Learning Beam Search Policies via Imitation Learning

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Abstract

Beam search is widely used for approximate decoding in structured prediction problems. Models often use a beam at test time but ignore its existence at train time, and therefore do not explicitly learn how to use the beam. We develop an unifying meta-algorithm for learning beam search policies using imitation learning. In our setting, the beam is part of the model, and not just an artifact of approximate decoding. Our meta-algorithm captures existing learning algorithms and suggests new ones. It also lets us show novel no-regret guarantees for learning beam search policies.

1 Introduction

Beam search is the dominant method for approximate decoding in structured prediction tasks such as machine translation [1], speech recognition [2], image captioning [3], and syntactic parsing [4]. Most models that use beam search at test time ignore the beam at train time and instead are learned via methods like likelihood maximization. They therefore suffer from two issues that we jointly address in this work: (1) learning ignores the existence of the beam and (2) learning uses only oracle trajectories. These issues lead to mismatches between the train and test settings that negatively affect performance. Our work addresses these two issues simultaneously by using imitation learning to develop novel beam-aware algorithms with no-regret guarantees. Our analysis is inspired by DAgger [5].

Beam-aware learning algorithms use beam search at both train and test time. These contrast with common two-stage learning algorithms that, first, at train time, learn a probabilistic model via maximum likelihood, and then, at test time, use beam search for approximate decoding. The insight behind beam-aware algorithms is that, if the model uses beam search at test time, then the model should be learned using beam search at train time. Resulting beam-aware methods run beam search at train time (i.e., roll-in) to collect losses that are then used to update the model parameters. The first proposed beam-aware algorithms are perceptron-based, updating the parameters either when the best hypothesis does not score first in the beam [6], or when it falls out of the beam [7].

While there is substantial prior work on beam-aware algorithms, none of the existing algorithms expose the learned model to its own consecutive mistakes at train time. When rolling in with the learned model, if a transition leads to a beam without the correct hypothesis, existing algorithms either stop [6, 8, 9] or reset to a beam with the correct hypothesis [7, 10, 11].[1] Additionally, existing beam-aware algorithms either do not have theoretical guarantees or only have perceptron-style guarantees [10]. We are the first to prove no-regret guarantees for an algorithm to learn beam search policies.

[1][12] take a different approach by training with a differentiable approximation of beam search, but decode with the standard (non-differentiable) search algorithm at test time.

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Imitation learning algorithms, such as DAgger [5], leverage the ability to query an oracle at train time to learn a model that is competitive (in the no-regret sense) to the best model in hindsight. Existing imitation learning algorithms such as SEARN [13], DAgger [5][2], AggreVaTe [15], and LOLS [16], execute the learned model at train time to collect data that is then labeled by the oracle and used for retraining. Nonetheless, these methods do not take the beam into account at train time, and therefore do not learn to use the beam effectively at test time.

We propose a new approach to learn beam search policies using imitation learning that addresses these two issues. We formulate the problem as learning a policy to traverse the combinatorial search space of beams. The learned policy is induced via a scoring function: the neighbors of the elements of a beam are scored and the top k are used to form the successor beam. We learn a scoring function to match the ranking induced by the oracle costs of the neighbors. We introduce training losses that capture this insight, among which are variants of the weighted all pairs loss [17] and existing beam-aware losses. As the losses we propose are differentiable with respect to the scores, our scoring function can be learned using modern online optimization algorithms, e.g. Adam [18].

In some problems (e.g., sequence labeling and syntactic parsing) we have the ability to compute oracle completions and oracle completion costs for non-optimal partial outputs. Within our imitation learning framework, we can use this ability to compute oracle completion costs for the neighbors of the elements of a beam at train time to induce an oracle that allows us to continue collecting supervision after the best hypothesis falls out of the beam. Using this oracle information, we are able to propose a DAgger-like beam-aware algorithm with no-regret guarantees.

We describe our novel learning algorithm as an instantiation of a meta-algorithm for learning beam search policies. This meta-algorithm sheds light into key design decisions that lead to more performant algorithms, e.g., the introduction of better training losses. Our meta-algorithm captures much of the existing literature on beam-aware methods (e.g., [7, 8]), allowing a clearer understanding of and comparison to existing approaches, for example, by emphasizing that they arise from specific choices of training loss function and data collection strategy, and by proving novel regret guarantees for them.

Our contributions are: an algorithm for learning beam search policies (Section 4.2) with accompanying regret guarantees (Section 5), a meta-algorithm that captures much of the existing literature (Section 4), and new theoretical results for the early update [6] and LaSO [7] algorithms (Section 5.3).

2 Preliminaries

Structured Prediction as Learning to Search We consider structured prediction in the learning to search framework [13, 5]. Input-output training pairs $D = \{(x_1, y_1), \ldots, (x_m, y_m)\}$ are drawn according to a data generating distribution $\mathcal{D}$ jointly over an input space $\mathcal{X}$ and an output space $\mathcal{Y}$. For each input $x \in \mathcal{X}$, there is an underlying search space $G_x = (V_x, E_x)$ encoded as a directed graph with nodes V_x and edges E_x. Each output $y \in \mathcal{Y}_x$ is encoded as a terminal node in G_x, where $\mathcal{Y}_x \subseteq \mathcal{Y}$ is the set of valid structured outputs for x.

In this paper, we deal with stochastic policies $\pi : V_x \to \Delta(V_x)$, where $\Delta(V_x)$ is the set of probability distributions over nodes in V_x. (For convenience and brevity of presentation, we make our policies deterministic later in the paper through the introduction of a tie-breaking total order over the elements of V_x, but our arguments and theoretical results hold more generally.) The goal is to learn a stochastic policy $\pi(\cdot, x, \theta) : V_x \to \Delta(V_x)$ parametrized by $\theta \in \Theta \subseteq \mathbb{R}^p$ that traverses the induced search spaces, generating outputs with small expected cost; i.e., ideally, we would want to minimize

$$c(\theta) = \mathbb{E}_{(x,y)\sim\mathcal{D}} \mathbb{E}_{\hat{y}\sim\pi(\cdot,x,\theta)} c_{x,y}(\hat{y}), \tag{1}$$

where $c_{x,y} : \mathcal{Y}_x \to \mathbb{R}$ is the cost function comparing the ground-truth labeling y to the predicted labeling $\hat{y}$. We are not able to optimize directly the loss in Equation (1), but we are able to find a mixture of policies $\theta_1, \ldots, \theta_m$, where $\theta_t \in \Theta$ for all $t \in [m]$, that is competitive with the best policy in Θ in the distribution of trajectories induced by the mixture of $\theta_1, \ldots, \theta_m$. We use notation $\hat{y} \sim \pi(\cdot, x, \theta)$ to mean that $\hat{y}$ is generated by sampling a trajectory $v_1, \ldots, v_h$ on G_x by executing policy $\pi(\cdot, x, \theta)$, and returning the labeling $\hat{y} \in \mathcal{Y}$ associated with terminal node $v_h \in T$. The search

[2] Scheduled sampling [14] is an instantiation of DAgger.

spaces, cost functions and policies depend on $x \in \mathcal{X}$ or $(x, y) \in \mathcal{X} \times \mathcal{Y}$—in the sequel, we omit indexing by example for conciseness.

Search Space, Cost, and Policies Each example $(x, y) \in \mathcal{X} \times \mathcal{Y}$ induces a search space $G = (V, E)$ and a cost function $c : \mathcal{Y} \to \mathbb{R}$. For all $v \in V$, we introduce its set of neighbors $N_v = \{v' \in V \mid (v, v') \in E\}$. We identify a single initial node $v_{(0)} \in V$. We define the set of terminal nodes $T = \{v \in V \mid N_v = \emptyset\}$. We assume without loss of generality that all nodes are reachable from $v_{(0)}$ and that all nodes have paths to terminal nodes. For clarity of exposition, we assume that G is a tree-structured directed graph where all terminals nodes are at distance h from the root $v_{(0)}$.[3]

Each terminal node $v \in T$ corresponds to a complete output $y \in \mathcal{Y}$, which can be compared to the ground-truth $y^* \in \mathcal{Y}$ via a cost function $c : T \to \mathbb{R}$ of interest (e.g., Hamming loss in sequence labeling or negative BLEU score [19] in machine translation). We define the optimal completion cost function $c^* : V \to \mathbb{R}$, which computes the cost of the best terminal node reachable from $v \in V$ as $c^*(v) = \min_{v' \in T_v} c(v')$, where T_v is the set of terminal nodes reachable from v.

The definition of $c^* : V \to \mathbb{R}$ naturally gives rise to an oracle policy $\pi^*(\cdot, c^*) : V \to \Delta(V)$. At $v \in V$, $\pi^*(v, c^*)$ can be any fixed distribution (e.g., uniform or one-hot) over $\arg\min_{v' \in N_v} c^*(v')$. For any state $v \in V$, executing $\pi^*(\cdot, c^*)$ until arriving at a terminal node achieves the lowest possible cost for completions of v.

At $v \in V$, a greedy policy $\pi : V \to \Delta(V)$ induced by a scoring function $s : V \to \mathbb{R}$ computes a fixed distribution $\pi(v, \theta)$ over $\arg\max_{v' \in N_v} s(v', \theta)$. When multiple elements are tied with the same highest score, we can choose an arbitrary distribution over them. If there is a single highest scoring element, the policy is deterministic. In this paper, we assume the existence of a total order over the elements of V that is used for breaking ties induced by a scoring function. The tie-breaking total ordering allows us to talk about a particular unique ordering, even when ties occur. The oracle policy $\pi^*(\cdot, c^*) : V \to \Delta(V)$ can be thought as being induced by the scoring function $-c^* : V \to \mathbb{R}$.

