# Discrete Latent Variables

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DeepBayes

1. Why Discreteness?
2. Problem
3. Relaxations
4. Variance Reduction
5. Conclusion

# Why Discreteness?

- Better interpretability
  - Easier to interpret discrete categories that continuous spectrum
- Manipulating control flow
  - Let the model make the discrete choice
- Inherent trait of the problem
  - Sometimes you need discrete predictions to have some properties

## Motivation



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- Discrete Variational Autoencoder
  - Assume observations can be described by some binary (or categorical) code
  - We want to learn both encoder and decoder for such code and observations
- Hard Attention
  - An attention module generates binary mask on where to look at
  - The network classifies masked images
  - We want attention module to attend only important ares of an image
- GANs for text
  - Generator outputs discrete text
  - Discriminator takes discrete text as input and classifies how real it is
  - We want generator to output text that fools the discriminator

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# Problem

Typical problems boil down to optimizing the following objective

$$\mathcal{L}(\phi) = \mathbb{E}_{q_\phi(\mathbf{z})} f(\mathbf{z}) \to \max_\phi$$

- We consider models where objective is continuous w.r.t. $\phi$
  - Hence the gradient $\frac{\partial}{\partial \phi}\mathcal{L}(\phi)$ exists
- Expectation is intractable, resort to *Stochastic Optimization*
- Stochastic Optimization requires stochastic (unbiased) estimate $g(\mathbf{z}, \phi)$ of the true gradient:

$$\mathbb{E}_{q_\phi(\mathbf{z})} g(\mathbf{z}, \phi) = \frac{\partial}{\partial \phi}\mathcal{L}(\phi)$$

- No continuous reparametrization is possible for $z$
  - Because $z$ is taking finitely many different values

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$$\frac{1}{M} \sum_{m=1}^{M} f(\mathbf{z}^{(m)}) \frac{\partial}{\partial \phi} \log q_\phi(\mathbf{z}^{(m)}), \qquad \mathbf{z}^{(m)} \sim q_\phi(\mathbf{z})$$

- Works for our case, discreteness does not get in the way
  - $f$ is not even required to be continuous
- Typically has large variance
- Requires sophisticated *Variance Reduction* methods
  - Just taking bigger $M$ won't help
  - Control Variates aka baselines, typically of the form

$$\frac{1}{M} \sum_{m=1}^{M} \left(f(\mathbf{z}^{(m)}) - b(\mathbf{z})\right) \frac{\partial}{\partial \phi} \log q_\phi(\mathbf{z}^{(m)}) + \frac{\partial}{\partial \phi} \mathbb{E}_{q_\phi(\mathbf{z})} b(\mathbf{z}),$$

for $b(\mathbf{z})$ s.t. the 2nd expectation is tractable and $\mathbf{z}^{(m)} \sim q_\phi(\mathbf{z})$

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# REINFORCE Estimator

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for $b(\mathbf{z})$ s.t. the 2nd expectation is tractable and $\mathbf{z}^{(m)} \sim q_\phi(\mathbf{z})$

Consider 1-sample estimate

$$g^{\text{REINFORCE}}(\mathbf{z}, \phi) = \overbrace{f(\mathbf{z})}^{\text{scalar}} \overbrace{\frac{\partial}{\partial \phi} \log q_\phi(\mathbf{z})}^{\text{vector}}, \qquad \mathbf{z} \sim q_\phi(\mathbf{z})$$

- Gradient estimate points in the direction of increasing probability of a given sample $\mathbf{z}$
  - Increases probability of $\mathbf{z}$ if it happened to be good
- The target function $f$ only enters as a scaling coefficient, and no gradient $\frac{\partial f}{\partial \mathbf{z}}$ is used
  - Has no idea where to move probability mass *systematically*
- **Random search in disguise!** [Rec18]

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# Relaxations

**Idea**: Relax the objective over discrete random samples into an objective oven continuous random samples during training and use the reparametrization trick:

$$\mathbb{E}_{q_\phi(\mathbf{z})} f(\mathbf{z}) \rightsquigarrow \mathbb{E}_{q_\phi(\mathbf{z})} f(\widetilde{\mathbf{z}}) \rightsquigarrow \mathbb{E}_{p(\gamma)} f(\widetilde{\mathbf{z}}(\gamma, \phi))$$

Keep the testing phase model unchanged

This requires $f$ to be able to work with relaxed values

- Limits the scope

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An old trick to sample Categorical random variables

$$z \sim \text{Categorical}(\pi_1, \dots, \pi_K),$$

Minimum of independent exponential distributions with carefully chosen probabilities has the same distribution:

$$z \stackrel{d}{=} \underset{k}{\text{argmin}} \frac{\xi_k}{\pi_k}, \qquad \xi_k \sim \text{Exp}(1)$$

Equivalently (applying $-\log$)

$$z \stackrel{d}{=} \underset{k}{\text{argmax}} \left[\log \pi_k - \log \xi_k\right], \qquad \xi_k \sim \text{Exp}(1)$$

Converts sampling $K$-ary discrete random variable into optimization by adding univariate noise $K$ times

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# Gumbel-Softmax Trick [JGP17], [MMT17]

Approximate argmax with softmax (with temperature)

$$\text{softmax}_\tau(x)_j = \frac{\exp(x_j/\tau)}{\sum_{k=1}^K \exp(x_k/\tau)}$$

Temperature controls "sharpness" of the softmax:

- $\tau = 0$ recovers argmax $= \text{softmax}_0$
- $\tau = \infty$ leads to uniform distribution ignoring any disparities

