# The Conditional Bernoulli and its Application to Speech Recognition

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## 1 Motivations

A major challenge in speech recognition involves converting a variable number of speech frames $\{x_t\}_{t\in[1,T]}$ into a variable number of transcription tokens $\{c_\ell\}_{\ell\in[1,L]}$, where $L \ll T$. In hybrid architectures, $c_\ell$ are generated as a by-product of transitioning between states $s_t$ in a weighted finite-state transducer. In end-to-end neural ASR, this process is commonly achieved either with Connectionist Temporal Classification (CTC) [9] or sequence-to-sequence (seq2seq) architectures [2]. The former introduces a special blank label; performs a one-to-many mapping $c_\ell \mapsto \tilde{c}_t^{(i)}$ by injecting blank tokens until the transcription matches length $T$ in all possible configurations $(i)$ during training; and removes all blank labels during testing. Seq2seq architectures first encode the speech frames $x_t$ into some encoding $h$, then some separate recurrent neural network conditions on $h$ to generate the token sequence $c_t$.

In 2017, Luo et al. developed a novel end-to-end speech recognizer. Given a prefix of acoustic feature frames including the current frame $\{x_{t'}\}_{t'\in[t,T]}$ and a prefix of Bernoulli samples excluding the current frame $\{b_{t'}\}_{t'\in[t+1,T]}$, the recognizer produces a Bernoulli sample for the current frame $B_t \sim P(b_t|x_{\leq t}, b_{<t})$, plus or minus some additional conditioned terms. Whenever $B_t = 1$, the model "emits" a token drawn from a class distribution conditioned on the same information $C_t \sim P(c_t|x_{\leq t}, b_{<t})$. The paper had two primary motivations. First, though it resembles a decoder in a *seq2seq* architecture [2], it does not need to encode the entire input sequence $x_t$ before it can start making decisions about what was said, making it suitable to online recognition. Second, we can interpret the emission points, or "highs," of the Bernoulli sequence $B_t = 1$ as a form of hard alignment: the token output according to $C_t$ is unaffected by speech $x_{>t}$[1].

Because of the stochasticity introduced by sampling $B_t$ discretely, the network cannot determine the exact gradient for parameterizations of $B_t$. Thus,

[1] This is not necessarily a synchronous alignment. $B_t = 1$ may occur well after whatever caused the emission. The last high $\arg\max_{t'<t} B_{t'} = 1$ cannot be assumed to bound the event to times after $t'$ for the same reason. Finite $t$ and vanishing gradients will force some synchronicity, however.

the authors rely on an estimate of the REINFORCE gradient [17]:

$$\frac{\partial R}{\partial \theta} = \mathbb{E}_b \left[ \sum_{t=1}^{T} \left( \frac{\partial R_t}{\partial \theta} + \left( \sum_{t' \geq t} R_{t'} \right) \frac{\partial}{\partial \theta} \log P(b_t | b_{<t}, c_{<\ell_t}) \right) \right] \tag{1}$$

where

$$R_t = \begin{cases} \log P(C_t = c_{\sum_{t'<t} b_{t'}} | x_{\leq t}, b_{<t}, c_{\sum_{t'<t-1} b_{t'}}) & \text{if } B_t = 1 \\ 0 & \text{if } B_t = 0 \end{cases} \tag{2}$$

The reward (eq. (2)) is the log probability of the $k$-th class label, where $k$ counts the number of high Bernoulli values up to and including time step $t$. The return for time step $t$ accumulates the instantaneous rewards for all non-past time steps $t' \geq t$.

In practice, using eq. (1) is very slow to train and yields mixed results. The authors found it was necessary to add a baseline function and an entropy function in order to converge. In a later publication [11], a bidirectional model[2] used Variational Inference to speed up convergence, though this failed to improve the overall performance of the model on the TIMIT corpus. The mixed performance and convergence of these models was blamed on the high-variance gradient estimate of eq. (1) [11].

We believe that the performance and convergence issues of these models are not due, at least in whole, to a high-variance estimate. Instead, we propose that the training objective has two other critical issues.

First, in order to ensure the total number of high Bernoulli values matched the total number of labels $L$ during training, i.e. $\sum_t b_t = L$, the authors would force later samples to some specific value. This implies that $B_t \not\sim P_B(b_t | \ldots)$, making the Monte Carlo estimate of eq. (1) biased.

Second, under the current regime, $B_t = 0$ maximizes the per-step reward by avoiding a negative reward associated with $\log P(c_t | \ldots)$. Equation (1) accumulates future rewards to mitigate this, but the choice to do so biases the system to emit as soon as possible to reduce the number of total frames accumulating negative rewards. This bias could explain why, without an additional "entropy penalty," the model would learn to emit entirely at the beginning of the utterance [12]. It could interact with the previous issue to produce a model that learns to immediately and repeatedly emit without stopping, since $b_{\geq L} = 0$, pushing $P_B(b_t | \ldots) \to 1$.