3 Beam search

Beam Search Space Given a search space G, we construct its beam search space $G_k = (V_k, E_k)$, where $k \in \mathbb{N}$ is the maximum beam capacity. V_k is the set of possible beams that can be formed along the search process, and E_k is the set of possible beam transitions. Nodes $b \in V_k$ correspond to nonempty sets of nodes of V with size upper bounded by k, i.e., $b = \{v_1, \ldots, v_{|b|}\}$ with $1 \leq |b| \leq k$ and $v_i \in V$ for all $i \in [|b|]$. The initial beam state $b_{(0)} \in V_k$ is the singleton set with the initial state $v_{(0)} \in V$. Terminal nodes in T_k are singleton sets with a single terminal node $v \in T$. For $b \in V_k$, we define $A_b = \cup_{v \in b} N_v$, i.e., the union of the neighborhoods of the elements in b.

Algorithm 1 Beam Search

function BEAMSEARCH(G, k, θ)
  $b \leftarrow \{v_{(0)}\} \equiv b_{(0)}$
  while BEST$(b, 1, s(\cdot, \theta)) \notin T$ **do**
    $b \leftarrow$ POLICY$(G, b, k, s(\cdot, \theta))$
  return BEST$(b, 1, s(\cdot, \theta))$

function POLICY(G, b, k, f)
  Let $A_b = \cup_{v \in b} N_v$
  return BEST(A_b, k, f)

function BEST(A, k, f)
  Let $A = \{v_1, \ldots, v_n\}$ be ordered
    such that $f(v_1) \geq \cdots \geq f(v_n)$
  Let $k' = \min(k, n)$
  return $v_1, \ldots, v_{k'}$

Algorithm 1 describes the beam search variant used in our paper. In this paper, all elements in the beam are simultaneously expanded when transitioning. It is possible to define different beam search space variants, e.g., by considering different expansion strategies or by handling terminals differently (in the case where terminals can be at different depths). The arguments developed in this paper can be extended to those variants in a straightforward manner.

Beam Costs We define the cost of a beam to be the cost of its lowest cost element, i.e., we have $c^* : V_k \to \mathbb{R}$ and, for $b \in V_k$, $c^*(b) = \min_{v \in b} c^*(v)$. We define the beam transition cost function

[3] We describe in Appendix A how to convert a directed graph search space to a tree-structured one with all terminals at the same depth.

$c : E_k \to \mathbb{R}$ to be $c(b, b') = c^*(b') - c^*(b)$, for $(b, b') \in E_k$, i.e., the difference in cost between the lowest cost element in b' and the lowest cost element in b.

A cost increase occurs on a transition $(b, b') \in E_k$ if $c^*(b') > c^*(b)$, or equivalently, $c(b, b') > 0$, i.e., b' dropped all the lowest cost neighbors of the elements of b. For all $b \in V_k$, we define $N_b^* = \{b' \in N_b \mid c(b, b') = 0\}$, i.e., the set of beams neighboring b that do not lead to cost increases. We will significantly overload notation, but usage will be clear from context and argument types, e.g., when referring to $c^* : V \to \mathbb{R}$ and $c^* : V_k \to \mathbb{R}$.

Beam Policies Let $\pi : V_k \to \Delta(V_k)$ be a policy induced by a scoring function $f : V \to \mathbb{R}$. To sample $b' \sim \pi(b)$ for a beam $b \in V_k$, form A_b, and compute scores $f(v)$ for all $v \in A_b$; let $v_1, \ldots, v_n$ be the elements of A_b ordered such that $f(v_1) \geq \ldots \geq f(v_n)$; if $v_1 \in T$, $b' = \{v_1\}$; if $v_1 \notin T$, let b' pick the k top-most elements from $A_b \setminus T$. At $b \in V_k$, if there are many orderings that sort the scores of the elements of A_b, we can choose a single one deterministically or sample one stochastically; if there is a single such ordering, the policy $\pi : V_k \to \Delta(V_k)$ is deterministic at b.

For each $x \in \mathcal{X}$, at train time, we have access to the optimal path cost function $c^* : V \to \mathbb{R}$, which induces the oracle policy $\pi^*(\cdot, c^*) : V_k \to \Delta(V_k)$. At a beam b, a successor beam $b' \in N_b$ is optimal if $c^*(b') = c^*(b)$, i.e., at least one neighbor with the smallest possible cost was included in b'. The oracle policy $\pi^*(\cdot, c^*) : V_k \to \Delta(V_k)$ can be seen as using scoring function $-c^* : V_k \to \mathbb{R}$ to transition in the beam search space G_k.

Algorithm 2 Meta-algorithm

function LEARN(D, θ_1, k)
  for each $t \in [|D|]$ **do**
    Induce G using x_t
    Induce $s(\cdot, \theta_t) : V \to \mathbb{R}$ using G and θ_t
    Induce $c^* : V \to \mathbb{R}$ using (x_t, y_t)
    $b_{1:j} \leftarrow$ BEAMTRAJECTORY($G, c^*, s(\cdot, \theta_t), k$)
    Incur losses $\ell(\cdot, b_1), \ldots, \ell(\cdot, b_{j-1})$
    Compute θ_{t+1} using $\sum_{i=1}^{j-1} \ell(\cdot, b_i)$, e.g., by SGD or Adam
  return best θ_t on validation

function BEAMTRAJECTORY(G, c^*, f, k)
  $b_1 \leftarrow \{v_{(0)}\} \equiv b_{(0)}$
  $j = 1$
  while BEST($b_j, 1, f$) $\notin T$ **do**
    if strategy is oracle **then**
      $b_{j+1} \leftarrow$ POLICY($G, b_j, k, -c^*$)
    else
      $b_{j+1} \leftarrow$ POLICY(G, b_j, k, f)
      if $c^*(b_{j+1}) > c^*(b_j)$ **then**
        if strategy is stop **then**
          break
        if strategy is reset **then**
          $b_{j+1} \leftarrow$ POLICY($G, b_j, 1, -c^*$)
    $j \leftarrow j + 1$
  return $b_{1:j}$

4 Meta-Algorithm

Our goal is to learn a policy $\pi(\cdot, \theta) : V_k \to \Delta(V_k)$ induced by a scoring function $s(\cdot, \theta) : V \to \mathbb{R}$ that achieves small expected cumulative transition cost along the induced trajectories. Algorithm 2 presents our meta-algorithm in detail. Instantiating our meta-algorithm requires choosing both a surrogate training loss function (Section 4.1) and a data collection strategy (Section 4.2). Table 1 shows how existing algorithms can be obtained as instances of our meta-algorithm with specific choices of loss function, data collection strategy, and beam size.

4.1 Surrogate Losses

Insight In the beam search space, a prediction $\hat{y} \in \mathcal{Y}_x$ for $x \in \mathcal{X}$ is generated by running $\pi(\cdot, \theta)$ on G_k. This yields a beam trajectory $b_{1:h}$, where $b_1 = b_{(0)}$ and $b_h \in T_k$. We have

$$c(\theta) = \mathbb{E}_{(x,y)\sim\mathcal{D}} \mathbb{E}_{\hat{y}\sim\pi(\cdot,\theta)} c(\hat{y}) = \mathbb{E}_{(x,y)\sim\mathcal{D}} \mathbb{E}_{b_{1:h}\sim\pi(\cdot,\theta)} c^*(b_h). \tag{2}$$

The term $c^*(b_h)$ can be written in a telescoping manner as

$$c^*(b_h) = c^*(b_1) + \sum_{i=1}^{h-1} c(b_i, b_{i+1}). \tag{3}$$

As $c^*(b_1)$ depends on an example $(x, y) \in \mathcal{X} \times \mathcal{Y}$, but not on the parameters $\theta \in \Theta$, the set of minimizers of $c : \Theta \to \mathbb{R}$ is the same as the set of minimizers of

$$c'(\theta) = \mathbb{E}_{(x,y)\sim\mathcal{D}} \mathbb{E}_{b_{1:h}\sim\pi(\cdot,\theta)} \left(\sum_{i=1}^{h-1} c(b_i, b_{i+1}) \right). \tag{4}$$

It is not easy to minimize the cost function in Equation (4) as, for example, $c(b, \cdot) : V_k \to \mathbb{R}$ is combinatorial. To address this issue, we observe the following by using linearity of expectation and the law of iterated expectations to decouple the term in the sum over the trajectory:

$$\begin{aligned} \mathbb{E}_{b_{1:h}\sim\pi(\cdot,\theta)} \left(\sum_{i=1}^{h-1} c(b_i, b_{i+1}) \right) &= \sum_{i=1}^{h-1} \mathbb{E}_{b_i\sim d_{\theta,i}} \mathbb{E}_{b_{i+1}\sim\pi(b_i,\theta)} c(b_i, b_{i+1}) \\ &= \mathbb{E}_{b_{1:h}\sim\pi(\cdot,\theta)} \left(\sum_{i=1}^{h-1} \mathbb{E}_{b'\sim\pi(b_i,\theta)} c(b_i, b') \right), \end{aligned} \tag{5}$$

where $d_{\theta,i}$ denotes the distribution over beams in V_k that results from following $\pi(\cdot, \theta)$ on G_k for i steps. We now replace $\mathbb{E}_{b'\sim\pi(b,\cdot)} c(b, b') : \Theta \to \mathbb{R}$ by a surrogate loss function $\ell(\cdot, b) : \Theta \to \mathbb{R}$ that is differentiable with respect to the parameters $\theta \in \Theta$, and where $\ell(\theta, b)$ is a surrogate loss for the expected cost increase incurred by following policy $\pi(\cdot, \theta)$ at beam b for one step.

Elements in A_b should be scored in a way that allows the best elements to be kept in the beam. Different surrogate losses arise from which elements we concern ourselves with, e.g., all the top k elements in A_b or simply one of the best elements in A_b. Surrogate losses are then large when the scores lead to discarding desired elements in A_b, and small when the scores lead to comfortably keeping the desired elements in A_b.

