EECE 571F: Deep Learning with Structures

Lecture 11: Stochastic Gradient Estimator for Discrete Latent Variable Models

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University of British Columbia

Winter, Term 1, 2022

Course Scope

- Brief Intro to Deep Learning

- Geometric Deep Learning

  - Deep Learning Models for Sets and Sequences: Deep Sets & Transformers
  - Deep Learning Models for Graphs: Graph Convolution & Message Passing GNNs
  - Expressiveness & Generalizations of GNNs
  - Unsupervised/Self-supervised Graph Representation Learning

- Probabilistic Deep Learning

  - Deep Generative Models:
    Auto-regressive models, GANs, VAEs, Diffusion/Score based models
  - Discrete/Hybrid Latent Variable Models: RBMs, Latent Graph Models
  - Stochastic Gradient Estimation

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    - **Stochastic Gradient Estimation**

Sampling Discrete (Categorical) Random Variables

Given a probability mass function of a discrete RV, how to draw samples?

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Probability Mass Function (PMF)

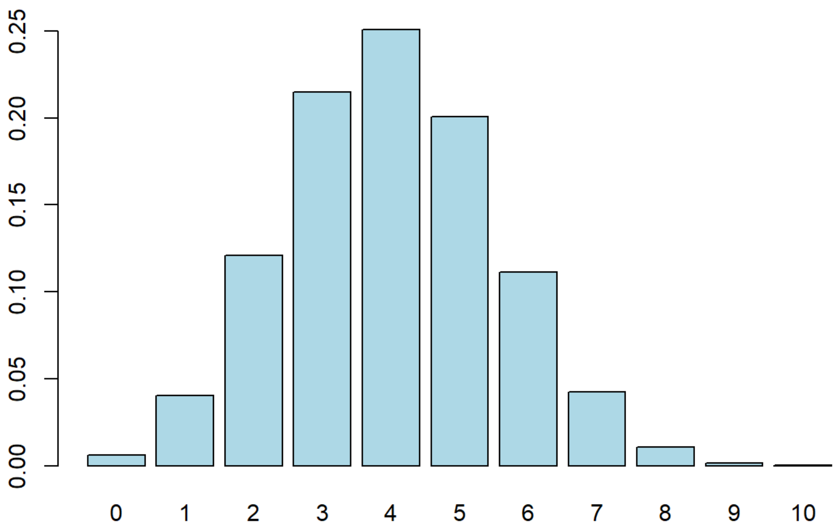

Image Credit: http://www.est.uc3m.es/icascos/eng/probability_notes/discrete-random-variables.html

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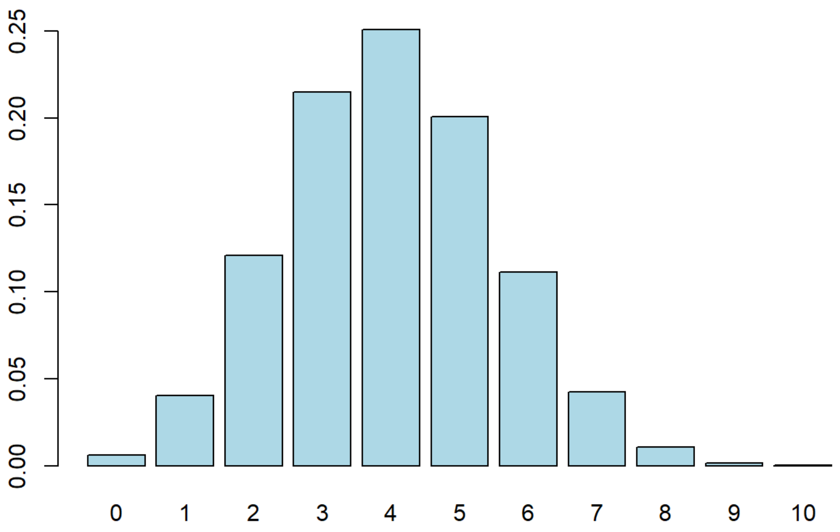
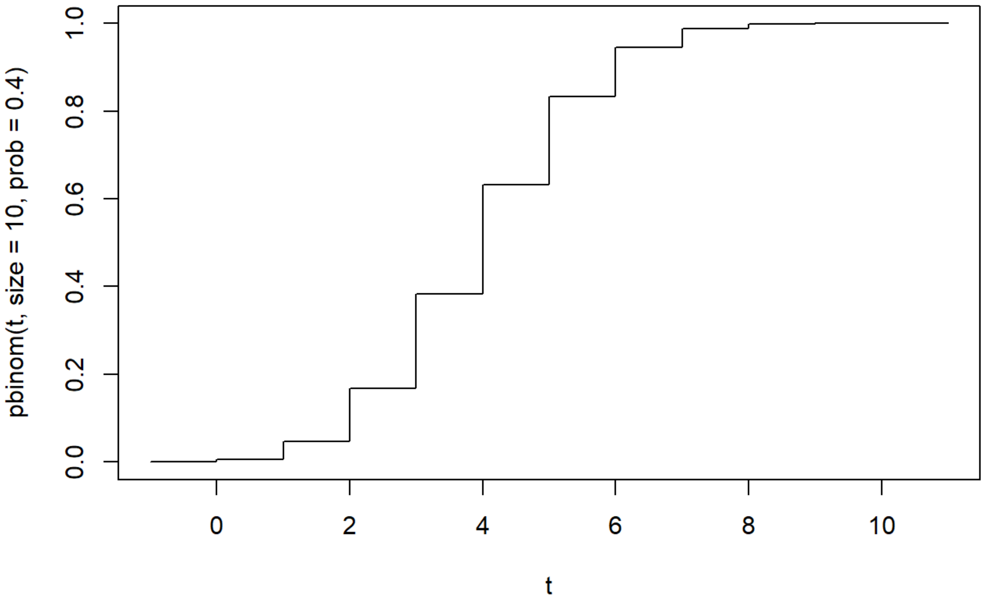