To solve both of these problems, we propose replacing the $T$ independent Bernoulli random variables $B_t$ sampled during training with a single sample $B$ from the Conditional Bernoulli (CB) distribution during training. The CB conditions on the required number of high trials, which will make the objective well-defined during testing and avoiding the first problem entirely. The CB can be decomposed into a series of $T$ Bernoulli trials that condition on past trial results, similar to eq. (2), but with an arbitrary ordering of trials. We can alternate forward and backward conditioning to mitigate the system's tendency to

[2] Forgoing the motivation for online speech recognition.

emit early. If we also train the model to fit a certain prior, CB training elegantly segues into the same Bernoulli testing scheme. In addition to modifying eq. (1), we will also show how the CB can be relaxed to a continuous variable for use in Straight-Through estimators [3, 10] or RELAX-like estimators [13, 8].

# 2 The Conditional Bernoulli

## 2.1 Definitions

The Conditional Bernoulli distribution [6, 5], sometimes called the Conditional Poisson distribution [1, 4], is defined as

$$P\left(b\middle|\sum_t b_t = k; w\right) = \frac{\prod_t w_t^{b_t}}{\sum_{\left\{b':\sum_t b'_t=k\right\}} \prod_t w_t^{b'_t}} \tag{3}$$

Where $w_t = p_t/(1-p_t)$ are the odds/weights of a Bernoulli random variable $B_t \sim P(b_t; w_t) = p_t^{b_t}(1-p_t)^{(1-b_t)} = w_t^{b_t}(1-p_t)$. Equation (3) reads as "what is the probability that Bernoulli random variables $B = \{B_t\}_{t\in[1,T]}$ have values $\{b_t\}_t$, given that exactly $k$ of them are high ($\sum_t b_t = k$)?" Letting $K = \sum_t B_t$, $K$ is a random variable that counts the total number of "highs" in a series of Bernoulli trials. $K$ is distributed according to the Poisson-Binomial (PB) distribution, a generalization of the Binomial distribution for when $p_i \neq p_j$. It is defined as

$$\begin{aligned} P(K=k;w) &= \sum_{\left\{b:\sum_t b_t=k\right\}} P(b;w) \\ &= \left(\prod_{t=1}^{T} 1-p_t\right) \sum_{\left\{b:\sum_t b_t=k\right\}} \prod_{t=1}^{T} w_t^{b_t} \end{aligned} \tag{4}$$

If we use eq. (4) to marginalize out $K$ from eq. (3), we recover the independent Bernoulli probabilities:

$$\begin{aligned} P(b;w) &= \sum_{k=0}^{T} P(b,k;w) = \sum_{k=0}^{T} P(b|k;w)P(k;w) \\ &= P(b|k';w)P(k';w) \text{ for exactly one } k' = \sum_t b_t \\ &= \left(\prod_t 1-p_t\right) \frac{\prod_{t=1}^{T} w_t^{b_t}}{\sum_{\left\{b':\sum_t b'_t=k'\right\}} \prod_{t=1}^{T} w_t^{b'_t}} \left(\sum_{\left\{b':\sum_t b'_t=k'\right\}} \prod_{t=1}^{T} w_t^{b'_t}\right) \\ &= \prod_{t=1}^{T} (1-p_t) w_t^{b_t} \end{aligned} \tag{5}$$

Which is to say that, if we do not have knowledge of the number of highs *a priori*, assuming a Poisson-Binomial prior, the probability of sample $B$ is the product of the probabilities of the outcomes of $T$ independent Bernoulli trials.

Direct calculation of equation eq. (3) involves summing over $T$-choose-$k$ products of $k$ odds, making it infeasible for large $T$ and $k$. To combat this, Chen and Liu [5] propose a number of alternative algorithms where the sample $B$ is constructed by iteratively deciding on the individual values of $B_i$. We will not only use these algorithms for efficiency: we will also use them to factor the CB distribution into useful forms for different objectives.

To better describe these algorithms, we define the set of indices $t \in [1, T] = I$ s.t. $B = \{B_t\}_{t \in I}$. The set $A \subseteq I$ maps to some sample $B$ such that all the high Bernoulli variables' indices can be found in $A$, i.e. $B_t = 1 \Leftrightarrow t \in A$. Then the CB can be restated as

$$P(A|k; w) = \frac{\prod_{a \in A} w_a}{R(k, I; w)} \tag{6}$$

where

$$R(v, S; w) = \sum_{\{A' \subseteq S : |A'| = v\}} \prod_{a \in A'} w_a \tag{7}$$

normalizes over all possible $k$-tuples of $w_i$ in some set $S$. Equation (7) can be considered a generalization of $T$-choose-$k$: $T$-choose-$k$ can be recovered by setting all $w_t = 1$. If we identify the product of weights from a set $A$ as a weight indexed by $A$ (i.e. $\prod_{a \in A} w_a \mapsto w'_A$), we can interpret eq. (6) as a categorical distribution.

