\partial}{\partial \phi} \int q(\epsilon) \log p_\theta(x| \overbrace{h^{-1}(\epsilon, \phi)}^{=z}) \, \mathrm{d}\epsilon$$

Inference Network – Reparametrised Gradient

$$= \frac{\partial}{\partial \phi} \int q_\phi(z|x) \log p_\theta(x|z) \, \mathrm{d}z$$

$$= \frac{\partial}{\partial \phi} \int q(\epsilon) \log p_\theta(x| \overbrace{h^{-1}(\epsilon, \phi)}^{=z}) \, \mathrm{d}\epsilon$$

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

Inference Network – Reparametrised Gradient

$$
\begin{aligned}
&= \frac{\partial}{\partial \phi} \int q_\phi(z|x) \log p_\theta(x|z)\, \mathrm{d}z \\
&= \frac{\partial}{\partial \phi} \int q(\epsilon) \log p_\theta(x|\overbrace{h^{-1}(\epsilon, \phi)}^{=z})\, \mathrm{d}\epsilon \\
&= \int q(\epsilon) \frac{\partial}{\partial \phi} \left[\log p_\theta(x|\overbrace{h^{-1}(\epsilon, \phi)}^{=z}) \right] \mathrm{d}\epsilon \\
&= \underbrace{\mathbb{E}_{q(\epsilon)} \left[\frac{\partial}{\partial \phi} \log p_\theta(x|h^{-1}(\epsilon, \phi)) \right] \mathrm{d}\epsilon}_{\text{expected gradient :D}}
\end{aligned}
$$

Reparametrised gradient estimate

$$= \underbrace{\mathbb{E}_{q(\epsilon)}\left[\frac{\partial}{\partial\phi}\log p_\theta(x|h^{-1}(\epsilon,\phi))\right]\mathrm{d}\epsilon}_{\text{expected gradient :D}}$$

Reparametrised gradient estimate

$$= \underbrace{\mathbb{E}_{q(\epsilon)}\left[\frac{\partial}{\partial\phi}\log p_\theta(x|h^{-1}(\epsilon,\phi))\right]\mathrm{d}\epsilon}_{\text{expected gradient :D}}$$

$$= \mathbb{E}_{q(\epsilon)}\left[\underbrace{\frac{\partial}{\partial z}\log p_\theta(x|\overbrace{h^{-1}(\epsilon,\phi)}^{=z}) \times \frac{\partial}{\partial\phi}h^{-1}(\epsilon,\phi)}_{\text{chain rule}}\right]$$

Reparametrised gradient estimate

$$= \underbrace{\mathbb{E}_{q(\epsilon)}\left[\frac{\partial}{\partial \phi} \log p_\theta(x|h^{-1}(\epsilon, \phi))\right] \mathrm{d}\epsilon}_{\text{expected gradient :D}}$$

$$= \mathbb{E}_{q(\epsilon)}\left[\underbrace{\frac{\partial}{\partial z} \log p_\theta(x|\overbrace{h^{-1}(\epsilon, \phi)}^{=z}) \times \frac{\partial}{\partial \phi} h^{-1}(\epsilon, \phi)}_{\text{chain rule}}\right]$$

$$\overset{\text{MC}}{\approx} \frac{1}{K} \sum_{k=1}^{K} \underbrace{\frac{\partial}{\partial z} \log p_\theta(x|\overbrace{h^{-1}(\epsilon^{(k)}, \phi)}^{=z}) \times \frac{\partial}{\partial \phi} h^{-1}(\epsilon^{(k)}, \phi)}_{\text{backprop's job}}$$

$$\epsilon^{(k)} \sim q(\epsilon)$$

Note that both models contribute with gradients

Gaussian KL

ELBO

$$\mathbb{E}_{q_\phi(z|x)}\left[\log p_\theta(x|z)\right] - \mathrm{KL}\left(q_\phi(z|x) \mid\mid p(z)\right)$$

Gaussian KL

ELBO

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

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

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

Gaussian KL

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$$\mathbb{E}_{q_\phi(z|x)}\left[\log p_\theta(x|z)\right] - \mathrm{KL}\left(q_\phi(z|x) \mid\mid p(z)\right)$$

