

# Gumbel-max trick derivation

## Notations

- $P(A)$ : The probability of event  $A$ .
- $P(A, B)$ : The probability of events  $A$  and  $B$  both occurring.
- $P(A|B)$ : The conditional probability of event  $A$  given the occurrence of event  $B$ .
- $f(x) = \exp[-(x + \exp(-x))]$ : The probability density function of the standard Gumbel distribution.
- $F(x) = \exp[-\exp(-x)]$ : The cumulative distribution function of the standard Gumbel distribution.
- $p_1, p_2, \dots, p_N$ : The unnormalized event probabilities of the target categorical distribution, assuming there are  $N$  categories.
- $x_1, x_2, \dots, x_N$ : Independent and identically distributed random variables from the standard Gumbel distribution.
- $\arg \max_m (x_m + \ln p_m)$ : A function that finds the index  $m$  which maximizes  $x_n + \ln p_n$ .

## Derivation

Consider calculating the probability of  $n$  being the index that maximizes  $x_n + \ln p_n$ , *i.e.*,  $P(n = \arg \max_m (x_m + \ln p_m))$ . In order to do so, we first express it in terms of a marginal probability:

$$\begin{aligned} & P\left(n = \arg \max_m (x_m + \ln p_m)\right) \\ &= \int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty} dx_2 \cdots \int_{-\infty}^{\infty} dx_N P\left(n = \arg \max_m (x_m + \ln p_m), x_1, x_2, \dots, x_N\right). \end{aligned} \quad (1)$$

The integrand in eq. (1) can be expanded using conditional probability

$$\begin{aligned} & P\left(n = \arg \max_m (x_m + \ln p_m), x_1, x_2, \dots, x_N\right) \\ &= P\left(n = \arg \max_m (x_m + \ln p_m) \middle| x_1, x_2, \dots, x_N\right) P(x_1, x_2, \dots, x_N). \end{aligned} \quad (2)$$

As  $x_1, x_2, \dots, x_N$  are independent of each other, both terms on the right-hand side of eq. (2) can be further expanded as products of probabilities:

$$P\left(n = \arg \max_m (x_m + \ln p_m) \middle| x_1, x_2, \dots, x_N\right) = \prod_{m=1}^N P(x_n + \ln p_n \geq x_m + \ln p_m | x_n, x_m), \quad (3)$$

$$P(x_1, x_2, \dots, x_N) = \prod_{m=1}^N P(x_m). \quad (4)$$

Plugging eqs. (2) to (4) into eq. (1) yields

$$\begin{aligned}
& P\left(n = \arg \max_m (x_m + \ln p_m)\right) \\
&= \int_{-\infty}^{\infty} dx_n P(x_n + \ln p_n \geq x_m + \ln p_m | x_n) P(x_n) \\
&\quad \times \prod_{\substack{m=1 \\ m \neq n}}^N \int_{-\infty}^{\infty} dx_m P(x_n + \ln p_n \geq x_m + \ln p_m | x_n, x_m) P(x_m).
\end{aligned} \tag{5}$$

Now that we have fully expanded the integrand in eq. (1), we are ready to proceed by specifying the mathematical form of each integrand of eq. (5). For each  $m = 1, 2, \dots, N$ , the event of  $x_n + \ln p_n \geq x_m + \ln p_m$  is a true-or-false question, so  $P(x_n + \ln p_n \geq x_m + \ln p_m | x_n, x_m)$  can only take 1 or 0 as its value. Therefore, we can express it in terms of the Heaviside step function:

$$P(x_n + \ln p_n \geq x_m + \ln p_m | x_n, x_m) = H(x_n + \ln p_n - x_m - \ln p_m). \tag{6}$$

Note that  $P(x_n + \ln p_n \geq x_n + \ln p_n | x_n)$  is always equal to 1. Moreover, as  $x_m$ 's are independently sampled from the standard Gumbel distribution, by definition,

$$P(x_m) = f(x_m). \tag{7}$$

Consequently, for any  $m \neq n$ ,

$$\begin{aligned}
& \int_{-\infty}^{\infty} dx_m P(x_n + \ln p_n \geq x_m + \ln p_m | x_n, x_m) P(x_m) \\
&= \int_{-\infty}^{\infty} dx_m H(x_n + \ln p_n - x_m - \ln p_m) f(x_m) = \int_{-\infty}^{x_n + \ln p_n - \ln p_m} dx_m f(x_m) \\
&= F(x) \Big|_{-\infty}^{x_n + \ln p_n - \ln p_m} = \exp[-\exp(-x_n - \ln p_n + \ln p_m)] \\
&= \exp\left[-\frac{p_m}{p_n} \exp(-x_n)\right].
\end{aligned} \tag{8}$$

It follows that

$$\prod_{\substack{m=1 \\ m \neq n}}^N \int_{-\infty}^{\infty} dx_m P(x_n + \ln p_n \geq x_m + \ln p_m | x_n, x_m) P(x_m) = \exp\left[-\frac{\sum_{m=1, m \neq n}^N p_m}{p_n} \exp(-x_n)\right] \tag{9}$$

Therefore,

$$\begin{aligned}
P\left(n = \arg \max_m (x_m + \ln p_m)\right) &= \int_{-\infty}^{\infty} dx_n f(x_n) \exp\left[-\frac{\sum_{m=1, m \neq n}^N p_m}{p_n} \exp(-x_n)\right] \\
&= \int_{-\infty}^{\infty} dx_n \exp(-x_n) \exp\left[-\exp(-x_n) - \frac{\sum_{m=1, m \neq n}^N p_m}{p_n} \exp(-x_n)\right] \\
&= \int_{-\infty}^{\infty} dx_n \exp(-x_n) \exp\left[-\frac{\sum_{m=1}^N p_m}{p_n} \exp(-x_n)\right].
\end{aligned} \tag{10}$$

At first this integral may seem intimidating, however, it can be evaluated through the simple substitution of  $u = \exp(-x_n)$ :

$$P\left(n = \arg \max_m (x_m + \ln p_m)\right) = \int_0^1 du \exp\left(-\frac{\sum_{m=1}^N p_m}{p_n} u\right) = \frac{p_n}{\sum_{m=1}^N p_m}. \tag{11}$$

From eq. (11), it is clear that the probability of  $n$  being the index that maximizes  $x_n + \ln p_n$  is equal to the normalized event probability of category  $n$ . In other words, to sample from a categorical distribution given the unnormalized log probabilities  $\ln p_1, \ln p_2, \dots, \ln p_N$ , we just need to independently sample  $N$  random variables from the standard Gumbel distribution,  $x_1, x_2, \dots, x_N$ , then return the category index  $n$  that maximizes  $x_n + \ln p_n$ .