Relaxations to Discrete Latent Variables

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

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1. Reparameterised Gradient

2. Biased Gradient Estimates for Discrete Variables

Change of density

For Gaussians

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

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
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  in particular, is it available for discrete variables?

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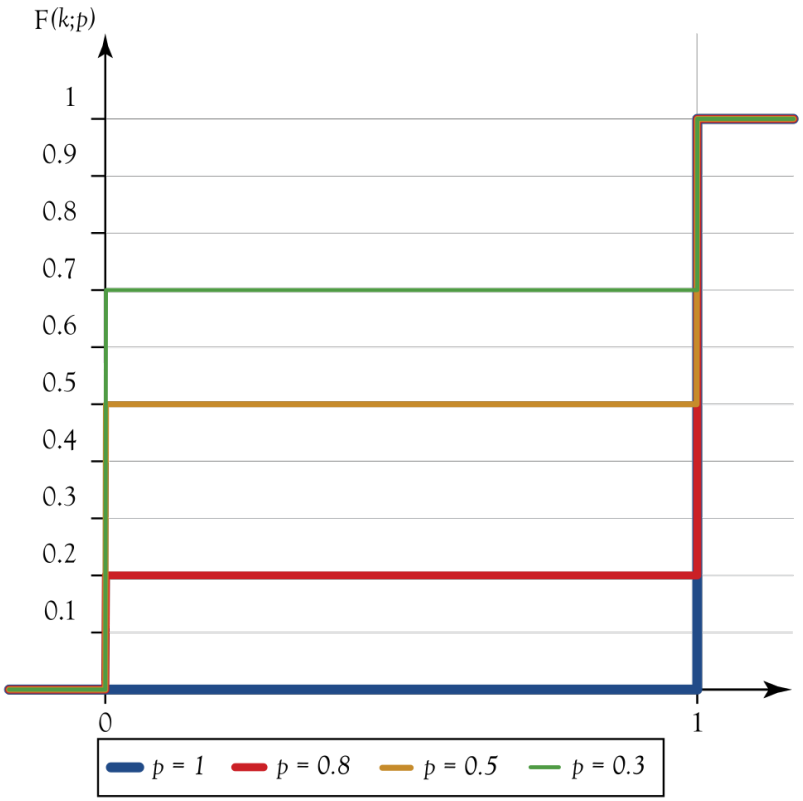
$$\underbrace{F_{Z|\lambda}(z)}_{\text{cdf}} \sim \mathcal{U}(\underbrace{0,1}_{\text{fixed}})$$

So, if I know the inverse cdf,

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

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

Let's reparameterise a Bernoulli



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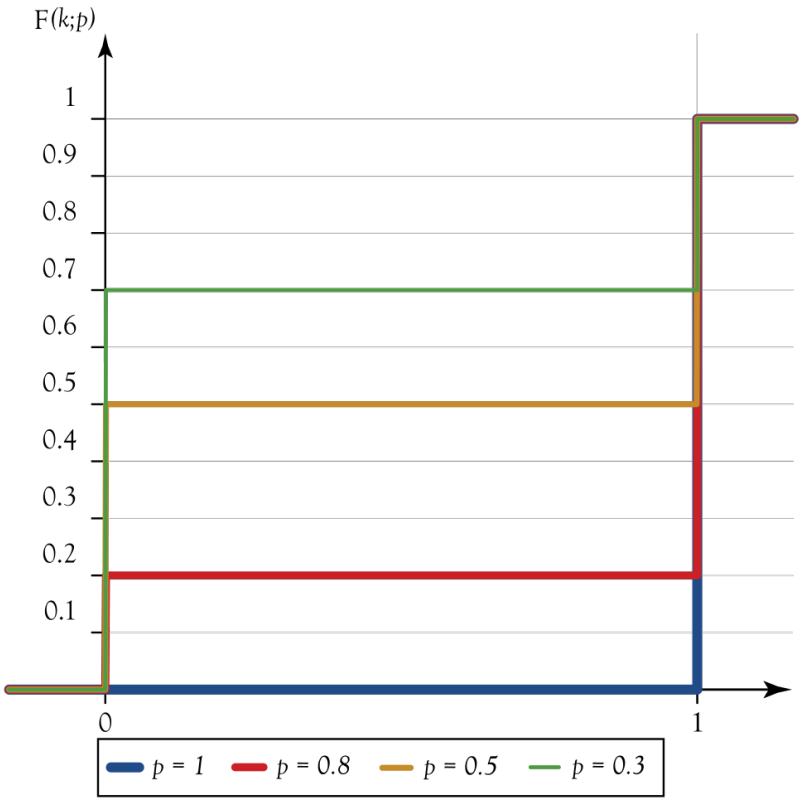