The Draft Sampling procedure [5] recursively builds $A$ by choosing a new weight to add to an ordered set. We use $j \in [1, T]$ to index elements of $I$ in the order in which they are drafted into $A$: $I = \{t_j\}_j$, $A_j = (t_1, t_2, \dots t_j)$, and $A_j^c = I \setminus A_j = \{t_{j+1}, t_{j+2}, \dots, t_T\}$. Then the probability that some $t \in A_{j-1}^c$ is the $j$-th sample to be drafted into $A$ is defined as

$$P(t \in A_j | A_{j-1}, k; w) = \frac{w_t R(k - j, A_{j-1}^c \setminus \{t\}; w)}{(k - j + 1) R(k - j + 1, A_{j-1}^c; w)} \tag{8}$$

Terms in both the numerator and denominator of eq. (8) sum over suffix sets of length $k - j + 1$ that could be appended to $A_{j-1}$ to get a $k$-tuple $A$. The numerator is the sum of products of odds including $w_t$. The conditional probability is conditioned on the remaining ("future") odds with respect to $j$, as well as whatever samples $t_j$ were chosen in the past. The total probability of a drafted

sample is

$$
\begin{aligned}
P(A_k|k;w) &= \prod_{j=1}^{k} P(t_j \in A_j|A_{j-1},k;w) \\
&= \prod_{j=1}^{k} \frac{w_{t_j} R(k-j, A_j^c, k)}{(k-j+1)R(k-j+1, A_{j-1}^c)} \\
&= \left(\prod_{j=1}^{k} w_{t_j}\right) \frac{R(0, A_k^c)}{k!R(k, I)} \\
&= \frac{1}{k!} P(A|k,w) \qquad (9)
\end{aligned}
$$

Section 2.1 produces almost the same probability as the Conditional Bernoulli, except for the factorial term. The factorial term accounts for the fact that samples are drafted into $A_k$ in some fixed order. Summing over the probabilities of the $k!$ possible permutations of $A_k$ yields the Conditional Bernoulli. We will call the distribution defined in the Draft Bernoulli (DB). Though the DB is not the same distribution as the CB, an expected value over the DB will be the same as that over the CB as long as the order of samples in $A_k$ is ignored by the value function.

The ID-Checking Sampling procedure [5] is another useful treatment of the CB. This procedure builds $A$ by iterating over Bernoulli trials and making binary decisions whether to include the trial in $A$. First, choose and fix an order $j$ in which samples $I$ will potentially be added to $A$. Let $A_{r_j,j} \subseteq A_j = (t_1, t_2, \ldots, t_j)$ be the subset of $r_j$ samples ($|A_{r_j,j}| = r_j$) that have been added to $A$. At every step $j$, we choose to either add $t_j$ to $A_{r_{j-1},j-1}$ and recurse on $A_{r_j,j} = A_{r_{j-1},j-1} \cup \{t_j\}$ or exclude $t_j$ and recurse on $A_{r_j,j} = A_{r_{j-1},j-1}$. The probability of including $t_j$ is

$$
P(t_j \in A_{r_j,j}|A_{r_{j-1},j-1},k;w) = \frac{w_{t_j} R(k-r_{j-1}-1, A_j^c; w)}{R(k-r_{j-1}, A_{j-1}u^c; w)} \qquad (10)
$$

From the perspective of Bernoulli trials, $P(t_j \in A_{r_j,j}|\ldots) = P(B_{t_j} = 1|k - r_j; w)$. Equation (10) can be interpreted as the probability that $B_{t_j}$ is high, given that $k - r_j$ remaining trials must be high. Like in eq. (8), the numerator and denominator of eq. (10) consist of products of weights of possible suffixes. The numerator only includes suffixes where $w_{t_j}$ is a multiplicand.

The joint probability of a prefix of Bernoulli trials $b_{t_{\leq j}} = (b_{t_1}, b_{t_2}, \ldots, b_{t_j})$ using eq. (10) equals

$$
\begin{aligned}
P(b_{t_{\leq j}}|k-r_j;w) &= \prod_{j'=1}^{j} P(b_{t_{j'}}|k-r_{j'};w) \\
&= \prod_{j'=1}^{j} \frac{w_{t_{j'}}^{b_{t_{j'}}} R(k-r_{j'}, A_j^c; w)}{R(k-r_{j'-1}, A_{j-1}^c; w)} \qquad (11)
\end{aligned}
$$

The dependence on prior trials is implicit in the $r_{j'}$ term. We will call the family of distributions over different prefixes the ID-checking Bernoulli (IDB). When the prefix is the length of the entire sequence $j = T$, $P(b_{t_{\leq T}}|k - r_T; w) = P(b|k; w)$ and the IDB distribution matches the CB distribution.

We will find a novel third decomposition useful. This method combines the ID-Checking and Drafting methods so that the draft at a given step must come from a bounded suffix of weights. Define $A_{r,j_r} \subseteq A_{j_r} = (t_1, t_2, \ldots t_{j_r})$ to be the $r$ samples of $A_{j_r}$ that have been added to $A$. Define the probability that the next sample $j$ is drafted from $A^c_{j_r}$ to be

$$P(t_j \in A_{r,j_r}|k - r, j_{r-1}; w) = \frac{w_{t_j} R(k - r, A^c_{t_j}; w)}{R(k - r + 1, A^c_{t_{j_{r-1}}}; w)} \tag{12}$$

