A. Proof of the Gumbel-Top-$k$ trick

**Theorem 1.** For $k \leq n$, let $I_1^*, ..., I_n^* = \arg\max_k G_{\phi_i}$. Then $I_1^*, ..., I_n^*$ is an (ordered) sample without replacement from the Categorical $\left( \frac{\exp \phi_i}{\sum_{j \in N_k^*} \exp \phi_j}, i \in N \right)$ distribution, e.g. for a realization $i_1^*, ..., i_k^*$ it holds that

$$P\left( I_1^* = i_1^*, ..., I_k^* = i_k^* \right) = \prod_{j=1}^{k} \frac{\exp \phi_{i_j^*}}{\sum_{\ell \in N_j^*} \exp \phi_{\ell}} \quad (15)$$

where $N_j^* = N \setminus \{i_1^*, ..., i_{j-1}^*\}$ is the domain (without replacement) for the $j$-th sampled element.

**Proof.** First note that

$$P\left( I_1^* = i_1^* | I_1^* = i_1^*, ..., I_{k-1}^* = i_{k-1}^* \right) = P\left( i_1^* = \arg\max_{i \in N_1^*} G_{\phi_i} | I_1^* = i_1^*, ..., I_{k-1}^* = i_{k-1}^* \right)$$

$$= P\left( i_1^* = \arg\max_{i \in N_1^*} \max_{i \in N_k^*} G_{\phi_i} < G_{\phi_i^*} \right) \quad (16)$$

$$= P\left( i_1^* = \arg\max_{i \in N_k^*} G_{\phi_i} \right) \quad (17)$$

$$= \frac{\exp \phi_{i_1^*}}{\sum_{\ell \in N_1^*} \exp \phi_{\ell}} \quad (18)$$

The step from (16) to (17) follows from the independence of the max and arg max (Section 2.3) and the step from (17) to (18) uses the Gumbel-Max trick. The proof follows by induction on $k$. The case $k = 1$ is the Gumbel-Max trick, while if we assume the result (15) proven for $k - 1$, then

$$P\left( I_k^* = i_k^* | I_1^* = i_1^*, ..., I_{k-1}^* = i_{k-1}^* \right)$$

$$= P\left( I_k^* = i_k^* | I_1^* = i_1^*, ..., I_{k-1}^* = i_{k-1}^* \right) \cdot P\left( I_1^* = i_1^*, ..., I_{k-1}^* = i_{k-1}^* \right)$$

$$= \frac{\exp \phi_{i_k^*}}{\sum_{\ell \in N_k^*} \exp \phi_{\ell}} \cdot \prod_{j=1}^{k-1} \frac{\exp \phi_{i_j^*}}{\sum_{\ell \in N_j^*} \exp \phi_{\ell}} \quad (19)$$

In (19) we have used Equation (18) and Equation (15) for $k - 1$ by induction.

B. Sampling set of Gumbels with maximum $T$

B.1. The truncated Gumbel distribution

A random variable $G'$ has a truncated Gumbel distribution with location $\phi$ and maximum $T$ (e.g. $G' \sim \text{TruncatedGumbel}(\phi, T)$) with CDF $F_{\phi, T}(g)$ if:

$$F_{\phi, T}(g) = P(G' \leq g) = P(G \leq g | G \leq T) = \frac{P(G \leq \min(g, T))}{P(G \leq T)} = \frac{F_{\phi}(\min(g, T))}{F_{\phi}(T)} = \exp(- \exp(\phi - \min(g, T)))$$

The inverse CDF is:

$$F_{\phi, T}^{-1}(u) = \phi - \log(\exp(\phi - T) - \log u). \quad (20)$$

B.2. Sampling set of Gumbels with maximum $T$

In order to sample a set of Gumbel variables $\{\tilde{G}_{\phi_i} \mid \max_i \tilde{G}_{\phi_i} = T\}$, e.g. with their maximum being exactly $T$, we can first sample the arg max, $i^*$ and then sample the Gumbels conditionally on both the max and arg max:

1. Sample $i^* \sim \text{Categorical}\left( \frac{\exp \phi_{i_j}}{\sum_{j \in N} \exp \phi_{j}} \right)$. We do not need to condition on $T$ since the arg max $i^*$ is independent of the max $T$ (Section 2.3).
2. Set $\tilde{G}_{\phi_{i^*}} = T$, since this follows from conditioning on the max $T$ and arg max $i^*$.
3. Sample $\tilde{G}_{\phi_i} \sim \text{TruncatedGumbel}(\phi_i, T)$ for $i \neq i^*$. This works because, conditioning on the max $T$ and arg max $i^*$, it holds that:

$$P(\tilde{G}_{\phi_i} < g \mid \max_i \tilde{G}_{\phi_i} = T, \text{arg max}_i \tilde{G}_{\phi_i} = i^*, i \neq i^*) = P(\tilde{G}_{\phi_i} < g \mid \tilde{G}_{\phi_i} < T).$$

Equivalently, we can let $G_{\phi_i} \sim \text{Gumbel}(\phi_i)$, let $Z = \max_i G_{\phi_i}$ and define

$$\tilde{G}_{\phi_i} = F_{\phi_i, T}^{-1}(F_{\phi_i, Z}(G_{\phi_i})) = \phi_i - \log(\exp(\phi_i - T) - \exp(\phi_i - Z) + \exp(-G_{\phi_i})). \quad (22)$$
Here we have used (20) and (21). Since the transformation (22) is monotonically increasing, it preserves the arg max and it follows from the Gumbel-Max trick (3) that

$$\arg \max_i \tilde{G}_{\phi_i} = \arg \max_i G_{\phi_i} \sim \text{Categorical} \left( \frac{\exp \phi_i}{\sum \exp \phi_j} \right).$$

We can think of this as using the Gumbel-Max trick for step 1 (sampling the argmax) in the sampling process described above. Additionally, for $i = \arg \max_i G_{\phi_i}$:

$$\tilde{G}_{\phi_i} = F_{\phi_i}^{-1}(F_{\phi_i}(G_{\phi_i})) = F_{\phi_i}^{-1}(F_{\phi_i}(Z)) = T$$

so here we recover step 2 (setting $\tilde{G}_{\phi_i} = T$). For $i \neq \arg \max_i G_{\phi_i}$, it holds that:

$$P(\tilde{G}_{\phi_i} \leq g) = E_{Z}(P(\tilde{G}_{\phi_i} \leq g | Z, i \neq \arg \max_i G_{\phi_i}))$$

$$= E_{Z}(P(\tilde{G}_{\phi_i} \leq g | Z, \tilde{G}_{\phi_i} < Z))$$

$$= E_{Z}(P(F_{\phi_i}(Z)) \leq g | Z, \tilde{G}_{\phi_i} < Z)$$

$$= E_{Z}(P(G_{\phi_i} \leq \exp(F_{\phi_i}(Z)) | Z, \tilde{G}_{\phi_i} < Z))$$

$$= E_{Z}(F_{\phi_i}(Z) \leq \exp(F_{\phi_i}(Z)) | Z, \tilde{G}_{\phi_i} < Z))$$

$$= E_{Z}(F_{\phi_i}(Z)) = F_{\phi_i}(Z).$$

This means that $\tilde{G}_{\phi_i} \sim \text{TruncatedGumbel}(\phi_i, T)$, so this is equivalent to step 3 (sampling $\tilde{G}_{\phi_i} \sim \text{TruncatedGumbel}(\phi_i, T)$ for $i \neq i^*$).

