Top-*k* Classification and Cardinality-Aware Prediction

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Abstract

We present a detailed study of top-k classification, the task of predicting the k most probable classes for an input, extending beyond single-class prediction. We demonstrate that several prevalent surrogate loss functions in multi-class classification, such as comp-sum and constrained losses, are supported by \mathcal{H} -consistency bounds with respect to the top-k loss. These bounds guarantee consistency in relation to the hypothesis set \mathcal{H} , providing stronger guarantees than Bayes-consistency due to their non-asymptotic and hypothesis-set specific nature. To address the trade-off between accuracy and cardinality k, we further introduce cardinality-aware loss functions through instance-dependent cost-sensitive learning. For these functions, we derive cost-sensitive comp-sum and constrained surrogate losses, establishing their \mathcal{H} -consistency bounds and Bayes-consistency. Minimizing these losses leads to new cardinality-aware algorithms for top-k classification. We report the results of extensive experiments on CIFAR-100, ImageNet, CIFAR-10, and SVHN datasets demonstrating the effectiveness and benefit of these algorithms.

1. Introduction

Top-k classification consists of predicting the k most likely classes for a given input, as opposed to solely predicting the single most likely class. Several compelling reasons support the adoption of top-k classification. First, it enhances accuracy by allowing the model to consider the top k predictions, accommodating uncertainty and providing a more comprehensive prediction. This proves particularly valuable in scenarios where multiple correct answers exist, such as image tagging, where a top-k classifier can identify all relevant objects in an image. Furthermore, top-k classification finds application in ranking and recommendation tasks, like suggesting the top k most relevant products in e-commerce based on user queries. The confidence scores associated with the top k predictions also serve as a means to estimate the model's uncertainty, a crucial aspect in applications requiring insight into the model's confidence level.

Ensembling can also benefit from top-k predictions as they can be combined from multiple models, contributing to improved overall performance by introducing a more robust and diverse set of predictions. In addition, top-k predictions can serve as input for downstream tasks like natural language generation or dialogue systems, enhancing the performance of these tasks by providing a broader range of potential candidates. Finally, the interpretability of the model's decision-making process is enhanced by examining the top k predicted classes, allowing users to gain insights into the rationale behind the model's predictions.

However, the top-k loss function is non-continuous and non-differentiable, and its direct optimization is intractable. Therefore, top-k classification algorithms typically resort to a surrogate loss (Lapin

et al., 2015, 2016; Berrada et al., 2018; Reddi et al., 2019; Yang and Koyejo, 2020; Thilagar et al., 2022). This raises critical questions: Which surrogate loss functions admit theoretical guarantees and efficient minimization properties? Can we design accurate top-k classification algorithms?

Unlike standard classification, this problem has been relatively unexplored. A crucial property in this context is *Bayes-consistency*, which has been extensively studied in binary and multi-class classification (Zhang, 2004a; Bartlett et al., 2006; Zhang, 2004b; Bartlett and Wegkamp, 2008). While Bayes-consistency has been explored for various top-k surrogate losses (Lapin et al., 2015, 2016, 2018; Yang and Koyejo, 2020; Thilagar et al., 2022), some face limitations. Non-convex "hinge-like" surrogates (Yang and Koyejo, 2020), inspired by ranking (Usunier et al., 2009), and polyhedral surrogates (Thilagar et al., 2022) cannot lead to effective algorithms as they cannot be efficiently computed and optimized. Negative results indicate that several convex "hinge-like" surrogates (Lapin et al., 2015, 2016, 2018) fail to achieve Bayes-consistency (Yang and Koyejo, 2020). Can we shed more light on these results?

On the positive side, it has been shown that the logistic loss (or cross-entropy loss used with the softmax activation) is a Bayes-consistent loss for top-k classification (Lapin et al., 2015; Yang and Koyejo, 2020). This prompts further inquiries: Which other smooth loss functions admit this property? More importantly, can we establish non-asymptotic and hypothesis set-specific guarantees for these surrogates, quantifying their effectiveness? Beyond top-k classification, it is important to consider the trade-off between accuracy and the cardinality k. This leads us to introduce and study cardinality-aware top-k classification algorithms, which aim to achieve a high accuracy while maintaining a small average cardinality.

This paper presents a detailed study of top-k classification. We first show that, remarkably, several widely used families of surrogate losses used in standard multi-class classification admit \mathcal{H} -consistency bounds (Awasthi et al., 2022a,b; Mao et al., 2023f,b) with respect to the top-k loss. These are strong consistency guarantees that are non-asymptotic and specific to the hypothesis set \mathcal{H} adopted, which further imply Bayes-consistency. In Section 3, we demonstrate this property for the broad family of comp-sum losses (Mao et al., 2023f), which includes the logistic loss, the sum-exponential loss, the mean absolute error loss, and the generalized cross-entropy loss. Further, in Section 4, we prove it for constrained losses, originally introduced for multi-class SVM (Lee et al., 2004), including the constrained exponential loss, constrained hinge loss and squared hinge loss, and the ρ -margin loss. These guarantees provide a strong foundation for principled algorithms in top-k classification, leveraging the minimization of these surrogate loss functions. Many of these loss functions are known for their smooth properties and favorable optimization solutions.

In Section 5, we further investigate cardinality-aware top-k classification, aiming to return an accurate top-k list with the lowest average cardinality k for each input instance. We introduce a target loss function tailored to this problem through instance-dependent cost-sensitive learning (Section 5.1). Subsequently, we present two novel surrogate loss families for optimizing this target loss: cost-sensitive comp-sum losses (Section 5.2) and cost-sensitive constrained losses (Section 5.3). These loss functions are obtained by augmenting their standard counterparts with instance-dependent cost terms. We establish \mathcal{H} -consistency bounds and thus Bayes-consistency for these cost-sensitive surrogate losses with respect to the cardinality-aware target loss. Minimizing these losses leads to new cardinality-aware algorithms for top-k classification. Section 6 presents experimental results on CIFAR-100, ImageNet, CIFAR-10, and SVHN datasets, demonstrating the effectiveness of these algorithms.

2. Preliminaries

We consider the learning task of top-k classification with $n \ge 2$ classes, that is seeking to ensure that the correct class label for a given input sample is among the top k predicted classes. We denote by $\mathfrak X$ the input space and $\mathfrak Y=[n]:=\{1,\ldots,n\}$ the label space. We denote by $\mathfrak D$ a distribution over $\mathfrak X\times \mathfrak Y$ and write $p(x,y)=\mathfrak D(Y=y\mid X=x)$ to denote the conditional probability of Y=y given X=x. We also write $p(x)=(p(x,1),\ldots,p(x,n))$ to denote the corresponding conditional probability vector.

We denote by $\ell: \mathcal{H}_{all} \times \mathcal{X} \times \mathcal{Y} \to \mathbb{R}$ a loss function defined for the family of all measurable functions \mathcal{H}_{all} . Given a hypothesis set $\mathcal{H} \subseteq \mathcal{H}_{all}$, the conditional error of a hypothesis h and the best-in-class conditional error are defined as follows:

$$\begin{split} & \mathcal{C}_{\ell}(h,x) = \underset{y|x}{\mathbb{E}} \big[\ell(h,x,y) \big] = \underset{y \in \mathcal{Y}}{\sum} p(x,y) \ell(h,x,y) \\ & \mathcal{C}^{\star}_{\ell}(\mathcal{H},x) = \inf_{h \in \mathcal{H}} \mathcal{C}_{\ell}(h,x) = \inf_{h \in \mathcal{H}} \underset{y \in \mathcal{Y}}{\sum} p(x,y) \ell(h,x,y). \end{split}$$

Accordingly, the generalization error of a hypothesis h and the best-in-class generalization error are defined by:

$$\mathcal{E}_{\ell}(h) = \underset{(x,y) \sim \mathcal{D}}{\mathbb{E}} [\ell(h,x,y)] = \mathbb{E}_{x} [\mathcal{C}_{\ell}(h,x)]$$

$$\mathcal{E}_{\ell}^{*}(\mathcal{H}) = \inf_{h \in \mathcal{H}} \mathcal{E}_{\ell}(h) = \inf_{h \in \mathcal{H}} \mathbb{E}_{x} [\mathcal{C}_{\ell}(h,x)].$$

Given a score vector $(h(x,1),\ldots,h(x,n))$ generated by hypothesis h, we sort its components in decreasing order and write $h_k(x)$ to denote the kth label, that is $h(x,h_1(x)) \geq h(x,h_2(x)) \geq \ldots \geq h(x,h_{n-1}(x)) \geq h(x,h_n(x))$. Similarly, for a given conditional probability vector $p(x) = (p(x,1),\ldots,p(x,n))$, we write $p_k(x)$ to denote the kth element in decreasing order, that is $p(x,p_1(x)) \geq p(x,p_2(x)) \geq \ldots \geq p(x,p_n(x))$. In the event of a tie for the k-th highest score or conditional probability, the label $h_k(x)$ or $p_k(x)$ is selected based on the highest index when considering the natural order of labels.

The target generalization error for top-k classification is given by the top-k loss, which is denoted by ℓ_k and defined, for any hypothesis h and $(x,y) \in \mathcal{X} \times \mathcal{Y}$ by

$$\ell_k(h, x, y) = 1_{y \notin \{h_1(x), \dots, h_k(x)\}}.$$

Thus, the loss takes value one when the correct label y is not included in the top-k predictions made by the hypothesis h, zero otherwise. In the special case where k=1, this is precisely the familiar zero-one classification loss. As with the zero-one loss, optimizing the top-k loss is NP-hard for common hypothesis sets. Therefore, an alternative surrogate loss is typically used to design learning algorithms.

A crucial property of these surrogate losses is *Bayes-consistency*. This requires that, asymptotically, nearly minimizing a surrogate loss over the family of all measurable functions leads to the near minimization of the top-k loss over the same family (Steinwart, 2007).

Definition 1 A surrogate loss ℓ is said to be Bayes-consistent with respect to the top-k loss ℓ_k if, for all given sequences of hypotheses $\{h_n\}_{n\in\mathbb{N}}\subset\mathcal{H}_{\mathrm{all}}$ and any distribution, $\lim_{n\to+\infty}\mathcal{E}_{\ell}(h_n)-\mathcal{E}_{\ell}^*(\mathcal{H}_{\mathrm{all}})=0$ implies $\lim_{n\to+\infty}\mathcal{E}_{\ell_k}(h_n)-\mathcal{E}_{\ell_k}^*(\mathcal{H}_{\mathrm{all}})=0$.

Bayes-consistency is an asymptotic guarantee and applies only to the family of all measurable functions. Recently, Awasthi, Mao, Mohri, and Zhong (2022a,b) proposed a stronger consistency guarantee, referred to as \mathcal{H} -consistency bounds. These are upper bounds on the target estimation error in terms of the surrogate estimation error that are non-asymptotic and hypothesis set-specific guarantees.

Definition 2 Given a hypothesis set \mathcal{H} , a surrogate loss ℓ is said to admit an \mathcal{H} -consistency bound with respect to the top-k loss ℓ_k if, for some non-decreasing function f, the following inequality holds for all $h \in \mathcal{H}$ and for any distribution:

$$f(\mathcal{E}_{\ell_k}(h) - \mathcal{E}_{\ell_k}^*(\mathcal{H})) \leq \mathcal{E}_{\ell}(h) - \mathcal{E}_{\ell}^*(\mathcal{H}).$$

We refer to $\mathcal{E}_{\ell_k}(h) - \mathcal{E}_{\ell_k}^*(\mathcal{H})$ as the target estimation error and $\mathcal{E}_{\ell}(h) - \mathcal{E}_{\ell}^*(\mathcal{H})$ as the surrogate estimation error. These bounds imply Bayes-consistency when $\mathcal{H} = \mathcal{H}_{all}$, by taking the limit on both sides.

We will study \mathcal{H} -consistency bounds for common surrogate losses in the multi-class classification, with respect to the top-k loss ℓ_k . A key quantity appearing in \mathcal{H} -consistency bounds is the *minimizability gap*, which measures the difference between the best-in-class generalization error and the expectation of the best-in-class conditional error, defined for a given hypothesis set \mathcal{H} and a loss function ℓ by:

$$\mathcal{M}_{\ell}(\mathcal{H}) = \mathcal{E}_{\ell}^{*}(\mathcal{H}) - \mathbb{E}_{x}[\mathcal{C}_{\ell}^{*}(\mathcal{H}, x)].$$

As shown by Mao et al. (2023f), the minimizability gap is non-negative and is upper bounded by the approximation error $\mathcal{A}_{\ell}(\mathcal{H}) = \mathcal{E}_{\ell}^*(\mathcal{H}) - \mathcal{E}_{\ell}^*(\mathcal{H}_{all})$: $0 \le \mathcal{M}_{\ell}(\mathcal{H}) \le \mathcal{A}_{\ell}(\mathcal{H})$. When $\mathcal{H} = \mathcal{H}_{all}$ or more generally $\mathcal{A}_{\ell_{log}}(\mathcal{H}) = 0$, the minimizability gap vanishes. However, in general, it is non-zero and provides a finer measure than the approximation error. Thus, \mathcal{H} -consistency bounds provide a stronger guarantee than the excess error bounds.