The draft is bound to the suffix $A^c_{t_{j_{r-1}}} = (t_{j_{r-1}+1}, t_{j_{r-1}+2}, \ldots, t_{j_T})$. Further, the draft requires that if $t_j$ is the $r$-th draft, the remaining drafts must come from indexed values $t_{>j}$. To balance the restriction, earlier $t_j$ will be more probable than later $t_j$ to be drafted earlier. Using the fact that $R(k - r + 1, A^c_{t_j}; w) = w_{t_{j+1}} R(k - r, A^c_{t_{j+1}}; w) + R(k - r + 1, A^c_{t_{j+1}}; w)$, it is easily shown via induction that $R(k-r+1, A^c_{t_{j_{r-1}}}; w) = \sum_{j=j_{r-1}+1}^{T} w_{t_j} R(k-r, A^c_{t_j}; w)$, proving that eq. (12) is a valid probability distribution. The probability of a draft prefix is calculated as

$$\begin{aligned} P(A_{r,j_r}|k - r; w) &= \prod_{r'=1}^{r} P(t_{j_{r'}} \in A_{r',j_{r'}}|k - r', j_{r'-1}; w) \\ &= \prod_{r'=1}^{r} \frac{w_{t_{j_{r'}}} R(k - r', A^c_{t_{j_{r'}}}; w)}{R(k - r' + 1, A^c_{t_{j_{r'-1}}}; w)} \\ &= \left( \prod_{r'=1}^{r} w_{t_{j_{r'}}} \right) \frac{R(k - r, A^c_{t_{j_r}}; w)}{R(k, I; w)} \end{aligned} \tag{13}$$

We call this distribution the Bounded Bernoulli (BB). When $r = k$, the BB matches the CB. The BB fixes the multiple orderings problem of the DB. The conditional probabilities of eq. (12) can be efficiently calculated using intermediate values when calculating $R$ using Method 2 from [5].

Outside of statistics, Swersky et al. [15] linked the CB distribution with the goal of choosing a subset of $k$ items from a set of $N$ alternatives. In this case, the $N$ alternatives are class labels, where one or more class labels may be active at a time. Models could be trained in a Maximum-Likelihood setting using the CB distribution: $B_n = 1$ implies class $n$ is present and the probability of the data can be estimated via eq. (3). The authors note that it was insufficient to rely on the implicit prior induced by training via eq. (3) and had to explicitly learn and condition on it.

Xie and Ermon [18] approximates the $T$-choose-$k$ sampling procedure by using a top-$k$ procedure called Weighted Reservoir Sampling. This procedure produces samples in an identical fashion to the Plackett-Luce (PL) distribution

[19], which has also been explored in the realm of gradient estimation [7]. While the PL distribution has a similar construction to the DB, its top-$k$ rankings do not have a uniform distribution over permutations and, as such, the PL does not match the expectation of the CB. Nonetheless, estimators involving the DB can be trivially modified to sample from the PL.

## 2.2 REINFORCE Objective

From section 1, we are interested in sampling $T$ Bernoulli random variables such that the total number of emissions/highs matches the number of tokens $L$ during training. We will start by considering the probability of a token sequence $c = \{c_\ell\}_{\ell \in [1,L]}$ under a model and work our way to a REINFORCE objective. For brevity, we supress conditioning on the acoustic data $\{x_t\}_{t \in [0,T]}$ and model parameters.

$$\begin{aligned} P(c) &= P(c, L) \\ &= \sum_b P(c, b, L) \\ &= P(L) \sum_b P(b|L) P(c|b, L) \\ &= P(L) \mathbb{E}_{b|L} \left[ P(c|b, L) \right] \end{aligned}$$

Where $P(c) = P(c, L)$ follows from the fact that $L$ is a deterministic function of $c$. Note that the expectation conditioning on $L$ requires that the individual samples $B_t$ are not entirely independent[3]. Taking the log, we get

$$\begin{aligned} \log P(c) &= \log P(L) + \log \mathbb{E}_{b|L} \left[ P(c|b, L) \right] \\ &\geq \log P(L) + \mathbb{E}_{b|L} \left[ \log P(c|b, L) \right] \end{aligned}$$

Where we have used Jensen's Inequality to establish a lower bound. Calling the bound $R$ and differentiating with respect to some parameter $\theta$, we get

$$\frac{\partial R}{\partial \theta} = \frac{\partial \log P(L)}{\partial \theta} + \frac{\partial}{\partial \theta} \mathbb{E}_{b|L} \left[ \log P(c|b, L) \right] \tag{14}$$

We have yet to make any assumptions about the distributions of any $P(\cdot)$, except to say that $|c| = L$. To recover the REINFORCE objective of eq. (1), we remove all mention of $L$ (including $P(L)$) and factor the conditional probability of the class labels as [11]:

$$P(c, b) = \prod_{t=1}^{T} P(c_{\ell_t} | b_{\leq t}, c_{< \ell_t})^{b_t} P(b_t | b_{\leq t}, c_{< \ell_t}) \tag{15}$$

where $\ell_t = \sum_{t'=0}^{t} b'_t$.

[3]Except the pathological case where exactly $P(B_t = 1) = 1$ for exactly $L$ of $T$ variables, and 0 otherwise.