Cumulative Distribution Function (CDF)



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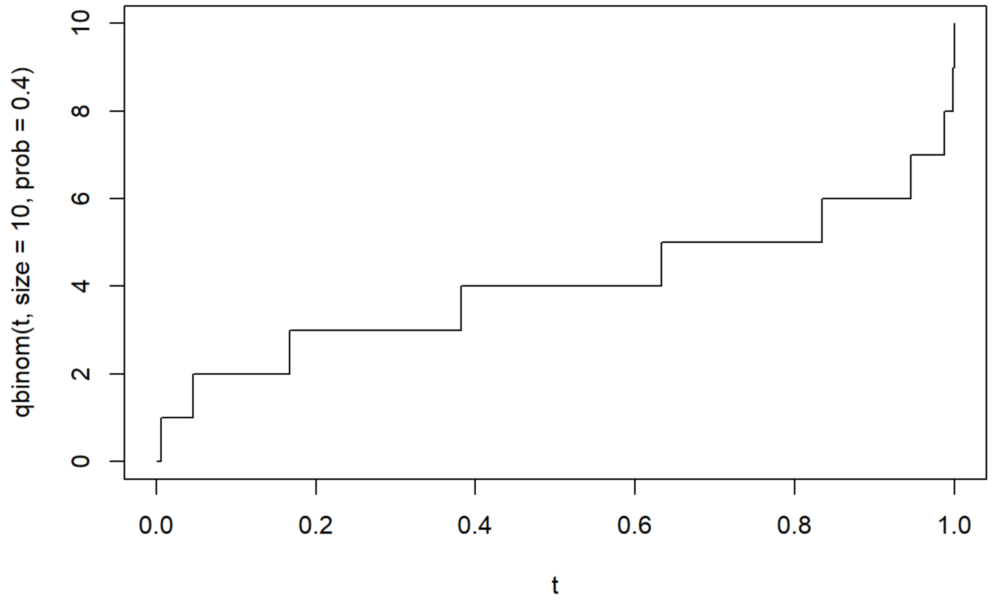

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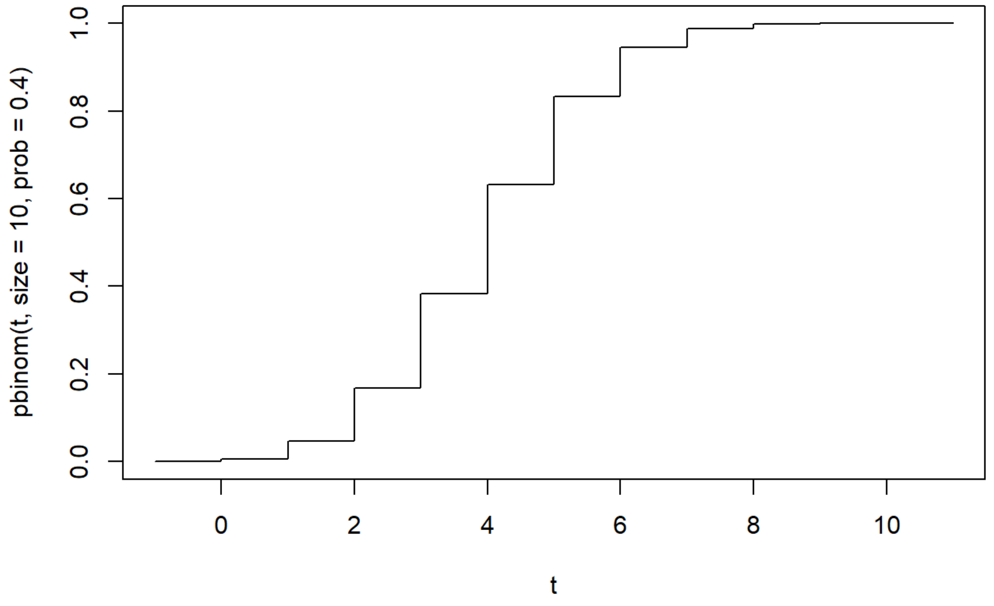

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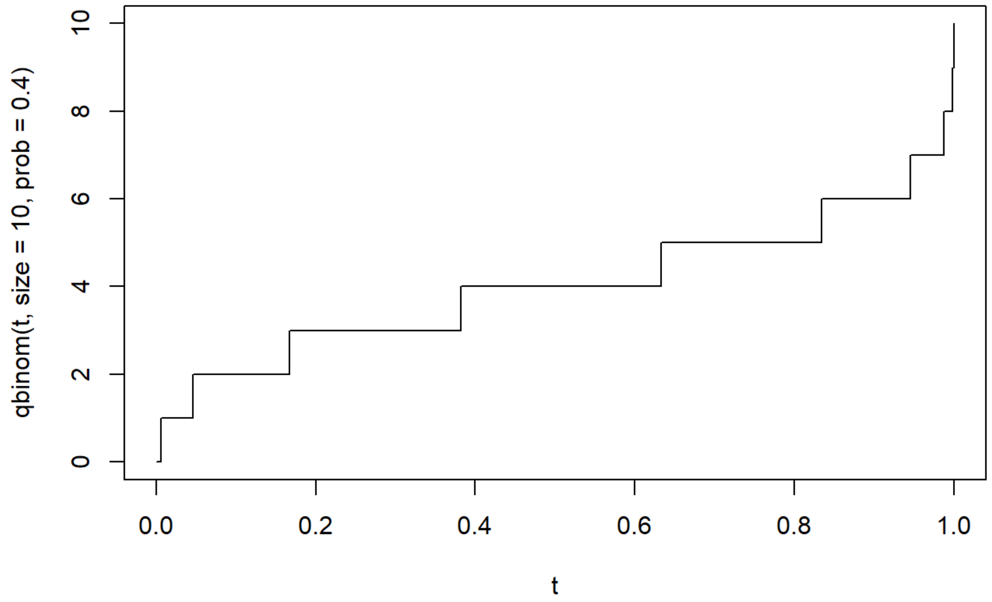

$$u \sim \text{Uniform}(0, 1)$$
$$x = \text{InverseCDF}(u)$$

CDF and its inverse are discontinuous (piece-wise constant)!

