Relaxations to Discrete Latent Variables

Philip Schulz and Wilker Aziz

VI Tutorial @ Host

Site

1. Reparameterised Gradient

2. Biased Gradient Estimates for Discrete Variables

Change of density

For Gaussians

$$z \sim \mathcal{N}(\mu, \sigma^2) \qquad\qquad \frac{z - \mu}{\sigma^2} \sim \mathcal{N}(0, 1)$$

Change of density

For Gaussians

$$z \sim \mathcal{N}(\underbrace{\mu, \sigma^2}_{\lambda}) \qquad \underbrace{\frac{z-\mu}{\sigma^2}}_{\epsilon = t^{-1}(z,\lambda)} \sim \mathcal{N}(0,1)$$

More generally

$$f_{Z|\lambda}(z) = s(\underbrace{t^{-1}(z,\lambda)}_{\epsilon})|\det J_{t^{-1}}(z,\lambda)|$$

Change of density

For Gaussians

$$z \sim \mathcal{N}(\underbrace{\mu, \sigma^2}_{\lambda}) \qquad \underbrace{\frac{z-\mu}{\sigma^2}}_{\epsilon = t^{-1}(z,\lambda)} \sim \mathcal{N}(0,1)$$

More generally

$$f_{Z|\lambda}(z) = s(\underbrace{t^{-1}(z,\lambda)}_{\epsilon})|\det J_{t^{-1}}(z,\lambda)|$$

$$\mathbb{E}_{f_{Z|\lambda}(z)}\left[\psi(z)\right] =$$

Change of density

For Gaussians

$$z \sim \mathcal{N}(\underbrace{\mu, \sigma^2}_{\lambda}) \qquad \underbrace{\frac{z-\mu}{\sigma^2}}_{\epsilon = t^{-1}(z,\lambda)} \sim \mathcal{N}(0,1)$$

More generally

$$f_{Z|\lambda}(z) = s(\underbrace{t^{-1}(z,\lambda)}_{\epsilon})|\det J_{t^{-1}}(z,\lambda)|$$

$$\mathbb{E}_{f_{Z|\lambda}(z)}\left[\psi(z)\right] = \underbrace{\mathbb{E}_{s(\epsilon)}\left[\psi(t(\epsilon,\lambda))\right]}_{\text{check class on ADVI}}$$

Reparameterised gradient

$$\frac{\partial}{\partial \lambda} \mathbb{E}_{f_{Z|\lambda}(z)} \left[\psi(z) \right] = \mathbb{E}_{s(\epsilon)} \left[\frac{\partial}{\partial \lambda} \psi(t(\epsilon, \lambda) \right]$$

Reparameterised gradient

$$\frac{\partial}{\partial \lambda}\mathbb{E}_{f_{Z|\lambda}(z)}\left[\psi(z)\right] = \mathbb{E}_{s(\epsilon)}\left[\frac{\partial}{\partial \lambda}\psi(t(\epsilon, \lambda))\right]$$
$$= \mathbb{E}_{s(\epsilon)}\left[\frac{\partial}{\partial z}\psi(z)\frac{\partial}{\partial \lambda}t(\epsilon, \lambda)\right]$$

Easy to MC estimate!

Comparing gradient estimators

Reparameterised gradient | Score function estimator

$$\mathbb{E}_{s(\epsilon)}\left[\underbrace{\frac{\partial}{\partial z}\psi(z)\frac{\partial}{\partial \lambda}t(\epsilon,\lambda)}_{\hat{g}_{\text{rep}}}\right] = \mathbb{E}_{f_\lambda(z)}\left[\underbrace{\psi(z)\frac{\partial}{\partial \lambda}f_{Z|\lambda}(z)}_{\hat{g}_{\text{sfe}}}\right]$$

- $\hat{g}_{\text{sfe}}$ is typically cursed with variance
- but is $\hat{g}_{\text{rep}}$ available in general?

Comparing gradient estimators

Reparameterised gradient | Score function estimator

$$\mathbb{E}_{s(\epsilon)}\left[\underbrace{\frac{\partial}{\partial z}\psi(z)\frac{\partial}{\partial \lambda}t(\epsilon,\lambda)}_{\hat{g}_{\text{rep}}}\right] = \mathbb{E}_{f_\lambda(z)}\left[\underbrace{\psi(z)\frac{\partial}{\partial \lambda}f_{Z|\lambda}(z)}_{\hat{g}_{\text{sfe}}}\right]$$

- $\hat{g}_{\text{sfe}}$ is typically cursed with variance
- but is $\hat{g}_{\text{rep}}$ available in general?
  in particular, is it available for discrete variables?

A general reparameterisation

What transformation will always absorb the parameters of a density?