### B.3. Numeric stability of truncated Gumbel computation

Direct computation of (22) can be unstable as large terms need to be exponentiated. Instead, we compute:

$$v_i = T - G_{\phi_i} + \log \text{1mexp}(G_{\phi_i} - Z)$$

$$\tilde{G}_{\phi_i} = T - \max(0, v_i) - \log \text{1pexp}(-|v_i|) \quad (23)$$

where we have defined

$$\log \text{1mexp}(a) = \log(1 - \exp(a)), \quad a \leq 0$$

$$\log \text{1pexp}(a) = \log(1 + \exp(a)).$$

This is equivalent as

$$T - \max(0, v_i) - \log(1 + \exp(-|v_i|))$$

$$= T - \log(1 + \exp(v_i))$$

$$= T - \log(1 + \exp(T - G_{\phi_i} + \log(1 - \exp(G_{\phi_i} - Z))))$$

$$= T - \log(1 + \exp(T - G_{\phi_i}(1 - \exp(G_{\phi_i} - Z))))$$

$$= T - \log(1 + \exp(T - G_{\phi_i}) - \exp(T - Z))$$

$$= -\log(\exp(-T) + \exp(-G_{\phi_i}) - \exp(-Z))$$

$$= \tilde{G}_{\phi_i}.$$

The first step can be easily verified by considering the cases $v_i < 0$ and $v_i \geq 0$. \text{log1mexp} and \text{log1pexp} can be computed accurately using (20) and (21) (Mächler, 2012):

$$\log \text{1mexp}(a) = \begin{cases} 
\log(-\exp(1)(a)) & a > -0.693 \\
\log(1 - \exp(a)) & \text{otherwise}
\end{cases}$$

$$\log \text{1pexp}(a) = \begin{cases} 
\log(1 + \exp(a)) & a < 18 \\
\log(1 + \exp(a)) & \text{otherwise}
\end{cases}$$

### C. Numerical stability of importance weights

We have to take care computing the importance weights as depending on the entropy the terms in the quotient $p_{\theta}(y_i|x)\frac{q_\theta(y_i|x)}{q_\theta(y_i|x)}$ can become very small, and in our case the computation of $P(G_{\phi_i} > \kappa) = 1 - \exp(-\exp(\phi_i - \kappa))$ can suffer from catastrophic cancellation. We can rewrite this expression using the more numerically stable implementation $\exp(1)(x) = \exp(x) - 1$ as $p(G_{\phi_i} > \kappa) = -\exp(1)(-\exp(\phi_i - \kappa))$ but in some cases this still suffers from instability as $\exp(\phi_i - \kappa)$ can underflow if $\phi_i - \kappa$ is small. Instead, for $\phi_i - \kappa < -10$ we use the identity

$$\log(1 - \exp(-z)) = \log(z) - \frac{z}{2} + \frac{z^2}{24} - \frac{z^4}{2880} + O(z^6)$$

to directly compute the log importance weight using $z = \exp(\phi_i - \kappa)$ and $\phi_i = \log p_{\theta}(y_i|x)$ (we assume $\phi_i$ is normalized):

$$\log \left( \frac{p_{\theta}(y_i|x)}{q_\theta(y_i|x)} \right) = \log p_{\theta}(y_i|x) - \log q_\theta(y_i|x)$$

$$= \log p_{\theta}(y_i|x) - \log(1 - \exp(-\exp(\phi_i - \kappa)))$$

$$= \log p_{\theta}(y_i|x) - \log(1 - \exp(-z))$$

$$= \log p_{\theta}(y_i|x) - \left( \log(z) - \frac{z}{2} + \frac{z^2}{24} - \frac{z^4}{2880} + O(z^6) \right)$$

$$= \log p_{\theta}(y_i|x) - \left( \phi_i - \kappa - \frac{z}{2} + \frac{z^2}{24} - \frac{z^4}{2880} + O(z^6) \right)$$

$$= \kappa + \frac{z}{2} - \frac{z^2}{24} + \frac{z^4}{2880} + O(z^6)$$

If $\phi_i - \kappa < -10$ then $0 < z < 10^{-6}$ so this computation will not lose any significant digits.
D. Proof of unbiasedness of priority sampling estimator

The following proof is adapted from the proofs by Duffield et al. (2007) and Vieira (2017). For generality of the proof, we write \( f(i) = f(y^i) \), \( p_i = p(y^i|x) \) and \( q_i(\kappa) = \theta_i(\kappa, y^i|x) \), and we consider general keys \( h_i \) (not necessarily Gumbel perturbations).