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Gumbel-Max Trick

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$$y = \arg\max_{i \in \{1, \cdots, K\}} x_i + z_i$$

where

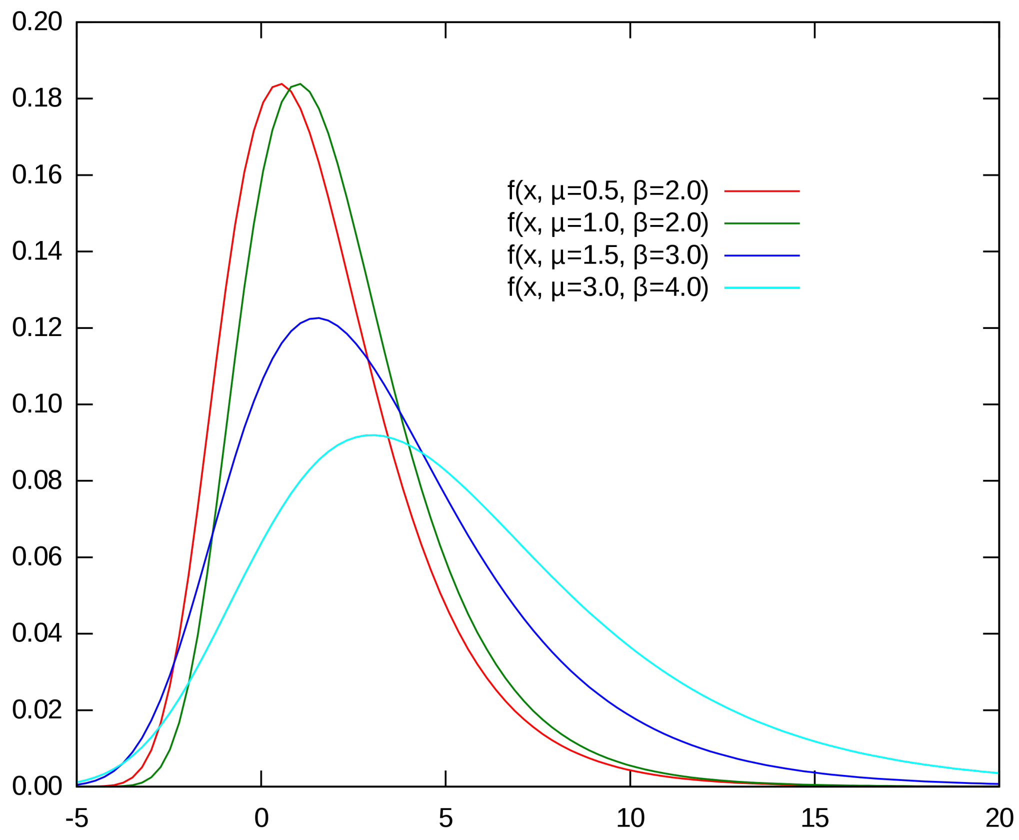
$$z_i \overset{iid}{\sim} \text{Gumbel}(0, 1)$$

Sampling Discrete (Categorical) Random Variables

Gumbel distribution $\text{Gumbel}(\mu, \beta)$

PDF:

$$p(x) = \frac{1}{\beta} \exp\left(- \left(\frac{x-\mu}{\beta} + \exp(-\frac{x-\mu}{\beta}) \right) \right)$$



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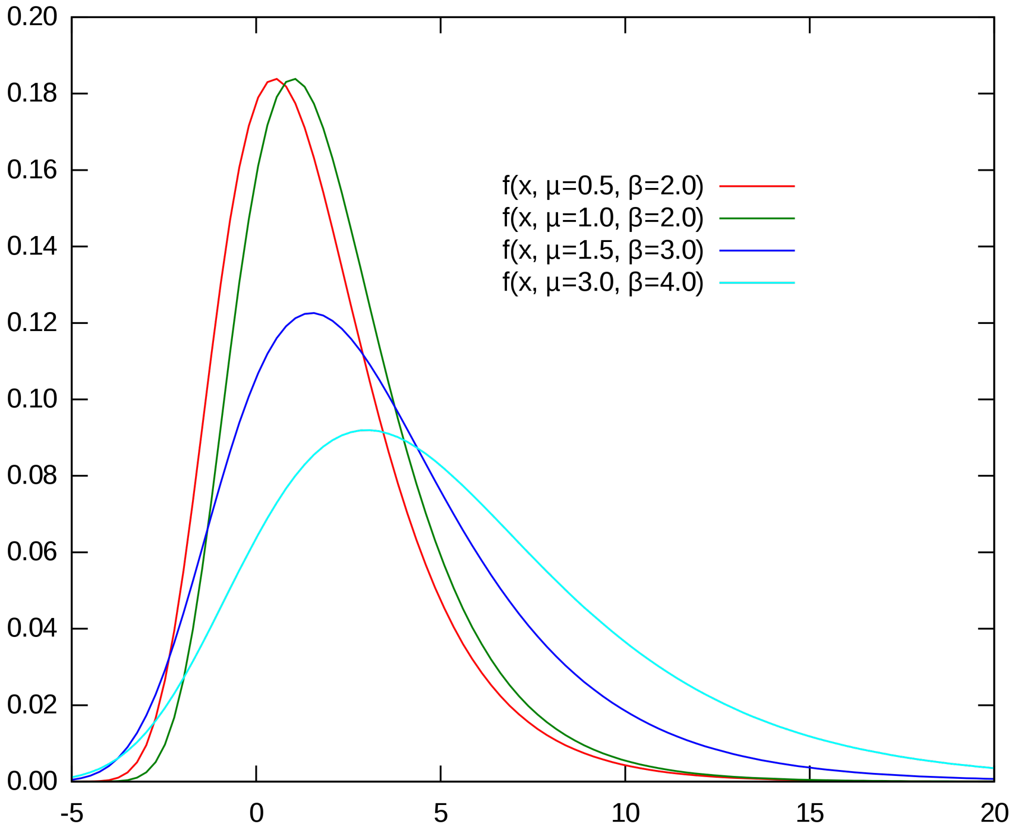
CDF:

$$F(x) = \exp\left(-\exp\left(-\frac{x-\mu}{\beta}\right)\right)$$

It is used to model the distribution of the maximum (or the minimum) of a number of samples of various distributions



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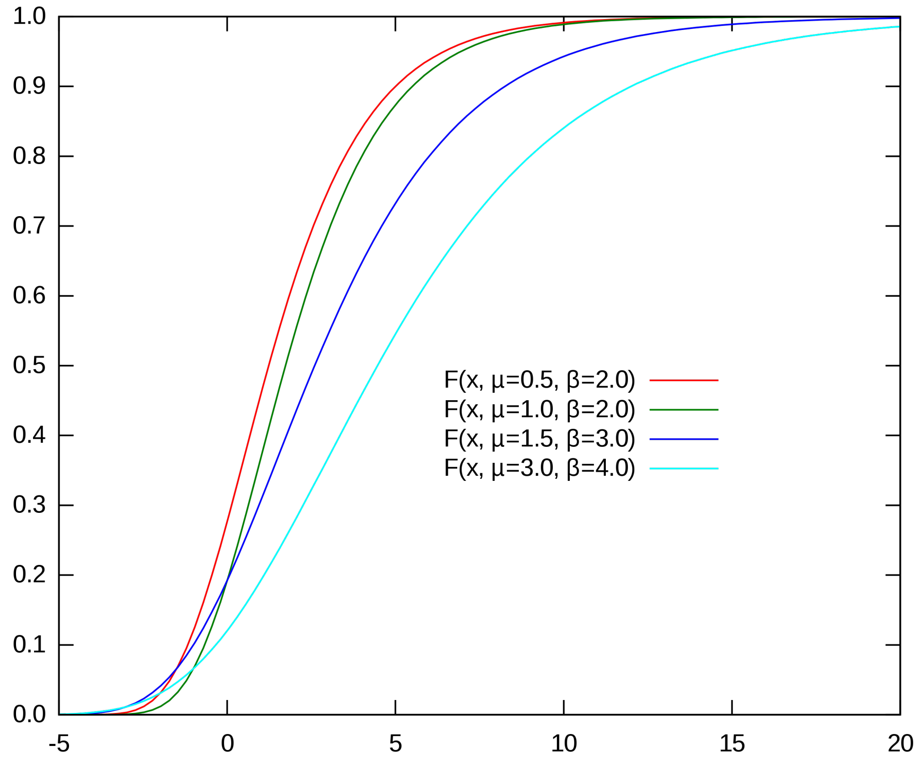
CDF:

$$F(x) = \exp\left(-\exp\left(-x\right)\right)$$



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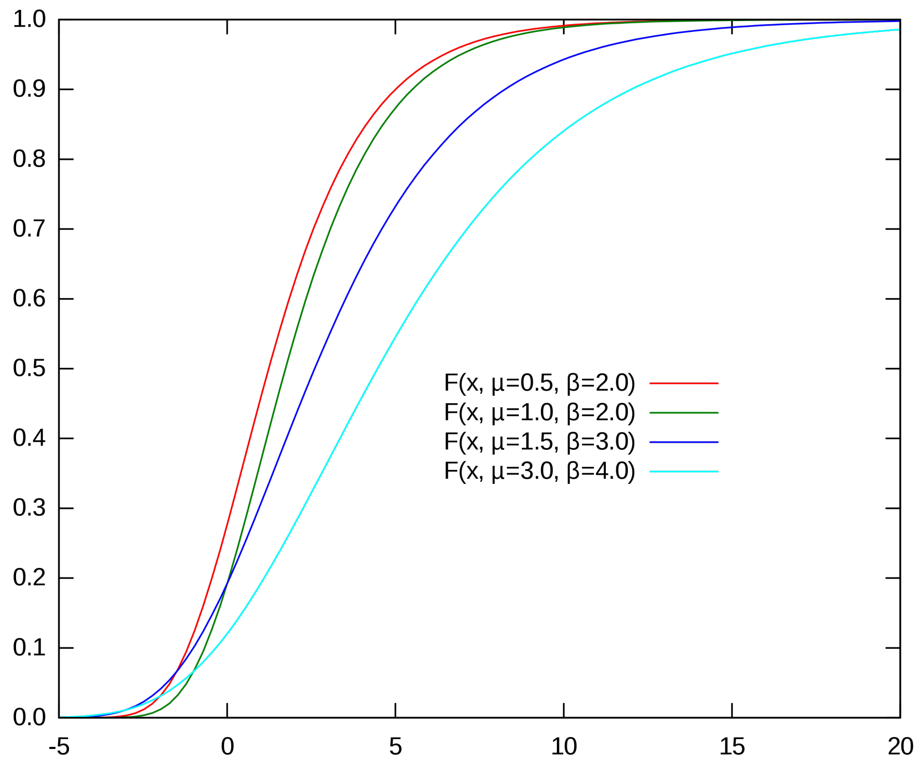
Inverse CDF:

$$F^{-1}(u) = -\log\left(-\log\left(u\right)\right)$$



Inverse Transform Sampling is efficient

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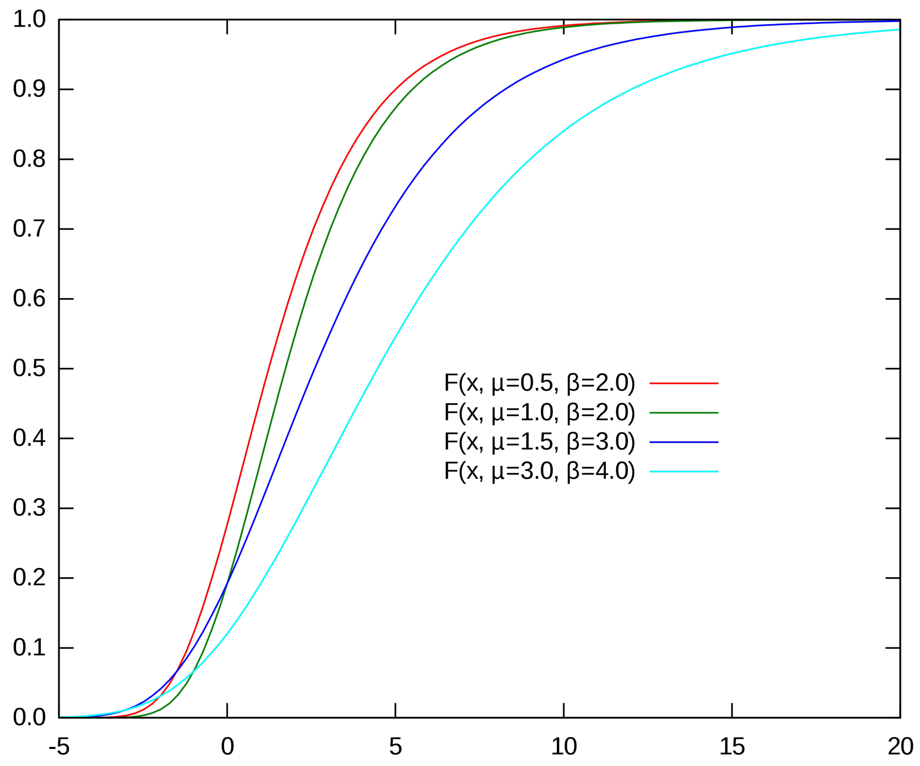

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Gumbel Max Trick

Given any real numbers $\{x_i | i = 1, \cdots, K\}$, we sample $z_i \overset{iid}{\sim} \mathrm{Gumbel}(0, 1)$

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Given any real numbers $\{x_i | i = 1, \cdots, K\}$, we sample $z_i \overset{iid}{\sim} \text{Gumbel}(0, 1)$

We have $x_i + z_i \overset{iid}{\sim} \text{Gumbel}(x_i, 1)$

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We have $x_i + z_i \overset{iid}{\sim} \text{Gumbel}(x_i, 1)$

The conditional probability that the index of maximum value of $\{x_i + z_i | i = 1, \cdots, K\}$ is i^* is

$$
\begin{aligned}
p\left(i^* = \underset{i \in \{1, \cdots, K\}}{\arg\max}\; x_i + z_i \,\middle|\, \{x_i + z_i | i = 1, \cdots, K\}\right) &= p\left(x_j + z_j \leq x_{i^*} + z_{i^*},\ \forall j \neq i^* | \{x_i + z_i | i = 1, \cdots, K\}\right) \\
&= \prod_{j \neq i^*} p\left(x_j + z_j \leq x_{i^*} + z_{i^*} | \{x_i + z_i | i = 1, \cdots, K\}\right) \\
&= \prod_{j \neq i^*} \text{CDF}_j\left(x_{i^*} + z_{i^*}\right) \\
&= \prod_{j \neq i^*} \exp\left(-\exp(-(x_{i^*} + z_{i^*} - x_j))\right)
\end{aligned}
$$

Sampling Discrete (Categorical) Random Variables

The marginal probability that the index of maximum value of $\{x_i + z_i | i = 1, \cdots, K\}$ is i^* is

$$
\begin{aligned}
&p\left(i^* = \operatorname*{arg\,max}_{i \in \{1,\cdots,K\}} x_i + z_i\right) \\
&= \int p\left(i^* = \operatorname*{arg\,max}_{i \in \{1,\cdots,K\}} x_i + z_i \middle| \{x_i + z_i | i = 1, \cdots, K\}\right) p(\{x_i + z_i\}) d\{x_i + z_i\} \\
&= \int \prod_{j \neq i^*} \exp\left(-\exp(-(x_{i^*} + z_{i^*} - x_j)\right) \prod_j \exp\left(-\left(z_j + \exp(-z_j)\right)\right) d\{z_i\} \\
&= \int \exp\left(-\left(z_{i^*} + \exp(-z_{i^*})\right)\right) \int \prod_{j \neq i^*} \exp\left(-\exp(-(x_{i^*} + z_{i^*} - x_j)\right) \\
&\qquad \exp\left(-\left(z_j + \exp(-z_j)\right)\right) d\{z_j | j \neq i^*\} dz_{i^*} \\
&= \int \exp\left(-\left(z_{i^*} + \exp(-z_{i^*})\right)\right) \prod_{j \neq i^*} \exp\left(-\exp(-(x_{i^*} + z_{i^*} - x_j)\right) dz_{i^*}
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The marginal probability that the index of maximum value of $\{x_i + z_i | i = 1, \cdots, K\}$ is i^* is

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$$= \int p\left(i^* = \underset{i \in \{1,\cdots,K\}}{\arg\max}\ x_i + z_i \middle| \{x_i + z_i | i = 1, \cdots, K\}\right) p(\{x_i + z_i\}) d\{x_i + z_i\}$$

$$= \int \prod_{j \neq i^*} \exp\left(-\exp(-(x_{i^*} + z_{i^*} - x_j)\right) \prod_j \exp\left(-\left(z_j + \exp(-z_j)\right)\right) d\{z_i\}$$

