Score function estimator and variance reduction techniques

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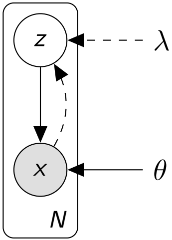
Outline

1. Recap
2. Score function estimator
3. Variance reduction

Variational inference for belief networks

Generative model with NN likelihood



Let $z \in \{0,1\}^d$ and

$$
\begin{aligned}
q_\lambda(z|x) &= \prod_{i=1}^{d} q_\lambda(z_i|x) \\
&= \prod_{i=1}^{d} \operatorname{Bern}(z_i|\operatorname{sigmoid}(f_\lambda(x)))
\end{aligned} \tag{1}
$$

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

Mnih and Gregor (2014)

Objective

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

Parameter estimation

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

Generative Network Gradient

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

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

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

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

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

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

Inference Network Gradient

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

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$$\begin{aligned}
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The first term again requires approximation by sampling, but there is a problem

Inference Network Gradient

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

Inference Network Gradient

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

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- 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

Outline

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2. Score function estimator
3. Variance reduction

Score function estimator

We can again use the log identity for derivatives

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&= \underbrace{\mathbb{E}_{q_\lambda(z|x)}\left[\log p_\theta(x|z)\frac{\partial}{\partial\lambda}\log q_\lambda(z|x)\right]}_{\text{expected gradient :)}}
\end{aligned}
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Score function estimator: high variance

We can now build an MC estimator

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but

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

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but **fully differentiable!**

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  and now it's time for it!

Example Model

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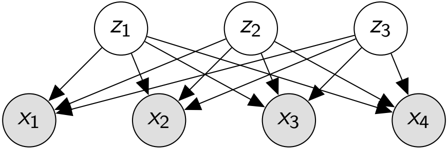
- a document $x = (x_1, \dots, x_n)$ consists of n i.i.d. categorical draws from that model
- the categorical distribution in turn depends on the binary latent factors $z = (z_1, \dots, z_k)$ which are also i.i.d.

$$\begin{aligned} z_j &\sim \text{Bernoulli}\,(\phi) && (1 \leq j \leq k) \\ x_i &\sim \text{Categorical}\,(g_\theta(z)) && (1 \leq i \leq n) \end{aligned}$$

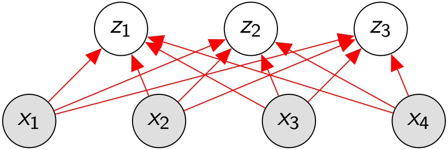
Here ϕ specifies a Bernoulli prior and $g_\theta(\cdot)$ is a function computed by neural network with softmax output.

Example Model



At inference time the latent variables are marginally dependent. For our variational distribution we are going to assume that they are not (recall: mean field assumption).

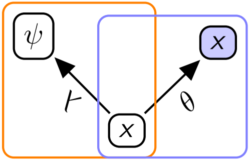
Inference Network



The inference network needs to predict k Bernoulli parameters ψ. Any neural network with sigmoid output will do that job.

$$q_\lambda(z|x) = \prod_{i=1}^{k} \text{Bern}(z_i|\psi_i) \quad \text{where } \psi = f_\lambda(x) \tag{2}$$

Computation Graph



inference model

generation model

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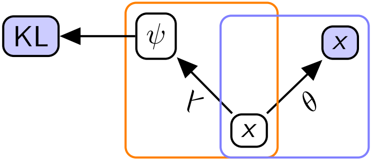

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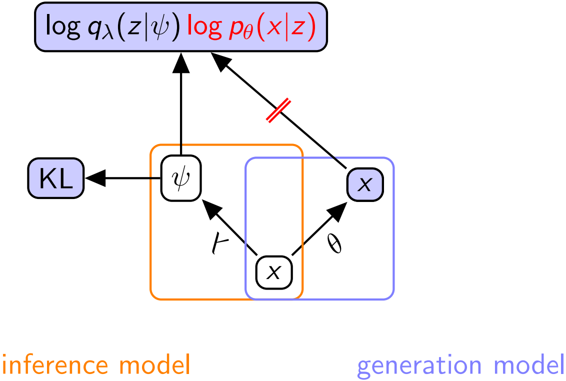

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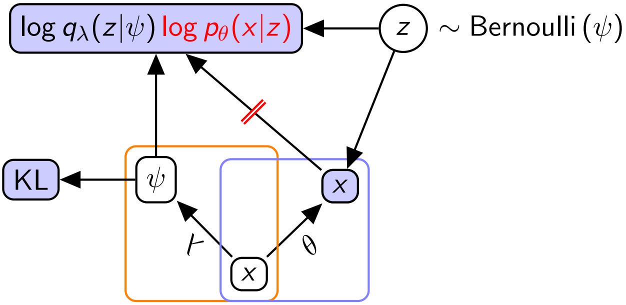