We will specifically study the surrogate loss families of *comp-sum losses* and *constrained losses* in multi-class classification, which have been shown in the past to benefit from \mathcal{H} -consistency bounds with respect to the zero-one classification loss, that is ℓ_k with k=1 (Awasthi et al., 2022b; Mao et al., 2023f) (see also (Mao et al., 2023c,d,e,a; Zheng et al., 2023; Mao et al., 2024a,c,b; Mohri et al., 2024)). We will significantly extend these results to top-k classification and prove \mathcal{H} -consistency bounds for these loss functions with respect to ℓ_k for any $1 \le k \le n$.

Note that another commonly used family of surrogate losses in multi-class classification is the *max losses*, which are defined through a convex function, such as the hinge loss function applied to the margin (Crammer and Singer, 2001; Awasthi et al., 2022b). However, as shown in (Awasthi et al., 2022b), no non-trivial \mathcal{H} -consistency guarantee holds for max losses with respect to ℓ_k , even when k=1.

We first characterize the best-in class conditional error and the conditional regret of top-k loss, which will be used in the analysis of \mathcal{H} -consistency bounds. We denote by $S^{[k]} = \{X \subset S \mid |X| = k\}$ the set of all k-subsets of a set S. We will study any hypothesis set that is regular.

Definition 3 Let A(n,k) be the set of ordered k-tuples with distinct elements in [n]. We say that a hypothesis set \mathcal{H} is regular for top-k classification, if the top-k predictions generated by the hypothesis set cover all possible outcomes:

$$\forall x \in \mathcal{X}, \{(\mathsf{h}_1(x), \dots, \mathsf{h}_k(x)) : h \in \mathcal{H}\} = A(n, k).$$

Common hypothesis sets such as that of linear models or neural networks, or the family of all measurable functions, are all regular for top-k classification.

Lemma 4 Assume that \mathcal{H} is regular. Then, for any $h \in \mathcal{H}$ and $x \in \mathcal{X}$, the best-in class conditional error and the conditional regret of the top-k loss can be expressed as follows:

$$\mathcal{C}_{\ell_k}^*(\mathcal{H}, x) = 1 - \sum_{i=1}^k p(x, \mathsf{p}_i(x))$$
$$\Delta \mathcal{C}_{\ell_k, \mathcal{H}}(h, x) = \sum_{i=1}^k (p(x, \mathsf{p}_i(x)) - p(x, \mathsf{h}_i(x))).$$

The proof is included in Appendix A. Note that, for k = 1, the result coincides with the known identities for standard multi-class classification with regular hypothesis sets (Awasthi et al., 2022b, Lemma 3).

As with (Awasthi et al., 2022b; Mao et al., 2023f), in the following sections, we will consider hypothesis sets that are symmetric and complete. This includes the class of linear models and neural networks typically used in practice, as well as the family of all measurable functions. We say that a hypothesis set \mathcal{H} is *symmetric* if it is independent of the ordering of labels. That is, for all $y \in \mathcal{Y}$, the scoring function $x \mapsto h(x,y)$ belongs to some real-valued family of functions \mathcal{F} . We say that a hypothesis set is *complete* if, for all $(x,y) \in \mathcal{X} \times \mathcal{Y}$, the set of scores h(x,y) can span over the real numbers, that is, $\{h(x,y): h \in \mathcal{H}\} = \mathbb{R}$. Note that any symmetric and complete hypothesis set is regular for top-k classification.

Next, we analyze the broad family of *comp-sum losses*, which includes the commonly used logistic loss (or cross-entropy loss used with the softmax activation) as a special case.

3. H-Consistency Bounds for Comp-Sum Losses

Comp-sum losses are defined as the composition of a function Φ with the sum exponential losses, as shown in (Mao et al., 2023f). For any $h \in \mathcal{H}$ and $(x, y) \in \mathcal{X} \times \mathcal{Y}$, they are expressed as

$$\ell^{\text{comp}}(h, x, y) = \Phi\left(\sum_{y'\neq y} e^{h(x, y') - h(x, y)}\right),$$

where $\Phi: \mathbb{R}_+ \to \mathbb{R}_+$ is non-decreasing. When Φ is chosen as the function $t \mapsto \log(1+t)$, $t \mapsto t$, $t \mapsto 1 - \frac{1}{1+t}$ and $t \mapsto \frac{1}{\alpha} \left(1 - \left(\frac{1}{1+t}\right)^{\alpha}\right)$, $\alpha \in (0,1)$, $\ell^{\mathrm{comp}}(h,x,y)$ coincides with the (multinomial) logistic loss ℓ_{\log} (Verhulst, 1838, 1845; Berkson, 1944, 1951), the sum-exponential loss $\ell_{\exp}^{\mathrm{comp}}$ (Weston and Watkins, 1998; Awasthi et al., 2022b), the mean absolute error loss ℓ_{mae} (Ghosh et al., 2017), and the generalized cross entropy loss ℓ_{gce} (Zhang and Sabuncu, 2018), respectively. We we will specifically study these loss functions and show that they benefit from \mathcal{H} -consistency bounds with respect to the top-k loss.

3.1. Logistic loss

We first show that the most commonly used logistic loss, defined as $\ell_{\log}(h, x, y) = \log(\sum_{y' \in \mathcal{Y}} e^{h(x, y') - h(x, y)})$, admits \mathcal{H} -consistency bounds with respect to ℓ_k .

Theorem 5 Assume that \mathcal{H} is symmetric and complete. Then, for any $1 \le k \le n$, the following \mathcal{H} -consistency bound holds for the logistic loss:

$$\mathcal{E}_{\ell_k}(h) - \mathcal{E}_{\ell_k}^*(\mathcal{H}) + \mathcal{M}_{\ell_k}(\mathcal{H}) \le k\psi^{-1} \Big(\mathcal{E}_{\ell_{\log}}(h) - \mathcal{E}_{\ell_{\log}}^*(\mathcal{H}) + \mathcal{M}_{\ell_{\log}}(\mathcal{H}) \Big),$$

where $\psi(t) = \frac{1-t}{2}\log(1-t) + \frac{1+t}{2}\log(1+t)$, $t \in [0,1]$. In the special case where $\mathcal{A}_{\ell_{\log}}(\mathcal{H}) = 0$, for any $1 \le k \le n$, the following upper bound holds:

$$\mathcal{E}_{\ell_k}(h) - \mathcal{E}_{\ell_k}^*(\mathcal{H}) \le k\psi^{-1} \Big(\mathcal{E}_{\ell_{\log}}(h) - \mathcal{E}_{\ell_{\log}}^*(\mathcal{H}) \Big).$$

The proof is included in Appendix B.1. The second part follows from the fact that when $\mathcal{A}_{\ell_{\log}}(\mathcal{H})=0$, the minimizability gap $\mathcal{M}_{\ell_{\log}}(\mathcal{H})$ vanishes. By taking the limit on both sides, Theorem 5 implies the \mathcal{H} -consistency and Bayes-consistency of logistic loss with respect to the top-k loss. It further shows that, when the estimation error of ℓ_{\log} is reduced to $\epsilon>0$, then the estimation error of ℓ_k is upper bounded by $k\psi^{-1}(\epsilon)$, which is approximately $k\sqrt{2\epsilon}$ for ϵ small.

3.2. Sum exponential loss

In this section, we prove \mathcal{H} -consistency bound guarantees for the sum-exponential loss, which is defined as $\ell_{\exp}^{\text{comp}}(h,x,y) = \sum_{y'\neq y} e^{h(x,y')-h(x,y)}$ and is widely used in multi-class boosting (Saberian and Vasconcelos, 2011; Mukherjee and Schapire, 2013; Kuznetsov et al., 2014).

Theorem 6 Assume that \mathcal{H} is symmetric and complete. Then, for any $1 \le k \le n$, the following \mathcal{H} -consistency bound holds for the sum exponential loss:

$$\mathcal{E}_{\ell_k}(h) - \mathcal{E}_{\ell_k}^*(\mathcal{H}) + \mathcal{M}_{\ell_k}(\mathcal{H}) \le k\psi^{-1} \Big(\mathcal{E}_{\ell_{\exp}}^{\text{comp}}(h) - \mathcal{E}_{\ell_{\exp}}^{*}(\mathcal{H}) + \mathcal{M}_{\ell_{\exp}}^{\text{comp}}(\mathcal{H}) \Big),$$

where $\psi(t) = 1 - \sqrt{1 - t^2}$, $t \in [0, 1]$. In the special case where $\mathcal{A}_{\ell_{\exp}^{\text{comp}}}(\mathcal{H}) = 0$, for any $1 \le k \le n$, the following bound holds:

$$\mathcal{E}_{\ell_k}(h) - \mathcal{E}_{\ell_k}^*(\mathcal{H}) \leq k\psi^{-1} \Big(\mathcal{E}_{\ell_{\text{even}}}^{\text{comp}}(h) - \mathcal{E}_{\ell_{\text{even}}}^{\text{comp}}(\mathcal{H}) \Big),$$

The proof is included in Appendix B.2. The second part follows from the fact that when $\mathcal{A}_{\ell_{\exp}^{\mathrm{comp}}}(\mathcal{H})=0$, the minimizability gap $\mathcal{M}_{\ell_{\exp}^{\mathrm{comp}}}(\mathcal{H})$ vanishes. As with the logistic loss, the sum exponential loss is Bayes-consistent and \mathcal{H} -consistent with respect to the top-k loss. Here too, when the estimation error of $\ell_{\exp}^{\mathrm{comp}}$ is reduced to ϵ , the estimation error of ℓ_k is upper bounded by $k\psi^{-1}(\epsilon)\approx k\sqrt{2\epsilon}$ for sufficiently small $\epsilon>0$.

3.3. Mean absolute error loss

The mean absolute error loss, defined as $\ell_{\text{mae}}(h, x, y) = 1 - \left[\sum_{y' \in \mathcal{Y}} e^{h(x, y') - h(x, y)}\right]^{-1}$, is known to be robust to label noise for training neural networks (Ghosh et al., 2017). The following shows that it benefits from \mathcal{H} -consistency bounds with respect to the top-k loss as well.

Theorem 7 Assume that \mathcal{H} is symmetric and complete. Then, for any $1 \le k \le n$, the following \mathcal{H} -consistency bound holds for the mean absolute error loss:

$$\mathcal{E}_{\ell_k}(h) - \mathcal{E}_{\ell_k}^*(\mathcal{H}) + \mathcal{M}_{\ell_k}(\mathcal{H}) \le kn \Big(\mathcal{E}_{\ell_{\text{mae}}}(h) - \mathcal{E}_{\ell_{\text{mae}}}^*(\mathcal{H}) + \mathcal{M}_{\ell_{\text{mae}}}(\mathcal{H}) \Big).$$

In the special case where $A_{\text{mae}}(\mathcal{H}) = 0$, for any $1 \le k \le n$, the following bound holds:

$$\mathcal{E}_{\ell_k}(h) - \mathcal{E}_{\ell_k}^*(\mathcal{H}) \le kn \left(\mathcal{E}_{\ell_{\text{mae}}}(h) - \mathcal{E}_{\ell_{\text{mae}}}^*(\mathcal{H})\right).$$

The proof is included in Appendix B.3. The second part follows from the fact that when $\mathcal{A}_{\ell_{\mathrm{mae}}}(\mathcal{H})=0$, the minimizability gap $\mathcal{M}_{\ell_{\mathrm{mae}}}(\mathcal{H})$ vanishes. As for the logistic loss and the sum exponential loss, the result implies Bayes-consistency. However, different from these losses, the bound for the mean absolute error loss is only linear: when the estimation error of ℓ_{ϵ} is reduced to ϵ , the estimation error of ℓ_{k} is upper bounded by $kn\epsilon$. The downside of this more favorable linear rate is the dependency in the number of classes and the fact that the mean absolute value loss is harder to optimize Zhang and Sabuncu (2018).

3.4. Generalized cross-entropy loss

Here, we provide \mathcal{H} -consistency bounds for the generalized cross-entropy loss, which is defined as $\ell_{\text{gce}}(h,x,y) = \frac{1}{\alpha} \Big[1 - \Big[\sum_{y' \in \mathcal{Y}} e^{h(x,y') - h(x,y)} \Big]^{-\alpha} \Big]$, $\alpha \in (0,1)$, and is a generalization of the logistic loss and mean absolute error loss for learning deep neural networks with noisy labels (Zhang and Sabuncu, 2018).

Theorem 8 Assume that \mathcal{H} is symmetric and complete. Then, for any $1 \le k \le n$, the following \mathcal{H} -consistency bound holds for the generalized cross-entropy:

$$\mathcal{E}_{\ell_k}(h) - \mathcal{E}_{\ell_k}^*(\mathcal{H}) + \mathcal{M}_{\ell_k}(\mathcal{H}) \le k\psi^{-1} \Big(\mathcal{E}_{\ell_{\text{gce}}}(h) - \mathcal{E}_{\ell_{\text{gce}}}^*(\mathcal{H}) + \mathcal{M}_{\ell_{\text{gce}}}(\mathcal{H}) \Big),$$

where $\psi(t) = \frac{1}{\alpha n^{\alpha}} \left[\left[\frac{(1+t)^{\frac{1}{1-\alpha}} + (1-t)^{\frac{1}{1-\alpha}}}{2} \right]^{1-\alpha} - 1 \right]$, for all $\alpha \in (0,1)$, $t \in [0,1]$. In the special case where $\mathcal{A}_{\ell_{\rm gce}}(\mathcal{H}) = 0$, for any $1 \le k \le n$, the following upper bound holds:

$$\mathcal{E}_{\ell_k}(h) - \mathcal{E}_{\ell_k}^*(\mathcal{H}) \le k\psi^{-1} (\mathcal{E}_{\ell_{gce}}(h) - \mathcal{E}_{\ell_{gce}}^*(\mathcal{H})),$$

The proof is presented in Appendix B.4. The second part follows from the fact that when $\mathcal{A}_{\ell_{\mathrm{gce}}}(\mathcal{H})=0$, the minimizability gap $\mathcal{M}_{\ell_{\mathrm{gce}}}(\mathcal{H})$ vanishes. The bound for the generalized crossentropy loss depends on both the number of classes n and the parameter α . When the estimation error of ℓ_{log} is reduced to ϵ , the estimation error of ℓ_k is upper bounded by $k\psi^{-1}(\epsilon)\approx k\sqrt{2n^{\alpha}\epsilon}$ for sufficiently small $\epsilon>0$. A by-product of this result is the Bayes-consistency of generalized cross-entropy.