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$$\exp\left(-\left(z_j + \exp(-z_j)\right)\right) d\{z_j | j \neq i^*\} dz_{i^*}$$

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$$\text{Gumbel}(0,1) \quad \int p(x) dx = \int \exp\left(-\left(x + \exp(-x)\right)\right) dx = 1$$

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&= \int \exp\left(-z_{i^*} - \exp(-z_{i^*}) - \sum_{j\neq i^*} \exp(-(x_{i^*} + z_{i^*} - x_j)\right) dz_{i^*} \\
&= \int \exp\left(-z_{i^*} - \sum_{j} \exp(-(x_{i^*} + z_{i^*} - x_j)\right) dz_{i^*} \\
&= \int \exp\left(-z_{i^*} - \exp(-z_{i^*}) \sum_{j} \exp(-x_{i^*} + x_j)\right) dz_{i^*} \\
&= \left(\sum_j \exp(-x_{i^*} + x_j)\right)^{-1} \\
&= \frac{\exp(x_{i^*})}{\sum_j \exp(x_j)}
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$$= \frac{\exp(x_{i^*})}{\sum_j \exp(x_j)}$$

$$\text{Gumbel}(\mu, \beta)$$

$$\int p(x) dx$$

$$= \int \frac{1}{\beta} \exp\left(-\left(\frac{x-\mu}{\beta} + \exp(-\frac{x-\mu}{\beta})\right)\right) dx$$

$$= 1$$

$$\mu = \log\left(\sum_j \exp(-x_{i^*} + x_j)\right)$$

$$\beta = 1$$

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We have derived *Gumbel-Max Trick*

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It can be used for efficient sampling from complicated probabilistic models like discrete MRFs [5]

Stochastic Gradient Estimation Again

Suppose we want to optimize $\mathcal{L}(\phi) = \mathbb{E}_{p_\phi(X)}[f(X)]$ and X is discrete

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Recall what we learned previously:

Reparameterization (path-derivative) gradient estimator $$\frac{\partial \mathcal{L}}{\partial \phi} = \frac{\partial}{\partial \phi}\mathbb{E}_{p(\epsilon)}[f(g(\phi, \epsilon))] = \mathbb{E}_{p(\epsilon)}\left[\frac{\partial f}{\partial g}\frac{\partial g}{\partial \phi}\right]$$

REINFORCE gradient estimator $$\frac{\partial \mathcal{L}}{\partial \phi} = \mathbb{E}_{p_\phi(X)}\left[\frac{\partial \log p_\phi(X)}{\partial \phi} f(X)\right]$$

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We use the reparameterization $X = g(\phi, \epsilon)$

However, for discrete X , we can not differentiate $g(\phi, \epsilon)$!

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However, for discrete X, we can not differentiate $g(\phi, \epsilon)$!

Can we find some differentiable approximation?

Straight-Through Estimator

Consider the binary (Bernoulli) case

$$X = g(\phi, \epsilon) = \begin{cases} 1 & \text{if } \epsilon \geq \phi \\ 0 & \text{otherwise} \end{cases}$$

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Since step-function is non-differentiable, we can approximate it using identity [7, 1] and sigmoid [1]

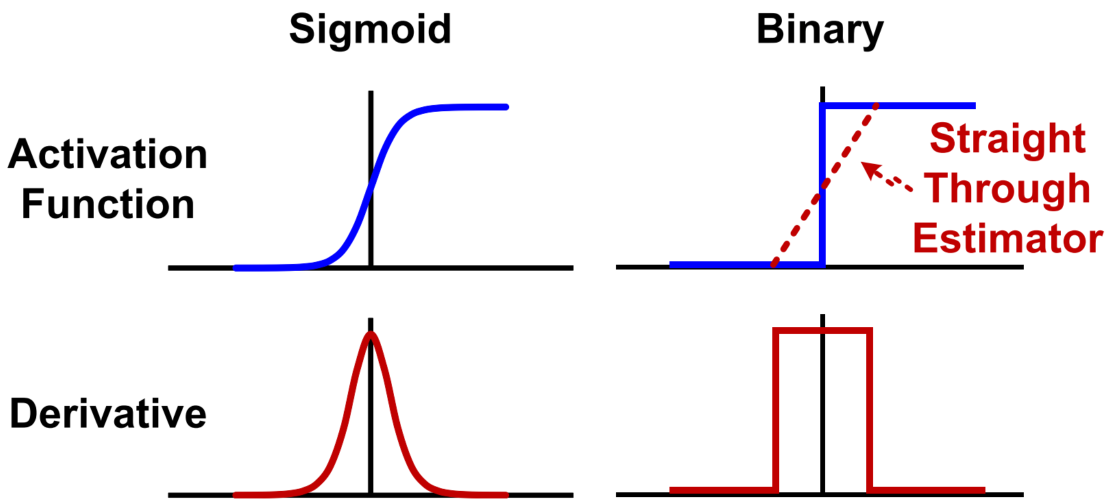

Image Credit: [8]