A general reparameterisation

What transformation will always absorb the parameters of a density?

$$Z \sim f_{Z|\lambda}(z)$$
$$F_{Z|\lambda}(z) \sim \mathcal{U}(0, 1)$$

A general reparameterisation

What transformation will always absorb the parameters of a density?

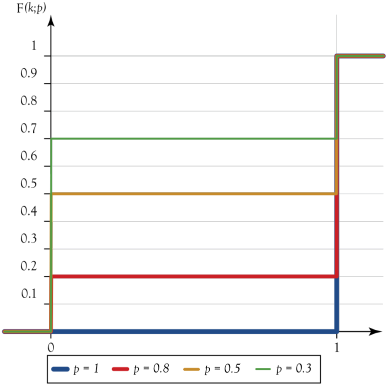
$$Z \sim f_{Z|\lambda}(z)$$
$$F_{Z|\lambda}(z) \sim \mathcal{U}(0, 1)$$

So, if I know the inverse cdf,

$$\epsilon \sim \mathcal{U}(0, 1)$$
$$z = F^{-1}_{Z|\lambda}(\epsilon)$$

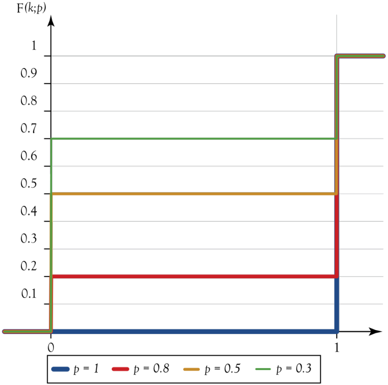
do I have access to $\hat{g}_{\text{rep}}$?

Let's reparameterise a Bernoulli



$$Z \sim \text{Bernoulli}(p)$$

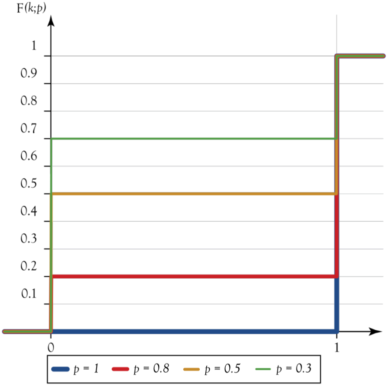
Let's reparameterise a Bernoulli



$$Z \sim \mathrm{Bernoulli}(p)$$

$$F^{-1}_{Z|p}(\epsilon) = \begin{cases} 0 & \text{if } \epsilon < 1 - p \\ 1 & \text{otherwise} \end{cases}$$

Let's reparameterise a Bernoulli

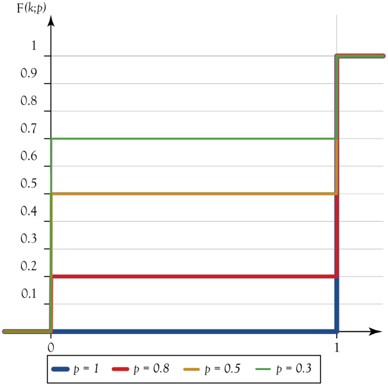


$$Z \sim \text{Bernoulli}(p)$$

$$F^{-1}_{Z|p}(\epsilon) = \begin{cases} 0 & \text{if } \epsilon < 1 - p \\ 1 & \text{otherwise} \end{cases}$$

How about $\frac{\partial}{\partial p} F^{-1}_{Z|p}(\epsilon)$?

Let's reparameterise a Bernoulli



$$Z \sim \text{Bernoulli}(p)$$

$$F^{-1}_{Z|p}(\epsilon) = \begin{cases} 0 & \text{if } \epsilon < 1 - p \\ 1 & \text{otherwise} \end{cases}$$

How about $\frac{\partial}{\partial p} F^{-1}_{Z|p}(\epsilon)$? Mostly 0, sometimes undefined!

Discrete case

Discrete variables do not admit a differentiable reparameterisation. The cells of the Jacobian are either 0 or undefined :/

Discrete case

Discrete variables do not admit a differentiable reparameterisation. The cells of the Jacobian are either 0 or undefined :/

The score function estimator is fully general, but very noisy.

Discrete case

Discrete variables do not admit a differentiable reparameterisation. The cells of the Jacobian are either 0 or undefined :/

The score function estimator is fully general, but very noisy.

Ask the deep learning literature for help :D

Discrete case

Discrete variables do not admit a differentiable reparameterisation. The cells of the Jacobian are either 0 or undefined :/

The score function estimator is fully general, but very noisy.

Ask the deep learning literature for help :D

Fake a Jacobian!

Straight-Through Estimator (STE)

In lack of a Jacobian, use the identity

$$J_{t^{-1}}(\epsilon, \lambda) = \mathrm{diag}(\mathbf{1})$$

STE is a biased gradient estimator that works in some cases, but unfortunately there are no general recipes.