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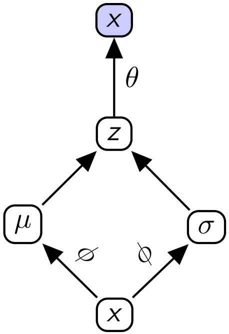
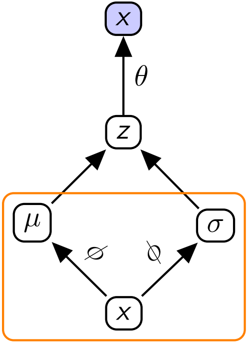
Thus backprop will compute $-\frac{\partial}{\partial\phi}\mathrm{KL}\left(q_\phi(z|x) \mid\mid p(z)\right)$ for us

Computation Graph



Computation Graph

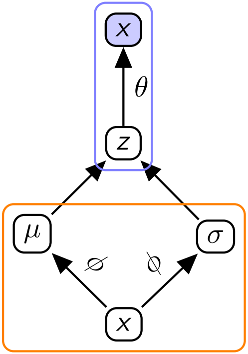
inference model



Computation Graph

generative model

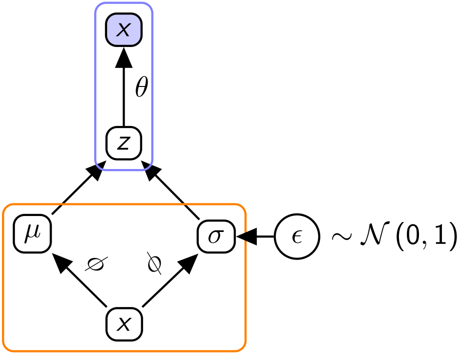
inference model



Computation Graph

generative model

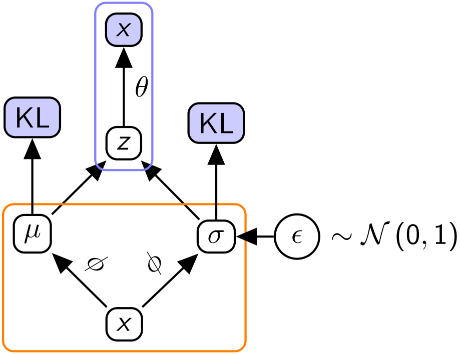
inference model



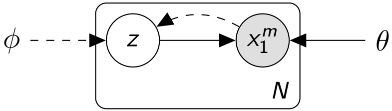
Computation Graph

generative model

inference model



Example



Generative model

- $Z \sim \mathcal{N}(0, I)$
- $X_i | z, x_{<i} \sim \text{Cat}(f_\theta(z, x_{<i}))$

Inference model

- $Z \sim \mathcal{N}(\mu_\phi(x_1^m), \sigma_\phi(x_1^m)^2)$

Bowman et al. (2016)

VAEs – Summary

Advantages

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

VAEs – Summary

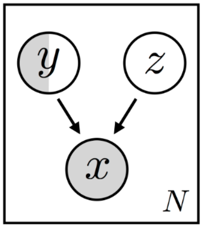
Advantages

- 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
- Location-scale families only
  but see Ruiz et al. (2016) and Kucukelbir et al. (2017)

Semi-supervised VAE



(Kingma et al., 2014)

Semi-supervised VAE

- Generative model:

$$\begin{aligned} p(y) &= \text{cat}(y|\boldsymbol{\pi}); \\ p(\mathbf{z}) &= \mathcal{N}(\mathbf{z}|\mathbf{0}, \mathbf{I}); \\ p_\theta(\mathbf{x}|y, \mathbf{z}) &= f(\mathbf{x}; y, \mathbf{z}, \boldsymbol{\theta}) \end{aligned} \tag{1}$$

- Inference model:

$$\begin{aligned} q_\phi(\mathbf{z}|y, \mathbf{x}) &= \mathcal{N}\left(\mathbf{z}|\boldsymbol{\mu}_\phi(y, \mathbf{x}), \text{diag}\left(\boldsymbol{\sigma}^2_\phi(\mathbf{x})\right)\right); \\ q_\phi(y|\mathbf{x}) &= \text{Cat}\left(y|\boldsymbol{\pi}_\phi(\mathbf{x})\right) \end{aligned} \tag{2}$$