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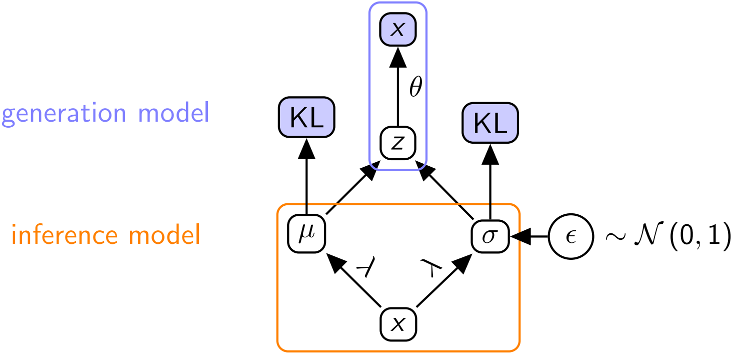
Reparametrisation Gradient



Pros and Cons

- Pros
    - Applicable to all distributions
    - Many libraries come with samplers for common distributions

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  - Applicable to all distributions
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- Cons
  - High Variance!

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Control variates

Suppose we want to estimate $\mathbb{E}[f(Z)]$ and we know the expected value of another function $\psi(z)$ on the same support.

Greensmith et al. (2004)

Control variates

Suppose we want to estimate $\mathbb{E}[f(Z)]$ and we know the expected value of another function $\psi(z)$ on the same support.

Then it holds that

$$\mathbb{E}[f(Z)] = \mathbb{E}[f(Z) - \psi(Z)] + \mathbb{E}[\psi(Z)] \tag{3}$$

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Then it holds that

$$\mathbb{E}[f(Z)] = \mathbb{E}[f(Z) - \psi(Z)] + \mathbb{E}[\psi(Z)] \tag{3}$$

If $\psi(z) = f(z)$, and we estimate the expected value of $f(x) - \psi(x)$, then we have reduced variance to 0. In general

$$\mathrm{Var}(f - \psi) = \mathrm{Var}(f) - 2\,\mathrm{Cov}(f, \psi) + \mathrm{Var}(\psi) \tag{4}$$

If f and ψ are strongly correlated and the covariance is greater than $\mathrm{Var}(\psi)$, then we improve on the original estimation problem.

Greensmith et al. (2004)

Reducing variance of score function estimator

Back to the score function estimator

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

Reducing variance of score function estimator

Back to the score function estimator

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

$$= \mathbb{E}_{q_\lambda(z|x)}\left[\underbrace{\log p_\theta(x|z)\frac{\partial}{\partial\lambda}\log q_\lambda(z|x)}_{f(z)} - \underbrace{C(x)\frac{\partial}{\partial\lambda}\log q_\lambda(z|x)}_{\psi(z)}\right]$$

$$+ \mathbb{E}_{q_\lambda(z|x)}\left[\underbrace{C(x)\frac{\partial}{\partial\lambda}\log q_\lambda(z|x)}_{\psi(z)}\right]$$

The last term is very simple!

$\mathbb{E}[\psi(Z)]$

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

$\mathbb{E}[\psi(Z)]$

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&= C(x)\mathbb{E}_{q_\lambda(z|x)}\left[\frac{\frac{\partial}{\partial\lambda}q_\lambda(z|x)}{q_\lambda(z|x)}\right]
\end{aligned}
$$

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= C(x)\frac{\partial}{\partial\lambda}1
\end{aligned}$$

$\mathbb{E}[\psi(Z)]$

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&= C(x)\int\frac{\partial}{\partial\lambda}q_\lambda(z|x)\,\mathrm{d}z = C(x)\frac{\partial}{\partial\lambda}\int q_\lambda(z|x)\,\mathrm{d}z\\
&= C(x)\frac{\partial}{\partial\lambda}1 = 0
\end{aligned}
$$

Improved estimator

Back to the score function estimator

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

Improved estimator

Back to the score function estimator

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

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

$$+ \mathbb{E}_{q_\lambda(z|x)}\left[C(x)\frac{\partial}{\partial\lambda}\log q_\lambda(z|x)\right]$$