In the proof of previous sections, we used the fact that the conditional regret of the top-k loss is the sum of k differences between two probabilities. We then upper bounded each difference with the conditional regret of the comp-sum loss, using a hypothesis based on the two probabilities. The final bound is derived by summing these differences.

3.5. Minimizability gaps and realizability

The key quantities in our \mathcal{H} -consistency bounds are the minimizability gaps, which can be upper bounded by the approximation error, or more refined terms, depending on the magnitude of the parameter space, as discussed by Mao et al. (2023f). As pointed out by these authors, these quantities, along with the functional form, can help compare different comp-sum loss functions.

Here, we further discuss the important role of minimizability gaps under the realizability assumption, and the connection with some negative results of Yang and Koyejo (2020).

Definition 9 (top-k- \mathcal{H} -realizability) A distribution \mathcal{D} over $\mathcal{X} \times \mathcal{Y}$ is top-k- \mathcal{H} -realizable, if there exists a hypothesis $h \in \mathcal{H}$ such that $\mathbb{P}_{(x,y) \sim \mathcal{D}}(h(x,y) > h(x,h_{k+1}(x))) = 1$.

This extends the \mathcal{H} -realizability definition from standard (top-1) classification (Long and Servedio, 2013) to top-k classification for any $k \ge 1$.

Definition 10 We say that a hypothesis set \mathcal{H} is closed under scaling, if it is a cone, that is for all $h \in \mathcal{H}$ and $\alpha \in \mathbb{R}_+$, $\alpha h \in \mathcal{H}$.

Definition 11 We say that a surrogate loss ℓ is realizable \mathcal{H} -consistent with respect to ℓ_k , if for all $k \in [1, n]$, and for any sequence of hypotheses $\{h_n\}_{n \in \mathbb{N}} \subset \mathcal{H}$ and top-k- \mathcal{H} -realizable distribution, $\lim_{n \to +\infty} \mathcal{E}_{\ell}(h_n) - \mathcal{E}_{\ell}^*(\mathcal{H}) = 0$ implies $\lim_{n \to +\infty} \mathcal{E}_{\ell_k}(h_n) - \mathcal{E}_{\ell_k}^*(\mathcal{H}) = 0$.

When \mathcal{H} is closed under scaling, for k=1 and all comp-sum loss functions $\ell=\ell_{\log}$, $\ell_{\exp}^{\mathrm{comp}}$, ℓ_{gce} and ℓ_{mae} , it can be shown that $\mathcal{E}_{\ell}^{*}(\mathcal{H})=\mathcal{M}_{\ell}(\mathcal{H})=0$ for any \mathcal{H} -realizable distribution. For example, for $\ell=\ell_{\log}$, by using the Lebesgue dominated convergence theorem,

$$\begin{split} \mathcal{M}_{\ell_{\log}}(\mathcal{H}) &\leq \mathcal{E}^*_{\ell_{\log}}(\mathcal{H}) \leq \lim_{\beta \to +\infty} \mathcal{E}_{\ell_{\log}}(\beta h^*) \\ &= \lim_{\beta \to +\infty} \log \left[1 + \sum_{y' \neq y} e^{\beta (h^*(x,y') - h^*(x,y))} \right] = 0 \end{split}$$

where h^* satisfies $\mathbb{P}_{(x,y)\sim \mathbb{D}}(h^*(x,y) > h^*(x,h_2(x))) = 1$ Therefore, Theorems 5, 6, 7 and 8 imply that all these loss functions are realizable \mathcal{H} -consistent with respect to ℓ_{0-1} (ℓ_k for k=1) when \mathcal{H} is closed under scaling.

Theorem 12 Assume that \mathcal{H} is closed under scaling. Then, ℓ_{log} , ℓ_{exp}^{comp} , ℓ_{gce} and ℓ_{mae} are realizable \mathcal{H} -consistent with respect to ℓ_{log} .

The formal proof is presented in Appendix C. However, for k > 1, since in the realizability assumption, h(x,y) is only larger than $h(x,\mathsf{h}_{k+1}(x))$ and can be smaller than $h(x,\mathsf{h}_1(x))$, there may exist an \mathcal{H} -realizable distribution \mathcal{D} such that $\mathcal{M}_{\ell_{\log}}(\mathcal{H}) > 0$. This explains the inconsistency of the logistic loss on top-k separable data with linear predictors, when k = 2 and n > 2, as shown in (Yang and Koyejo, 2020). More generally, the exact same example in (Yang and Koyejo, 2020, Proposition 5.1) can be used to show that all the comp-sum losses, ℓ_{\log} , $\ell_{\exp}^{\text{comp}}$, ℓ_{gce} and ℓ_{mae} are not realizable \mathcal{H} -consistent with respect to ℓ_k . Nevertheless, as previously shown, when the hypothesis set \mathcal{H} adopted is sufficiently rich such that $\mathcal{M}_{\ell}(\mathcal{H}) = 0$ or even $\mathcal{A}_{\ell}(\mathcal{H}) = 0$, they are guaranteed to be \mathcal{H} -consistent. This is typically the case in practice when using deep neural networks.

4. H-Consistency Bounds for Constrained Losses

Constrained losses are defined as a summation of a function Φ applied to the scores, subject to a constraint, as shown in (Lee et al., 2004; Awasthi et al., 2022b). For any $h \in \mathcal{H}$ and $(x, y) \in \mathcal{X} \times \mathcal{Y}$, they are expressed as

$$\ell^{\text{cstnd}}(h, x, y) = \sum_{y' \neq y} \Phi(-h(x, y')),$$

with the constraint $\sum_{y \in \mathbb{Y}} h(x,y) = 0$, where $\Phi \colon \mathbb{R} \to \mathbb{R}_+$ is non-increasing. When Φ is chosen as the function $t \mapsto e^{-t}$, $t \mapsto \max\{0, 1 - t\}^2$, $t \mapsto \max\{0, 1 - t\}$ and $t \mapsto \min\{\max\{0, 1 - t/\rho\}, 1\}$, $\rho > 0$, $\ell^{\mathrm{cstnd}}(h, x, y)$ are referred to as the constrained exponential loss $\ell^{\mathrm{cstnd}}_{\mathrm{exp}}$, the constrained squared hinge loss $\ell_{\mathrm{sq-hinge}}$, the constrained hinge loss ℓ_{hinge} , and the constrained ρ -margin loss ℓ_{ρ} , respectively (Awasthi et al., 2022b). We now study these loss functions and show that they benefit from \mathcal{H} -consistency bounds with respect to the top-k loss.

4.1. Constrained exponential loss

We first consider the constrained exponential loss, defined as $\ell_{\exp}^{\operatorname{cstnd}}(h, x, y) = \sum_{y' \neq y} e^{h(x, y')}$. The following result provide \mathcal{H} -consistency bounds for $\ell_{\exp}^{\operatorname{cstnd}}$.

Theorem 13 Assume that \mathcal{H} is symmetric and complete. Then, for any $1 \le k \le n$, the following \mathcal{H} -consistency bound holds for the constrained exponential loss:

$$\mathcal{E}_{\ell_k}(h) - \mathcal{E}_{\ell_k}^*(\mathcal{H}) + \mathcal{M}_{\ell_k}(\mathcal{H}) \leq 2k \left(\mathcal{E}_{\ell_{\exp}^{\text{cstnd}}}(h) - \mathcal{E}_{\ell_{\exp}^{\text{cstnd}}}^*(\mathcal{H}) + \mathcal{M}_{\ell_{\exp}^{\text{cstnd}}}(\mathcal{H}) \right)^{\frac{1}{2}}.$$

In the special case where $A_{\ell_{\exp}^{\operatorname{cstnd}}}(\mathfrak{H}) = 0$, for any $1 \leq k \leq n$, the following bound holds:

$$\mathcal{E}_{\ell_k}(h) - \mathcal{E}_{\ell_k}^*(\mathcal{H}) \le 2k \left(\mathcal{E}_{\ell_{\exp}}^{\text{cstnd}}(h) - \mathcal{E}_{\ell_{\exp}}^*(\mathcal{H})\right)^{\frac{1}{2}}.$$

The proof is included in Appendix D.1. The second part follows from the fact that when $\mathcal{A}_{\ell_{\exp}^{\text{estnd}}}(\mathcal{H})=0$, we have $\mathcal{M}_{\ell_{\exp}^{\text{estnd}}}(\mathcal{H})=0$. Therefore, the constrained exponential loss is \mathcal{H} -consistent and Bayes-consistent with respect to ℓ_k . If the surrogate estimation error $\mathcal{E}_{\ell_{\exp}^{\text{estnd}}}(h)-\mathcal{E}_{\ell_{\exp}^{\text{estnd}}}^*(\mathcal{H})$ is ϵ , then, the target estimation error satisfies $\mathcal{E}_{\ell_k}(h)-\mathcal{E}_{\ell_k}^*(\mathcal{H})\leq 2k\sqrt{\epsilon}$.

4.2. Constrained squared hinge loss

Here, we consider the constrained squared hinge loss, defined as $\ell_{\text{hinge}}(h, x, y) = \sum_{y' \neq y} \max\{0, 1 + h(x, y')\}^2$. The following result shows that $\ell_{\text{sq-hinge}}$ admits an \mathcal{H} -consistency bound with respect to ℓ_k .

Theorem 14 Assume that \mathcal{H} is symmetric and complete. Then, for any $1 \le k \le n$, the following \mathcal{H} -consistency bound holds for the constrained squared hinge loss:

$$\mathcal{E}_{\ell_k}(h) - \mathcal{E}_{\ell_k}^*(\mathcal{H}) + \mathcal{M}_{\ell_k}(\mathcal{H}) \leq 2k \left(\mathcal{E}_{\ell_{\text{sq-hinge}}}(h) - \mathcal{E}_{\ell_{\text{sq-hinge}}}^*(\mathcal{H}) + \mathcal{M}_{\ell_{\text{sq-hinge}}}(\mathcal{H}) \right)^{\frac{1}{2}}.$$

In the special case where $A_{\ell_{sq-hinge}}(\mathcal{H}) = 0$, for any $1 \le k \le n$, the following bound holds:

$$\mathcal{E}_{\ell_k}(h) - \mathcal{E}_{\ell_k}^*(\mathcal{H}) \le 2k \left(\mathcal{E}_{\ell_{\text{sq-hinge}}}(h) - \mathcal{E}_{\ell_{\text{sq-hinge}}}^*(\mathcal{H})\right)^{\frac{1}{2}}.$$

The proof is included in Appendix D.2. The second part follows from the fact that when the hypothesis set \mathcal{H} is sufficiently rich such that $\mathcal{A}_{\ell_{\operatorname{sq-hinge}}}(\mathcal{H}) = 0$, we have $\mathcal{M}_{\ell_{\operatorname{sq-hinge}}}(\mathcal{H}) = 0$. As with the constrained exponential loss, the bound is square root: $\mathcal{E}_{\ell_{\operatorname{sq-hinge}}}(h) - \mathcal{E}_{\ell_{\operatorname{sq-hinge}}}^*(\mathcal{H}) \leq \epsilon \Rightarrow \mathcal{E}_{\ell_k}(h) - \mathcal{E}_{\ell_k}^*(\mathcal{H}) \leq 2k\sqrt{\epsilon}$. This also implies that $\ell_{\operatorname{sq-hinge}}$ is Bayes-consistent with respect to ℓ_k .

4.3. Constrained hinge loss and ρ -margin loss

Similarly, in Appendix D.3 and D.4, we study the constrained hinge loss and the constrained ρ -margin loss, respectively. Both are shown to admit a linear \mathcal{H} -consistency bound and are Bayes-consistent with respect to ℓ_k (See Theorems 18 and 19)

5. Cardinality-Aware Loss Functions

The strong theoretical results of the previous sections demonstrate that for common hypothesis sets used in practice, comp-sum losses and constrained losses can be effectively used as surrogate losses for the target top-k loss. Nonetheless, the algorithms seeking to minimize these surrogate losses offer no guidance on the crucial task of determining the optimal cardinality k for top-k classification applications. This selection is essential for practical performance, as it directly influences the number of predicted positives.

In this section, our goal is to select a suitable top-k classifier for each input instance x. For easier input instances, the top-k set with a smaller k contains the accurate label, while it may be necessary to resort to larger k values for harder input instances. Choosing k optimally for each instance allows us to maintain accuracy while reducing the average cardinality used.

