Score function estimator and variance reduction techniques

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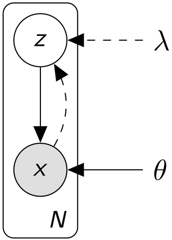
Outline

Variational inference for belief networks

Generative model with NN likelihood



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

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

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

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

Parameter estimation

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

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

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

Score function estimator

We can again use the log identity for derivatives

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&= \int q_\lambda(z|x) \frac{\partial}{\partial \lambda} (\log q_\lambda(z|x)) \log p_\theta(x|z) \, \mathrm{d}z \\
&= \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 :)}}
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Score function estimator: high variance

We can now build an MC estimator

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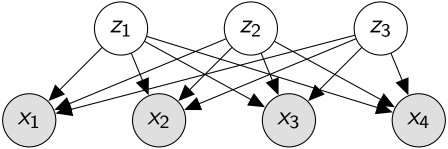
- a document $x = (x_1, \ldots, x_n)$ consists of n i.i.d. categorical draws from that model
- the categorical distribution in turn depends on the binary latent factors $z = (z_1, \ldots, z_k)$ which are also i.i.d.

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

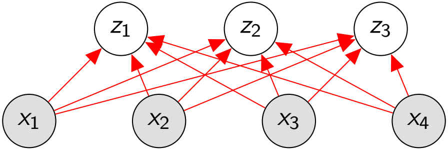
Here ϕ specifies a Bernoulli prior and $g_\theta(\cdot)$ is a function computed by neural network with softmax output.

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).

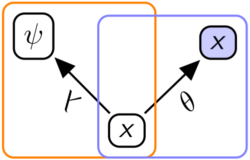
Inference Network



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

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

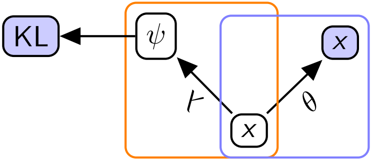
Computation Graph



inference model

generation model

Computation Graph



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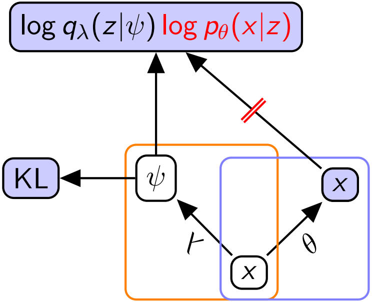

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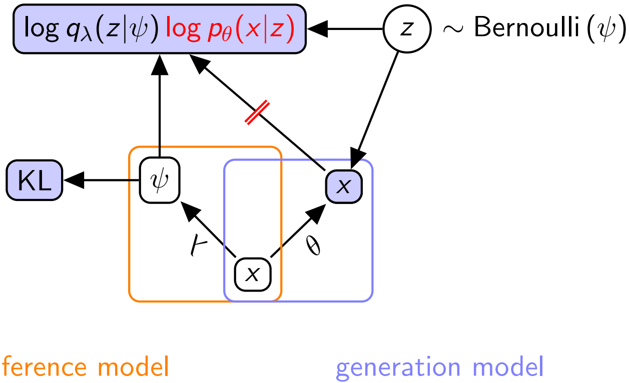
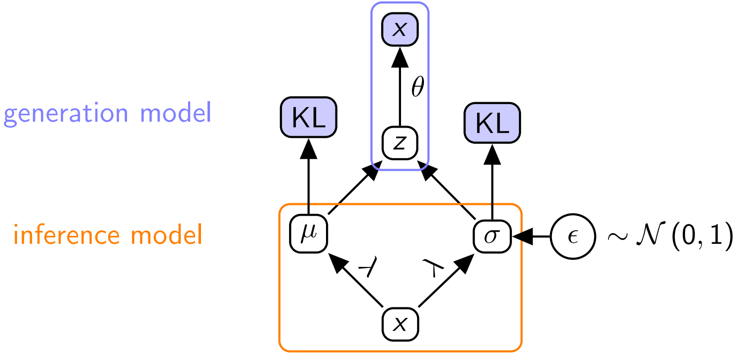


Reparametrisation Gradient



Pros and Cons

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

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- Pros
  - Applicable to all distributions
  - Many libraries come with samplers for common distributions
- Cons
  - High Variance!

Outline

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

Baselines

$$
\begin{aligned}
&\mathbb{E}_{q_\lambda(z|x)}\left[\log p_\theta(x|z)\frac{\partial}{\partial\lambda}\log q_\lambda(z|x)\right]\\
&=\mathbb{E}_{q_\lambda(z|x)}\left[\left(\log p_\theta(x|z)-C(x)\right)\frac{\partial}{\partial\lambda}\log q_\lambda(z|x)\right]\\
&+\mathbb{E}_{q_\lambda(z|x)}\left[C(x)\frac{\partial}{\partial\lambda}\log q_\lambda(z|x)\right]\\
&=\mathbb{E}_{q_\lambda(z|x)}\left[\left(\log p_\theta(x|z)-C(x)\right)\frac{\partial}{\partial\lambda}\log q_\lambda(z|x)\right]+C(x)
\end{aligned}
\tag{3}
$$

Baselines

We attempt to centre the gradient estimate. To do this we learn a quantity C that we subtract from the reconstruction loss.

$$\log q(z|\lambda) \left(\log p(x|z, \theta) - C\right)$$

We call C a baseline. It does not change the expected gradient (Williams, 1992).

Baselines

We can make baselines input-depdendent to make them more flexible.

$$\log q(z|\lambda) \left(\log p(x|z, \theta) - C(x)\right)$$

However, baselines may not depend on the random value z!
Quantities that may depend on the random value ($C(z)$) are called **control variates**. See Blei et al. (2012); Ranganath et al. (2014); Gregor et al. (2014).

Baselines

Baselines are predicted by a regression model (e.g. a neural net).
The model is trained using an L_2-loss.

$$\min \left(C(x) - \log p(x|z, \theta) \right)^2$$

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

Literature I

David M. Blei, Michael I. Jordan, and John W. Paisley. Variational bayesian inference with stochastic search. In *ICML*, 2012. URL http://icml.cc/2012/papers/687.pdf.

Karol Gregor, Ivo Danihelka, Andriy Mnih, Charles Blundell, and Daan Wierstra. Deep autoregressive networks. In Eric P. Xing and Tony Jebara, editors, *ICML*, pages 1242–1250, 2014. URL http://proceedings.mlr.press/v32/gregor14.html.

Andriy Mnih and Karol Gregor. Neural variational inference and learning in belief networks. *arXiv preprint arXiv:1402.0030*, 2014.

Rajesh Ranganath, Sean Gerrish, and David Blei. Black Box Variational Inference. In Samuel Kaski and Jukka Corander, editors, *AISTATS*, pages 814–822, 2014. URL http://proceedings.mlr.press/v33/ranganath14.pdf.

Literature II

Ronald J. Williams. Simple statistical gradient-following algorithms for connectionist reinforcement learning. *Machine Learning*, 8(3-4): 229–256, 1992. URL https://doi.org/10.1007/BF00992696.