CATEGORICAL REPARAMETERIZATION WITH GUMBEL-SOFTMAX

Eric Jang, Shixiang Gu, Ben Poole

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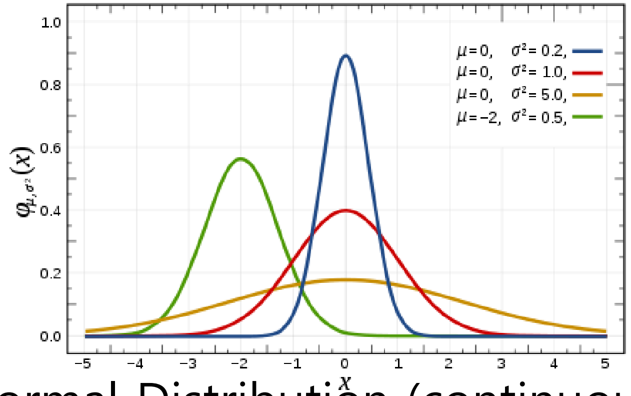
Introduction

Presents an efficient **gradient estimator** that replaces
the **non-differentiable sample** from a categorical distribution
with a **differentiable sample** from a novel Gumbel-Softmax distribution

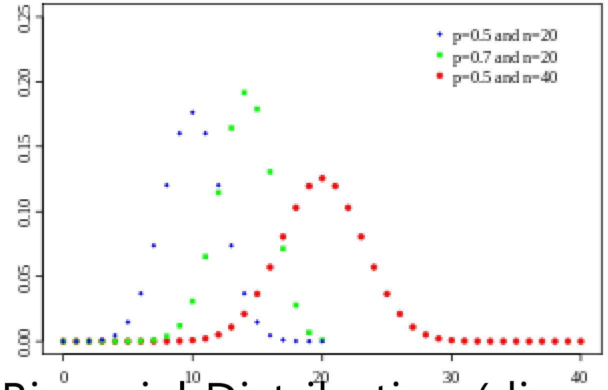
Introduction

- Discrete Stochastic Node
  - Sampling 할 때 discrete distribution을 사용
    - variational autoencoder with discrete latent variable
  - discrete variable을 사용하면 해석이 쉽다
  - label 정보를 추가하고 싶을 때 사용 가능

→ sampling process of discrete data from a categorical distribution is not differentiable



Normal Distribution (continuous)

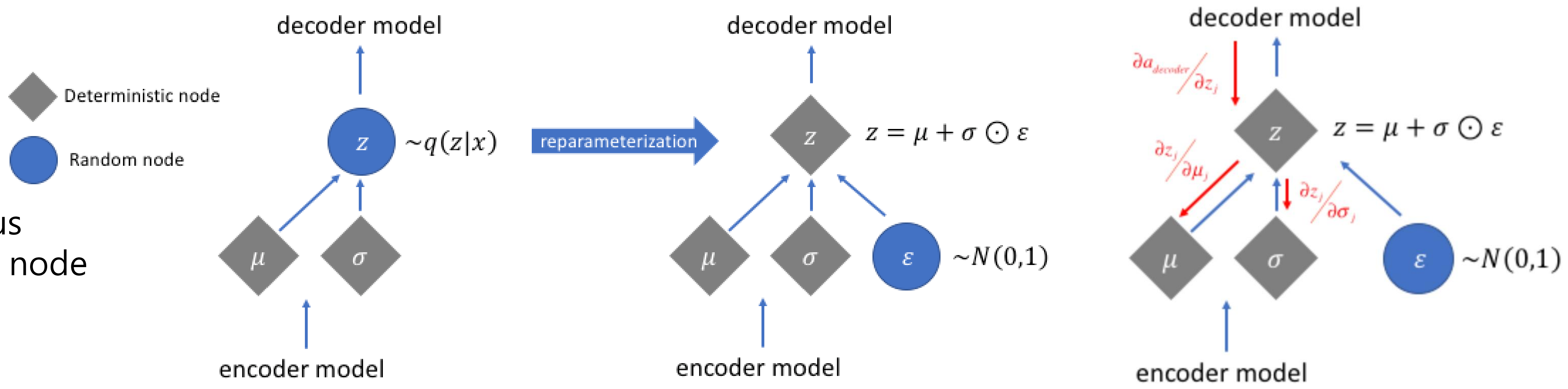


Binomial Distribution (discrete)