To tackle this problem, we introduce target cardinality-aware loss functions for top-k classification through instance-dependent cost-sensitive learning. Then, we propose two novel families of instance-dependant cost-sensitive surrogate losses. These loss functions are derived by augmenting the standard comp-sum losses and constrained loss with the corresponding cost. We show the benefits of these surrogate losses by proving that they admit \mathcal{H} -consistency bounds with respect to the target cardinality-aware loss functions. Minimizing these loss functions leads to a family of new cardinality-aware algorithms for top-k classification.

5.1. Instance-Dependent Cost-Sensitive Learning

Given a pre-fixed subset $\mathcal{K} = \{k_1, \dots, k_m\} \subset [n]$ of all possible choices for cardinality k, our goal is to select the best k in the sample such that the top-k loss is minimized while using a small cardinality. More precisely, let $c: \mathcal{X} \times \mathcal{K} \times \mathcal{Y}$ be a instance-dependent cost function, defined as

$$c(x,k,y) = \ell_k(h,x,y) + \lambda \mathcal{C}(k)$$

$$= 1_{y \notin \{h_1(x),\dots,h_k(x)\}} + \lambda \mathcal{C}(k)$$
(1)

for some function \mathcal{C} : $[n] \to \mathbb{R}_+$ and parameter $\lambda > 0$. Let \mathcal{R} be a hypothesis set of functions mapping from $\mathcal{X} \times \mathcal{K}$ to \mathbb{R} . The prediction of a cardinality selector $r \in \mathcal{R}$ is defined as the cardinality corresponding to the highest score, that is $\mathbf{r}(x) = \operatorname{argmax}_{k \in \mathcal{K}} r(x, k)$. In the event of a tie for the highest score, the cardinality $\mathbf{r}(x)$ is selected based on the highest index when considering the natural order of labels.

Then, our target cardinality aware loss function $\widetilde{\ell}$ can be defined as follows: for all $r \in \mathbb{R}$, $x \in \mathcal{X}$ and $y \in \mathcal{Y}$,

$$\widetilde{\ell}(r, x, y) = c(x, \mathsf{r}(x), y). \tag{2}$$

For example, when the function \mathbb{C} is chosen as $t \mapsto \log(t)$, the learner will select a cardinality selector $r \in \mathbb{R}$ that selects the best k among \mathcal{K} for each instance x, in terms of balancing the top-k loss with the magnitude of $\log(k)$.

Note that our work focuses on determining the optimal cardinality k for top-k classification, and thus the cost function defined in (1) is based on the top-k sets. However, it can potentially be generalized to other settings, such as those described in (Denis and Hebiri, 2017), by using confidence sets and learning a model r to select the optimal confidence set based on the instance.

(2) is an instance-dependent cost-sensitive learning problem. However, directly minimizing this target loss is intractable. In the next sections, we will propose novel surrogate losses to address this

problem. As a useful tool, we characterized the conditional regret of the target cardinality-aware loss function in Lemma 20, which can be found in Appendix E.

Without loss of generality, assume that $0 \le c(x, k, y) \le 1$, which can be achieved by normalizing the cost function.

5.2. Cost-Sensitive Comp-Sum Losses

We first introduce a new family of surrogate losses, that we called *cost-sensitive comp-sum losses*. They are defined as follows: for all $(r, x, y) \in \mathbb{R} \times \mathbb{X} \times \mathbb{Y}$:

$$\widetilde{\ell}^{\text{comp}}(r, x, y) = \sum_{k \in \mathcal{K}} (1 - c(x, k, y)) \ell^{\text{comp}}(r, x, k).$$

For example, when $\ell^{\rm comp}$ = $\ell_{\rm log}$, we obtain the cost-sensitive logistic loss as follows:

$$\widetilde{\ell}_{\log}(r, x, y) = \sum_{k \in \mathcal{K}} (1 - c(x, k, y)) \ell_{\log}(r, x, k)
= \sum_{k \in \mathcal{K}} (1 - c(x, k, y)) \log \left(\sum_{k' \in \mathcal{K}} e^{r(x, k') - r(x, k)} \right).$$
(3)

Similarly, we will use $\widetilde{\ell}_{exp}^{comp}$, $\widetilde{\ell}_{gce}$ and $\widetilde{\ell}_{mae}$ to denote the corresponding cost-sensitive counterparts for the sum-exponential loss, generalized cross-entropy loss and mean absolute error loss, respectively. Next, we show that these cost-sensitive surrogate loss functions benefit from \mathcal{R} -consistency bounds with respect to the target loss $\widetilde{\ell}$.

Theorem 15 Assume that \Re is symmetric and complete. Then, the following \Re -consistency bound holds for the cost-sensitive comp-sum loss:

$$\mathcal{E}_{\widetilde{\ell}}(r) - \mathcal{E}_{\widetilde{\ell}}^{*}(\mathcal{R}) + \mathcal{M}_{\widetilde{\ell}}(\mathcal{R}) \leq \gamma \left(\mathcal{E}_{\widetilde{\ell}^{\text{comp}}}(r) - \mathcal{E}_{\widetilde{\ell}^{\text{comp}}}^{*}(\mathcal{R}) + \mathcal{M}_{\widetilde{\ell}^{\text{comp}}}(\mathcal{R})\right);$$

In the special case where $\Re = \Re_{all}$, *the following holds:*

$$\mathcal{E}_{\widetilde{\ell}}(r) - \mathcal{E}_{\widetilde{\ell}}^*(\mathcal{R}_{all}) \leq \gamma \left(\mathcal{E}_{\widetilde{\ell}^{comp}}(r) - \mathcal{E}_{\widetilde{\ell}^{comp}}^*(\mathcal{R}_{all})\right),$$

where $\gamma(t) = 2\sqrt{t}$ when $\widetilde{\ell}^{comp}$ is either $\widetilde{\ell}_{log}$ or $\widetilde{\ell}^{comp}_{exp}$; $\gamma(t) = 2\sqrt{n^{\alpha}t}$ when $\widetilde{\ell}^{comp}$ is $\widetilde{\ell}_{gce}$; and $\gamma(t) = nt$ when $\widetilde{\ell}^{comp}$ is $\widetilde{\ell}_{mae}$.

The proof is included in Appendix E.1. The second part follows from the fact that when $\Re = \Re_{\text{all}}$, all the minimizability gaps vanish. In particular, Theorem 15 implies the Bayes-consistency of cost-sensitive comp-sum losses. The bounds for cost-sensitive generalized cross-entropy and mean absolute error loss depend on the number of classes, making them less favorable when n is large. As pointed out earlier, while the cost-sensitive mean absolute error loss admits a linear rate, it is difficult to optimize even in the standard classification, as reported by Zhang and Sabuncu (2018) and Mao et al. (2023f).

In the proof, we represented the comp-sum loss as a function of the softmax and introduced a softmax-dependent function S_{μ} to upper bound the conditional regret of the target cardinality-aware loss function by that of the cost-sensitive comp-sum loss. This technique is novel and differs from the approach used in the standard scenario (Section 3).

5.3. Cost-Sensitive Constrained Losses

Motivated by the formulation of constrained loss functions in the standard multi-class classification, we introduce a new family of surrogate losses, termed *cost-sensitive constrained losses*, which are defined, for all $(r, x, y) \in \mathbb{R} \times \mathbb{X} \times \mathcal{Y}$, by

$$\widetilde{\ell}^{\mathrm{cstnd}}(r, x, y) = \sum_{k \in \mathcal{K}} c(x, k, y) \Phi(-r(x, k)),$$

with the constraint that $\sum_{y \in \mathcal{Y}} r(x, y) = 0$, where $\Phi: \mathbb{R} \to \mathbb{R}_+$ is non-increasing. For example, when $\Phi(t) = e^{-t}$, we obtain the cost-sensitive constrained exponential loss as follows:

$$\widetilde{\ell}_{\mathrm{exp}}^{\mathrm{cstnd}}(r, x, y) = \sum_{k \in \mathcal{K}} c(x, k, y) e^{r(x, k)},$$

with the constraint that $\sum_{y \in \mathcal{Y}} r(x,y) = 0$. Similarly, we will use $\widetilde{\ell}_{\text{sq-hinge}}$, $\widetilde{\ell}_{\text{hinge}}$ and $\widetilde{\ell}_{\rho}$ to denote the corresponding cost-sensitive counterparts for the constrained squared hinge loss, constrained hinge loss and constrained ρ -margin loss, respectively. Next, we show that these cost-sensitive surrogate loss functions benefit from \Re -consistency bounds with respect to the target loss $\widetilde{\ell}$.

Theorem 16 Assume that \Re is symmetric and complete. Then, the following \Re -consistency bound holds for the cost-sensitive constrained loss:

$$\mathcal{E}_{\widetilde{\ell}}(r) - \mathcal{E}_{\widetilde{\ell}}^{*}(\mathcal{R}) + \mathcal{M}_{\widetilde{\ell}}(\mathcal{R}) \leq \gamma \Big(\mathcal{E}_{\widetilde{\ell}^{\operatorname{cstnd}}}(r) - \mathcal{E}_{\widetilde{\ell}^{\operatorname{cstnd}}}^{*}(\mathcal{R}) + \mathcal{M}_{\widetilde{\ell}^{\operatorname{cstnd}}}(\mathcal{R}) \Big);$$

In the special case where $\Re = \Re_{all}$ *, the following holds:*

$$\mathcal{E}_{\widetilde{\ell}}(r) - \mathcal{E}_{\widetilde{\ell}}^*(\mathcal{R}_{\mathrm{all}}) \le \gamma \left(\mathcal{E}_{\widetilde{\ell}^{\mathrm{cstnd}}}(r) - \mathcal{E}_{\widetilde{\ell}^{\mathrm{cstnd}}}^*(\mathcal{R}_{\mathrm{all}})\right),$$

where
$$\gamma(t) = 2\sqrt{t}$$
 when $\widetilde{\ell}^{cstnd}$ is either $\widetilde{\ell}^{cstnd}_{exp}$ or $\widetilde{\ell}_{sq-hinge}$; $\gamma(t) = t$ when $\widetilde{\ell}^{cstnd}$ is either $\widetilde{\ell}_{hinge}$ or $\widetilde{\ell}_{\rho}$.

The proof is included in Appendix E.2. The second part follows from the fact that when $\Re = \Re_{\rm all}$, all the minimizability gaps vanish. In particular, Theorem 16 implies the Bayes-consistency of cost-sensitive constrained losses. Note that while the constrained hinge loss and ρ -margin loss have a more favorable linear rate in the bound, their optimization may be more challenging compared to other smooth loss functions.

6. Experiments

Here, we report empirical results for our cardinality-aware algorithm and show that it consistently outperforms top-k classifiers on benchmark datasets CIFAR-10, CIFAR-100 (Krizhevsky, 2009), SVHN (Netzer et al., 2011) and ImageNet (Deng et al., 2009).

We adopted a linear model for the base model h to classify the extracted features from the datasets. We used the outputs of the second-to-last layer of ResNet (He et al., 2016) as features for the CIFAR-10, CIFAR-100 and SVHN datasets. For the ImageNet dataset, we used the CLIP (Radford et al., 2021) model to extract features. We used a two-hidden-layer feedforward neural network with ReLU activation functions (Nair and Hinton, 2010) for the cardinality selector r. Both the base model h and the cardinality selector r were trained using the Adam optimizer (Kingma and Ba, 2014), with a learning rate of 1×10^{-3} , a batch size of 128, and a weight decay of 1×10^{-5} .

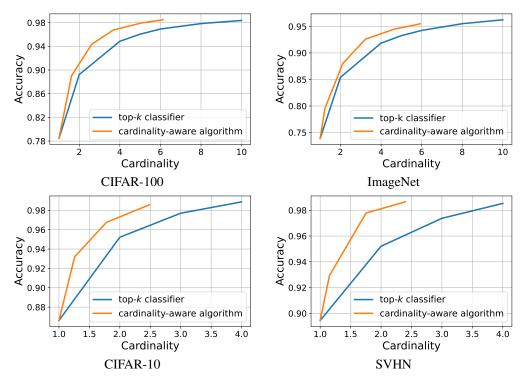


Figure 1: Accuracy versus cardinality on various datasets.

Figure 1 compares the accuracy versus cardinality curve of the cardinality-aware algorithm with that of top-k classifiers. The accuracy of a top-k classifier is measured by $\mathbb{E}_{(x,y)\sim S}[1-\ell_k(h,x,y)]$, that is the fraction of the sample in which the top-k predictions include the true label. It naturally grows as the cardinality k increases, as shown in Figure 1. The accuracy of the carnality-aware algorithms is measured by $\mathbb{E}_{(x,y)\sim S}[1-\ell_{\mathsf{r}(x)}(h,x,y)]$, that is the fraction of the sample in which the predictions selected by the model r include the true label, and the corresponding cardinality is measured by $\mathbb{E}_{(x,y)\sim S}[\mathsf{r}(x)]$, that is the average size of the selected predictions. The cardinality selector r was trained by minimizing the cost-sensitive logistic loss $\widetilde{\ell}_{\log}$ (Eq. (3)) with the cost c(x,k,y) defined as $\ell_k(h,x,y)+\lambda\mathcal{C}(k)$, where $\lambda=0.05$ and $\mathcal{C}(k)=\log(k)$. We began with a set $\mathcal{K}=\{1\}$ for the loss function and then progressively expanded it by adding choices of larger cardinality, each of which doubles the largest value currently in \mathcal{K} . In Figure 1, the largest set \mathcal{K} for the CIFAR-100 and ImageNet datasets is $\{1,2,4,8,16,32,64\}$, whereas for the CIFAR-10 and SVHN datasets, it is $\{1,2,4,8\}$. As the set \mathcal{K} expands, there is an increase in both the average cardinality and the accuracy.

