Discrete Latent Variables: Variance Reduction

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VI Tutorial @ University of Alicante https://vitutorial.github.io/tour/ua2020

Recap: Score Function Estimator

Control Variates and Baselines

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

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

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

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

We can now build an MC estimator

$$\frac{\partial}{\partial \lambda} \mathbb{E}_{q(z|x,\lambda)} \left[\log p(x|z,\theta) \right] \\
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Empirically this estimator often exhibits high variance.

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

Idea: standardize the "reward" $r(z) := \log p(x|z, \theta)$ to have a mean at 0 and a variance of 1

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$$\begin{split} \frac{\partial}{\partial \lambda} \mathbb{E}_{q(z|x,\lambda)} \left[\log p(x|z,\theta) \right] &= \mathbb{E}_{q(z|x,\lambda)} \left[\log p(x|z,\theta) \frac{\partial}{\partial \lambda} \log q(z|x,\lambda) \right] \\ &\approx E_{q(z|x,\lambda)} \left[\hat{r}(z) \frac{\partial}{\partial \lambda} \log q(z|x,\lambda) \right] \end{split}$$

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- We can show that using these baselines do not bias the estimator.
- More generally, we can design more sophisticated control variates that further reduce the variance.

Recap: Score Function Estimator

Control Variates and Baselines

Control variates

Intuition

To estimate $\mathbb{E}[f(z)]$ via Monte Carlo we compute the empirical average of $\hat{f}(z)$ where $\hat{f}(z)$ is chosen so that $\mathbb{E}[\hat{f}(z)] = \mathbb{E}[f(z)]$ and $Var(f) > Var(\hat{f})$.

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- say we know $\bar{c} = \mathbb{E}[c(z)]$
- then for $\hat{f}(z) \triangleq f(z) b(c(z) \mathbb{E}[c(z)])$ it holds that $\mathbb{E}[\hat{f}(z)] = \mathbb{E}[f(z)]$
- and $Var(\hat{f}) = Var(f) 2b Cov(f, c) + b^2 Var(c)$

- $\hat{f}(z) \triangleq f(z) b(c(z) \mathbb{E}[c(z)])$

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How do we choose b and c(z)?

- If f(z) and c(z) are positively correlated, then we may reduce variance
- solving $\frac{\partial}{\partial b} \operatorname{Var}(\hat{f}) = 0$ yields $b^* = \frac{\operatorname{Cov}(f,c)}{\operatorname{Var}(c)}$

Of course, $\mathbb{E}[c(z)]$ must be known!

MC

We then use the estimate

$$ar{f} \stackrel{\mathsf{MC}}{pprox} rac{1}{S} \left(\sum_{s=1}^S f(z^{(s)}) - bc(z^{(s)})
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And recall that for us

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

and $z^{(s)} \sim q(z|x,\lambda)$

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

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Expected score

The Expectation of the score function is 0.

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

$$= \int q(z|x,\lambda) \frac{\partial}{\partial \lambda} \log q(z|x,\lambda) dz$$

$$= \int \frac{\partial}{\partial \lambda} q(z|x,\lambda) dz$$

$$= \frac{\partial}{\partial \lambda} \int q(z|x,\lambda) dz$$

$$= \frac{\partial}{\partial \lambda} 1 = 0$$

Baselines

With

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

and

$$c(z) = \frac{\partial}{\partial \lambda} \log q(z|x,\lambda)$$

we have

$$\hat{f}(z) =$$

Baselines

With

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

and

$$c(z) = \frac{\partial}{\partial \lambda} \log q(z|x,\lambda)$$

we have

$$\hat{f}(z) = (\log p(x|z, \theta) - b) \frac{\partial}{\partial \lambda} \log q(z|x, \lambda)$$

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

and

$$c(z) = \frac{\partial}{\partial \lambda} \log q(z|x,\lambda)$$

we have

$$\hat{f}(z) = (\log p(x|z, \theta) - b) \frac{\partial}{\partial \lambda} \log q(z|x, \lambda)$$

b is known as baseline in RL literature.

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- A trainable constant b
- A neural network prediction based on x e.g. $b(x; \omega)$
- The likelihood assessed at a deterministic point, e.g. $b(x) = \log p(x|z^*, \theta)$ where $z^* = \arg \max_z q(z|x, \lambda)$

Trainable baselines

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

The model is trained using an L_2 -loss.

$$\min_{\omega} (b(x; \omega) - \log p(x|z, \theta))^2$$

Summary

 In practice the score function estimator leads to high variance gradient estimates.

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- In practice the score function estimator leads to high variance gradient estimates.
- We can design control variates that reduce estimator variance, yet do not bias the estimator!

Literature I

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

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.