Improved estimator

Back to the score function estimator

$$\begin{aligned}
&\mathbb{E}_{q_\lambda(z|x)}\left[\log p_\theta(x|z)\frac{\partial}{\partial\lambda}\log q_\lambda(z|x)\right]\\
&=\mathbb{E}_{q_\lambda(z|x)}\left[\log p_\theta(x|z)\frac{\partial}{\partial\lambda}\log q_\lambda(z|x)-C(x)\frac{\partial}{\partial\lambda}\log q_\lambda(z|x)\right]\\
&\quad+\mathbb{E}_{q_\lambda(z|x)}\left[C(x)\frac{\partial}{\partial\lambda}\log q_\lambda(z|x)\right]\\
&=\mathbb{E}_{q_\lambda(z|x)}\left[\log p_\theta(x|z)\frac{\partial}{\partial\lambda}\log q_\lambda(z|x)-C(x)\frac{\partial}{\partial\lambda}\log q_\lambda(z|x)\right]
\end{aligned}$$

Improved estimator

Back to the score function estimator

$$\begin{aligned}
&\mathbb{E}_{q_\lambda(z|x)}\left[\log p_\theta(x|z)\frac{\partial}{\partial\lambda}\log q_\lambda(z|x)\right]\\
&=\mathbb{E}_{q_\lambda(z|x)}\left[\log p_\theta(x|z)\frac{\partial}{\partial\lambda}\log q_\lambda(z|x) - C(x)\frac{\partial}{\partial\lambda}\log q_\lambda(z|x)\right]\\
&\quad+\mathbb{E}_{q_\lambda(z|x)}\left[C(x)\frac{\partial}{\partial\lambda}\log q_\lambda(z|x)\right]\\
&=\mathbb{E}_{q_\lambda(z|x)}\left[\log p_\theta(x|z)\frac{\partial}{\partial\lambda}\log q_\lambda(z|x) - C(x)\frac{\partial}{\partial\lambda}\log q_\lambda(z|x)\right]\\
&=\mathbb{E}_{q_\lambda(z|x)}\left[\left(\log p_\theta(x|z) - C(x)\right)\frac{\partial}{\partial\lambda}\log q_\lambda(z|x)\right]
\end{aligned}$$

$C(x)$ is called a **baseline**

Baselines

Baselines can be constant

$$\mathbb{E}_{q_\lambda(z|x)}\left[\left(\log p_\theta(x|z) - C\right)\frac{\partial}{\partial\lambda}\log q_\lambda(z|x)\right] \tag{5}$$

Williams (1992)

Baselines

Baselines can be constant

$$\mathbb{E}_{q_\lambda(z|x)}\left[\left(\log p_\theta(x|z) - C\right)\frac{\partial}{\partial\lambda}\log q_\lambda(z|x)\right] \tag{5}$$

or input-dependent

$$\mathbb{E}_{q_\lambda(z|x)}\left[\left(\log p_\theta(x|z) - C(x)\right)\frac{\partial}{\partial\lambda}\log q_\lambda(z|x)\right] \tag{6}$$

Williams (1992)

Baselines

Baselines can be constant

$$\mathbb{E}_{q_\lambda(z|x)}\left[\left(\log p_\theta(x|z) - C\right)\frac{\partial}{\partial\lambda}\log q_\lambda(z|x)\right] \tag{5}$$

or input-dependent

$$\mathbb{E}_{q_\lambda(z|x)}\left[\left(\log p_\theta(x|z) - C(x)\right)\frac{\partial}{\partial\lambda}\log q_\lambda(z|x)\right] \tag{6}$$

or both

$$\mathbb{E}_{q_\lambda(z|x)}\left[\left(\log p_\theta(x|z) - C - C(x)\right)\frac{\partial}{\partial\lambda}\log q_\lambda(z|x)\right] \tag{7}$$

Williams (1992)

Full power of control variates

If we design $C(\cdot)$ to depend on the variable of integration z, we exploit the full power of **control variates**, but designing and using those require more careful treatment

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Blei et al. (2012); Ranganath et al. (2014); Gregor et al. (2014)

Learning baselines

Baselines are predicted by a regression model (e.g. a neural net).

One idea is to "centre the learning signal", in which case we train the baseline with an L_2-loss:

$$\rho = \arg\min_{\rho} \left(C_\rho(x) - \log p(x|z) \right)^2$$

Gu et al. (2015)

Putting it together

Parameter estimation

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

Variance reduction

$$\arg\min_{\rho} \left(C_\rho(x) - \log p(x|z)\right)^2$$

Generative gradient

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

Inference gradient

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

Summary

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- Reparametrisation not available for discrete variables.

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- High variance.

Summary

- Reparametrisation not available for discrete variables.
- Use score function estimator.
- High variance.
- Always use baselines for variance reduction!

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