Figure 1 shows that the cardinality-aware algorithm is superior across the CIFAR-100, ImageNet, CIFAR-10 and SVHN datasets. For a given cardinality k, the cardinality-aware algorithm always achieves higher accuracy than a top-k classifier. In other words, to achieve the same level of accuracy, the predictions made by the cardinality-aware algorithm can be significantly smaller in size compared to those made by the corresponding top-k classifier. In particular, on the CIFAR-100, CIFAR-10 and SVHN datasets, the cardinality-aware algorithm achieves the same accuracy (98%) as the top-k classifier while using roughly only half of the cardinality. As with the ImageNet dataset, it achieves the same accuracy (95%) as the top-k classifier with only two-thirds of the cardinality. This illustrates the effectiveness of our cardinality-aware algorithm.

7. Conclusion

We gave a series of results demonstrating that several common surrogate loss functions, including comp-sum losses and constrained losses in standard classification, benefit from \mathcal{H} -consistency bounds with respect to the top-k loss. These findings establish a theoretical and algorithmic foundation for top-k classification with a fixed cardinality k. We further introduced a cardinality-aware framework for top-k classification through cost-sensitive learning, for which we proposed cost-sensitive compsum losses and constrained losses that benefit from \mathcal{H} -consistency guarantees within this framework. This leads to principled and practical cardinality-aware algorithms for top-k classification, which we showed empirically to be very effective. Our analysis and algorithms are likely to be applicable to other similar scenarios.

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Appendix A. Proof of Lemma 4

Lemma 17 Assume that \mathcal{H} is regular. Then, for any $h \in \mathcal{H}$ and $x \in \mathcal{X}$, the best-in class conditional error and the conditional regret of the top-k loss can be expressed as follows:

$$\begin{split} & \mathcal{C}^{\star}_{\ell_k}(\mathcal{H},x) = 1 - \sum_{i=1}^k p(x,\mathsf{p}_i(x)) \\ & \Delta \mathcal{C}_{\ell_k,\mathcal{H}}(h,x) = \sum_{i=1}^k (p(x,\mathsf{p}_i(x)) - p(x,\mathsf{h}_i(x))). \end{split}$$

Proof By definition, for any $h \in \mathcal{H}$ and $x \in \mathcal{X}$, the conditional error of top-k loss can be written as

$$\mathcal{C}_{\ell_k}(h, x) = \sum_{y \in \mathcal{Y}} p(x, y) 1_{y \notin \{h_1(x), \dots, h_k(x)\}} = 1 - \sum_{i=1}^k p(x, h_i(x)).$$

By definition of the labels $p_i(x)$, which are the most likely top-k labels, $\mathcal{C}_{\ell_k}(h, x)$ is minimized for $h_i(x) = k_{\min}(x)$, $i \in [k]$. Since \mathcal{H} is regular, this choice is realizable for some $h \in \mathcal{H}$. Thus, we have

$$\mathcal{C}_{\ell_k}^*(\mathcal{H}, x) = \inf_{h \in \mathcal{H}} \mathcal{C}_{\ell_k}(h, x) = 1 - \sum_{i=1}^k p(x, \mathsf{p}_i(x)).$$

Furthermore, the calibration gap can be expressed as

$$\Delta \mathcal{C}_{\ell_k,\mathcal{H}}(h,x) = \mathcal{C}_{\ell_k}(h,x) - \mathcal{C}_{\ell_k}^*(\mathcal{H},x) = \sum_{i=1}^k (p(x,\mathsf{p}_i(x)) - p(x,\mathsf{h}_i(x))),$$

which completes the proof.

Appendix B. Proofs of \mathcal{H} -consistency bounds for comp-sum losses

B.1. Proof of Theorem 5

Theorem 5 Assume that \mathcal{H} is symmetric and complete. Then, for any $1 \le k \le n$, the following \mathcal{H} -consistency bound holds for the logistic loss:

$$\mathcal{E}_{\ell_k}(h) - \mathcal{E}_{\ell_k}^*(\mathcal{H}) + \mathcal{M}_{\ell_k}(\mathcal{H}) \le k\psi^{-1} \Big(\mathcal{E}_{\ell_{\log}}(h) - \mathcal{E}_{\ell_{\log}}^*(\mathcal{H}) + \mathcal{M}_{\ell_{\log}}(\mathcal{H}) \Big),$$

where $\psi(t) = \frac{1-t}{2}\log(1-t) + \frac{1+t}{2}\log(1+t)$, $t \in [0,1]$. In the special case where $\mathcal{A}_{\ell_{\log}}(\mathcal{H}) = 0$, for any $1 \le k \le n$, the following upper bound holds:

$$\mathcal{E}_{\ell_k}(h) - \mathcal{E}_{\ell_k}^*(\mathcal{H}) \le k\psi^{-1} \Big(\mathcal{E}_{\ell_{\log}}(h) - \mathcal{E}_{\ell_{\log}}^*(\mathcal{H})\Big).$$

Proof For logistic loss ℓ_{\log} , the conditional regret can be written as

$$\Delta C_{\ell_{\log}, \mathcal{H}}(h, x) = \sum_{y=1}^{n} p(x, y) \ell_{\log}(h, x, y) - \inf_{h \in \mathcal{H}} \sum_{y=1}^{n} p(x, y) \ell_{\log}(h, x, y)$$

$$\geq \sum_{y=1}^{n} p(x, y) \ell_{\log}(h, x, y) - \inf_{\mu \in \mathbb{R}} \sum_{y=1}^{n} p(x, y) \ell_{\log}(h_{\mu, i}, x, y),$$

where for any
$$i \in [k]$$
, $h_{\mu,i}(x,y) = \begin{cases} h(x,y), & y \notin \{p_i(x),h_i(x)\} \\ \log(e^{h(x,p_i(x))} + \mu) & y = h_i(x) \\ \log(e^{h(x,h_i(x))} - \mu) & y = p_i(x). \end{cases}$ Note that such a

choice of $h_{\mu,i}$ leads to the following equality holds:

$$\sum_{y \notin \{\mathsf{h}_i(x),\mathsf{p}_i(x)\}} p(x,y) \ell_{\log}(h,x,y) = \sum_{y \notin \{\mathsf{h}_i(x),\mathsf{p}_i(x)\}} p(x,y) \ell_{\log}(h_{\mu,i},x,y).$$

Therefore, for any $i \in [k]$, the conditional regret of logistic loss can be lower bounded as

$$\begin{split} \Delta \mathcal{C}_{\ell_{\log},\mathcal{H}}(h,x) &\geq -p(x,\mathsf{h}_i(x)) \log \left(\frac{e^{h(x,\mathsf{h}_i(x))}}{\sum_{y \in \mathcal{Y}} e^{h(x,y)}} \right) - p(x,\mathsf{p}_i(x)) \log \left(\frac{e^{h(x,\mathsf{p}_i(x))}}{\sum_{y \in \mathcal{Y}} e^{h(x,y)}} \right) \\ &+ \sup_{\mu \in \mathbb{R}} \left(p(x,\mathsf{h}_i(x)) \log \left(\frac{e^{h(x,\mathsf{p}_i(x))} + \mu}{\sum_{y \in \mathcal{Y}} e^{h(x,y)}} \right) + p(x,\mathsf{p}_i(x)) \log \left(\frac{e^{h(x,\mathsf{h}_i(x))} - \mu}{\sum_{y \in \mathcal{Y}} e^{h(x,y)}} \right) \right) \\ &= \sup_{\mu \in \mathbb{R}} \left(p(x,\mathsf{h}_i(x)) \log \left(\frac{e^{h(x,\mathsf{p}_i(x))} + \mu}{e^{h(x,\mathsf{h}_i(x))}} \right) + p(x,\mathsf{p}_i(x)) \log \left(\frac{e^{h(x,\mathsf{h}_i(x))} - \mu}{e^{h(x,\mathsf{p}_i(x))}} \right) \right). \end{split}$$

By the concavity of the function, differentiate with respect to μ , we obtain that the supremum is achieved by $\mu^* = \frac{p(x, \mathsf{h}_i(x))e^{h(x, \mathsf{h}_i(x))} - p(x, \mathsf{p}_i(x))e^{h(x, \mathsf{p}_i(x))}}{p(x, \mathsf{h}_i(x)) + p(x, \mathsf{p}_i(x))}$. Plug in μ^* , we obtain

$$\begin{split} &\Delta \mathcal{C}_{\ell_{\log},\mathcal{H}}(h,x) \\ &\geq p(x,\mathsf{h}_i(x)) \log \left(\frac{p(x,\mathsf{h}_i(x))}{p(x,\mathsf{h}_i(x)) + p(x,\mathsf{p}_i(x))} \frac{e^{h(x,\mathsf{h}_i(x))} + e^{h(x,\mathsf{p}_i(x))}}{e^{h(x,\mathsf{h}_i(x))}} \right) \\ &\quad + p(x,\mathsf{p}_i(x)) \log \left(\frac{p(x,\mathsf{p}_i(x))}{p(x,\mathsf{h}_i(x)) + p(x,\mathsf{p}_i(x))} \frac{e^{h(x,\mathsf{h}_i(x))} + e^{h(x,\mathsf{p}_i(x))}}{e^{h(x,\mathsf{h}_i(x))}} \right) \\ &\geq p(x,\mathsf{h}_i(x)) \log \left(\frac{2p(x,\mathsf{h}_i(x))}{p(x,\mathsf{h}_i(x)) + p(x,\mathsf{p}_i(x))} \right) + p(x,\mathsf{p}_i(x)) \log \left(\frac{2p(x,\mathsf{p}_i(x))}{p(x,\mathsf{h}_i(x)) + p(x,\mathsf{p}_i(x))} \right). \end{split}$$
(minimum is achieved when $h(x,\mathsf{h}_i(x)) = h(x,\mathsf{p}_i(x))$

let $S_i = p(x, p_i(x)) + p(x, h_i(x))$ and $\Delta_i = p(x, p_i(x)) - p(x, h_i(x))$, we have

$$\begin{split} \Delta \mathcal{C}_{\ell_{\log},\mathcal{H}}(h,x) &\geq \frac{S_i - \Delta_i}{2} \log(\frac{S_i - \Delta_i}{S_i}) + \frac{S_i + \Delta_i}{2} \log(\frac{S_i + \Delta_i}{S_i}) \\ &\geq \frac{1 - \Delta_i}{2} \log(1 - \Delta_i) + \frac{1 + \Delta_i}{2} \log(1 + \Delta_i) \quad \text{(minimum is achieved when } S_i = 1) \\ &= \psi(p(x,\mathsf{p}_i(x)) - p(x,\mathsf{h}_i(x))), \end{split}$$

where $\psi(t) = \frac{1-t}{2}\log(1-t) + \frac{1+t}{2}\log(1+t)$, $t \in [0,1]$. Therefore, the conditional regret of the top-k loss can be upper bounded as follows:

$$\Delta \mathcal{C}_{\ell_k,\mathcal{H}}(h,x) = \sum_{i=1}^k (p(x,\mathsf{p}_i(x)) - p(x,\mathsf{h}_i(x))) \le k\psi^{-1} (\Delta \mathcal{C}_{\ell_{\log},\mathcal{H}}(h,x)).$$

By the concavity of ψ^{-1} , take expectations on both sides of the preceding equation, we obtain

$$\mathcal{E}_{\ell_k}(h) - \mathcal{E}_{\ell_k}^*(\mathcal{H}) + \mathcal{M}_{\ell_k}(\mathcal{H}) \le k\psi^{-1} \Big(\mathcal{E}_{\ell_{\log}}(h) - \mathcal{E}_{\ell_{\log}}^*(\mathcal{H}) + \mathcal{M}_{\ell_{\log}}(\mathcal{H}) \Big).$$

The second part follows from the fact that when $\mathcal{A}_{\ell_{\log}}(\mathcal{H}) = 0$, the minimizability gap $\mathcal{M}_{\ell_{\log}}(\mathcal{H})$ vanishes.