Surrogate Loss Functions The following additional notation allows us to define losses precisely. Let $A_b = \{v_1, \ldots, v_n\}$ be an arbitrary ordering of the neighbors of the elements in b. Let $c = c_1, \ldots, c_n$ be the corresponding costs, where $c_i = c^*(v_i)$ for all $i \in [n]$, and $s = s_1, \ldots, s_n$ be the corresponding scores, where $s_i = s(v_i, \theta)$ for all $i \in [n]$. Let $\sigma^* : [n] \to [n]$ be a permutation such that $c_{\sigma^*(1)} \leq \ldots \leq c_{\sigma^*(n)}$, i.e., $v_{\sigma^*(1)}, \ldots, v_{\sigma^*(n)}$ are ordered in increasing order of cost. Note that $c^*(b) = c_{\sigma^*(1)}$. Similarly, let $\hat{\sigma} : [n] \to [n]$ be a permutation such that $s_{\hat{\sigma}(1)} \geq \ldots \geq s_{\hat{\sigma}(n)}$, i.e., $v_{\hat{\sigma}(1)}, \ldots, v_{\hat{\sigma}(n)}$ are ordered in decreasing order of score. We assume unique $\sigma^* : [n] \to [n]$ and $\hat{\sigma} : [n] \to [n]$ for simplifying the presentation of the loss functions (which can be guaranteed via the tie-breaking total order on V). In this case, at $b \in V_k$, the successor beam $b' \in N_b$ is uniquely determined by the scores of the elements of A_b.

For each $(x, y) \in \mathcal{X} \times \mathcal{Y}$, the corresponding cost function $c^* : V \to \mathbb{R}$ is independent of the parameters $\theta \in \Theta$. We define a loss function $\ell(\cdot, b) : \Theta \to \mathbb{R}$ at a beam $b \in V_k$ in terms of the oracle costs of the elements of A_b. We now introduce some well-motivated surrogate loss functions. Perceptron and large-margin inspired losses have been used in early update [6], LaSO [7], and BSO [11]. We also introduce two log losses.

perceptron (first) Penalizes the lowest cost element in A_b not being put at the top of the beam. When applied on the first cost increase, this is equivalent to an "early update" [6].

$$\ell(s, c) = \max\left(0, s_{\hat{\sigma}(1)} - s_{\sigma^*(1)}\right). \tag{6}$$

perceptron (last) Penalizes the lowest cost element in A_b falling out of the beam.

$$\ell(s, c) = \max\left(0, s_{\hat{\sigma}(k)} - s_{\sigma^*(1)}\right). \tag{7}$$

margin (last) Prefers the lowest cost element to be scored higher than the last element in the beam by a margin. This yields updates that are similar but not identical to the approximate large-margin variant of LaSO [7].

$$\ell(s, c) = \max\left(0, 1 + s_{\hat{\sigma}(k)} - s_{\sigma^*(1)}\right) \tag{8}$$

cost-sensitive margin (last) Weights the margin loss by the cost difference between the lowest cost element and the last element in the beam. When applied on a LaSO-style cost increase, this is equivalent to the BSO update of [11].

$$\ell(s, c) = (c_{\hat{\sigma}(k)} - c_{\sigma^*(1)}) \max\left(0, 1 + s_{\hat{\sigma}(k)} - s_{\sigma^*(1)}\right). \tag{9}$$

upper bound Convex upper bound to the expected beam transition cost, $\mathbb{E}_{b' \sim \pi(b,\cdot)} c(b, b') : \Theta \to \mathbb{R}$, where b' is induced by the scores $s \in \mathbb{R}^n$.

$$\ell(s, c) = \max(0, \delta_{k+1}, \ldots, \delta_n) \tag{10}$$

where $\delta_j = (c_{\sigma^*(j)} - c_{\sigma^*(1)})(s_{\sigma^*(j)} - s_{\sigma^*(1)} + 1)$ for $j \in \{k + 1, \ldots, n\}$. Intuitively, this loss imposes a cost-weighted margin between the best neighbor $v_{\sigma^*(1)} \in A_b$ and the neighbors $v_{\sigma^*(k+1)}, \ldots, v_{\sigma^*(n)} \in A_b$ that ought not to be included in the best successor beam b'. We prove in Appendix B that this loss is a convex upper bound for the expected beam transition cost.

log loss (beam) Normalizes only over the top k neighbors of a beam according to the scores s.

$$\ell(s, c) = -s_{\sigma^*(1)} + \log\left(\sum_{i \in I} \exp(s_i)\right), \tag{11}$$

where $I = \{\sigma^*(1), \hat{\sigma}(1), \ldots, \hat{\sigma}(k)\}$. The normalization is only over the correct element $v_{\sigma^*(1)}$ and the elements included in the beam. The set of indices $I \subseteq [n]$ encodes the fact that the score vector $s \in \mathbb{R}^n$ may not place $v_{\sigma^*(1)}$ in the top k, and therefore it has to also be included in that case. This loss is used in [9], albeit introduced differently.

log loss (neighbors) Normalizes over all elements in A_b.

$$\ell(s, c) = -s_{\sigma^*(1)} + \log\left(\sum_{i=1}^{n} \exp(s_i)\right) \tag{12}$$

Discussion The losses here presented directly capture the purpose of using a beam for prediction—ensuring that the best hypothesis stays in the beam, i.e., that, at $b \in V_k$, $v_{\sigma^*(1)} \in A_b$ is scored sufficiently high to be included in the successor beam $b' \in N_b$. If full cost information is not accessible, i.e., if are not able to evaluate $c^* : V \to \mathbb{R}$ for arbitrary elements in V, it is still possible to use a subset of these losses, provided that we are able to identify the lowest cost element among the neighbors of a beam, i.e., for all $b \in V_k$, an element $v \in A_b$, such that $c^*(v) = c^*(b)$.

While certain losses do not appear beam-aware (e.g., those in Equation (6) and Equation (12)), it is important to keep in mind that all losses are collected by executing a policy on the beam search space G_k. Given a beam $b \in V_k$, the score vector $s \in \mathbb{R}^n$ and cost vector $c \in \mathbb{R}^n$ are defined for the elements of A_b. The losses incurred depend on the specific beams visited. Losses in Equation (6), (10), and (12) are convex. The remaining losses are non-convex. For $k = 1$, we recover well-known losses, e.g., loss in Equation (12) becomes a simple log loss over the neighbors of a single node, which is precisely the loss used in typical log-likelihood maximization models; loss in Equation (7) becomes a perceptron loss. In Appendix C we discuss convexity considerations for different types of losses. In Appendix D, we present additional losses and expand on their connections to existing work.

4.2 Data Collection Strategy

Our meta-algorithm requires choosing a train time policy $\pi : V_k \to \Delta(V_k)$ to traverse the beam search space G_k to collect supervision. Sampling a trajectory to collect training supervision is done by BEAMTRAJECTORY in Algorithm 2.

oracle Our simplest policy follows the oracle policy $\pi^* : V_k \to \Delta(V_k)$ induced by the optimal completion cost function $c^* : V \to \mathbb{R}$ (as in Section 3). Using the terminology of Algorithm 1, we can write $\pi^*(b, c^*) = \textsc{Policy}(G, b, k, -c^*)$. This policy transitions using the negated sorted costs of the elements in A_b as scores.

The oracle policy does not address the distribution mismatch problem. At test time, the learned policy will make mistakes and visit beams for which it has not collected supervision at train time, leading to error compounding. Imitation learning tells us that it is necessary to collect supervision at train time with the learned policy to avoid error compounding at test time [5].

We now present data collection strategies that use the learned policy. For brevity, we only cover the case where the learned policy is always used (except when the transition leads to a cost-increase),

Table 1: Existing and novel beam-aware algorithms as instances of our meta-algorithm. Our theoretical guarantees require the existence of a deterministic no-regret online learning algorithm for the resulting problem.

Algorithm	**Meta-algorithm choices**		
	data collection	surrogate loss	k
log-likelihood	oracle	log loss (neighbors)	1
DAGGER [5]	continue	log loss (neighbors)	1
early update [6]	stop	perceptron (first)	> 1
LaSO (perceptron) [7]	reset	perceptron (first)	> 1
LaSO (large-margin) [7]	reset	margin (last)	> 1
BSO [11]	reset	cost-sensitive margin (last)	> 1
globally normalized [9]	stop	log loss (beam)	> 1
Ours	continue	[choose a surrogate loss]	> 1

and leave the discussion of additional possibilities (e.g., probabilistic interpolation of learned and oracle policies) to Appendix E.3. When an edge $(b, b') \in E_k$ incurring cost increase is traversed, different strategies are possible:

stop Stop collecting the beam trajectory. The last beam in the trajectory is b', i.e., the beam on which we arrive in the transition that led to a cost increase. This data collection strategy is used in structured perceptron training with early update [6].

reset Reset the beam to contain only the best state as defined by the optimal completion cost function: $b' = \text{BEST}(b, 1, -c^*)$. In the subsequent steps of the policy, the beam grows back to size k. LaSO [7] uses this data collection strategy. Similarly to the oracle data collection strategy, rather than committing to a specific $b' \in N_b^*$, we can sample $b' \sim \pi^*(b, c^*)$ where $\pi^*(b, c^*)$ is any distribution over N_b^*. The reset data collection strategy collects beam trajectories where the oracle policy π is executed conditionally, i.e., when the roll-in policy $\pi(\cdot, \theta_t)$ would lead to a cost increase.

continue We can ignore the cost increase and continue following policy π_t. This is the strategy taken by DAgger [5]. The continue data collection strategy has not been considered in the beam-aware setting, and therefore it is a novel contribution of our work. Our stronger theoretical guarantees apply to this case.

5 Theoretical Guarantees

We state regret guarantees for learning beam search policies using the continue, reset, or stop data collection strategies. One of the main contributions of our work is framing the problem of learning beam search policies in a way that allows us to obtain meaningful regret guarantees. Detailed proofs are provided in Appendix E. We begin by analyzing the continue collection strategy. As we will see, regret guarantees are stronger for continue than for stop or reset.