Reparameterization trick

- VAE
  - Reparameterization trick
    - Sampling할 때 backpropagation을 할 수 있게 하는 trick
    - VAE 에서는 continuous stochastic node를 사용

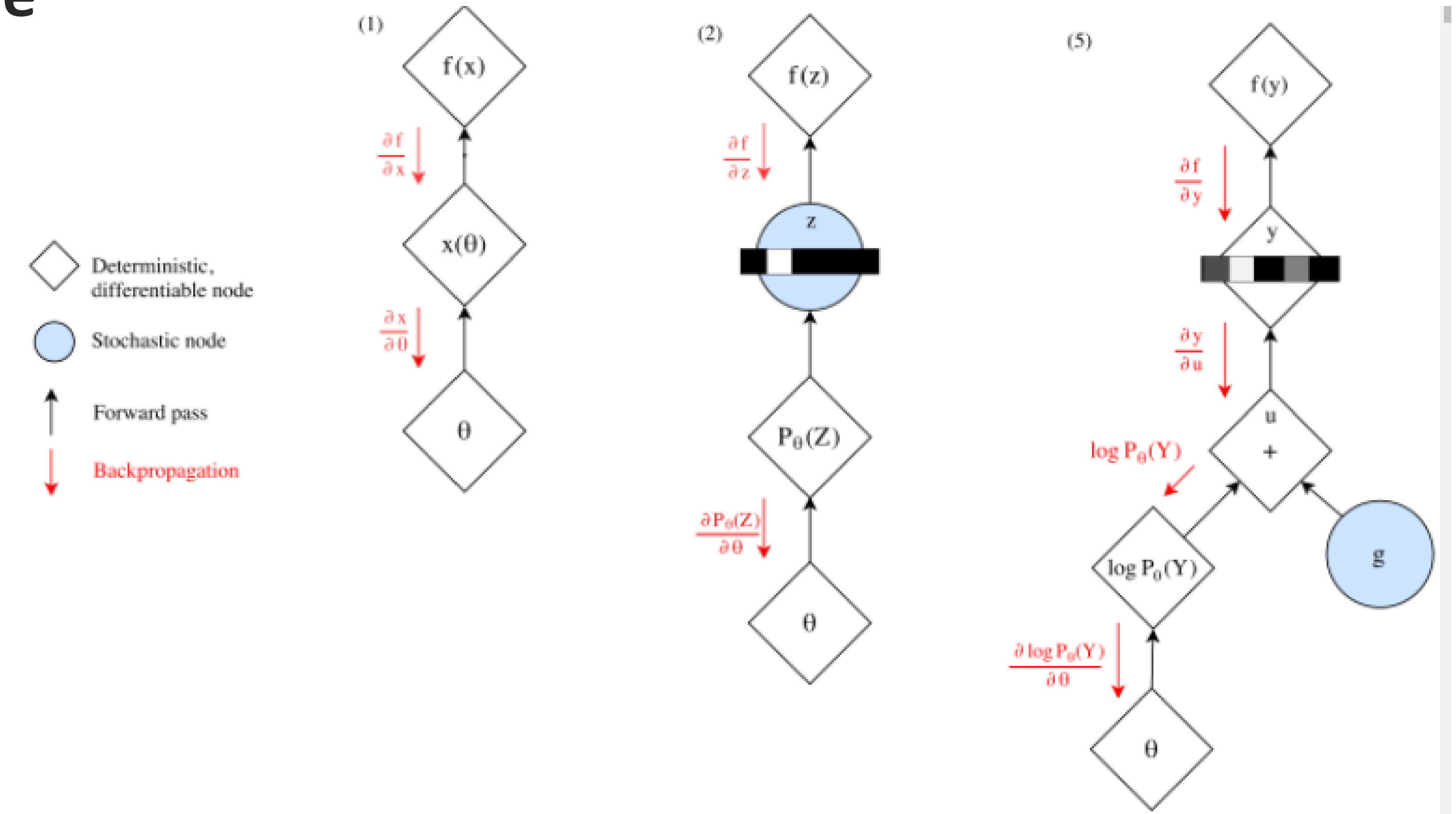
Continuous
stochastic node



z 미분 가능해야 back propagation이 가능하다
→ discrete distribution인 경우 미분 가능하지 않다.