B.2. Proof of Theorem 6

Theorem 6 Assume that \mathcal{H} is symmetric and complete. Then, for any $1 \leq k \leq n$, the following \mathcal{H} -consistency bound holds for the sum exponential loss:

$$\mathcal{E}_{\ell_k}(h) - \mathcal{E}_{\ell_k}^*(\mathcal{H}) + \mathcal{M}_{\ell_k}(\mathcal{H}) \leq k\psi^{-1} \Big(\mathcal{E}_{\ell_{\exp}}^{\text{comp}}(h) - \mathcal{E}_{\ell_{\exp}}^*(\mathcal{H}) + \mathcal{M}_{\ell_{\exp}}^{\text{comp}}(\mathcal{H}) \Big),$$

where $\psi(t) = 1 - \sqrt{1 - t^2}$, $t \in [0, 1]$. In the special case where $\mathcal{A}_{\ell_{\exp}^{\text{comp}}}(\mathcal{H}) = 0$, for any $1 \le k \le n$, the following bound holds:

$$\mathcal{E}_{\ell_k}(h) - \mathcal{E}_{\ell_k}^*(\mathcal{H}) \le k\psi^{-1} \Big(\mathcal{E}_{\ell_{\exp}}^{\text{comp}}(h) - \mathcal{E}_{\ell_{\exp}}^{\text{comp}}(\mathcal{H}) \Big),$$

Proof For sum exponential loss $\ell_{\rm exp}^{\rm comp}$, the conditional regret can be written as

$$\begin{split} \Delta \mathcal{C}_{\ell_{\exp}^{\text{comp}},\mathcal{H}}(h,x) &= \sum_{y=1}^{n} p(x,y) \ell_{\exp}^{\text{comp}}(h,x,y) - \inf_{h \in \mathcal{H}} \sum_{y=1}^{n} p(x,y) \ell_{\exp}^{\text{comp}}(h,x,y) \\ &\geq \sum_{y=1}^{n} p(x,y) \ell_{\exp}^{\text{comp}}(h,x,y) - \inf_{\mu \in \mathbb{R}} \sum_{y=1}^{n} p(x,y) \ell_{\exp}^{\text{comp}}(h_{\mu,i},x,y), \end{split}$$

where for any
$$i \in [k]$$
, $h_{\mu,i}(x,y) = \begin{cases} h(x,y), & y \notin \{\mathsf{p}_i(x),\mathsf{h}_i(x)\} \\ \log \left(e^{h(x,\mathsf{p}_i(x))} + \mu\right) & y = \mathsf{h}_i(x) \\ \log \left(e^{h(x,\mathsf{h}_i(x))} - \mu\right) & y = \mathsf{p}_i(x). \end{cases}$ Note that such a

choice of $h_{\mu,i}$ leads to the following equality holds:

$$\sum_{y \notin \{\mathsf{h}_i(x),\mathsf{p}_i(x)\}} p(x,y) \ell_{\exp}^{\mathrm{comp}}(h,x,y) = \sum_{y \notin \{\mathsf{h}_i(x),\mathsf{p}_i(x)\}} p(x,y) \ell_{\exp}^{\mathrm{comp}}(h_{\mu,i},x,y).$$

Therefore, for any $i \in [k]$, the conditional regret of sum exponential loss can be lower bounded as

$$\Delta \mathcal{C}_{\ell_{\exp}^{\text{comp}},\mathcal{H}}(h,x) \geq \sum_{y' \in \mathcal{Y}} \exp(h(x,y')) \left[\frac{p(x,\mathsf{h}_i(x))}{\exp(h(x,\mathsf{h}_i(x)))} + \frac{p(x,\mathsf{p}_i(x))}{\exp(h(x,\mathsf{p}_i(x)))} \right] \\ + \sup_{\mu \in \mathbb{R}} \left(-\sum_{y' \in \mathcal{Y}} \exp(h(x,y')) \left[\frac{p(x,\mathsf{h}_i(x))}{\exp(h(x,\mathsf{p}_i(x))) + \mu} + \frac{p(x,\mathsf{p}_i(x))}{\exp(h(x,\mathsf{h}_i(x))) - \mu} \right] \right).$$

By the concavity of the function, differentiate with respect to μ , we obtain that the supremum is achieved by $\mu^* = \frac{\exp[h(x, \mathsf{h}_i(x))]\sqrt{p(x, \mathsf{h}_i(x))} - \exp[h(x, \mathsf{p}_i(x))]\sqrt{p(x, \mathsf{p}_i(x))}}{\sqrt{p(x, \mathsf{h}_i(x))} + \sqrt{p(x, \mathsf{p}_i(x))}}$. Plug in μ^* , we obtain

$$\Delta \mathcal{C}_{\ell_{\exp}^{\text{comp}},\mathcal{H}}(h,x)$$

$$\geq \sum_{y' \in \mathcal{Y}} \exp\left(h(x,y')\right) \left[\frac{p(x,\mathsf{h}_i(x))}{\exp(h(x,\mathsf{h}_i(x)))} + \frac{p(x,\mathsf{p}_i(x))}{\exp(h(x,\mathsf{p}_i(x)))} - \frac{\left(\sqrt{p(x,\mathsf{h}_i(x))} + \sqrt{p(x,\mathsf{p}_i(x))}\right)^2}{\exp(h(x,\mathsf{p}_i(x))) + \exp(h(x,\mathsf{h}_i(x)))} \right] \\ \geq \left[1 + \frac{\exp(h(x,\mathsf{p}_i(x)))}{\exp(h(x,\mathsf{h}_i(x)))} \right] p(x,\mathsf{h}_i(x)) + \left[1 + \frac{\exp(h(x,\mathsf{h}_i(x)))}{\exp(h(x,\mathsf{p}_i(x)))} \right] p(x,\mathsf{p}_i(x)) - \left(\sqrt{p(x,\mathsf{h}_i(x))} + \sqrt{p(x,\mathsf{p}_i(x))}\right)^2 \\ \left(\sum_{y' \in \mathcal{Y}} \exp(h(x,y')) \geq \exp(h(x,\mathsf{p}_i(x))) + \exp(h(x,\mathsf{h}_i(x))) + \exp(h(x,\mathsf{h}_i(x))) \right) \\ \geq 2p(x,\mathsf{h}_i(x)) + 2p(x,\mathsf{p}_i(x)) - \left(\sqrt{p(x,\mathsf{h}_i(x))} + \sqrt{p(x,\mathsf{p}_i(x))}\right)^2.$$
(minimum is attained when $\frac{\exp(h(x,\mathsf{p}_i(x)))}{\exp(h(x,\mathsf{h}_i(x)))} = 1$)

let $S_i = p(x, p_i(x)) + p(x, h_i(x))$ and $\Delta_i = p(x, p_i(x)) - p(x, h_i(x))$, we have

$$\begin{split} \Delta \mathcal{C}_{\ell_{\exp}^{\text{comp}},\mathcal{H}}(h,x) &\geq 2S_i - \left(\sqrt{\frac{S_i + \Delta_i}{2}} + \sqrt{\frac{S_i - \Delta_i}{2}}\right)^2 \\ &\geq 2 \left[1 - \left[\frac{\left(1 + \Delta_i\right)^{\frac{1}{2}} + \left(1 - \Delta_i\right)^{\frac{1}{2}}}{2}\right]^2\right] \qquad \text{(minimum is achieved when } S_i = 1) \\ &= 1 - \sqrt{1 - (\Delta_i)^2} \\ &= \psi(p(x, \mathsf{p}_i(x)) - p(x, \mathsf{h}_i(x))), \end{split}$$

where $\psi(t) = 1 - \sqrt{1 - t^2}$, $t \in [0, 1]$. Therefore, the conditional regret of the top-k loss can be upper bounded as follows:

$$\Delta \mathcal{C}_{\ell_k,\mathcal{H}}(h,x) = \sum_{i=1}^k (p(x,\mathsf{p}_i(x)) - p(x,\mathsf{h}_i(x))) \le k\psi^{-1} \Big(\Delta \mathcal{C}_{\ell_{\exp}^{\mathrm{comp}},\mathcal{H}}(h,x)\Big).$$

By the concavity of ψ^{-1} , take expectations on both sides of the preceding equation, we obtain

$$\mathcal{E}_{\ell_k}(h) - \mathcal{E}_{\ell_k}^*(\mathcal{H}) + \mathcal{M}_{\ell_k}(\mathcal{H}) \leq k\psi^{-1} \Big(\mathcal{E}_{\ell_{\exp}}^{\text{comp}}(h) - \mathcal{E}_{\ell_{\exp}}^{\text{comp}}(\mathcal{H}) + \mathcal{M}_{\ell_{\exp}}^{\text{comp}}(\mathcal{H}) \Big).$$

The second part follows from the fact that when $\mathcal{A}_{\ell_{\exp}^{\text{comp}}}(\mathcal{H}) = 0$, the minimizability gap $\mathcal{M}_{\ell_{\exp}^{\text{comp}}}(\mathcal{H})$ vanishes.

B.3. Proof of Theorem 7

Theorem 7 Assume that \mathcal{H} is symmetric and complete. Then, for any $1 \le k \le n$, the following \mathcal{H} -consistency bound holds for the mean absolute error loss:

$$\mathcal{E}_{\ell_k}(h) - \mathcal{E}_{\ell_k}^*(\mathcal{H}) + \mathcal{M}_{\ell_k}(\mathcal{H}) \leq kn \Big(\mathcal{E}_{\ell_{\mathrm{mae}}}(h) - \mathcal{E}_{\ell_{\mathrm{mae}}}^*(\mathcal{H}) + \mathcal{M}_{\ell_{\mathrm{mae}}}(\mathcal{H})\Big).$$

In the special case where $A_{\text{mae}}(\mathcal{H}) = 0$, for any $1 \le k \le n$, the following bound holds:

$$\mathcal{E}_{\ell_k}(h) - \mathcal{E}_{\ell_k}^*(\mathcal{H}) \le kn \left(\mathcal{E}_{\ell_{\text{mae}}}(h) - \mathcal{E}_{\ell_{\text{mae}}}^*(\mathcal{H})\right).$$

Proof For mean absolute error loss ℓ_{mae} , the conditional regret can be written as

$$\begin{split} \Delta \mathcal{C}_{\ell_{\text{mae}},\mathcal{H}}(h,x) &= \sum_{y=1}^{n} p(x,y) \ell_{\text{mae}}(h,x,y) - \inf_{h \in \mathcal{H}} \sum_{y=1}^{n} p(x,y) \ell_{\text{mae}}(h,x,y) \\ &\geq \sum_{y=1}^{n} p(x,y) \ell_{\text{mae}}(h,x,y) - \inf_{\mu \in \mathbb{R}} \sum_{y=1}^{n} p(x,y) \ell_{\text{mae}}(h_{\mu,i},x,y), \end{split}$$

where for any $i \in [k]$, $h_{\mu,i}(x,y) = \begin{cases} h(x,y), & y \notin \{\mathsf{p}_i(x),\mathsf{h}_i(x)\} \\ \log \left(e^{h(x,\mathsf{p}_i(x))} + \mu\right) & y = \mathsf{h}_i(x) \\ \log \left(e^{h(x,\mathsf{h}_i(x))} - \mu\right) & y = \mathsf{p}_i(x). \end{cases}$ Note that such a

choice of $h_{\mu,i}$ leads to the following equality holds:

$$\sum_{y \notin \{\mathsf{h}_i(x),\mathsf{p}_i(x)\}} p(x,y) \ell_{\mathrm{mae}}(h,x,y) = \sum_{y \notin \{\mathsf{h}_i(x),\mathsf{p}_i(x)\}} p(x,y) \ell_{\mathrm{mae}}(h_{\mu,i},x,y).$$

Therefore, for any $i \in [k]$, the conditional regret of mean absolute error loss can be lower bounded as

$$\begin{split} &\Delta \mathcal{C}_{\ell_{\text{mae}},\mathcal{H}}(h,x) \\ &\geq p(x,\mathsf{h}_i(x)) \bigg(1 - \frac{\exp(h(x,\mathsf{h}_i(x)))}{\sum_{y' \in \mathcal{Y}} \exp(h(x,y'))} \bigg) + p(x,\mathsf{p}_i(x)) \bigg(1 - \frac{\exp(h(x,\mathsf{p}_i(x)))}{\sum_{y' \in \mathcal{Y}} \exp(h(x,y'))} \bigg) \\ &+ \sup_{\mu \in \mathbb{R}} \bigg(-p(x,\mathsf{p}_i(x)) \bigg(1 - \frac{\exp(h(x,\mathsf{h}_i(x))) - \mu}{\sum_{y' \in \mathcal{Y}} \exp(h(x,y'))} \bigg) - p(x,\mathsf{h}_i(x)) \bigg(1 - \frac{\exp(h(x,\mathsf{p}_i(x))) + \mu}{\sum_{y' \in \mathcal{Y}} \exp(h(x,y'))} \bigg) \bigg). \end{split}$$

By the concavity of the function, differentiate with respect to μ , we obtain that the supremum is achieved by $\mu^* = -\exp[h(x, p_i(x))]$. Plug in μ^* , we obtain

$$\begin{split} &\Delta \mathcal{C}_{\ell_{\text{mae}},\mathcal{H}}(h,x) \\ &\geq p(x,\mathsf{p}_i(x)) \frac{\exp(h(x,\mathsf{h}_i(x)))}{\sum_{y' \in \mathcal{Y}} \exp(h(x,y'))} - p(x,\mathsf{h}_i(x)) \frac{\exp(h(x,\mathsf{h}_i(x)))}{\sum_{y' \in \mathcal{Y}} \exp(h(x,y'))} \\ &\geq \frac{1}{n} (p(x,\mathsf{p}_i(x)) - p(x,\mathsf{h}_i(x))) \qquad \qquad \qquad (\frac{\exp(h(x,\mathsf{h}_i(x)))}{\sum_{y' \in \mathcal{Y}} \exp(h(x,y'))} \geq \frac{1}{n}) \end{split}$$

Therefore, the conditional regret of the top-k loss can be upper bounded as follows:

$$\Delta \mathcal{C}_{\ell_k,\mathcal{H}}(h,x) = \sum_{i=1}^k (p(x,\mathsf{p}_i(x)) - p(x,\mathsf{h}_i(x))) \le kn \big(\Delta \mathcal{C}_{\ell_{\mathrm{mae}},\mathcal{H}}(h,x)\big).$$

Take expectations on both sides of the preceding equation, we obtain

$$\mathcal{E}_{\ell_k}(h) - \mathcal{E}_{\ell_k}^*(\mathcal{H}) + \mathcal{M}_{\ell_k}(\mathcal{H}) \leq kn (\mathcal{E}_{\ell_{\max}}(h) - \mathcal{E}_{\ell_{\max}}^*(\mathcal{H}) + \mathcal{M}_{\ell_{\max}}(\mathcal{H})).$$

The second part follows from the fact that when $\mathcal{A}_{\ell_{\mathrm{mae}}}(\mathcal{H}) = 0$, the minimizability gap $\mathcal{M}_{\ell_{\mathrm{mae}}}(\mathcal{H})$ vanishes.