No-regret online learning algorithms have an important role in the proofs of our guarantees. Let $\ell_1, \ldots, \ell_m$ be a sequence of loss functions with $\ell_t : \Theta \to \mathbb{R}$ for all $t \in [m]$. Let $\theta_1, \ldots, \theta_m$ be a sequence of iterates with $\theta_t \in \Theta$ for all $t \in [m]$. The loss function ℓ_t can be chosen according to an arbitrary rule (e.g., adversarially). The online learning algorithm chooses the iterate θ_t. Both ℓ_t and θ_t are chosen online, as functions of loss functions $\ell_1, \ldots, \ell_{t-1}$ and iterates $\theta_1, \ldots, \theta_{t-1}$.

Definition 1. *An online learning algorithm is no-regret if for any sequence of functions $\ell_1, \ldots, \ell_m$ chosen according to the conditions above we have*

$$\frac{1}{m}\sum_{t=1}^{m} \ell_t(\theta_t) - \min_{\theta \in \Theta} \frac{1}{m}\sum_{t=1}^{m} \ell_t(\theta) = \gamma_m, \tag{13}$$

where γ_m goes to zero as m goes to infinity.

Many no-regret online learning algorithms, especially for convex loss functions, have been proposed in the literature, e.g., [20, 21, 22]. Our proofs of the theoretical guarantees require the no-regret online learning algorithm to be deterministic, i.e., θ_t to be a deterministic rule of previous observed iterates $\theta_1, \ldots, \theta_{t-1}$ and loss functions $\ell_1, \ldots, \ell_{t-1}$, for all $t \in [m]$. Online gradient descent [20] is an example of such an algorithm.

In Theorem 1, we prove no-regret guarantees for the case where the no-regret online algorithm is presented with explicit expectations for the loss incurred by a beam search policy. In Theorem 2, we upper bound the expected cost incurred by a beam search policy as a function of its expected loss. This result holds in cases where, at each beam, the surrogate loss is an upper bound on the expected cost increase at that beam. In Theorem 3, we use Azuma-Hoeffding to prove no-regret high probability bounds for the case where we only have access to empirical expectations of the loss incurred by a policy, rather than explicit expectations. In Theorem 4, we extend Theorem 3 for the case where the data collection policy is different from the policy that we are evaluating. These results allow us to give regret guarantees that depend on how frequently is the data collection policy different from the policy that we are evaluating.

In this section we simply state the results of the theorems alongside some discussion. All proofs are presented in detail in Appendix E. Our analysis closely follows that of DAgger [5], although the results need to be interpreted in the beam search setting. Our regret guarantees for beam-aware algorithms with different data collection strategies are novel.

5.1 No-Regret Guarantees with Explicit Expectations

The sequence of functions $\ell_1, \ldots, \ell_m$ can be chosen in a way that applying a no-regret online learning algorithm to generate the sequence of policies $\theta_1, \ldots, \theta_m$ leads to no-regret guarantees for the performance of the mixture of $\theta_1, \ldots, \theta_m$. The adversary presents the no-regret online learning algorithm with $\ell_t = \ell(\cdot, \theta_t)$ at time $t \in [m]$. The adversary is able to play $\ell(\cdot, \theta_t)$ because it can anticipate θ_t, as the adversary knows the deterministic rule used by the no-regret online learning algorithm to pick iterates. Paraphrasing Theorem 1, on the distribution of trajectories induced by the the uniform stochastic mixture of $\theta_1, \ldots, \theta_m$, the best policy in Θ for this distribution performs as well (in the limit) as the uniform mixture of $\theta_1, \ldots, \theta_m$.

Theorem 1. *Let $\ell(\theta, \theta') = \mathbb{E}_{(x,y)\sim\mathcal{D}}\mathbb{E}_{b_{1:h}\sim\pi(\cdot,\theta')}\left(\sum_{i=1}^{h-1} \ell(\theta, b_i)\right)$. If the sequence $\theta_1, \ldots, \theta_m$ is chosen by a deterministic no-regret online learning algorithm, we have $\frac{1}{m}\sum_{t=1}^{m} \ell(\theta_t, \theta_t) - \min_{\theta\in\Theta} \frac{1}{m}\sum_{t=1}^{m} \ell(\theta, \theta_t) = \gamma_m$, where γ_m goes to zero when m goes to infinity.*

Furthermore, if for all $(x, y) \in \mathcal{X} \times \mathcal{Y}$ the surrogate loss $\ell(\cdot, b) : \Theta \to \mathbb{R}$ is an upper bound on the expected cost increase $\mathbb{E}_{b'\sim\pi(b,\cdot)}c(b, b') : \Theta \to \mathbb{R}$ for all $b \in V_k$, we can transform the surrogate loss no-regret guarantees into performance guarantees in terms of $c : \mathcal{Y} \to \mathbb{R}$. Theorem 2 tells us that if the best policy along the trajectories induced by the mixture of $\theta_1, \ldots, \theta_m$ in Θ incurs small surrogate loss, then the expected cost resulting from labeling examples $(x, y) \in \mathcal{X} \times \mathcal{Y}$ sampled from $\mathcal{D}$ with the uniform mixture of $\theta_1, \ldots, \theta_m$ is also small. It is possible to transform the results about the uniform mixture of $\theta_1, \ldots, \theta_m$ on results about the best policy among $\theta_1, \ldots, \theta_m$, e.g., following the arguments of [23], but for brevity we do not present them in this paper. Proofs of Theorem 1 and Theorem 2 are in Appendix E.1

Theorem 2. *Let all the conditions in Definition 1 be satisfied. Additionally, let $c(\theta) = c^*(b_1) + \mathbb{E}_{(x,y)\sim\mathcal{D}}\mathbb{E}_{b_{1:h}\sim\pi(\cdot,\theta)}\left(\sum_{i=1}^{h-1} c(b_i, b_{i+1})\right) = \mathbb{E}_{(x,y)\sim\mathcal{D}}\mathbb{E}_{b_{1:h}\sim\pi(\cdot,\theta)}c^*(b_h)$. Let $\ell(\cdot, b) : \Theta \to \mathbb{R}$ be an upper bound on $\mathbb{E}_{b'\sim\pi(b,\cdot)}c(b, b') : \Theta \to \mathbb{R}$, for all $b \in V_k$. Then, $\frac{1}{m}\sum_{t=1}^{m} c(\theta_t) \leq \mathbb{E}_{(x,y)\sim\mathcal{D}}c^*(b_1) + \min_{\theta\in\Theta} \frac{1}{m}\sum_{t=1}^{m} \ell(\theta, \theta_t) + \gamma_m$, where γ_m goes to zero as m goes to infinity.*

5.2 Finite Sample Analysis

Theorem 1 and Theorem 2 are for the case where the adversary presents explicit expectations, i.e., the loss function at time $t \in [m]$ is $\ell_t(\cdot) = \mathbb{E}_{(x,y)\sim\mathcal{D}}\mathbb{E}_{b_{1:h}\sim\pi(\cdot,\theta_t)}\left(\sum_{i=1}^{h-1} \ell(\cdot, b_i)\right)$. We most likely only have access to a sample estimator $\hat{\ell}(\cdot, \theta_t) : \Theta \to \mathbb{R}$ of the true expectation: we first sample an example $(x_t, y_t) \sim \mathcal{D}$, sample a trajectory $b_{1:h}$ according to $\pi(\cdot, \theta_t)$, and obtain $\hat{\ell}(\cdot, \theta_t) = \sum_{i=1}^{h-1} \ell(\cdot, b_i)$. We prove high probability no-regret guarantees for this case. Theorem 3 tells us that the population surrogate loss of the mixture of policies $\theta_1, \ldots, \theta_m$ is, with high probability, not much larger than its empirical surrogate loss. Combining this result with Theorem 1 and

Theorem 2 allows us to give finite sample high probability results for the performance of the mixture of policies $\theta_1, \ldots, \theta_m$. The proof of Theorem 3 is found in Appendix E.2.

Theorem 3. *Let $\hat{\ell}(\cdot, \theta') = \sum_{i=1}^{h-1} \ell(\cdot, b_i)$ which is generated by sampling (x, y) from $\mathcal{D}$ (which induces the corresponding beam search space G_k and cost functions), and sampling a beam trajectory using $\pi(\cdot, \theta')$. Let $|\sum_{i=1}^{h-1} \ell(\theta, b_i)| \leq u$ for a constant $u \in \mathbb{R}$, for all $(x, y) \in \mathcal{X} \times \mathcal{Y}$, beam trajectories $b_{1:h}$, and $\theta \in \Theta$. Let the iterates be chosen by a no-regret online learning algorithm, based on the sequence of losses $\ell_t = \hat{\ell}(\cdot, \theta_t) : \Theta \to \mathbb{R}$, for $t \in [m]$, then we have $\mathbb{P}\left(\frac{1}{m}\sum_{t=1}^{m} \ell(\theta_t, \theta_t) \leq \frac{1}{m}\sum_{t=1}^{m} \hat{\ell}(\theta_t, \theta_t) + \eta(\delta, m)\right) \geq 1 - \delta$, where $\delta \in (0, 1]$ and $\eta(\delta, m) = u\sqrt{2\log(1/\delta)/m}$.*

5.3 Finite Sample Analysis for Arbitrary Data Collection Policies

All the results stated so far are for the continue data collection strategy where, at time $t \in [m]$, the whole trajectory $b_{1:h}$ is collected using the current policy $\pi(\cdot, \theta_t)$. Stop and reset data collection strategies do not necessarily collect the full trajectory under $\pi(\cdot, \theta_t)$. If the data collection policy $\pi' : V_k \to \Delta(V_k)$ is other than the learned policy, the analysis can be adapted by accounting for the difference in distribution of trajectories induced by the learned policy and the data collection policy. The insight is that $\sum_{i=1}^{h-1} \ell(\theta, b_i)$ only depends on $b_{1:h-1}$, so if no cost increases occur in this portion of the trajectory, we are effectively sampling the trajectory using $\pi(\cdot, \theta)$ when using the stop and reset data collection strategies.