Gumbel Softmax

sampling process of discrete data from a categorical distribution is **not differentiable**



Reparameterization Trick

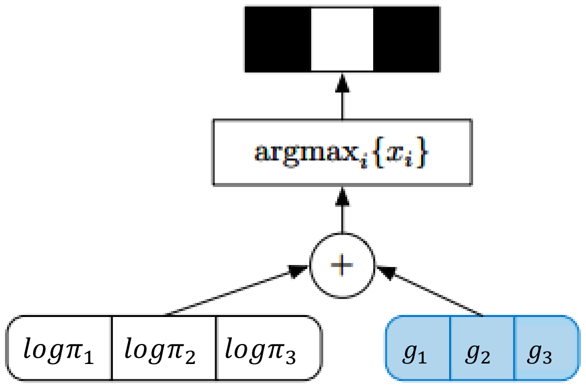
Gumbel Softmax

Gumbel Max

discrete stochastic node에 reparameterization trick 적용

z : categorical variable with class probabilities $\pi_1, \pi_2, \pi_3, \ldots, \pi_k$

categorical samples as k-dimensional one-hot vector



$$z = \mathtt{one\_hot}\left(\arg\max_i \left[g_i + \log \pi_i\right]\right)$$

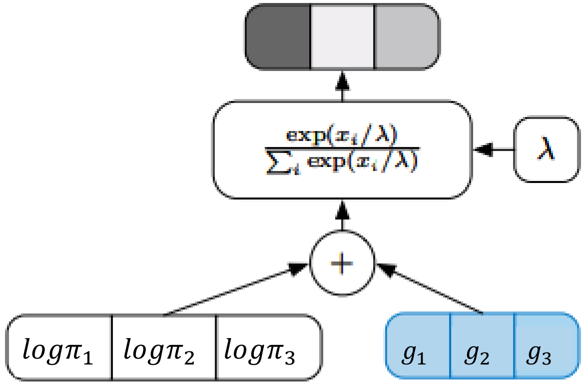
$$g_1, g_2, \ldots, g_k \sim \mathrm{Gumbel}(0,1)$$

→ argmax의 non-differentiable을 해결하기 위해 continuous function인 softmax 사용

Gumbel Softmax

Gumbel Softmax

z : categorical variable with class probabilities $\pi_1, \pi_2, \pi_3, \ldots, \pi_k$



$$y_i = \frac{\exp((\log(\pi_i) + g_i)/\tau)}{\sum_{j=1}^{k} \exp((\log(\pi_j) + g_j)/\tau)} \qquad \text{for } i = 1, \ldots, k.$$

temperature(τ) controls how closely the new samples approximate discrete

$\tau \rightarrow 0$, softmax computation smoothly approaches the argmax, sample vectors approach one-hot