B.4. Proof of Theorem 8

Theorem 8 Assume that \mathcal{H} is symmetric and complete. Then, for any $1 \leq k \leq n$, the following \mathcal{H} -consistency bound holds for the generalized cross-entropy:

$$\mathcal{E}_{\ell_k}(h) - \mathcal{E}_{\ell_k}^*(\mathcal{H}) + \mathcal{M}_{\ell_k}(\mathcal{H}) \le k\psi^{-1} \Big(\mathcal{E}_{\ell_{\text{gce}}}(h) - \mathcal{E}_{\ell_{\text{gce}}}^*(\mathcal{H}) + \mathcal{M}_{\ell_{\text{gce}}}(\mathcal{H}) \Big),$$

where $\psi(t) = \frac{1}{\alpha n^{\alpha}} \left[\left[\frac{(1+t)^{\frac{1}{1-\alpha}} + (1-t)^{\frac{1}{1-\alpha}}}{2} \right]^{1-\alpha} - 1 \right]$, for all $\alpha \in (0,1)$, $t \in [0,1]$. In the special case where $\mathcal{A}_{\ell_{gce}}(\mathcal{H}) = 0$, for any $1 \le k \le n$, the following upper bound holds:

$$\mathcal{E}_{\ell_k}(h) - \mathcal{E}_{\ell_k}^*(\mathcal{H}) \le k\psi^{-1} \left(\mathcal{E}_{\ell_{gce}}(h) - \mathcal{E}_{\ell_{gce}}^*(\mathcal{H})\right),$$

Proof For generalized cross-entropy loss $\ell_{\rm gce}$, the conditional regret can be written as

$$\begin{split} &\Delta \mathcal{C}_{\ell_{\text{gce}},\mathcal{H}}(h,x) \\ &= \sum_{y=1}^{n} p(x,y) \ell_{\text{gce}}(h,x,y) - \inf_{h \in \mathcal{H}} \sum_{y=1}^{n} p(x,y) \ell_{\text{gce}}(h,x,y) \\ &\geq \sum_{y=1}^{n} p(x,y) \ell_{\text{gce}}(h,x,y) - \inf_{\mu \in \mathbb{R}} \sum_{y=1}^{n} p(x,y) \ell_{\text{gce}}(h_{\mu,i},x,y), \end{split}$$

where for any $i \in [k]$, $h_{\mu,i}(x,y) = \begin{cases} h(x,y), & y \notin \{\mathsf{p}_i(x),\mathsf{h}_i(x)\} \\ \log \left(e^{h(x,\mathsf{p}_i(x))} + \mu\right) & y = \mathsf{h}_i(x) \\ \log \left(e^{h(x,\mathsf{h}_i(x))} - \mu\right) & y = \mathsf{p}_i(x). \end{cases}$ Note that such a

choice of $h_{\mu,i}$ leads to the following equality holds

$$\sum_{y \notin \{\mathsf{h}_i(x),\mathsf{p}_i(x)\}} p(x,y) \ell_{\mathrm{gce}}(h,x,y) = \sum_{y \notin \{\mathsf{h}_i(x),\mathsf{p}_i(x)\}} p(x,y) \ell_{\mathrm{gce}}(h_{\mu,i},x,y).$$

Therefore, for any $i \in [k]$, the conditional regret of generalized cross-entropy loss can be lower bounded as

$$\begin{split} &\alpha\Delta\mathcal{C}_{\ell_{\text{gce}},\mathcal{H}}(h,x)\\ &\geq p(x,\mathsf{h}_{i}(x))\bigg(1-\bigg[\frac{\exp(h(x,\mathsf{h}_{i}(x)))}{\sum_{y'\in\mathcal{Y}}\exp(h(x,y'))}\bigg]^{\alpha}\bigg)+p(x,\mathsf{p}_{i}(x))\bigg(1-\bigg[\frac{\exp(h(x,\mathsf{p}_{i}(x)))}{\sum_{y'\in\mathcal{Y}}\exp(h(x,y'))}\bigg]^{\alpha}\bigg)\\ &+\sup_{\mu\in\mathbb{R}}\bigg(-p(x,\mathsf{h}_{i}(x))\bigg(1-\bigg[\frac{\exp(h(x,\mathsf{p}_{i}(x)))+\mu}{\sum_{y'\in\mathcal{Y}}\exp(h(x,y'))}\bigg]^{\alpha}\bigg)-p(x,\mathsf{p}_{i}(x))\bigg(1-\bigg[\frac{\exp(h(x,\mathsf{h}_{i}(x)))-\mu}{\sum_{y'\in\mathcal{Y}}\exp(h(x,y'))}\bigg]^{\alpha}\bigg)\bigg). \end{split}$$

By the concavity of the function, differentiate with respect to μ , we obtain that the supremum is achieved by $\mu^* = \frac{\exp[h(x,\mathsf{h}_i(x))]p(x,\mathsf{p}_i(x))^{\frac{1}{\alpha-1}} - \exp[h(x,\mathsf{p}_i(x))]p(x,\mathsf{h}_i(x))^{\frac{1}{\alpha-1}}}{p(x,\mathsf{h}_i(x))^{\frac{1}{\alpha-1}} + p(x,\mathsf{p}_i(x))^{\frac{1}{\alpha-1}}}$. Plug in μ^* , we obtain

$$\alpha \Delta \mathcal{C}_{\ell_{\text{gce}},\mathcal{H}}(h,x)$$

$$\geq p(x,\mathsf{h}_i(x)) \Bigg[\frac{[\exp(h(x,\mathsf{h}_i(x))) + \exp(h(x,\mathsf{p}_i(x)))]p(x,\mathsf{p}_i(x))^{\frac{1}{\alpha-1}}}{\sum_{y' \in \mathbb{Y}} \exp(h(x,y')) \Big[p(x,\mathsf{h}_i(x))^{\frac{1}{\alpha-1}} + p(x,\mathsf{p}_i(x))^{\frac{1}{\alpha-1}}\Big]}^{\alpha} - p(x,\mathsf{h}_i(x)) \Big[\frac{\exp(h(x,\mathsf{h}_i(x)))}{\sum_{y' \in \mathbb{Y}} \exp(h(x,y'))} \Big]^{\alpha} \\ + p(x,\mathsf{p}_i(x)) \Bigg[\frac{[\exp(h(x,\mathsf{h}_i(x))) + \exp(h(x,\mathsf{p}_i(x)))]p(x,\mathsf{h}_i(x))^{\frac{1}{\alpha-1}}}{\sum_{y' \in \mathbb{Y}} \exp(h(x,y')) \Big[p(x,\mathsf{h}_i(x))^{\frac{1}{\alpha-1}} + p(x,\mathsf{p}_i(x))^{\frac{1}{\alpha-1}}\Big]}^{\alpha} - p(x,\mathsf{p}_i(x)) \Bigg[\frac{\exp(h(x,\mathsf{p}_i(x)))}{\sum_{y' \in \mathbb{Y}} \exp(h(x,y'))} \Big]^{\alpha} \\ \geq \frac{1}{n^{\alpha}} \Bigg(p(x,\mathsf{h}_i(x)) \Bigg[\frac{2p(x,\mathsf{p}_i(x))^{\frac{1}{\alpha-1}}}{p(x,\mathsf{h}_i(x))^{\frac{1}{\alpha-1}} + p(x,\mathsf{p}_i(x))^{\frac{1}{\alpha-1}}} \Big]^{\alpha} - p(x,\mathsf{h}_i(x)) \Bigg) \\ + \frac{1}{n^{\alpha}} \Bigg(p(x,\mathsf{p}_i(x)) \Bigg[\frac{2p(x,\mathsf{h}_i(x))^{\frac{1}{\alpha-1}} + p(x,\mathsf{p}_i(x))^{\frac{1}{\alpha-1}}}{p(x,\mathsf{h}_i(x))^{\frac{1}{\alpha-1}} + p(x,\mathsf{p}_i(x))^{\frac{1}{\alpha-1}}} \Bigg]^{\alpha} - p(x,\mathsf{p}_i(x)) \Bigg) \\ + \frac{1}{n^{\alpha}} \Bigg(p(x,\mathsf{p}_i(x)) \Bigg[\frac{2p(x,\mathsf{h}_i(x))^{\frac{1}{\alpha-1}} + p(x,\mathsf{p}_i(x))^{\frac{1}{\alpha-1}}}{p(x,\mathsf{h}_i(x))^{\frac{1}{\alpha-1}} + p(x,\mathsf{p}_i(x))^{\frac{1}{\alpha-1}}} \Bigg]^{\alpha} - p(x,\mathsf{p}_i(x)) \Bigg) \\ + \frac{1}{n^{\alpha}} \Bigg(p(x,\mathsf{p}_i(x)) \Bigg[\frac{2p(x,\mathsf{h}_i(x))^{\frac{1}{\alpha-1}} + p(x,\mathsf{p}_i(x))^{\frac{1}{\alpha-1}}}{p(x,\mathsf{h}_i(x))^{\frac{1}{\alpha-1}} + p(x,\mathsf{p}_i(x))^{\frac{1}{\alpha-1}}} \Bigg]^{\alpha} - p(x,\mathsf{p}_i(x)) \Bigg) \\ + \frac{1}{n^{\alpha}} \Bigg(p(x,\mathsf{p}_i(x)) \Bigg[\frac{2p(x,\mathsf{h}_i(x))^{\frac{1}{\alpha-1}} + p(x,\mathsf{p}_i(x))^{\frac{1}{\alpha-1}}}{p(x,\mathsf{h}_i(x))^{\frac{1}{\alpha-1}} + p(x,\mathsf{p}_i(x))^{\frac{1}{\alpha-1}}} \Bigg]^{\alpha} - p(x,\mathsf{p}_i(x)) \Bigg] \\ + \frac{1}{n^{\alpha}} \Bigg(p(x,\mathsf{p}_i(x)) \Bigg[\frac{2p(x,\mathsf{h}_i(x))^{\frac{1}{\alpha-1}} + p(x,\mathsf{p}_i(x))^{\frac{1}{\alpha-1}}}{p(x,\mathsf{h}_i(x))^{\frac{1}{\alpha-1}} + p(x,\mathsf{p}_i(x))^{\frac{1}{\alpha-1}}} \Bigg]^{\alpha} - p(x,\mathsf{p}_i(x)) \Bigg]$$

let $S_i = p(x, p_i(x)) + p(x, h_i(x))$ and $\Delta_i = p(x, p_i(x)) - p(x, h_i(x))$, we have

$$\Delta \mathcal{C}_{\ell_{\text{gce}},\mathcal{H}}(h,x) \ge \frac{1}{\alpha n^{\alpha}} \left(\left[\frac{\left(S_{i} + \Delta_{i}\right)^{\frac{1}{1-\alpha}} + \left(S_{i} - \Delta_{i}\right)^{\frac{1}{1-\alpha}}}{2} \right]^{1-\alpha} - S_{i} \right)$$

$$\ge \frac{1}{\alpha n^{\alpha}} \left(\left[\frac{\left(1 + \Delta_{i}\right)^{\frac{1}{1-\alpha}} + \left(1 - \Delta_{i}\right)^{\frac{1}{1-\alpha}}}{2} \right]^{1-\alpha} - 1 \right)$$

(minimum is achieved when $S_i = 1$)

$$= \psi(p(x, \mathsf{p}_i(x)) - p(x, \mathsf{h}_i(x))),$$

where $\psi(t) = \frac{1}{\alpha n^{\alpha}} \left[\left[\frac{(1+t)^{\frac{1}{1-\alpha}} + (1-t)^{\frac{1}{1-\alpha}}}{2} \right]^{1-\alpha} - 1 \right], t \in [0,1].$ Therefore, the conditional regret of the top-k loss can be upper bounded as follows:

$$\Delta \mathcal{C}_{\ell_k,\mathcal{H}}(h,x) = \sum_{i=1}^k (p(x,\mathsf{p}_i(x)) - p(x,\mathsf{h}_i(x))) \le k\psi^{-1} (\Delta \mathcal{C}_{\ell_{\mathrm{gce}},\mathcal{H}}(h,x)).$$

By the concavity of ψ^{-1} , take expectations on both sides of the preceding equation, we obtain

$$\mathcal{E}_{\ell_k}(h) - \mathcal{E}_{\ell_k}^*(\mathcal{H}) + \mathcal{M}_{\ell_k}(\mathcal{H}) \le k\psi^{-1} \Big(\mathcal{E}_{\ell_{\text{gce}}}(h) - \mathcal{E}_{\ell_{\text{gce}}}^*(\mathcal{H}) + \mathcal{M}_{\ell_{\text{gce}}}(\mathcal{H}) \Big).$$

The second part follows from the fact that when $\mathcal{A}_{\ell_{\rm gce}}(\mathcal{H}) = 0$, the minimizability gap $\mathcal{M}_{\ell_{\rm gce}}(\mathcal{H})$ vanishes.