Prior work presented only perceptron-style results for these settings [6, 7]—we are the first to present regret guarantees. Our guarantee depends on the probability with which $b_{1:h-1}$ is collected solely with $\pi(\cdot, \theta)$. We state the finite sample analysis result for the case where these probabilities are not known explicitly, but we are able to estimate them. The proof of Theorem 4 is found in Appendix E.3.

Theorem 4. *Let $\pi_t : V_k \to \Delta(V_k)$ be the data collection policy for example $t \in [m]$, which uses either the stop or reset data collection strategies. Let $\hat{\alpha}(\theta_t)$ be the empirical estimate of the probability of $\pi(\cdot, \theta_t)$ incurring at least one cost increase up to time $h - 1$. Then,*

$$\mathbb{P}\left(\frac{1}{m}\sum_{t=1}^{m} \ell(\theta_t, \theta_t) \leq \frac{1}{m}\sum_{t=1}^{m} \hat{\ell}(\theta_t, \pi_t) + u\left(1 - \frac{1}{m}\sum_{t=1}^{m} \hat{\alpha}(\theta_t)\right) + 2\eta(\delta, m)\right) \geq 1 - \delta,$$

where $\delta \in (0, 1]$ and $\eta(\delta, m) = u\sqrt{2\log(1/\delta)/m}$.

If the probability of stopping or resetting goes to zero as m goes to infinity, then the term captures the discrepancy between the distributions of induced by $\pi(\cdot, \theta_t)$ and π_t vanishes, and we recover a guarantee similar to Theorem 3. If the probability of stopping or resetting does not go completely to zero, it is still possible to provide regret guarantees for the performance of this algorithm but now with a term that does not vanish with increasing m. These regret guarantees for the different data collection strategies are novel.

6 Conclusion

We propose a framework for learning beam search policies using imitation learning. We provide regret guarantees for both new and existing algorithms for learning beam search policies. One of the main contributions is formulating learning beam search policies in the learning to search framework. Policies for beam search are induced via a scoring function. The intuition is that the best neighbors in a beam should be scored sufficiently high, allowing them to be kept in the beam when transitioning using these scores. Based on this insight, we motivate different surrogate loss functions for learning scoring functions. We recover existing algorithms in the literature through specific choices for the loss function and data collection strategy. Our work is the first to provide a beam-aware algorithm with no-regret guarantees.

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A Conversion to Tree-Structured Search Spaces

We define a search space as an arbitrary finite directed graph $G = (V, E)$, where V is the set of nodes and $E \subset V \times V$ is the set of directed edges. Every directed graph $G = (V, E)$ has associated a tree-structured directed graph $G_p = (V_p, E_p)$ encoding all possible paths through G. An important reason to do this transformation is that, in practice, policies often incorporate history features, so they are functions of the whole path leading to a node in G, rather than just a single node in G. A policy becomes a function of single nodes of G_p. If G is tree-structured, G_p is isomorphic to G, i.e., they are the same search space.

The set of terminal nodes T_p contains all paths from the initial node $v_{(0)} \in V$ to terminal nodes $v \in T$. For $v \in V_p$, we denote the length of the sequence encoding a path by $|v|$. The length of a path $v \in V_p$ is $|v| - 1$. We write v_i for the i-th element of a path $v \in V_p$. For all $v \in V$, $v_i \in V$ for all $i \in [|v|]$ and $v_1 = v_{(0)}$. The sets $N_{p,v}, R_{p,v}, T_{p,v}$ for $v \in V_p$ are defined analogously to the sets N_v, R_v, T_v for $v \in V$. For a path $v \in V_p$, $v' \in N_{p,v}$ if $v'_{1:|v|} = v$, $|v| = |v'| - 1$, and $v'_{|v'|} \in N_{v'_{|v|}}$, i.e., a path $v' \in V_p$ neighbors $v \in V_p$ if it can be written as v followed by an additional node in $N_{v_{|v|}}$. For $v \in V_p$, $v' \in R_{p,v}$ if v is a prefix of v' and $v' \in T_{p,v}$ if v is a prefix of v' and $v'_{|v'|} \in T$. As G_p is tree-structured, we can define the depth d_v of a path $v \in V_p$ as its length, i.e., $d_v = |v| - 1$. If path $v \in V_p$, then prefix $v_{1:i} \in V_p$, for all $i \in [|v|]$, i.e., path prefixes are themselves paths.

Tree-structured search spaces are common in practice. They often occur in write-only search spaces, where once an action is taken, its effects are irreversible. Typical search spaces for sequence tagging and machine translation are tree-structured: given a sequence to tag or translate, at each step we commit to a token and never get to change it. When the search space G is not naturally seen as being tree-structured, the construction described makes it natural to work with an equivalent tree-structured search space of paths G_p.

If G has cycles, G_p would be infinite. Infinite cycling in G_p can be prevented by, for example, introducing a maximum path length or a maximum number of times that any given node $v \in V$ can be visited. In this paper, we also assumed that all nodes in T_p have distance h to the root. It is possible to transform G_p into a new tree-structured graph G'_p by padding shorter paths to length h. Let h be the maximum distance of any terminal in T_p to the root. For each terminal node $v \in T_p$ with distance $d_v < h$ to the root, we extend the path to v by appending a linear chain of $h - d_v$ additional nodes. Node v is no longer a terminal node in G'_p, and all the nodes in G'_p that resulted from extending the path are identified with v.

B Convex Upper Bound Surrogate for Expected Beam Transition Cost

In this appendix, we design a convex upper bound surrogate loss $\ell(\cdot, b) : \Theta \to \mathbb{R}$ for the expected beam transition cost $\mathbb{E}_{b' \sim \pi(b,\cdot)} c(b, b') : \Theta \to \mathbb{R}$. Let $A_b = \{v_1, \ldots, v_n\}$ be an arbitrary ordering of the neighbors of b, with corresponding costs $c_1, \ldots, c_n$, with $c_i = c^*(v_i)$ for all $i \in [n]$. Let $s_1, \ldots, s_n$ be the corresponding scores, with $s_i = s(v_i, \theta)$ for all $i \in [n]$. Let $\sigma^* : [n] \to [n]$ and $\hat{\sigma} : [n] \to [n]$ be the unique permutations such that $c_{\sigma^*(1)} \leq \ldots \leq c_{\sigma^*(n)}$ and $s_{\hat{\sigma}(1)} \geq \ldots \geq s_{\hat{\sigma}(n)}$, respectively, with ties broken according to the total order on V. We have $c^*(b) = c_{\sigma^*(1)}$. Let $k \in \mathbb{N}$ be the maximum beam capacity. Let b' be the beam induced by the scores $s_1, \ldots, s_n$, i.e., $b' = \{v_{\hat{\sigma}(1)}, \ldots, v_{\hat{\sigma}(k')}\}$, with $k' = \min(k, n)$ and ties broken according to the total order.

Consider the *upper bound* loss function (repeated here from Equation (10))

$$\ell(s, c) = \max\left(0, \delta_{k+1}, \ldots, \delta_n\right), \tag{14}$$

where $\delta_j = (c_{\sigma^*(j)} - c_{\sigma^*(1)})(s_{\sigma^*(j)} - s_{\sigma^*(1)} + 1)$ for $j \in \{k+1, \ldots, n\}$.

This loss function is lower bounded by zero, so we only need to show that it upper bounds $c(b, b')$ when there is a cost increase, i.e., when $c(b, b') > 0$. A cost increase $c(b, b') > 0$ implies that the best element $v_{\sigma^*(1)}$ fell off the beam, meaning that $b' = \{v_{\hat{\sigma}(1)}, \ldots, v_{\hat{\sigma}(k)}\} \neq \{v_{\sigma^*(1)}, \ldots, v_{\sigma^*(k)}\}$, and therefore $b' \cap \{v_{\sigma^*(k+1)}, \ldots, v_{\sigma^*(n)}\} \neq \emptyset$. Let $v_{\sigma^*(j)} \in b' \cap \{v_{\sigma^*(k+1)}, \ldots, v_{\sigma^*(n)}\}$, then

$s_{\sigma^*(j)} \geq s_{\sigma^*(1)}$ and $c(b, b') \leq c_{\sigma^*(j)} - c_{\sigma^*(1)}$, with $j \in \{k+1, \ldots, n\}$. We have

$$\begin{aligned} \max\left(0, \delta_{k+1}, \ldots, \delta_n\right) &\geq \delta_j \\ &= (c_{\sigma^*(j)} - c_{\sigma^*(1)})(s_{\sigma^*(j)} - s_{\sigma^*(1)} + 1) \\ &\geq c_{\sigma^*(j)} - c_{\sigma^*(1)} \\ &\geq c(b, b'), \end{aligned}$$

proving the upper bound property of the loss in Equation (14).

This loss is the maximum of a finite number of affine functions of the scores, and therefore convex with respect to the score vector $s \in \mathbb{R}^n$. The resulting optimization problem is convex with respect to the parameters of the scoring function if, for example, the scoring function is linear with respect to the parameters $\theta \in \Theta$, i.e., $s(v, \theta) = \theta^T \phi(v, x)$, where $\phi : V \times \mathcal{X} \to \mathbb{R}^p$ is a fixed feature function of the state. If A_b has no more than k elements, this surrogate loss is identically zero, i.e., for $k \geq n$, $\ell(s, c) = 0$, for all $s \in \mathbb{R}^n$ and $c \in \mathbb{R}^n$. If $k = 1$, we recover a greedy decoding algorithm and the loss in Equation (14) becomes a weighted hinge loss.

C Convexity Considerations for Surrogate Loss Functions

It is common in the literature to update the parameters only when a cost increase occurs [10, 8, 9]. We show that the resulting loss surrogate functions are, in general, non-convex in the scores.