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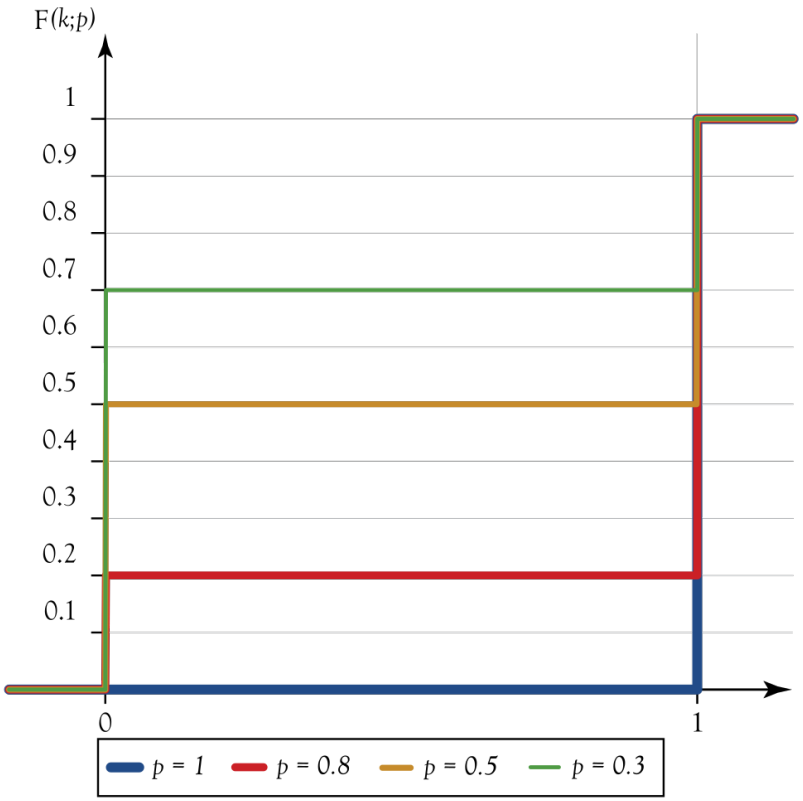

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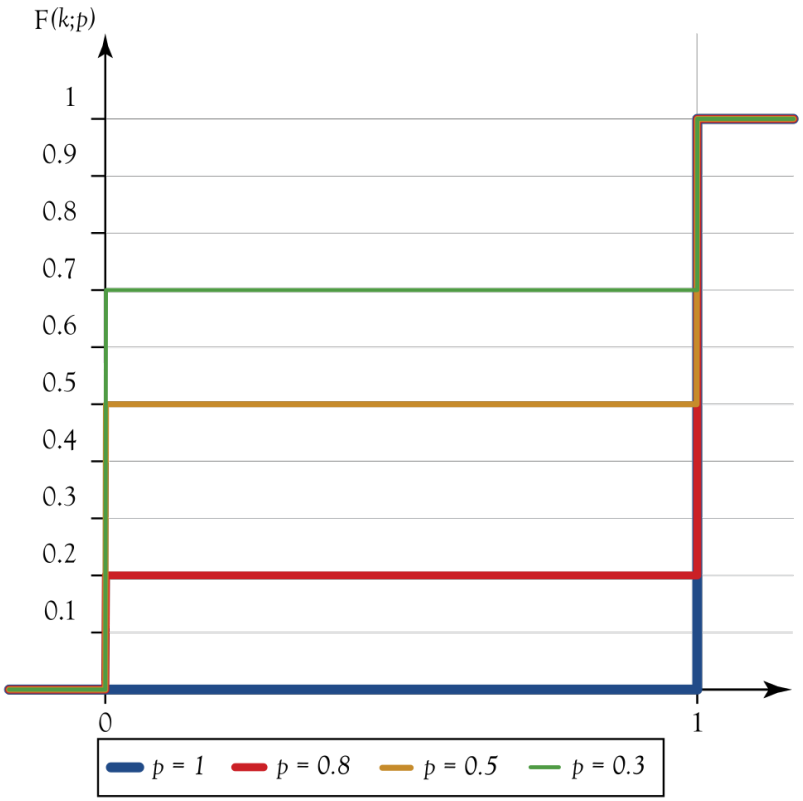

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How about $\frac{\partial}{\partial p} F^{-1}_{Z|p}(\epsilon)$? Mostly 0, sometimes undefined!

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Fake a Jacobian!

Straight-Through Estimator (STE)

In lack of a Jacobian, use the identity

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

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:

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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

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

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

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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).

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