Gumbel Softmax Algorithm Description

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February 2021

One can use Gumbel-Softmax to sample a continuous approximation of a m hot vector. Assume that we are given a categorical distribution with probabilities $p_1, \ldots, p_k$. If we wish to generate a single sample of a one-hot vector based on this categorical distribution, then the first step is to generate k perturbations from a uniform distribution, i.e., each perturbation is generated with

$$\epsilon_i = -\log(-\log u_i), u_i \sim \text{Uniform}(0,1). \tag{1}$$

The output of these k perturbations becomes $[\epsilon_1, ..., \epsilon_k]$. The i^{th} element of the one-hot vector is then computed with

$$C_i = \frac{e^{(\log p_i + \epsilon_i)/\tau}}{\sum_{j=1}^{D} e^{(\log p_j + \epsilon_j)/\tau}} \tag{2}$$

where τ is a parameter that control the sharpness of the one-hot vectors. Note that since the Gumbe-Softmax method results in a differentiable one-hot vectors, the values produced by Eq. (2) are not exactly 1s and 0s, but an approximation. The τ value controls the sharpness of these approximations where a small τ of approximately 0 yield a very sharp of nearly 1 and 0; the common default value is 0.1.

By repeating Eq. (2) for each of the k groups, a one-hot vector can be generated for feature j can be denoted as $\mathbf{C}_j$ where

$$\mathbf{C}_j = [C_1, C_2, ..., C_k]^T. \tag{3}$$

We again repeated Eq. (3) for each of the d features to generate the columns of $G \in \mathbb{R}^{k \times d}$ as

$$G = [\mathbf{C_1}, \mathbf{C_2}, ..., \mathbf{C_d}]. \tag{4}$$

To generate samples for S where m elements are 1s, we repeat Gumbel-softmax m times to create a matrix V where

$$V = [\mathbf{C_1}, ..., \mathbf{C_m}]. \tag{5}$$

By setting the k^{th} row of V as $\bar{V}_k$, the k^{th} element of S can be set to the maximum value in $\bar{V}_k$ where

$$S_k = \max \bar{V}_k. \tag{6}$$

Note that in the event where the newly generated $\mathbf{C_j}$ is a repeat of a previous column, it is discarded, and a new $\mathbf{C_j}$ is generated in its place.