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, \ldots, p_N : The unnormalized event probabilities of the target categorical distribution, assuming there are N categories.
- x_1, x_2, \ldots, 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:

$$P\left(n = \underset{m}{\operatorname{arg\,max}} (x_m + \ln p_m)\right)$$

$$= \int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty} dx_2 \cdots \int_{-\infty}^{\infty} dx_N P\left(n = \underset{m}{\operatorname{arg\,max}} (x_m + \ln p_m), x_1, x_2, \dots, x_N\right). \tag{1}$$

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

$$P\left(n = \arg\max_{m} (x_{m} + \ln p_{m}), x_{1}, x_{2}, \dots, x_{N}\right)$$

$$= P\left(n = \arg\max_{m} (x_{m} + \ln p_{m}) \middle| x_{1}, x_{2}, \dots, x_{N}\right) P\left(x_{1}, x_{2}, \dots, x_{N}\right). \tag{2}$$

As x_1, x_2, \ldots, 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:

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

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

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

$$P\left(n = \underset{m}{\operatorname{arg\,max}} (x_m + \ln p_m)\right)$$

$$= \int_{-\infty}^{\infty} dx_n P\left(x_n + \ln p_n \ge x_n + \ln p_n | x_n\right) P\left(x_n\right)$$

$$\times \prod_{\substack{m=1\\m \ne n}}^{N} \int_{-\infty}^{\infty} dx_m P\left(x_n + \ln p_n \ge x_m + \ln p_m | x_n, x_m\right) P\left(x_m\right). \tag{5}$$

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 $m=1,2,\ldots,N$, the event of $x_n+\ln p_n\geq x_m+\ln p_m$ is a true-or-false question, so $P\left(x_n+\ln p_n\geq x_m+\ln p_m|x_n,x_m\right)$ can only take 1 or 0 as its value. Therefore, we can express it in terms of the Heaviside step function:

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

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

$$P\left(x_{m}\right) = f\left(x_{m}\right). \tag{7}$$

Consequently, for any $m \neq n$,

$$\int_{-\infty}^{\infty} dx_m P(x_n + \ln p_n \ge x_m + \ln p_m | x_n, x_m) P(x_m)$$

$$= \int_{-\infty}^{\infty} dx_m H(x_n + \ln p_n - x_m - \ln p_m) f(x_m) = \int_{-\infty}^{x_n + \ln p_n - \ln p_m} dx_m f(x_m)$$

$$= F(x) \Big|_{-\infty}^{x_n + \ln p_n - \ln p_m} = \exp\left[-\exp\left(-x_n - \ln p_n + \ln p_m\right)\right]$$

$$= \exp\left[-\frac{p_m}{p_n} \exp\left(-x_n\right)\right].$$
(8)

It follows that

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

Therefore,

$$P\left(n = \operatorname*{arg\,max}_{m}\left(x_{m} + \ln p_{m}\right)\right) = \int_{-\infty}^{\infty} \mathrm{d}x_{n} f\left(x_{n}\right) \exp\left[-\frac{\sum_{m=1, m \neq n}^{N} p_{m}}{p_{n}} \exp\left(-x_{n}\right)\right]$$

$$= \int_{-\infty}^{\infty} \mathrm{d}x_{n} \exp\left(-x_{n}\right) \exp\left[-\exp\left(-x_{n}\right) - \frac{\sum_{m=1, m \neq n}^{N} p_{m}}{p_{n}} \exp\left(-x_{n}\right)\right]$$

$$= \int_{-\infty}^{\infty} \mathrm{d}x_{n} \exp\left(-x_{n}\right) \exp\left[-\frac{\sum_{m=1}^{N} p_{m}}{p_{n}} \exp\left(-x_{n}\right)\right]. \tag{10}$$

At first this integral may seem intimidating, however, it can be evaluated through the simple substitution of $u = \exp(-x_n)$, and the final result is what we are looking for:

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