The following loss is an upper bound on the beam transition loss $c : E_k \to \mathbb{R}$, but is non-convex in the scores:

$$\ell(s, c) = (c_{\hat{\sigma}(k)} - c_{\sigma^*(1)}) \max(0, s_{\hat{\sigma}(k)} - s_{\sigma^*(1)} + 1). \tag{15}$$

The upper bound property for this loss is easy to verify: if $s \in \mathbb{R}^n$ at $b \in V_k$ induces $b' \in V_k$ with $c(b, b') > 0$, then $s_{\hat{\sigma}(k)} \geq s_{\sigma^*(1)}$ and $c_{\hat{\sigma}(k)} > c_{\sigma^*(1)}$, leading to

$$\begin{aligned} (c_{\hat{\sigma}(k)} - c_{\sigma^*(1)}) \max(0, s_{\hat{\sigma}(k)} - s_{\sigma^*(1)} + 1) &\geq c_{\hat{\sigma}(k)} - c_{\sigma^*(1)} \\ &\geq c(b, b'), \end{aligned}$$

as $v_{\hat{\sigma}(k)} \in b'$. This loss is used in [11]. The same reasoning holds when substituting k in Equation (15) by any $i \in [k]$.

We now show that two aspects commonly present in the beam-aware literature lead to non-convexity of the surrogate losses. The first aspect is updating the parameters only when there is a cost increase. This amounts to defining a new loss function $\ell' : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$ from $\ell : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$ of the form

$$\ell'(s, c) = \ell(s, c)\mathbb{1}[c(b, b') > 0],$$

where b' is induced by $s \in \mathbb{R}^n$. The second aspect that leads to non-convexity is indexing the score vector $s \in \mathbb{R}^n$ or cost vector $c \in \mathbb{R}^n$ with a function of the parameters, e.g., permutation $\hat{\sigma} : [n] \to [n]$ depends on the scores $s \in \mathbb{R}^n$ and therefore, on the parameters $\theta \in \Theta$. We show non-convexity with respect to the scores through two simple counter examples.

For the first aspect, let $k = 2$ and $n = 3$, with v_1, v_2, v_3 having costs $c_1 = 0, c_2 = 1, c_3 = 1$. Any beam that keeps v_1 has no cost increase. Consider the scores $s_1 = 1, s_2 = 10, s_3 = 0$ and $s'_1 = 1, s'_2 = 0, s'_3 = 10$. Both s and s' lead to no cost increase, as both score vectors keep v_1 in the beam. For $\ell' : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$ to be convex in the scores, we must have $\ell'(\alpha s + (1 - \alpha)s', c) \leq \alpha\ell'(s, c) + (1 - \alpha)\ell'(s', c)$, for all $\alpha \in [0, 1]$. As both s and s' lead to no cost increase, we have $\ell'(s, c) = \ell'(s', c) = 0$, yielding the following necessary condition for convexity: $\ell(\alpha s + (1 - \alpha)s', c) \leq 0$ for all $\alpha \in [0, 1]$. For $\alpha = 0.5$, we have $\overline{s}_1 = 1, \overline{s}_2 = 5, \overline{s}_3 = 5$, which leads to a cost increase, and therefore to loss $\ell'(\overline{s}, c) > 0$, implying that $\ell' : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$ is non-convex in the scores.

For the second aspect, consider the loss in Equation (15). Ignore the multiplicative term involving the costs and consider only the hinge part $\max(0, s_{\hat{\sigma}(k)} - s_{\sigma^*(k)} + 1)$. Let $k = 2$ and $n = 3$. Consider that the elements v_1, v_2, v_3 are sorted in increasing order of cost; let $s_1 = 2, s_2 = 1, s_3 = 0$, and $s'_1 = 2, s'_2 = 4, s'_3 = 0$. In both cases, the hinge part of loss in Equation (15) is zero, but if we take a convex combination of the scores with $\alpha = 0.5$, we get $\overline{s}_1 = 2, \overline{s}_2 = 2.5, \overline{s}_3 = 0$, for which the surrogate loss is nonzero (assuming that the costs of v_1, v_2, v_3 are unique).

D Additional Loss Functions

We present additional loss functions that were omitted in Section 4.1 and discuss their connections to previous work.

cost sensitive margin (beam) Prefers the lowest cost element to be scored higher than best runner-up in the beam by a cost-weighted margin. With unbounded beam capacity, we recover the structured max-margin loss of [24] for M^{3}Ns.

$$\ell(s, c) = -s_{\sigma^*(1)} + \max_{i \in \{1, \ldots, k\}} \left(c_{\hat{\sigma}(i)} + s_{\hat{\sigma}(i)}\right) \tag{16}$$

softmax margin (beam) Log loss that can be understood as smoothing the $\max$ in *cost sensitive margin (beam)*. With unbounded beam capacity, we recover the softmax-margin loss of [25] for CRFs.

$$\ell(s, c) = -s_{\sigma^*(1)} + \log \left(\sum_{i=1}^{k} \exp\left(c_{\hat{\sigma}(i)} + s_{\hat{\sigma}(i)}\right) \right) \tag{17}$$

weighted pairs (all) Reduces the problem of producing the correct ranking over the neighbors to $n(n-1)/2$ weighted binary classification problems. Hinge terms for pairs with the same cost cancel, effectively expressing that we are indifferent to the relative order of the elements of the pair.

$$\ell(s, c) = \sum_{i=1}^{n} \sum_{j=i+1}^{n} \left(c_{\sigma^*(j)} - c_{\sigma^*(i)}\right) \max\left(0, s_{\sigma^*(j)} - s_{\sigma^*(1)} + 1\right) \tag{18}$$

weighted pairs (bipartite) Only weighted pairs between elements than ought to be included in the beam and those that ought to excluded from the beam. A similar loss has been proposed for bipartite ranking, where the goal is to order all positive examples before all negative examples

$$\ell(s, c) = \sum_{i=1}^{k} \sum_{j=k+1}^{n} \left(c_{\sigma^*(j)} - c_{\sigma^*(i)}\right) \max\left(0, s_{\sigma^*(j)} - s_{\sigma^*(1)} + 1\right) \tag{19}$$

weighted pairs (hybrid) Similar to weighted pairs bipartite but we also include the pairs for the elements that ought to be included in the beam

$$\ell(s, c) = \sum_{i=1}^{k} \sum_{j=i+1}^{n} \left(c_{\sigma^*(j)} - c_{\sigma^*(i)}\right) \max\left(0, s_{\sigma^*(j)} - s_{\sigma^*(1)} + 1\right) \tag{20}$$

The *weighted pairs (all)* loss provides many different variants as exemplified by *weighted pairs (bipartite)* and *weighted pairs (hybrid)*. We believe that exploring the ranking literature can lead to interesting insights on what losses to use for learning beam search policies in our framework.

E No-Regret Guarantees

This section presents analysis that leads to proofs of theorems 1, 2, 3, and 4. We analyze

$$c(\theta) = \mathbb{E}_{(x,y) \sim \mathcal{D}} \mathbb{E}_{\hat{y} \sim \pi(\cdot, \theta)} c_{x,y}(\hat{y}).$$

The prediction cost $c_{x,y}(\hat{y})$ is generated by sampling a beam trajectory $b_{1:h}$ with policy $\pi(\cdot, \theta)$. The prediction $\hat{y}$ is extracted from b_h. We have

$$c(\theta) = \mathbb{E}_{(x,y) \sim \mathcal{D}} \mathbb{E}_{b_{1:h} \sim \pi(\cdot, \theta)} \left(c^*(b_1) + \sum_{i=1}^{h-1} c(b_i, b_{i+1}) \right).$$

As b_1 depends only on $x \in \mathcal{X}$, $c^*(b_1)$ does not depend on the parameters θ and therefore can be ignored for optimization purposes. We analyze instead the surrogate

$$\ell(\theta, \theta') = \mathbb{E}_{(x,y) \sim \mathcal{D}} \mathbb{E}_{b_{1:h} \sim \pi(\cdot, \theta')} \left(\sum_{i=1}^{h-1} \ell(\theta, b_i) \right), \tag{21}$$

where $\ell(\cdot, b) : \Theta \to \mathbb{R}$ is a surrogate for $\mathbb{E}_{b' \sim \pi(b, \cdot)} c(b, b') : \Theta \to \mathbb{R}$. See Section 4.1 for extended discussion on the motivation behind surrogate loss $\ell(\cdot, b)$. It is convenient to assume that the policy $\pi(\cdot, \theta') : V_k \to \Delta(V_k)$ used to collect the beam trajectory $b_{1:h}$ can be different than the policy $\pi(\cdot, \theta) : V_k \to \Delta(V_k)$ used to evaluate the surrogate losses at the visited beams. The surrogate loss function $\ell : \Theta \times V_k \to \mathbb{R}$ depends on the sampled example $(x, y) \in \mathcal{X} \times \mathcal{Y}$, but we omit this dependency for conciseness.