Under these assumptions, the rightmost expectation in eq. (14) decomposes into[4]

$$\begin{aligned}
\frac{\partial}{\partial\theta}\mathbb{E}_b\left[\log P(c|b)\right] &= \frac{\partial}{\partial\theta}\mathbb{E}_b\left[\sum_{t=1}^{T} b_t \log P(c_{\ell_t}|b_{\leq t}, c_{<\ell_t})\right] \\
&= \sum_{t=1}^{T}\frac{\partial}{\partial\theta}\mathbb{E}_b\left[R_t\right] \text{ from eq. (2)} \\
&= \sum_{t=1}^{T}\frac{\partial}{\partial\theta}\mathbb{E}_{b_{\leq t}}\left[R_t\right] \text{ since } R_t \text{ not based on } b_{>t} \\
&= \sum_{t=1}^{T}\mathbb{E}_{b_{\leq t}}\left[\frac{\partial R_t}{\partial\theta} + R_t\frac{\partial}{\partial\theta}\log P(b_{\leq t}|c_{<\ell_t})\right] \\
&= \sum_{t=1}^{T}\mathbb{E}_{b_{\leq t}}\left[\frac{\partial R_t}{\partial\theta} + R_t\sum_{t'\leq t}\frac{\partial}{\partial\theta}\log P(b_{t'}|b_{t'-1}, c_{<\ell_{t'}})\right] \\
&= \mathbb{E}_b\left[\sum_{t=1}^{T}\left(\frac{\partial R_t}{\partial\theta} + \left(\sum_{t'\geq t} R_{t'}\right)\frac{\partial}{\partial\theta}\log P(b_t|b_{<t}, c_{<\ell_t})\right)\right]
\end{aligned}$$

The expectation of the sum of frame-wise objectives is the same as the expectation of the "global" objective, where no subset of $B$ are attributed to a given class label $c_\ell$:

$$\frac{\partial}{\partial\theta}\mathbb{E}_b\left[\log P(c|b)\right] = \mathbb{E}_{b|L}\left[\sum_{\ell=1}^{L}\left(\frac{\partial\log P(c_\ell|b)}{\partial\theta} + \log P(c_\ell|b)\frac{\partial}{\partial\theta}\log P(b)\right)\right]$$

However, the frame-wise - or "local" - signal is expected to be less noisy [14].

We can see the two issues with the above REINFORCE objective discussed in section 1 by observing eq. (15). First, $c_{\ell_t}$ is undefined when $\ell_t$ exceeds $L$. Second, $P(c, b)$ is maximized whenever $B_t = 0$ for all $t$. The second problem (a tendency to emit early) may be solved by skipping the factorization of class label probabilities and using the aforementioned global objective. However, in this case, $L$ is still ignored and the first problem is still a problem. Furthermore, we would lose the ability to attribute credit to the $t$-th frame for classifying label $c_{\ell_t}$. Alternatively, we could remove the auto-regressive property of the network and make the Bernoulli trials independent $P(b) = \prod_{t=1}^{T} P(b_t)$, but all the "low" Bernoulli trials would receive no gradient updates.

The primary concerns above may be addressed by assuming $P(L)$ is PB-distributed and $P(b|L)$ is CB-distributed. Letting $t_\ell$ be the inverse mapping of $\ell_t$, we define

$$P(c, b|L) = P(c|b, L)P(b|L) = \left(\prod_{\ell=1}^{L} P(c_\ell|b_{t_{\leq\ell}})\right)P(b|L) \tag{16}$$

[4]Thanks to Dieterich Lawson for this derivation.

and plug the conditional probability $P(c|b, L)$ into the expectation in eq. (14) to get the "global" CB REINFORCE gradient:

$$\frac{\partial R}{\partial \theta} = \frac{\partial \log P(L)}{\partial \theta} + \mathbb{E}_{b|L}\left[\sum_{\ell=1}^{L}\left(\frac{\partial R_\ell}{\partial \theta} + R_\ell \frac{\partial}{\partial \theta}\log P(b|L)\right)\right] \tag{17}$$

Where $R_\ell = \log P(c_\ell|b_{t_{\leq \ell}})$.

Since the set of all samples $B \sim P(b|L)$ will have exactly $L$ highs $\sum_t B_t = L$, the decomposition of the class label sequence probability is well-defined. The pathological case where reward is maximized when $B_t$ is no longer a problem because we have switched to a global reward rather than a per-frame reward.

There are, however, two new issues introduced by eq. (17). The first is the same as if we stopped using a per-frame reward in eq. (1): we can no longer use the error signal for a specific $c_\ell$ to optimize a subset of $B$. The second problem is that $P(b|L)$ can no longer be auto-regressive. Equation (3) uses the entire set of odds from all frames. While there are ways to decompose eq. (3) into a fixed-order series of binary decisions [5], the current trial $B_t$ would still be distributed according to the log-odds of non-past trials $w_{\geq t}$. While we will propose an alternate per-frame estimate to combat the first issue, the second is an unavoidable consequence of the dependencies across trial outcomes imposed by the CB.

In Section 2.1, we mentioned that an expectation over a DB variable will yield the same expected value as the same expectation over a CB variable assuming that the value function in the expectation is not conditioned on the order in which samples are drafted. The total reward in eq. (17) satisfies this criterion. Thus the global DB REINFORCE objective maximizes the same expectation as the CB REINFORCE objective:

$$\frac{\partial R}{\partial \theta} = \frac{\partial \log P(L)}{\partial \theta} + \mathbb{E}_{A_L|L}\left[\sum_{\ell=1}^{L}\left(\frac{\partial R_\ell}{\partial \theta} + R_\ell \frac{\partial}{\partial \theta}\log P(A_L|L)\right)\right] \tag{18}$$

The advantage of the DB REINFORCE objective over the CB REINFORCE objective is it can leverage the relaxation of the DB, discussed in section 2.3.