We assume we have a probability distribution over a finite domain \( 1, \ldots, n \) with normalized probabilities \( p_i \), e.g. \( \sum_{i=1}^n p_i = 1 \). For a given function \( f(i) \) we want to estimate the expectation

\[
\mathbb{E}[f(i)] = \sum_{i=1}^n p_i f(i).
\]

Each element \( i \) has an associated random key \( h_i \) and we define \( q_i(a) = P(h_i > a) \). This way, if we know the threshold \( a \) it holds that \( q_i(a) = P(i \in S) \) is the probability that element \( i \) is in the sample \( S \). As noted by Vieira (2017), the actual distribution of the key does not influence the unbiasedness of the estimator but does determine the effective sampling scheme. Using the Gumbel perturbed log-probabilities as keys (e.g. \( h_i = G_{\phi_i} \)) is equivalent to the PPSWOR scheme described by Vieira (2017).

We define shorthand notation \( h_{1:n} = \{h_1, \ldots, h_n\} \), \( h_{-i} = \{h_1, \ldots, h_{i-1}, h_{i+1}, \ldots, h_n\} = h_{1:n} \setminus \{h_i\} \). For a given sample size \( k \), let \( \kappa \) be the \((k+1)\)-th largest element of \( h_{1:n} \), so \( \kappa \) is the empirical threshold. Let \( \kappa'_i \) be the \( k \)-th largest element of \( h_{-i} \) (the \( k \)-th largest of all other elements).

Similar to Duffield et al. (2007) we will show that every element \( i \) in our sample contributes an unbiased estimate of \( \mathbb{E}[f(i)] \), so that the total estimator is unbiased. Formally, we will prove that

\[
\mathbb{E}_{h_{1:n}} \left[ \frac{1_{\{i \in S\}}}{q_i(\kappa)} \right] = 1 \tag{25}
\]

from which the result follows:

\[
\mathbb{E}_{h_{1:n}} \left[ \sum_{i \in S} \frac{p_i f(i)}{q_i(\kappa)} \right] = \mathbb{E}_{h_{1:n}} \left[ \sum_{i=1}^n \frac{p_i f(i)}{q_i(\kappa)} 1_{\{i \in S\}} \right] = \sum_{i=1}^n p_i f(i) \cdot \mathbb{E}_{h_{1:n}} \left[ \frac{1_{\{i \in S\}}}{q_i(\kappa)} \right] = \sum_{i=1}^n p_i f(i) = \mathbb{E}[f(i)]
\]

To prove (25), we make use of the observation (slightly rephrased) by Duffield et al. (2007) that conditioning on \( h_{-i} \), we know \( \kappa'_i \) and the event \( i \in S \) implies that \( \kappa = \kappa'_i \) since \( i \) will only be in the sample if \( h_i > \kappa'_i \) which means that \( \kappa'_i \) is the \( k \)-th largest element of \( h_{-i} \cup \{h_i\} = h_{1:n} \). The reverse is also true (if \( \kappa = \kappa'_i \) then \( h_i \) must be larger than \( \kappa'_i \) since otherwise the \( k \)-th largest element of \( h_{1:n} \) will be smaller than \( \kappa'_i \)).

\[
\mathbb{E}_{h_{1:n}} \left[ \frac{1_{\{i \in S\}}}{q_i(\kappa)} \right] = \mathbb{E}_{h_{-i}} \left[ \mathbb{E}_{h_i} \left[ \frac{1_{\{i \in S\}}}{q_i(\kappa)} \right] \right] = \mathbb{E}_{h_{-i}} \left[ \frac{1_{\{i \in S\}}}{q_i(\kappa)} \right] = \mathbb{E}_{h_{-i}} [1] = 1
\]