E.1 No-Regret Guarantees with Explicit Expectations

Here we present the proofs of Theorem 1 and Theorem 2. It is informative to consider the case where we have access to both explicit expectations. In this case, the no-regret algorithm is run on the sequence of losses $\ell(\theta_1, \theta_1), \ldots, \ell(\theta_m, \theta_m)$ yielding average regret

$$\gamma_m = \frac{1}{m} \sum_{t=1}^{m} \ell(\theta_t, \theta_t) - \min_{\theta \in \Theta} \frac{1}{m} \sum_{t=1}^{m} \ell(\theta, \theta_t).$$

As the sequence $\theta_1, \ldots, \theta_m$ is generated by a no-regret algorithm, the average regret goes to zero as m goes to infinity. This result tells us that the uniform mixture obtained by sampling uniformly at random one of $\theta_1, \ldots, \theta_m$ and acting according to it for the full trajectory, is competitive with the best policy in Θ along the same induced trajectories. Note that

$$\frac{1}{T} \sum_{t=1}^{T} \ell(\theta_t, \theta_t) - \min_{\theta \in \Theta} \frac{1}{T} \sum_{t=1}^{T} \ell(\theta, \theta_t) = \mathbb{E}_{t \sim U(1,T)} \ell(\theta_t, \theta_t) - \min_{\theta \in \Theta} \mathbb{E}_{t \sim U(1,T)} \ell(\theta, \theta_t),$$

where $U(1, T)$ denotes the uniform distribution over $[T]$. Performance guarantees are obtained from the rearrangement

$$\frac{1}{m} \sum_{t=1}^{m} \ell(\theta_t, \theta_t) = \epsilon_m + \gamma_m,$$

where

$$\epsilon_m = \min_{\theta \in \Theta} \frac{1}{m} \sum_{t=1}^{m} \ell(\theta, \theta_t),$$

$$\gamma_m = \frac{1}{m} \sum_{t=1}^{m} \ell(\theta_t, \theta_t) - \min_{\theta \in \Theta} \frac{1}{m} \sum_{t=1}^{m} \ell(\theta, \theta_t).$$

Furthermore, if the surrogate loss $\ell(\cdot, b) : \Theta \to \mathbb{R}$ upper bounds the expected beam transition cost $\mathbb{E}_{b' \sim \pi(b, \cdot)} c(b, b') : \Theta \to \mathbb{R}$, i.e., $\ell(\theta, b) \geq \mathbb{E}_{b' \sim \pi(b, \theta)} c(b, b')$ for all $b \in V_k$ and all $\theta \in \Theta$, we have

$$\mathbb{E}_{b_{1:h} \sim \pi(\cdot, \theta)} \left(\sum_{i=1}^{h-1} c(b_i, b_{i+1}) \right) \leq \mathbb{E}_{b_{1:h} \sim \pi(\cdot, \theta)} \left(\sum_{i=1}^{h-1} \ell(\theta, b_i) \right),$$

and consequently,

$$\frac{1}{m} \sum_{t=1}^{m} c(\theta_t) \leq \frac{1}{m} \sum_{t=1}^{m} \ell(\theta_t, \theta_t) + \mathbb{E}_{(x,y) \sim \mathcal{D}} c^*(b_1),$$

i.e, we are able to use the expected surrogate loss incurred by the uniform mixture of $\theta_1, \ldots, \theta_m$ to upper bound the expected labeling cost resulting from labeling examples $(x, y) \sim \mathcal{D}$ with the uniform mixture of $\theta_1, \ldots, \theta_m$.

As the sequence $\theta_1, \ldots, \theta_m$ is chosen by a no-regret algorithm, γ_m goes to zero as m goes to infinity. The term ϵ_m is harder to characterize as m goes to infinity. We are guaranteed that the uniform mixture of $\theta_1, \ldots, \theta_m$ and, as result the best policy in $\theta_1, \ldots, \theta_m$, is competitive with the best policy in hindsight $\theta^*_m \in \arg\min_{\theta \in \Theta} 1/m \sum_{t=1}^{m} \ell(\theta, \theta_t)$. For the performance guarantees to be interesting, it is necessary for ϵ_m to remain small as m goes to infinity, i.e., there must exist a policy in Θ that performs well on the distribution of trajectories induced by the uniform mixture of $\theta_1, \ldots, \theta_m$. We think that this remark is often not adequately discussed in the literature. Nonetheless, for expressive policy classes, e.g., neural networks, it is reasonable to assume the existence of such a policy.

E.2 Finite Sample Analysis

Next we provide a proof of Theorem 3. We typically do not have access to the explicit expectations in Equation (21). What we do have access to is an estimator

$$\hat{\ell}(\theta, \theta') = \sum_{i=1}^{h-1} \ell(\theta, b_i),$$

which is obtained by sampling an example (x, y) from the data generating distribution $\mathcal{D}$, and executing policy $\pi(\cdot, \theta')$ to collect a trajectory $b_{1:h}$.

Our no-regret algorithm is then run on the sequence of sampled losses, yielding the sequence $\theta_1, \ldots, \theta_m$ and average regret

$$\hat{\gamma}_m = \frac{1}{m} \sum_{t=1}^{m} \hat{\ell}(\theta_t, \theta_t) - \min_{\theta \in \Theta} \frac{1}{m} \sum_{t=1}^{m} \hat{\ell}(\theta, \theta_t).$$

We show that the true population loss of the uniform mixture of $\theta_1, \ldots, \theta_m$ is, with high probability, not much larger than the empirical loss observed on the sampled trajectories, i.e.,

$$\mathbb{P}\left(\frac{1}{m} \sum_{t=1}^{m} \ell(\theta_t, \theta_t) \leq \frac{1}{m} \sum_{t=1}^{m} \hat{\ell}(\theta_t, \theta_t) + \eta(\delta, m) \right) \geq 1 - \delta, \tag{22}$$

where $\delta \in (0, 1]$ is related to the probability of the statement, and $\eta(\delta, m)$ depends only on δ and m. Given this result, we are able to give performance guarantees for the uniform mixture of $\theta_1, \ldots, \theta_m$ as

$$\mathbb{P}\left(\frac{1}{m} \sum_{t=1}^{m} \ell(\theta_t, \theta_t) \leq \hat{\epsilon}_m + \hat{\gamma}_m + \eta(\delta, m) \right) \geq 1 - \delta. \tag{23}$$

Proof. Define a function on beam trajectories. Assume that we have $0 \leq \ell(\theta, b_{1:h}) \leq u$, with $u \in \mathbb{R}$, for all $(x, y) \in \mathcal{X} \times \mathcal{Y}$ and for all beam trajectories $b_{1:h}$ through G_k, i.e., $b_1 = b_{(0)}$, $b_h \in T_k$, $b_i \in V_k$ for all $i \in [n]$, and $b_{i+1} \in N_{b_i}$ for $i \in [h-1]$. As a result, $0 \leq \ell(\theta, \theta') \leq u$ and $0 \leq \hat{\ell}(\theta, \theta') \leq u$, for all $\theta, \theta' \in \Theta$ and all $(x, y) \in \mathcal{X} \times \mathcal{Y}$. In our case,

$$\ell(\theta, b_{1:h}) = \sum_{i=1}^{h-1} \ell(\theta, b_i). \tag{24}$$

Construct the martingale sequence

$$z_t = \sum_{j=1}^{t} \left(\ell(\theta_j, \theta_j) - \hat{\ell}(\theta_j, \theta_j) \right), \tag{25}$$

for $t \in [m]$. It is simple to verify that the sequence $z_1, \ldots, z_m$ is a martingale, i.e., that we have $\mathbb{E}_{z_t | z_1, \ldots, z_{t-1}} z_t = z_{t-1}$ for all $t \in [m]$. Furthermore, we have $|z_t - z_{t-1}| \leq u$ for all $t \in [m]$, where $z_0 = 0$. The high probability result is obtained by applying the Azuma-Hoeffding inequality to the martingale sequence z_t, for $t \in \mathbb{N}$, which yields

$$\mathbb{P}\left(\frac{1}{m} \sum_{t=1}^{m} \ell(\theta_t, \theta_t) \leq \frac{1}{m} \sum_{t=1}^{m} \hat{\ell}(\theta_t, \theta_t) + u \sqrt{\frac{2 \log(1/\delta)}{m}} \right) \geq 1 - \delta. \tag{26}$$

Revisiting Equation (23), for fixed $\delta \in (0, 1]$, as m goes to infinity, we have that both $\hat{\gamma}_m$ and $\eta(\delta, m)$ go to zero, proving high probability no-regret guarantees for this setting. $\square$

E.3 Finite Sample Analysis for Arbitrary Data Collection Policies

Finally, in this section, we provide a proof of Theorem 4. All the results stated so far are for the continue data collection strategy where, at time $t \in [m]$, the whole trajectory $b_{1:h}$ is collected using the current policy $\pi(\cdot, \theta_t)$. Stop and reset data collection strategies do not necessarily collect the full trajectory under $\pi(\cdot, \theta_t)$. If a transition $(b, b') \sim \pi(\cdot, \theta_t)$ leads to a cost increase, then, the stop data collection strategy stops collecting the trajectory at b', and the reset data collection strategy, the oracle policy $\pi^*(\cdot, c^*)$ is used to sample the transition at b instead.

In this section, we relate the expected loss of $\pi(\cdot, \theta)$ on trajectories collected by a different policy π' to the expected loss of $\pi(\cdot, \theta)$ on its own trajectories. Consider the following auxiliary lemma:

Lemma 1. *Let $f : X \to \mathbb{R}$ be a function such that $f(x) \in [a, a + r]$, for $a, r \in \mathbb{R}$ and $r \geq 0$ for all $x \in X$, that can be either discrete or continuous. Let d, d' be two probability distributions over X. We have*

$$|\mathbb{E}_{x \sim d} f(x) - \mathbb{E}_{x \sim d'} f(x)| \leq r/2 ||d - d'||_1. \tag{27}$$

Proof. We prove the result for the case where X is discrete, i.e., d and d' are discrete probability distributions. The result for discrete distributions is sufficient for our purposes. Let $|X| = e$, with $e \in \mathbb{N}$, then $d, d' \in \mathbb{R}^e$. We have

$$\begin{aligned}
|\mathbb{E}_{x \sim d} f(x) - \mathbb{E}_{x \sim d'} f(x)| &= \left| \sum_{x \in X} d(x) f(x) - \sum_{x \in X} d'(x) f(x) \right| \\
&= \left| \sum_{x \in X} d(x)(f(x) - c) - \sum_{x \in X} d'(x)(f(x) - c) \right| \\
&= \left| (d - d')^T (f - c) \right| \\
&\leq ||f - c||_\infty ||d - d'||_1,
\end{aligned}$$

where c is an arbitrary constant in $\mathbb{R}$ and $f \in \mathbb{R}^e$ is the vector representation of the function. In the second equality, we use $\sum_{x \in X} d(x) = \sum_{x \in X} d'(x) = 1$. In the third equality, we express the expectations as inner products and slightly abuse notation by denoting the coordinate-wise subtraction of c from f as $f - c$. In the final inequality, we use the generalized Cauchy–Schwarz inequality for the pair of dual norms $|| \cdot ||_1$ and $|| \cdot ||_\infty$. The desired result is obtained by choosing $c = a + r/2$. $\square$