Bernoulli-STE

Consider a VAE where $q(z|x) = \mathrm{Bern}(z|g(x;\lambda))$.

Bernoulli-STE

Consider a VAE where $q(z|x) = \text{Bern}(z|g(x;\lambda))$.
We sample z via a reparameterisation that absorbs λ:

$$\epsilon \sim \mathcal{U}(0,1) \qquad p = g(x;\lambda) \qquad z = \underbrace{\mathbb{1}_{(0,p)}(\epsilon)}_{t}$$

Bernoulli-STE

Consider a VAE where $q(z|x) = \text{Bern}(z|g(x;\lambda))$.
We sample z via a reparameterisation that absorbs λ:

$$\epsilon \sim \mathcal{U}(0,1) \qquad p = g(x;\lambda) \qquad z = \underbrace{\mathbb{1}_{(0,p)}(\epsilon)}_{t}$$

A gradient estimate of the ELBO involves computing:

$$\frac{\partial}{\partial\lambda}\log p(x|z = t(\epsilon,\lambda)) = \frac{\partial}{\partial z}\log p(x|z)\frac{\partial}{\partial\lambda}t(\epsilon,\lambda)$$

Bernoulli-STE

Consider a VAE where $q(z|x) = \text{Bern}(z|g(x;\lambda))$.
We sample z via a reparameterisation that absorbs λ:

$$\epsilon \sim \mathcal{U}(0,1) \qquad p = g(x;\lambda) \qquad z = \underbrace{\mathbb{1}_{(0,p)}(\epsilon)}_{t}$$

A gradient estimate of the ELBO involves computing:

$$\frac{\partial}{\partial \lambda} \log p(x|z = t(\epsilon,\lambda)) = \frac{\partial}{\partial z} \log p(x|z) \frac{\partial}{\partial \lambda} t(\epsilon,\lambda)$$

and we use our *pseudo gradient*

$$\frac{\partial}{\partial \lambda} t(\epsilon,\lambda) = \frac{\partial}{\partial \lambda} g(x;\lambda) \cancel{\frac{\partial}{\partial p} \mathbb{1}_{(0,p)}(\epsilon)} \overset{\text{def}}{=} 1$$

Concrete (Gumbel-Softmax) Distribution

We can sample from a Categorical distribution via

$$
\begin{aligned}
\epsilon_k &\sim \mathrm{Gumbel}(0, 1) \\
\underbrace{\arg\max_k \; \{\lambda_k + \epsilon_k\}_{k=1}^{K}}_{z = t(\epsilon, \lambda)} &\sim \mathrm{Cat}(\mathrm{softmax}(\lambda))
\end{aligned}
$$

Concrete (Gumbel-Softmax) Distribution

We can sample from a Categorical distribution via

$$\epsilon_k \sim \text{Gumbel}(0, 1)$$
$$\underbrace{\arg\max_k \ \{\lambda_k + \epsilon_k\}_{k=1}^K}_{z=t(\epsilon,\lambda)} \sim \text{Cat}(\text{softmax}(\lambda))$$

The problem is that $t(\epsilon, \lambda)$ is not differentiable, but note

$$\text{onehot}(z) \approx \text{softmax}\left(\frac{\lambda + \epsilon}{\tau}\right) \qquad \text{as } \tau \to 0$$

and now the transformation is differentiable, but the outcome is dense. For sparsity, use (biased) STE.

Summary

- The inverse cdf is a general reparameterisation procedure
- In the discrete case, its inverse is piecewise constant
- Relaxations of Categorical variables are based on the idea of relaxing the one-hot representation of the outcome
- Dense relaxations are mapped to sparse (one-hot) representations via a discontinuity which is ignored in backpropagation (STE).

Literature I

Yoshua Bengio, Nicholas Léonard, and Aaron Courville. Estimating or propagating gradients through stochastic neurons for conditional computation. *arXiv preprint arXiv:1308.3432*, 2013.

Chris J. Maddison, Andriy Mnih, and Yee Whye Teh. The concrete distribution: A continous relaxation of discrete random variables. In *ICLR*, 2017.

Eric Jang, Shixiang Gu, and Ben Poole. Categorical reparameterization with gumbel-softmax. In *ICLR*, 2017.

Literature II

Jason Tyler Rolfe. Discrete variational autoencoders. In *ICLR*, 2017.

Christos Louizos, Max Welling, and Diederik P Kingma. Learning sparse neural networks through l_0 regularization. In *ICLR*, 2018.

Joost Bastings, Wilker Aziz, and Ivan Titov. Interpretable neural predictions with differentiable binary variables. In *ACL*, July 2019.