

Discrete Latent Variables: Variance Reduction

Bryan Eikema and Wilker Aziz

VI Tutorial @ University of Alicante

<https://vitutorial.github.io/tour/ua2020>

1 Recap: Score Function Estimator

2 Control Variates and Baselines

Score Function Estimator

We are interested in computing

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

Score Function Estimator

We are interested in computing

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

Score Function Estimator

We are interested in computing

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

Score Function Estimator

We are interested in computing

$$\begin{aligned}
 & \frac{\partial}{\partial \lambda} \mathbb{E}_{q_{\lambda}(z|x)} [\log p_{\theta}(x|z)] \\
 &= \sum_z \frac{\partial}{\partial \lambda} (q(z|x, \lambda)) \log p(x|z, \theta) \\
 &= \sum_z q(z|x, \lambda) \frac{\partial}{\partial \lambda} (\log q(z|x, \lambda)) \log p(x|z, \theta) \\
 &= \underbrace{\mathbb{E}_{q(z|x, \lambda)} \left[\log p(x|z, \theta) \frac{\partial}{\partial \lambda} \log q(z|x, \lambda) \right]}_{\text{expected gradient :)}}
 \end{aligned}$$

Score Function Estimator

We can now build an MC estimator

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

Score Function Estimator

We can now build an MC estimator

$$\begin{aligned}
 & \frac{\partial}{\partial \lambda} \mathbb{E}_{q(z|x, \lambda)} [\log p(x|z, \theta)] \\
 &= \mathbb{E}_{q(z|x, \lambda)} \left[\log p(x|z, \theta) \frac{\partial}{\partial \lambda} \log q(z|x, \lambda) \right] \\
 &\stackrel{\text{MC}}{\approx} \frac{1}{S} \sum_{s=1}^S \log p(x|z^{(s)}, \theta) \frac{\partial}{\partial \lambda} \log q(z^{(s)}|x, \lambda)
 \end{aligned}$$

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

Score Function Estimator: Variance

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

Empirically this estimator often exhibits high variance.

Score Function Estimator: Variance

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

Empirically this estimator often exhibits high variance.

- the magnitude of $\log p(x|z, \theta)$ varies widely

Score Function Estimator: Variance

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

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

Score Function Estimator: Variance

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

Score Function Estimator: Variance

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

- Keep a moving average of the mean and variance $\log p(x|z, \theta)$: $\hat{\mu}$ and $\hat{\sigma}^2$.

Score Function Estimator: Variance

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

- Keep a moving average of the mean and variance $\log p(x|z, \theta)$: $\hat{\mu}$ and $\hat{\sigma}^2$.
- $$\hat{r}(z) = \frac{\log p(x|z, \theta) - \hat{\mu}}{\sqrt{\hat{\sigma}^2}}$$

Score Function Estimator: Variance

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

- Keep a moving average of the mean and variance $\log p(x|z, \theta)$: $\hat{\mu}$ and $\hat{\sigma}^2$.

- $\hat{r}(z) = \frac{\log p(x|z, \theta) - \hat{\mu}}{\sqrt{\hat{\sigma}^2}}$

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

Score Function Estimator: Variance

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

- Keep a moving average of the mean and variance $\log p(x|z, \theta)$: $\hat{\mu}$ and $\hat{\sigma}^2$.

- $\hat{r}(z) = \frac{\log p(x|z, \theta) - \hat{\mu}}{\sqrt{\hat{\sigma}^2}}$

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

Score Function Estimator: Variance

- We can show that using these *baselines* do not bias the estimator.

Score Function Estimator: Variance

- 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.

1 Recap: Score Function Estimator

2 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 $\text{Var}(f) > \text{Var}(\hat{f})$.

Equivalent expectations

Let $\bar{f} = \mathbb{E}[f(z)]$ be an expectation of interest

Equivalent expectations

Let $\bar{f} = \mathbb{E}[f(z)]$ be an expectation of interest

- say we know $\bar{c} = \mathbb{E}[c(z)]$

Equivalent expectations

Let $\bar{f} = \mathbb{E}[f(z)]$ be an expectation of interest

- say we know $\bar{c} = \mathbb{E}[c(z)]$
- then for $\hat{f}(z) \triangleq f(z) - b(c(z) - \mathbb{E}[c(z)])$