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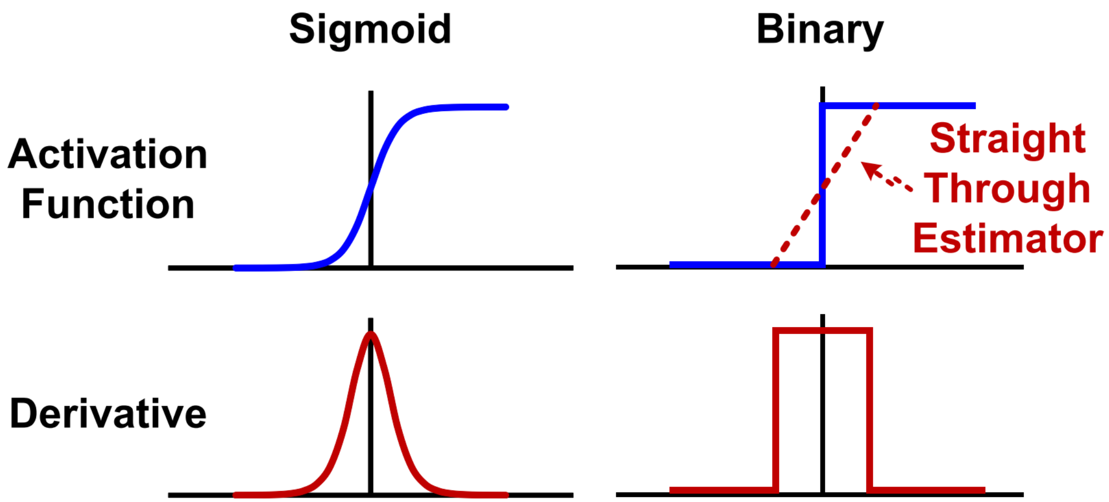

We use discrete samples in forward pass and differentiable approximations in backward pass!

Image Credit: [8]

Gumbel-Softmax Estimator

We know *Gumbel-Max Trick* can sample from categorical distributions

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However, argmax is non-differentiable!

Softmax is a differentiable approximation of argmax!

Gumbel-Softmax Estimator

Recall in Gumbel-Max trick, we have $$y = \arg\max_{i \in \{1, \cdots, K\}} x_i + z_i$$

$$z_i \overset{iid}{\sim} \text{Gumbel}(0, 1)$$

Use softmax instead of argmax (adding temperature τ), we have

$$y = \frac{\exp\left((x_k + z_k)/\tau\right)}{\sum_{i=1}^{K} \exp\left((x_i + z_i)/\tau\right)}$$

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The Gumbel-Softmax distribution (concrete distribution) [2, 3] is then

$$p(y_1, \cdots, y_K) = \Gamma(K)\tau^{K-1} \left(\sum_{i=1}^{K} \frac{\pi_i}{y_i^{\tau}} \right)^{-K} \prod_{i=1}^{K} \frac{\pi_i}{y_i^{\tau+1}} \qquad \pi_i = \frac{\exp(x_k)}{\sum_{i=1}^{K} \exp(x_i)}$$

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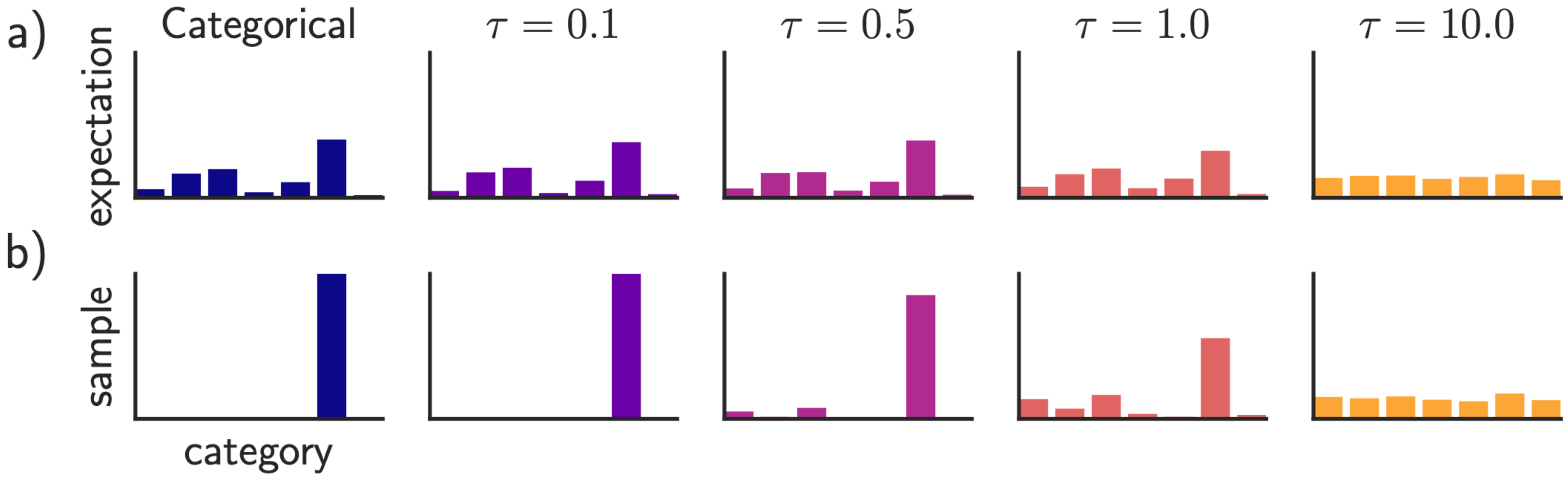

Histogram View

Image Credit: [2]

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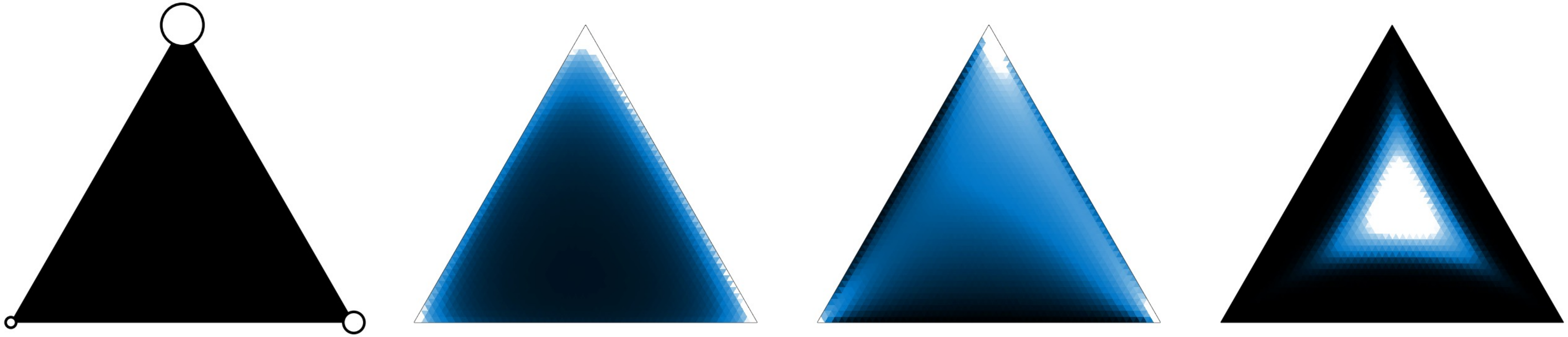