Our first frame-wise objective is courtesy of the IDB decomposition of the CB from eq. (11). Though a given trial sample $B_{t_j}$ is conditioned on non-past weights $w_{t_{\geq j}}$, it is only conditioned on samples from the past $b_{t_{<j}}$. Setting $t_j = j$, we decompose the joint probability of the class label sequence and the CB sample as

$$P(c, b|L) = P(c|b, L)P(B|L) = \prod_{t=1}^{T} P(c_{\ell_t}|b_{\leq t})^{b_t} P(b_t|L - r_t) \tag{19}$$

Equation (19) is very similar to eq. (15), except the conditioning on the number of class labels $L$ forces $\ell_t$ to be well-defined whenever $B_t = 1$. The derivation of the IDB REINFORCE gradient is almost identical to that for

eq. (1), yielding

$$\frac{\partial R}{\partial \theta} = \mathbb{E}_b \left[ \sum_{t=1}^{T} \left( \frac{\partial R_t}{\partial \theta} + \left( \sum_{t' \geq t} R_{t'} \right) \frac{\partial}{\partial \theta} \log P(b_t | L - r_t) \right) \right] \tag{20}$$

where $R_t = b_t \log P(c_{\ell_t} | b_{\leq t})$.

The IDB REINFORCE gradient solves the problem of ill-defined $\ell_t$, provides a frame-wise gradient update, and avoids the pathological case of maximum probability when $\forall t.B_t = 0$. However, were we to use eqs. (19) and (20) on their own, the model would likely still learn to emit early so as to minimize future accumulated (negative) rewards.

To mitigate this tendency, we can leverage the fact that the IDB factors the CB in a fixed but arbitrary order of trials $\{t_j\}_j$. Denoting eq. (19) as the forward IDB joint probability, we define the backward IDB joint probability as

$$P(c, b | L) = \prod_{t=1}^{T} P(c_{L-\ell_t} | b_{>t})^{b_t} P(b_t | L - r_{T-t}) \tag{21}$$

where we use the mapping $t_j = T - j + 1$. We define the backward IDB reinforce gradient analogously. To perform the backward gradient updates, we need merely to reverse the Bernoulli sequence of weights $w_t \mapsto w_{T-t+1}$ and classes $c_\ell \mapsto c_{L-\ell+1}$ and perform the forward update.

We hypothesize that, though the forward and backward objectives tend to emit at the beginning and end of the utterance, respectively, alternating between them will cancel out the tendencies. By alternating directions, on average, every weight $w_t$ should receive a signal from $L/2$ nonzero rewards $R_t$.

While alternating between eqs. (19) and (21) should mitigate or solve the problem of emitting too early or late, the IDB REINFORCE objective can still be trimmed. The IDB REINFORCE expectation for class label $\ell_t$ requires conditioning on all Bernoulli samples $b_{\leq t}$. However, the knowledge of which exact Bernoulli trials were high up to time $t$ is superfluous: all we need to know to determine a distribution over the $\ell$-th class label is the time $t$ at which the $\ell$-th high Bernoulli (ordered by time $t$) occurred. This is the $t_\ell$ term in eq. (16). $t_\ell$ is a sufficient statistic for $P(c_\ell | \ldots)$ with respect to the Bernoulli trials $B$. Decomposing $P(b|L)$ in eq. (16) in terms of that statistic, we get

$$\begin{aligned} P(c, b | L) &= \prod_{\ell=1}^{L} P(c_\ell | t_\ell) P(P(t_\ell | t_{<\ell}, L)) \\ &= \prod_{\ell=1}^{L} P(c_\ell | t_\ell) P(t_\ell | t_{\ell-1}, L - \ell) \end{aligned} \tag{22}$$

The first line is a simple application of the chain rule of probabilities. $t_\ell \perp\!\!\!\perp t_{\ell-2} | t_{\ell-1}$ follows from the fact that $t_\ell > t_{\ell-1} > t_{\ell-2}$, so $t_{\ell-1} + 1$ will be the minimum value that $t_\ell$ can take.

The $P(t_\ell|t_{\ell-1}, L-\ell)$ term is identical in definition to the step function of the BB from eq. (12): $t_\ell$ must be drafted from $t \in [t_{\ell-1}+1, T]$ subject to the condition that $T-\ell-1$ more samples must be drafted after $t_\ell$. The joint probability of $t_{\leq \ell}$ is the BB, matching the CB when $\ell = L$.

Deriving the BB REINFORCE gradient is similar to before. Letting $R_\ell = \log P(c_\ell|t_\ell)$,

$$\begin{aligned}
\frac{\partial}{\partial\theta}\mathbb{E}_b[\log P(c|b)] &= \sum_{\ell=1}^{L} \frac{\partial}{\partial\theta}\mathbb{E}_b[R_\ell] \\
&= \sum_{\ell=1}^{L} \frac{\partial}{\partial\theta}\mathbb{E}_{\{t_1,t_2,\ldots t_\ell\}|L-\ell}[R_\ell] \\
&\cdots \\
&= \mathbb{E}_b\left[\sum_{\ell=1}^{L}\left(\frac{\partial R_\ell}{\partial\theta} + \left(\sum_{\ell'\geq\ell} R_{\ell'}\right)\frac{\partial}{\partial\theta}\log P(t_\ell|t_{\ell-1}, L-\ell)\right)\right]
\end{aligned} \tag{23}$$

Equation (23), like eqs. (1) and (20), must accumulate future rewards due to $t_\ell$'s dependency on past drafted samples $t_{<\ell}$. A critical difference of eq. (23), however, is that it does not assign a reward to a non-event - a low Bernoulli trial - directly. This will avoid the tendency to emit early in order to maximize future non-events.