$\tau \rightarrow \infty$, sample vectors become uniform

Gumbel Softmax

discrete
distribution

sample vector

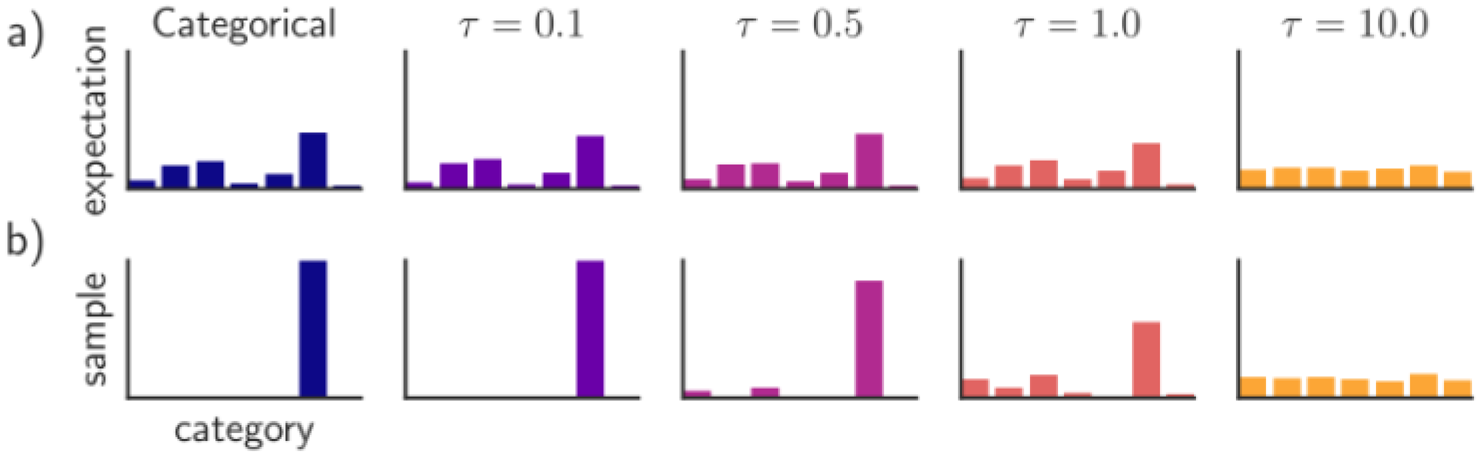
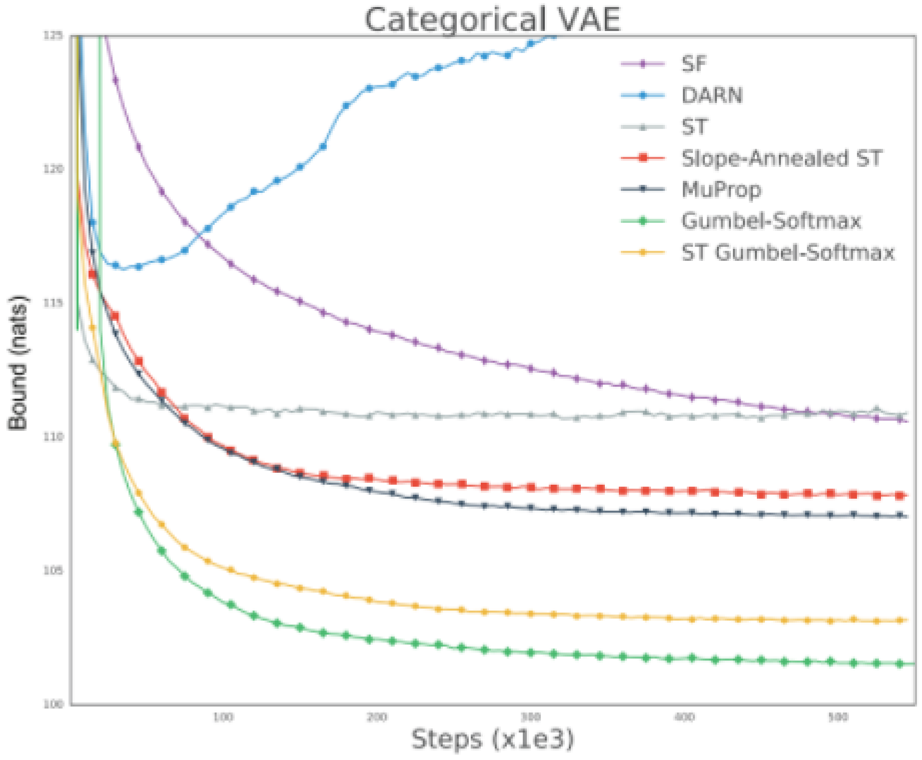


Figure 1: The Gumbel-Softmax distribution interpolates between discrete one-hot-encoded categorical distributions and continuous categorical densities. (a) For low temperatures ($\tau = 0.1, \tau = 0.5$), the expected value of a Gumbel-Softmax random variable approaches the expected value of a categorical random variable with the same logits. As the temperature increases ($\tau = 1.0, \tau = 10.0$), the expected value converges to a uniform distribution over the categories. (b) Samples from Gumbel-Softmax distributions are identical to samples from a categorical distribution as $\tau \to 0$. At higher temperatures, Gumbel-Softmax samples are no longer one-hot, and become uniform as $\tau \to \infty$.

Experiments

- Categorical VAE
  - 20 categorical latent variables

Negative variational lower bound of MNIST data



Appendix

- Gumbel Distribution
  - is used to model the distribution of the maximum (or the minimum) of a number of samples of various distributions.
  - In the latent variable formulation of the multinomial logit model — common in discrete choice theory — the errors of the latent variables follow a Gumbel distribution.