(a) $\lambda = 0$ (b) $\lambda = 1/2$ (c) $\lambda = 1$ (d) $\lambda = 2$

Simplex View

Image Credit: [3]

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Sampling operator is

$$y = \frac{\exp\left((x_k + z_k)/\tau\right)}{\sum_{i=1}^{K}\exp\left((x_i + z_i)/\tau\right)}$$

Since samples are not discrete anymore, it is a biased estimator $\mathcal{L}(\phi) = \mathbb{E}_{p_\phi(X)}\left[f(X)\right]$

Image Credit: [3]

Gumbel-Softmax Estimator

The Gumbel-Softmax distribution (concrete distribution) [2, 3] is then

$$p(y_1, \cdots, y_K) = \Gamma(K)\tau^{K-1} \left(\sum_{i=1}^{K} \frac{\pi_i}{y_i^\tau} \right)^{-K} \prod_{i=1}^{K} \frac{\pi_i}{y_i^{\tau+1}}$$

Sampling operator is

$$y = \frac{\exp\left((x_k + z_k)/\tau\right)}{\sum_{i=1}^{K} \exp\left((x_i + z_i)/\tau\right)}$$

Since samples are not discrete anymore, it is a biased estimator $\mathcal{L}(\phi) = \mathbb{E}_{p_\phi(X)}\left[f(X)\right]$

But samples are differentiable, so we can use reparameterization trick!

Empirically, it has low variances with a reasonable temperature!

Gumbel-Top K for Sequences

For random processes like sequences of discrete random variables, we are interested in sampling most probable sequences, e.g., in language models

(Deterministic) beam search is typically used!

Gumbel Top K Trick:

$$y_1, \cdots, y_m = \text{argtop m}_{i \in \{1, \cdots, K\}} x_i + z_i$$

$$z_i \overset{iid}{\sim} \text{Gumbel}(0, 1)$$

We can generalize Gumbel-Softmax to Gumbel-TopK to construct stochastic beam search [4]!

Gumbel-Top K for Sequences

Stochastic beam search

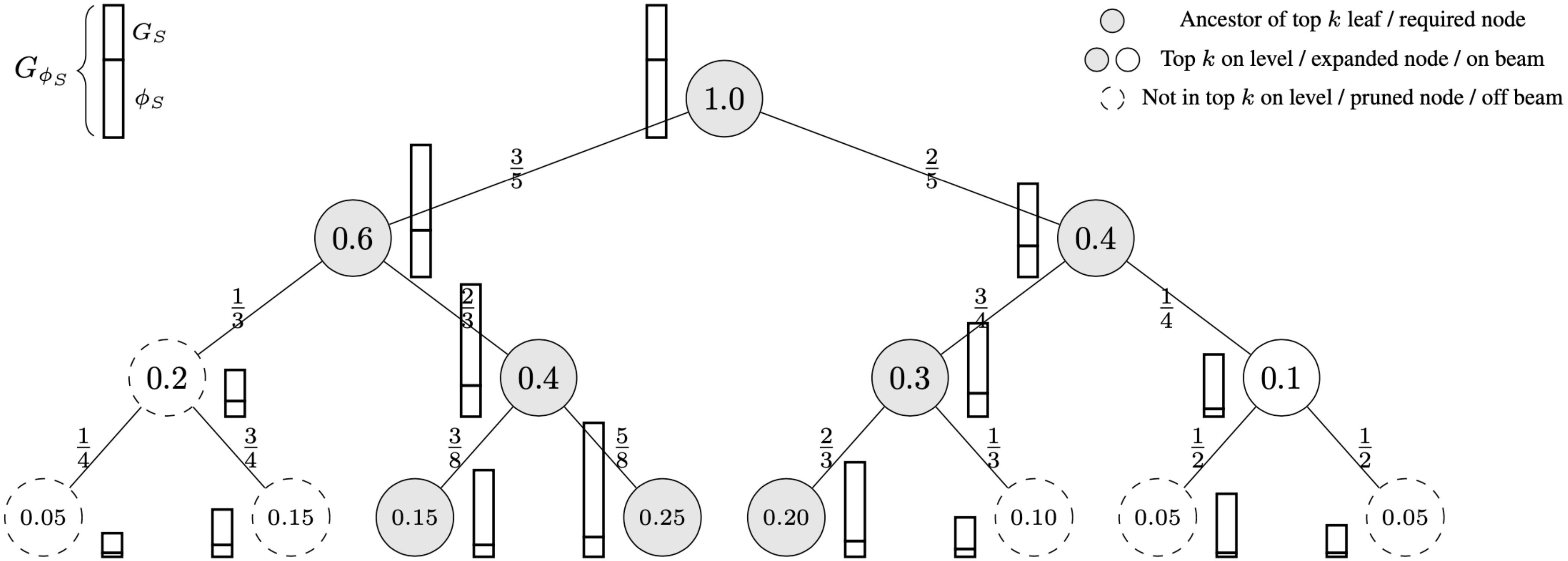

Image Credit: [4]

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Questions?