The sum of future rewards reflects the uncertainty of the impact of the current decision on future ones. We expect earlier $t_\ell$ to receive a higher variance, higher magnitude signal than later ones because of this sum. We can spread out this variance in the BB REINFORCE objective by alternating between forward and backward decompositions of $P(c, b|L)$, just like we did for the IDB REINFORCE objective.

## 2.3 Continuous relaxations

A continuous relaxation is a continuous random variable that approximates (relaxes) some discrete random variable. Of particular note is the Concrete/Gumbel-Softmax distribution [13, 10], which approximates a categorical random variable $B \in [1, N]$ with odds $\{w_n\}_{n\in[1,N]}$, Gumbel noise $G_n = -\log(-\log U_n), U_n \sim Uniform(0,1)$, and a scalar temperature $\lambda \in \mathbb{R}^+$. The Concrete random variable $Z \in \{x \in [0,1]^N; \sum_n x_n = 1\}$ is defined as

$$Z_n = \frac{\exp((\log w_n + G_n)/\lambda)}{\sum_{n'=1}^{N}\exp((\log w_{n'} + G_{n'})/\lambda)} \tag{24}$$

A categorical sample $B \sim P(n; N)$ can be recovered from a Concrete sample in two equivalent manners. First, by the Gumbel-Max trick [19]:

$$P(\forall n'.Z_n \geq Z_{n'}) = \frac{w_n}{\sum_{n'=1}^{N} w_{n'}} = P(B = n) \tag{25}$$

Which implies that $B = H(Z) = \arg_n \max(Z_n)$ is a Categorical sample. Alternatively, $Z$ approaches a one-hot representation of $B$ as $\lambda \to 0$:

$$P(\lim_{\lambda \to 0} Z_n = 1) = \frac{w_n}{\sum_{n'=1}^{N} w_{n'}} = P(B = n) \tag{26}$$

When $N = 2$, $P(B = n)$ is Bernoulli, the Concrete variable is defined as

$$Z = \frac{1}{1 + \exp(-(\log w + D)/\lambda)}, D = \log U - \log(1 - U) \tag{27}$$

and the deterministic mapping $B = H(Z) = 1_{Z>0.5}$.

Using the mapping $\prod_{a \in A} w_a = w'$, the CB can be considered a categorical distribution and suitable for a Concrete relaxation. Unfortunately, using this mapping directly would convert an $N$-length vector of weights $w_n$ to a vector of $N$-choose-$k$ weights, which is intractable for large $N$. The numerator in eq. (24) cannot be teased into a combination of random variables $W_1(w_1), W_2(w_2), \ldots$, because the Gumbel noise $G_n$, which would now represent the combination of noise of the $W_a$ terms, would no longer be independent of $G_{n'}, n' \neq n$. Thus, the CB is not directly suited to continuous relaxation.

However, reframing the CB in terms of intermediate variables defined in the DB and IDB recursive definitions will allow us a tractable number of independent, non-identical random variables to relax. Specifically, we will relax the recursive step distributions in eqs. (8) and (10). The drafting procedure in eq. (8) can be reframed as a categorical distribution over $T - j$, where $P(i \in A_j | \ldots) \mapsto w'_i$. We can use the Concrete distribution to relax the draft and repeat the relaxation $L$ times, with a combined representation of size $\sum_{\ell=1}^{L} T - \ell + 1$ values. Similarly, the choice of including $t_j$ in the sample $A_{r_j,j}$ from eq. (10) is a binary decision and can be reframed as a Bernoulli distribution where $P(t_j \in A_{r_j,j} | \ldots) \mapsto p_{t_j}$. Again, the Concrete distribution can be used to relax each of the $T$ decisions, with a combined representation of size $T$. The BB relaxation is similar to the draft relaxation, but involves $\sum_{\ell=1}^{L} T - t_{\ell-1} \leq \sum_{\ell=1}^{L} T - \ell + 1$ values.

While the DB, IDB, and BB relaxations are continuous within a single step, discontinuities will arise between steps. This is because the probabilities of the next step are conditioned on a discrete decision $H(Z)$ made in the previous step. Better continuous relaxations that smooth the decision function across steps may exist, and are left for future work.

When the objective can be reframed in terms of the relaxation $Z$, a network can start by optimizing a high temperature $\lambda$, then slowly lower it over the course of training so that $Z$ approaches the discrete distribution. At test time, the deterministic mapping $H(Z)$ can be used. For our objective, a relaxed emission does not make sense. We need to come up with $L$ distinct distributions for each of the class labels $c_\ell$.