Equivalent expectations

Let $\bar{f} = \mathbb{E}[f(z)]$ be an expectation of interest

- 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 $\mathbb{E}[\hat{f}(z)] = \mathbb{E}[f(z)]$

Equivalent expectations

Let $\bar{f} = \mathbb{E}[f(z)]$ be an expectation of interest

- 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 $\text{Var}(\hat{f}) = \text{Var}(f) - 2b \text{Cov}(f, c) + b^2 \text{Var}(c)$

Choosing the control variate

- 1 $\hat{f}(z) \triangleq f(z) - b(c(z) - \mathbb{E}[c(z)])$
- 2 $\text{Var}(\hat{f}) = \text{Var}(f) - 2b \text{Cov}(f, c) + b^2 \text{Var}(c)$

How do we choose b and $c(z)$?

Choosing the control variate

- 1 $\hat{f}(z) \triangleq f(z) - b(c(z) - \mathbb{E}[c(z)])$
- 2 $\text{Var}(\hat{f}) = \text{Var}(f) - 2b \text{Cov}(f, c) + b^2 \text{Var}(c)$

How do we choose b and $c(z)$?

- If $f(z)$ and $c(z)$ are positively correlated, then we may reduce variance

Choosing the control variate

- 1 $\hat{f}(z) \triangleq f(z) - b(c(z) - \mathbb{E}[c(z)])$
- 2 $\text{Var}(\hat{f}) = \text{Var}(f) - 2b \text{Cov}(f, c) + b^2 \text{Var}(c)$

How do we choose b and $c(z)$?

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

Choosing the control variate

- 1 $\hat{f}(z) \triangleq f(z) - b(c(z) - \mathbb{E}[c(z)])$
- 2 $\text{Var}(\hat{f}) = \text{Var}(f) - 2b \text{Cov}(f, c) + b^2 \text{Var}(c)$

How do we choose b and $c(z)$?

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

Choosing the control variate

- 1 $\hat{f}(z) \triangleq f(z) - b(c(z) - \mathbb{E}[c(z)])$
- 2 $\text{Var}(\hat{f}) = \text{Var}(f) - 2b \text{Cov}(f, c) + b^2 \text{Var}(c)$

How do we choose b and $c(z)$?

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

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

MC

We then use the estimate

$$\bar{f} \stackrel{\text{MC}}{\approx} \frac{1}{S} \left(\sum_{s=1}^S f(z^{(s)}) - bc(z^{(s)}) \right) + b\bar{c}$$

MC

We then use the estimate

$$\bar{f} \stackrel{\text{MC}}{\approx} \frac{1}{S} \left(\sum_{s=1}^S f(z^{(s)}) - bc(z^{(s)}) \right) + b\bar{c}$$

And recall that for us

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

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

Expected score

The Expectation of the score function is 0.

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

Expected score

The Expectation of the score function is 0.

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

Expected score

The Expectation of the score function is 0.

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

Expected score

The Expectation of the score function is 0.

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

Expected score

The Expectation of the score function is 0.

$$\begin{aligned} & \mathbb{E}_{q(z|x, \lambda)} \left[\frac{\partial}{\partial \lambda} \log q(z|x, \lambda) \right] \\ &= \int q(z|x, \lambda) \frac{\partial}{\partial \lambda} \log q(z|x, \lambda) dz \\ &= \int \frac{\partial}{\partial \lambda} q(z|x, \lambda) dz \\ &= \frac{\partial}{\partial \lambda} \int q(z|x, \lambda) dz \\ &= \frac{\partial}{\partial \lambda} 1 = 0 \end{aligned}$$

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

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

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

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

b is known as *baseline* in RL literature.

Examples of baselines

- Moving average of $\log p(x|z, \theta)$ based on previous batches

Examples of baselines

- Moving average of $\log p(x|z, \theta)$ based on previous batches
- A trainable constant b

Examples of baselines

- Moving average of $\log p(x|z, \theta)$ based on previous batches
- A trainable constant b
- A neural network prediction based on x e.g. $b(x; \omega)$

Examples of baselines

- Moving average of $\log p(x|z, \theta)$ based on previous batches
- 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

- The score function estimator inhibits high variance.

Summary

- The score function estimator inhibits high variance.
- We can design control variates that reduce estimator variance, yet do not bias the estimator!

Literature I

iiiiiii HEAD ===== iiiiiiii
c9d66c768b8484311dcf5667a54fdd4b6549ecbe

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>.