Objective

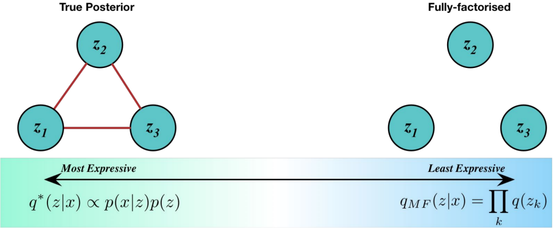
- Labelled data:

$$\log p_\theta(\mathbf{x}, y) \geq \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x},y)} [\log p_\theta(\mathbf{x}|y, \mathbf{z}) + \log p_\theta(y) + \log p(\mathbf{z}) - \log q_\phi \tag{3}$$

- Unlabelled data:

$$\begin{aligned} \log p_\theta(\mathbf{x}) &\geq \mathbb{E}_{q_\phi(y,\mathbf{z}|\mathbf{x})} [\log p_\theta(\mathbf{x}|y, \mathbf{z}) + \log p_\theta(y) + \log p(\mathbf{z}) - \log q_\phi(y \\ &= \sum_y q_\phi(y|\mathbf{x})(-\mathcal{L}(\mathbf{x}, y)) + \mathcal{H}\left(q_\phi(y|\mathbf{x})\right) = -\mathcal{U}(\mathbf{x}) \end{aligned} \tag{4}$$

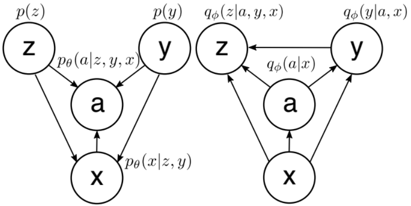
Beyond the mean field



Mohamed S. 2017, Deep Generative Models Tutorial

Auxiliary variable

The mean field assumption might result in models that do not capture all dependencies in the observations:



(a) Generative model P. (b) Inference model Q.

(Maaløe et al., 2016)

Auxiliary variable

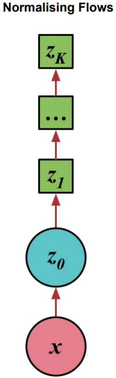
- Generative model:

$$\begin{aligned} p(z) &= \mathcal{N}(z|0, \mathrm{I}) \\ p(y) &= \mathrm{Cat}(y|\pi) \\ p_\theta(a|z, y, x) &= f(a; z, y, x, \theta) \\ p_\theta(x|z, y) &= f(x; z, y, \theta) \end{aligned} \tag{5}$$

- Inference model:

$$\begin{aligned} q_\phi(a|x) &= \mathcal{N}\left(a|\mu_\phi(x), \mathrm{diag}\left(\sigma^2_\phi(x)\right)\right) \\ q_\phi(y|a, x) &= \mathrm{Cat}\left(y|\pi_\phi(a, x)\right) \\ q_\phi(z|a, y, x) &= \mathcal{N}\left(z|\mu_\phi(a, y, x), \mathrm{diag}\left(\sigma^2_\phi(a, y, x)\right)\right) \end{aligned} \tag{6}$$

Normalizing flow



NF for NLP

- (Pelsmaeker and Aziz, 2019) tackle issues present in VAE models for language.
- Annealing
- Expressive posterior

Summary

Deep learning in NLP

- task-driven feature extraction
- models with more realistic assumptions

Probabilistic modelling

- better (or at least more explicit) statistical assumptions
- compact models
- semi-supervised learning

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Lars Maaløe, Casper Kaae Sønderby, Søren Kaae Sønderby, and Ole Winther. Auxiliary deep generative models. In Maria Florina Balcan and Kilian Q. Weinberger, editors, *Proceedings of The 33rd International Conference on Machine Learning*, volume 48 of *Proceedings of Machine Learning Research*, pages 1445–1453, New York, New York, USA, 20–22 Jun 2016. PMLR. URL `http://proceedings.mlr.press/v48/maaloe16.html`.

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