We focus on two uses of continuous relaxations with a discrete objective. The first is to use a RELAX-based gradient estimator [8]. RELAX-based gradient estimators augment the REINFORCE estimator with some additional terms

that are intendent to reduce its variance. Letting $B$ be a discrete random variable of a continuous relaxation $Z$, the gradient of the expected value of some $f$ (where $f$ can be a reward, e.g.) is defined as

$$\frac{\partial \mathbb{E}_b[f(b)]}{\partial \theta} = \mathbb{E}_b\left[\left(f(b) - \mathbb{E}_{z|b}[c(z)]\right)\frac{\partial \log P(b)}{\partial \theta} - \frac{\partial \mathbb{E}_{z|b}[c(z)]}{\partial \theta}\right] + \frac{\partial \mathbb{E}_z[c(z)]}{\partial \theta} \quad (28)$$

Where $c(z)$ is a control variate, e.g. a neural network trained on the values of the relaxation to minimize the difference between the objective $f(b)$ and itself. $P(z|b)$ is the truncated distribution over $Z$ such that the value of $Z$ obeys the relationship $H(Z) = b$. If $c(z)$ is the concrete distribution parameterized by a learnable $\lambda$, eq. (28) is the REBAR gradient [16].

The second is the so-called Straight-Through (ST) estimator [3, 10]. An ST estimator uses the discrete sample $H(X)$ during the forward pass, and estimates the partial derivative of $H(X)$ in the backward pass with that of $X$, i.e. $\frac{\partial H(X)}{\partial \theta} \approx \frac{\partial X}{\partial \theta}$. This estimator is biased, but can work well in practice. If we output a one-hot representation $H(X^{(\ell)}) = b^{(\ell)} \in \{0,1\}^T, b_t^{(\ell)} = 1_{t=n^{(\ell)}}$ for the $\ell$-th drafted (DB or BB) sample, adding them together $b = \sum_{\ell=1}^{L} b^{(\ell)}$ produces our CB sample. If we substitute $\frac{\partial b_t^{(\ell)}}{\partial \theta} \approx \frac{\partial X_t^{(\ell)}}{\partial \theta}$ then $\frac{\partial b_t}{\partial \theta} = \sum_\ell \frac{\partial b_t^{(\ell)}}{\partial \theta}$ is well-defined. Alternatively, we can construct $b$ by concatenating together the relaxed Bernoulli trials of the IDB, $b = [b^{(1)}, b^{(2)}, \ldots, b^{(T)}], b^{(t)} = H(X^{(t)})$. Again, the partial derivatives are well-defined: $\frac{\partial b_t}{\partial \theta} = \frac{\partial b^{(t)}}{\partial \theta}$. From there, we maximize the likelihood of the data using the conditional distribution derived from eq. (15):

$$P(c|b, L) = \prod_{t=1}^{T} P(c_{\ell_t}|h_t, b_{\leq t})^{b_t} \quad (29)$$

where $h_t$ is a hidden state of the network at timestep $t$. Conditioning on $b_{\leq t}$ is implicit in the definition of $c_{\ell_t}$, though this conditioning is ignored by the ST estimator.

By taking the log-probability, only the timesteps where $B_t = 1$ will have nonzero loss. Were the relaxation a series of independent Bernoulli trials, only the odds $w_t$ of those trials would be updated in backpropagation. Since eqs. (8), (10) and (12) involve all "future" odds, the CB-based ST estimators will update more weights with the likelihood of the data. The DB has a clear advantage in this regard: drafting involves $T - j + 1$ odds for the $j$-th draft, whereas the BB involves $T - t_j$, and the IDB involves only $T - t + 1$ odds. Since the ST estimators already ignore conditioning on past labels, we can ensure that, on average, the each weight receives $L/2$ updates from the data by shuffling the order in which timesteps are processed $t_j$. In any case, optimizing the PB term $\frac{\partial P(L)}{\partial \theta}$ will give a blanket update to all weights.

## 2.4 Exact values

Sample estimates of the expectations in section 2.2 should only be used when the value in the expectation is not differentiable or it is infeasible to marginalize out

the sample variable. In the case of the model proposed in [12], the distribution $\log P(c_t|\ldots)$ is calculated by a simple linear transformation of the RNN hidden state $h_t$ followed by a softmax. These calculations can be parallelized across $t$. Further, they are fully differentiable. Therefore if the latent variable $B$ can be efficiently marginalized and that process is differentiable, we can use $P(c)$ to directly maximize the data log likelihood. To show this is possible, we will use the BB distribution:

$$\begin{aligned}
P(c) &= P(L)\sum_b P(b|L)P(c|b) \\
&= P(L)\sum_b P(b|L)\prod_{\ell=1}^{L} P(c_\ell|b) \\
&= P(L)\sum_{\{t_1,t_2,\ldots,t_\ell\}} P(t_1,t_2,\ldots,t_\ell|L)\prod_{\ell=1}^{L} P(c_\ell|t_\ell) \\
&= P(L)\sum_{\ell=1}^{L}\sum_{t_\ell=t_{\ell-1}+1}^{T-L+\ell} P(t_\ell|t_{\ell-1},L-\ell)P(c_\ell|t_\ell) \\
&= \sum_{\ell=1}^{L}\sum_{t_\ell=1}^{T} P(t_\ell|t_{\ell-1},L-\ell)P(c_\ell|t_\ell) \qquad (30)
\end{aligned}$$

where the last line follows assuming $P(t_\ell|t_{\ell-1},L-\ell)=0$ when $t_\ell \le t_{\ell-1}$.

Treating $P(t_\ell|t_{\ell-1},L)$ as the transition probability between states $t\in[1,T]$ and $P(c_\ell|t_\ell)$ as the emission probability, eq. (30) can be considered a Hidden Markov Model. Thus, $P(c)$ can be efficiently calculated using the forward algorithm.

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