We then replace discrete $z$ with their continuous relaxations $\widetilde{z}$

$$\widetilde{z}(\gamma, \pi) = \text{softmax}_\tau\left(\log \pi_1 + \gamma_1, \dots, \log \pi_K + \gamma_K\right)$$

Where $\gamma_k \sim \text{Gumbel}(0, 1)$ is a standard Gumbel random variable, and can be generated from uniform noise $u_k$ as

$$\gamma_k \stackrel{d}{=} -\log(-\log u_k), \qquad u_k \sim \text{Uniform}(0, 1)$$

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$$\mathcal{L}(\phi) = \mathbb{E}_\gamma f(\widetilde{\mathbf{z}}(\gamma, \phi)), \qquad \gamma_{dk} \sim \text{Gumbel}(0, 1)$$

Gradient estimate is obtained simply by exchanging $\frac{\partial}{\partial \phi}$ and $\mathbb{E}$:

$$g^{\text{Rep}}(\gamma, \phi) = \frac{\partial}{\partial \phi} f(\widetilde{z}(\gamma, \pi(\phi)))$$

Similar to stochastic discrete nodes replaced by their expectation (softmax), but has **noise injected into log-probabilities**

- Rooted in (Approximate) Bayesian Inference
- Noise helps exploration and regularizes
- Right kind of noise makes $\widetilde{z}$ similar to one-hot vectors
  - Reducing train-test mismatch

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In a special case of $K = 2$ we can write a bit more sample-efficient scheme.

$$\widetilde{z} = \sigma_\tau\left(\log \tfrac{p}{1-p} + \upsilon\right), \qquad \upsilon \sim \text{Logistic}(0, 1)$$

where Logistic(0, 1) is the distribution of difference of 2 Gumbels:

$$\upsilon \overset{d}{=} \gamma_1 - \gamma_2$$

You can easily see this by yourself by simplifying the formula of the softmax over 2 classes.

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# Gumbel-Softmax Trick: Binary Case

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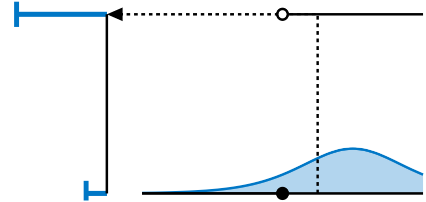
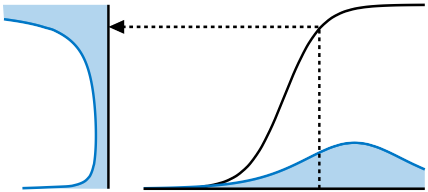
# Gumbel-Softmax Trick: Temperature

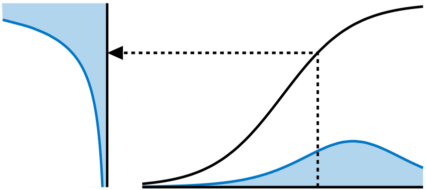




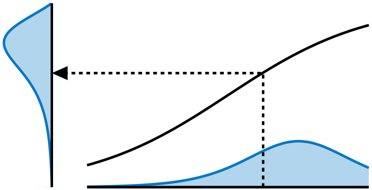
$\tau = 0$



$\tau = 1/2$



$\tau = 1$



$\tau = 2$

For $K$-ary categorical r.v. it has been shown that for $\tau \leqslant \frac{1}{K-1}$ there are no modes in the interior of the probability simplex

- All modes are in the vertices, which are one-hot vectors
  - (or edges, which is still good, since at least one component is close to zero)
- This makes relaxed samples more likely to be *contrastive*
  - Similar to actual discrete samples
  - Forces the model to adapt to the corresponding mode

How to choose the temperature?

- Small temperature leads to high variances, but resembles discrete case well
- Large temperatures have lower variance, but deviates away from the discrete case
- In practice grid search over a couple possible values

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- Small temperature leads to high variances, but resembles discrete case well
- Large temperatures have lower variance, but deviates away from the discrete case
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- Gumbel-Softmax relaxes discrete random variables into continuous, enabling the reparametrization trick
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Consider some $b(\mathbf{z})$ with **tractable** expectation $\mu = \mathbb{E}_{q(\mathbf{z})} b(\mathbf{z})$

$$\frac{1}{M} \sum_{m=1}^{M} (f(\mathbf{z}_m) - b(\mathbf{z}_m)) + \mu$$

Might be a better (low-variance) estimate if $f(\mathbf{z})$ and $b(\mathbf{z})$ have positive correlation.

- Unbiased estimator
- $b(\mathbf{z})$ is called *Control Variate*
- Especially convenient if $b(\mathbf{z})$ is zero-mean
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$$(f(\mathbf{z}) - c)\frac{\partial}{\partial\phi}\log q_\phi(\mathbf{z}) + \overbrace{\frac{\partial}{\partial\phi}\mathbb{E}_{q_\phi(\mathbf{z})} c}^{=0}$$

Just centers the learning signal, optimal c is

$$c = \frac{\text{Cov}\left[f(\mathbf{z})\frac{\partial}{\partial\phi}\log q_\phi(\mathbf{z}), \frac{\partial}{\partial\phi}\log q_\phi(\mathbf{z})\right]}{\text{Var}\left[\frac{\partial}{\partial\phi}\log q_\phi(\mathbf{z})\right]}$$

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Use Gumbel-relaxed $f$ as a baseline

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- Work well in practice
- Have hyperparameters to tune
- Have biased gradients aka introduce train-test mismatch

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- Cumbersome
- Not clear if their results are worth added complexity
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- Allow you to tune baseline to minimize variance
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