Relaxations to Discrete Latent Variables

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

1. Reparameterised Gradient

2. Biased Gradient Estimates for Discrete Variables

Change of density

For Gaussians

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

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

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

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?

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

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

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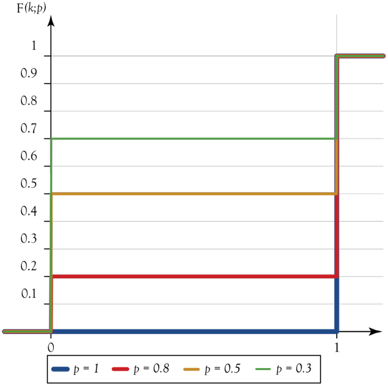
$$\underbrace{F_{Z|\lambda}(z)}_{\text{cdf}} \sim \mathcal{U}(\underbrace{0,1}_{\text{fixed}})$$

So, if I know the inverse cdf,

$$\begin{aligned} \epsilon &\sim \mathcal{U}(0,1) \\ F^{-1}_{Z|\lambda}(\epsilon) &\sim Z \end{aligned}$$

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

Let's reparameterise a Bernoulli



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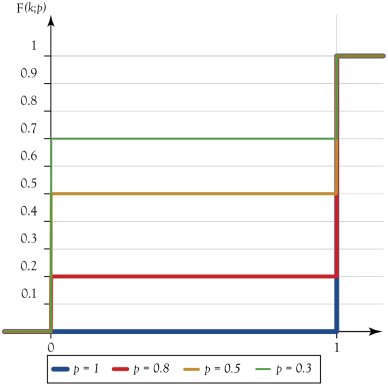

$$Z \sim \text{Bernoulli}(p)$$

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

$$= \mathbb{1}_{(0,p)}(\epsilon)$$

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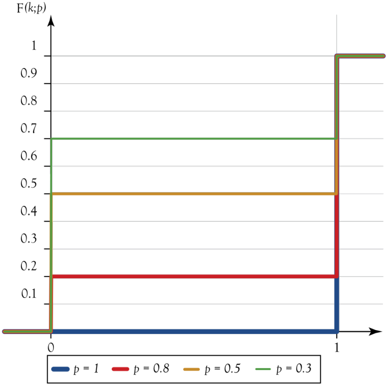

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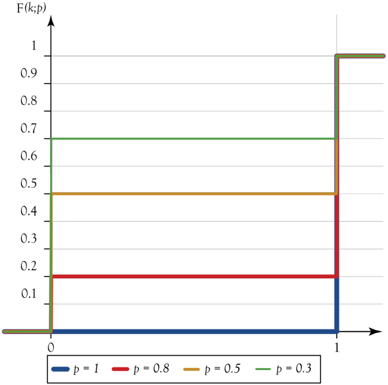

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How about $\frac{\partial}{\partial p} F^{-1}_{Z|p}(\epsilon)$? Mostly 0, sometimes undefined!

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Fake a Jacobian!

Straight-Through Estimator (STE)

In lack of a Jacobian, use the identity

$$J_t(\epsilon, \lambda) = \mathrm{diag}(\mathbf{1})$$

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

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A gradient estimate of the ELBO involves computing:

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

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

and we use our *pseudo gradient*

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

Concrete (Gumbel-Softmax) Distribution

We can sample from a Categorical distribution via

$$\epsilon_k \sim \text{Gumbel}(0, 1)$$

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

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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.