Often, $\pi' = (1 - \beta)\pi(\cdot, \theta) + \beta\pi^*(\cdot, c^*)$ for $\beta \in [0, 1]$, i.e., a probabilistic interpolation of the learned policy and the oracle policy. We do a more general analysis that will be useful to provide regret guarantees for the stop and reset data collection strategies. It is not necessarily the case that, for a roll-in policy $\pi' : V_k \to \Delta(V_k)$, there exists $\theta' \in \Theta$ such that $\pi' = \pi(\cdot, \theta')$. We modify the notation in Equation (21) to capture this fact and write

$$\ell(\theta, \pi') = \mathbb{E}_{(x,y) \sim \mathcal{D}} \mathbb{E}_{b_{1:h} \sim \pi'} \left(\sum_{i=1}^{h-1} \ell(\theta, b_i) \right). \tag{28}$$

The roll-in policies $\pi' : V_k \to \Delta(V_k)$ that we consider induce distributions over beam trajectories in G_k that have a component where the beam trajectory up to $h - 1$ can be thought as coming from $\pi(\cdot, \theta)$. For a policy π' that is somehow derived from the learned policy $\pi(\cdot, \theta)$, we write $d_{\pi'} = \alpha(\theta, x, y) d_\theta + (1 - \alpha(\theta, x, y))q$, where $d_{\pi'}$ is the distribution over trajectories induced by the roll-in policy π', d_θ is the distribution over trajectories induced by the learned policy $\pi(\cdot, \theta)$, q is the residual distribution over trajectories of the component that is not captured by d_θ, and $\alpha(\theta, x, y)$ is the probability that the trajectory up to b_{h-1} is drawn solely from $\pi(\cdot, \theta)$. For example, for the policy $\pi' = (1 - \beta)\pi(\cdot, \theta) + \beta\pi^*(\cdot, c^*)$, we have $\alpha(\theta, x, y) = (1 - \beta)^{h-2}$, where $\alpha(\theta, x, y)$ is independent of θ in this case. In this example, π', at each step of the trajectory of length h, flips a biased coin and acts with probability $1 - \beta$ according to $\pi(\cdot, \theta)$ and with probability β according to $\pi(\cdot, c^*)$.

Relating expectations We use Lemma 1 to relate $\mathbb{E}_{b_{1:h} \sim \pi(\cdot, \theta)} \left(\sum_{i=1}^{h-1} \ell(\theta, b_i) \right)$ and $\mathbb{E}_{b_{1:h} \sim \pi'} \left(\sum_{i=1}^{h-1} \ell(\theta, b_i) \right)$. We have

$$\begin{aligned}
||d_{\pi'} - d_\theta||_1 &= ||\alpha(\theta, x, y) d_\theta + (1 - \alpha(\theta, x, y))q - d_\theta||_1 \\
&= (1 - \alpha(\theta, x, y))||q - d_\theta||_1 \\
&\leq 2(1 - \alpha(\theta, x, y)),
\end{aligned}$$

where we used that $||d_1 - d_2||_1 \leq 2$ for any two distributions d_1, d_2. Revisiting Equation (27), we have

$$\mathbb{E}_{b_{1:h} \sim \pi(\cdot, \theta)} \left(\sum_{i=1}^{h-1} \ell(\theta, b_i) \right) \leq \mathbb{E}_{b_{1:h} \sim \pi'} \left(\sum_{i=1}^{h-1} \ell(\theta, b_i) \right) + u(1 - \alpha(\theta, x, y)),$$

and as a result

$$\begin{aligned} \ell(\theta, \theta) &= \mathbb{E}_{(x,y) \sim \mathcal{D}} \mathbb{E}_{b_{1:h} \sim \pi(\cdot, \theta)} \left(\sum_{i=1}^{h-1} \ell(\theta, b_i) \right) \\ &\leq \mathbb{E}_{(x,y) \sim \mathcal{D}} \left(\mathbb{E}_{b_{1:h} \sim \pi'} \left(\sum_{i=1}^{h-1} \ell(\theta, b_i) \right) + u(1 - \alpha(\theta, x, y) \right) \\ &= \ell(\theta, \pi') + u(1 - \alpha(\theta)), \end{aligned} \tag{29}$$

where we defined $\alpha(\theta) = \mathbb{E}_{(x,y) \sim \mathcal{D}} \alpha(\theta, x, y)$, i.e., the probability of sampling the beam trajectory up to time $h - 1$ solely with $\pi(\cdot, \theta)$, or equivalently, the probability of $\pi(\cdot, \theta)$ incurring no cost increases up to time $h - 1$.

Finite sample analysis with known schedules We now consider the finite sample analysis for the setting considered in this section. By arguments similar to those in Appendix E.2, we have

$$\mathbb{P} \left(\frac{1}{m} \sum_{t=1}^{m} \ell(\theta_t, \pi_t) \leq \frac{1}{m} \sum_{t=1}^{m} \hat{\ell}(\theta_t, \pi_t) + u \sqrt{\frac{2 \log(1/\delta)}{m}} \right) \geq 1 - \delta,$$

which, combining with Equation (29) implies

$$\mathbb{P} \left(\frac{1}{m} \sum_{t=1}^{m} \ell(\theta_t, \theta_t) \leq \frac{1}{m} \sum_{t=1}^{m} \hat{\ell}(\theta_t, \pi_t) + u \sqrt{\frac{2 \log(1/\delta)}{m}} + u \left(1 - \frac{1}{m} \sum_{t=1}^{m} \alpha(\theta_t) \right) \right) \geq 1 - \delta, \tag{30}$$

Equation (30) can be simplified for roll-in policies $\pi_t = (1 - \beta_t) \pi(\cdot, \theta) + \beta_t \pi^*(\cdot, c^*)$ with fixed interpolation schedules β_t, for $t \in \mathbb{N}$. For example, for $\beta_1 = 1$ for $t \in [t_0]$, for some $t_0 \in \mathbb{N}$, and $\beta_t = 0$ for $t > t_0$, we have

$$\mathbb{P} \left(\frac{1}{m} \sum_{t=1}^{m} \ell(\theta_t, \theta_t) \leq \frac{1}{m} \sum_{t=1}^{m} \hat{\ell}(\theta_t, \pi_t) + u \sqrt{\frac{2 \log(1/\delta)}{m}} + u \min \left(1, \frac{t_0}{m} \right) \right) \geq 1 - \delta. \tag{31}$$

Guarantees for the stop and reset data collection strategies The previous analysis allows us to provide regret guarantees for the reset data collection strategy. Steps in the trajectory are sampled using the learned policy $\pi(\cdot, \theta)$ when they do not result in cost increase, and sampled from $\pi^*(\cdot, c^*)$ otherwise, i.e., while sampling a trajectory $b_1, \ldots, b_i$ with $\pi(\cdot, \theta)$, if a cost increase would occur on the transition from b_i to $b' \sim \pi(b_i, \theta)$, then rather than transitioning to $b_{i+1} = b'$, we transition to $b_{i+1} \sim \pi^*(b_i, c^*)$, and continue from b_{i+1} until a terminal beam $b_h \in T_k$ is reached. In this case, $\alpha(\theta, x, y)$ is interpreted as the probability that the trajectory $b_{1:h-1}$ on the beam search G_k induced by x is sampled using only $\pi(\cdot, \theta)$, i.e., no cost increases occur up to time $h - 1$.

We can use this fact along with the previous results to obtain a regret statement for both the explicit expectation and the finite sample cases. The main difficulty is that $\alpha(\theta, x, y)$ and $\alpha(\theta)$ are not known. Again, the only way that we have access to them is through a sample estimate $\hat{\alpha}(\theta)$. We construct a martingale for this case involving both the randomness of the loss function and the reset probability.

We can use this information along with Azuma-Hoeffding inequality to give a joint concentration result. The martingale sequence that we now construct is

$$z_t = \sum_{j=1}^{t} \left(\ell(\theta_j, \pi_j) - \hat{\ell}(\theta_j, \pi_j) + u \left(1 - \alpha(\theta_j) \right) - u \left(1 - \hat{\alpha}(\theta_j) \right) \right), \tag{32}$$

which now includes the random variables of the estimator of the probability that we will reset at least once. Note that $\hat{\alpha}(\theta)$ also depends on $x, y, b_{1:h}$, which we omit for simplicity. Similarly to the martingale arguments in Equation (25), Equation (32) defines a martingale. In this case, we have $|z_t - z_{t-1}| \leq 2u$ for all $t \in [m]$, and $z_0 = 0$. Applying Azuma-Hoeffding yields a result similar to Equation (30), i.e.,

$$\mathbb{P}\left(\frac{1}{m}\sum_{t=1}^{m}\ell(\theta_t, \theta_t) \leq \frac{1}{m}\sum_{t=1}^{m}\hat{\ell}(\theta_t, \pi_t) + 2u\sqrt{\frac{2\log(1/\delta)}{m}} + u\left(1 - \frac{1}{m}\sum_{t=1}^{m}\hat{\alpha}(\theta_t)\right)\right) \geq 1 - \delta, \tag{33}$$

Even if $1/m\sum_{t=1}^{m}\hat{\alpha}(\theta_t)$ remains at some nonzero quantity as m goes to infinity, we can still give a guarantee with respect to this reset probability. Namely, if we observe that we are most of the time sampling the full trajectory with the learned policy, then we guarantee that we are not too far away from the true loss of the mixture policy.