Appendix C. Proofs of realizable \mathcal{H} -consistency for comp-sum losses

Theorem 12 Assume that \mathcal{H} is closed under scaling. Then, ℓ_{log} , ℓ_{exp}^{comp} , ℓ_{gce} and ℓ_{mae} are realizable \mathcal{H} -consistent with respect to ℓ_{0-1} .

Proof Since the distribution is realizable, there exists a hypothesis $h \in \mathcal{H}$ such that

$$\mathbb{P}_{(x,y)\sim\mathcal{D}}(h^*(x,y) > h^*(x,h_2(x))) = 1.$$

Therefore, for the logistic loss, by using the Lebesgue dominated convergence theorem,

$$\mathcal{M}_{\ell_{\log}}(\mathcal{H}) \leq \mathcal{E}_{\ell_{\log}}^*(\mathcal{H}) \leq \lim_{\beta \to +\infty} \mathcal{E}_{\ell_{\log}}(\beta h) = \lim_{\beta \to +\infty} \log \left[1 + \sum_{y' \neq y} e^{\beta(h^*(x,y') - h^*(x,y))} \right] = 0.$$

For the sum exponential loss, by using the Lebesgue dominated convergence theorem,

$$\mathcal{M}_{\ell_{\exp}^{\mathrm{comp}}}(\mathcal{H}) \leq \mathcal{E}_{\ell_{\exp}^{\mathrm{comp}}}^{*}(\mathcal{H}) \leq \lim_{\beta \to +\infty} \mathcal{E}_{\ell_{\exp}^{\mathrm{comp}}}(\beta h) = \lim_{\beta \to +\infty} \sum_{y' \neq y} e^{\beta (h^{*}(x,y') - h^{*}(x,y))} = 0.$$

For the generalized cross entropy loss, by using the Lebesgue dominated convergence theorem,

$$\mathcal{M}_{\ell_{\text{gce}}}(\mathcal{H}) \leq \mathcal{E}_{\ell_{\text{gce}}}^{*}(\mathcal{H}) \leq \lim_{\beta \to +\infty} \mathcal{E}_{\ell_{\text{gce}}}(\beta h) = \lim_{\beta \to +\infty} \frac{1}{\alpha} \left[1 - \left[\sum_{y' \in \mathcal{Y}} e^{\beta (h^{*}(x,y') - h^{*}(x,y))} \right]^{-\alpha} \right] = 0.$$

For the mean absolute error loss, by using the Lebesgue dominated convergence theorem,

$$\mathcal{M}_{\ell_{\text{mae}}}(\mathcal{H}) \leq \mathcal{E}_{\ell_{\text{mae}}}^{*}(\mathcal{H}) \leq \lim_{\beta \to +\infty} \mathcal{E}_{\ell_{\text{mae}}}(\beta h) = \lim_{\beta \to +\infty} 1 - \left[\sum_{y' \in \mathcal{Y}} e^{\beta (h^{*}(x,y') - h^{*}(x,y))} \right]^{-1} = 0.$$

Therefore, by Theorems 5, 6, 7 and 8, the proof is completed.

Appendix D. Proofs of \mathcal{H} -consistency bounds for constrained losses

D.1. Proof of Theorem 13

The conditional error for the constrained loss can be expressed as follows:

$$C_{\ell^{\text{cstnd}}}(h,x) = \sum_{y=1}^{n} p(x,y) \ell^{\text{cstnd}}(h,x,y) = \sum_{y=1}^{n} p(x,y) \sum_{y'\neq y} \Phi(-h(x,y')) = \sum_{y\in \S} (1-p(x,y)) \Phi(-h(x,y)).$$

Theorem 13 Assume that \mathcal{H} is symmetric and complete. Then, for any $1 \le k \le n$, the following \mathcal{H} -consistency bound holds for the constrained exponential loss:

$$\mathcal{E}_{\ell_k}(h) - \mathcal{E}_{\ell_k}^*(\mathcal{H}) + \mathcal{M}_{\ell_k}(\mathcal{H}) \leq 2k \left(\mathcal{E}_{\ell_{\exp}^{\text{cstnd}}}(h) - \mathcal{E}_{\ell_{\exp}^{\text{cstnd}}}^*(\mathcal{H}) + \mathcal{M}_{\ell_{\exp}^{\text{cstnd}}}(\mathcal{H})\right)^{\frac{1}{2}}.$$

In the special case where $A_{\ell_{\exp}^{\operatorname{cstnd}}}(\mathfrak{H})=0$, for any $1\leq k\leq n$, the following bound holds:

$$\mathcal{E}_{\ell_k}(h) - \mathcal{E}_{\ell_k}^*(\mathcal{H}) \le 2k \left(\mathcal{E}_{\ell_{\exp}}^{\text{cstnd}}(h) - \mathcal{E}_{\ell_{\exp}}^{\text{cstnd}}(\mathcal{H})\right)^{\frac{1}{2}}$$

Proof For the constrained exponential loss $\ell_{\rm exp}^{\rm cstnd}$, the conditional regret can be written as

$$\Delta \mathcal{C}_{\ell_{\exp}^{\text{cstnd}},\mathcal{H}}(h,x) = \sum_{y=1}^{n} p(x,y) \ell_{\exp}^{\text{cstnd}}(h,x,y) - \inf_{h \in \mathcal{H}} \sum_{y=1}^{n} p(x,y) \ell_{\exp}^{\text{cstnd}}(h,x,y)$$
$$\geq \sum_{y=1}^{n} p(x,y) \ell_{\exp}^{\text{cstnd}}(h,x,y) - \inf_{\mu \in \mathbb{R}} \sum_{y=1}^{n} p(x,y) \ell_{\exp}^{\text{cstnd}}(h_{\mu,i},x,y),$$

where for any $i \in [k]$, $h_{\mu,i}(x,y) = \begin{cases} h(x,y), & y \notin \{\mathsf{p}_i(x),\mathsf{h}_i(x)\} \\ h(x,\mathsf{p}_i(x)) + \mu & y = \mathsf{h}_i(x) \end{cases}$ Note that such a choice $h(x,\mathsf{h}_i(x)) - \mu & y = \mathsf{p}_i(x).$

of $h_{\mu,i}$ leads to the following equality holds

$$\sum_{y \notin \{\mathsf{h}_i(x),\mathsf{p}_i(x)\}} p(x,y) \ell_{\exp}^{\mathrm{cstnd}}(h,x,y) = \sum_{y \notin \{\mathsf{h}_i(x),\mathsf{p}_i(x)\}} p(x,y) \ell_{\exp}^{\mathrm{cstnd}}(h_{\mu,i},x,y).$$

Let $q(x, p_i(x)) = 1 - p(x, p_i(x))$ and $q(x, h_i(x)) = 1 - p(x, h_i(x))$. Therefore, for any $i \in [k]$, the conditional regret of constrained exponential loss can be lower bounded as

$$\begin{split} &\Delta \mathcal{C}_{\ell_{\exp}^{\text{estnd}},\mathcal{H}}(h,x) \\ &\geq \inf_{h \in \mathcal{H}} \sup_{\mu \in \mathbb{R}} \left\{ q(x,\mathsf{p}_i(x)) \Big(e^{h(x,\mathsf{p}_i(x))} - e^{h(x,\mathsf{h}_i(x)) - \mu} \Big) + q(x,\mathsf{h}_i(x)) \Big(e^{h(x,\mathsf{h}_i(x))} - e^{h(x,\mathsf{p}_i(x)) + \mu} \Big) \right\} \\ &= \Big(\sqrt{q(x,\mathsf{p}_i(x))} - \sqrt{q(x,\mathsf{h}_i(x))} \Big)^2 \qquad \qquad \text{(differentiating with respect to } \mu, \, h \text{ to optimize)} \\ &= \left(\frac{q(x,\mathsf{h}_i(x)) - q(x,\mathsf{p}_i(x))}{\sqrt{q(x,\mathsf{p}_i(x))} + \sqrt{q(x,\mathsf{h}_i(x))}} \right)^2 \\ &\geq \frac{1}{4} (q(x,\mathsf{h}_i(x)) - q(x,\mathsf{p}_i(x)))^2 \\ &= \frac{1}{4} (p(x,\mathsf{p}_i(x)) - p(x,\mathsf{h}_i(x)))^2. \end{split}$$

Therefore, by Lemma 4, the conditional regret of the top-k loss can be upper bounded as follows:

$$\Delta \mathcal{C}_{\ell_k,\mathcal{H}}(h,x) = \sum_{i=1}^k (p(x,\mathsf{p}_i(x)) - p(x,\mathsf{h}_i(x))) \le 2k \Big(\Delta \mathcal{C}_{\ell_{\exp}}^{\mathrm{cstnd}},\mathcal{H}}(h,x)\Big)^{\frac{1}{2}}.$$

By the concavity, take expectations on both sides of the preceding equation, we obtain

$$\mathcal{E}_{\ell_k}(h) - \mathcal{E}_{\ell_k}^*(\mathcal{H}) + \mathcal{M}_{\ell_k}(\mathcal{H}) \leq 2k \Big(\mathcal{E}_{\ell_{\exp}^{\text{cstnd}}}(h) - \mathcal{E}_{\ell_{\exp}^{\text{cstnd}}}^*(\mathcal{H}) + \mathcal{M}_{\ell_{\exp}^{\text{cstnd}}}(\mathcal{H})\Big)^{\frac{1}{2}}.$$

The second part follows from the fact that when $\mathcal{A}_{\ell_{\exp}^{\text{cstnd}}}(\mathcal{H}) = 0$, we have $\mathcal{M}_{\ell_{\exp}^{\text{cstnd}}}(\mathcal{H}) = 0$.

D.2. Proof of Theorem 14

Theorem 14 Assume that \mathcal{H} is symmetric and complete. Then, for any $1 \le k \le n$, the following \mathcal{H} -consistency bound holds for the constrained squared hinge loss:

$$\mathcal{E}_{\ell_k}(h) - \mathcal{E}_{\ell_k}^*(\mathcal{H}) + \mathcal{M}_{\ell_k}(\mathcal{H}) \leq 2k \left(\mathcal{E}_{\ell_{\text{sq-hinge}}}(h) - \mathcal{E}_{\ell_{\text{sq-hinge}}}^*(\mathcal{H}) + \mathcal{M}_{\ell_{\text{sq-hinge}}}(\mathcal{H}) \right)^{\frac{1}{2}}.$$

In the special case where $A_{\ell_{sq-hinge}}(\mathcal{H}) = 0$, for any $1 \le k \le n$, the following bound holds:

$$\mathcal{E}_{\ell_k}(h) - \mathcal{E}_{\ell_k}^*(\mathcal{H}) \le 2k \left(\mathcal{E}_{\ell_{\text{sq-hinge}}}(h) - \mathcal{E}_{\ell_{\text{sq-hinge}}}^*(\mathcal{H}) \right)^{\frac{1}{2}}.$$

Proof For the constrained squared hinge loss $\ell_{\text{sq-hinge}}$, the conditional regret can be written as

$$\Delta \mathcal{C}_{\ell_{\text{sq-hinge}},\mathcal{H}}(h,x) = \sum_{y=1}^{n} p(x,y) \ell_{\text{sq-hinge}}(h,x,y) - \inf_{h \in \mathcal{H}} \sum_{y=1}^{n} p(x,y) \ell_{\text{sq-hinge}}(h,x,y)$$

$$\geq \sum_{y=1}^{n} p(x,y) \ell_{\text{sq-hinge}}(h,x,y) - \inf_{\mu \in \mathbb{R}} \sum_{y=1}^{n} p(x,y) \ell_{\text{sq-hinge}}(h_{\mu,i},x,y),$$

where for any
$$i \in [k]$$
, $h_{\mu,i}(x,y) = \begin{cases} h(x,y), & y \notin \{\mathsf{p}_i(x),\mathsf{h}_i(x)\} \\ h(x,\mathsf{p}_i(x)) + \mu & y = \mathsf{h}_i(x) \\ h(x,\mathsf{h}_i(x)) - \mu & y = \mathsf{p}_i(x). \end{cases}$ Note that such a choice

of $h_{\mu,i}$ leads to the following equality holds:

$$\sum_{y \notin \{\mathsf{h}_i(x), \mathsf{p}_i(x)\}} p(x, y) \ell_{\text{sq-hinge}}(h, x, y) = \sum_{y \notin \{\mathsf{h}_i(x), \mathsf{p}_i(x)\}} p(x, y) \ell_{\text{sq-hinge}}(h_{\mu, i}, x, y).$$

Let $q(x, p_i(x)) = 1 - p(x, p_i(x))$ and $q(x, h_i(x)) = 1 - p(x, h_i(x))$. Therefore, for any $i \in [k]$, the conditional regret of the constrained squared hinge loss can be lower bounded as

$$\Delta \mathcal{C}_{\ell_{\text{sq-hinge}},\mathcal{H}}(h,x) \geq \inf_{h \in \mathcal{H}} \sup_{\mu \in \mathbb{R}} \left\{ q(x,\mathsf{p}_{i}(x)) \left(\max\{0,1+h(x,\mathsf{p}_{i}(x))\}^{2} - \max\{0,1+h(x,\mathsf{h}_{i}(x)) - \mu\}^{2} \right) \right. \\ \left. + q(x,\mathsf{h}_{i}(x)) \left(\max\{0,1+h(x,\mathsf{h}_{i}(x))\}^{2} - \max\{0,1+h(x,\mathsf{p}_{i}(x)) + \mu\}^{2} \right) \right\} \\ \geq \frac{1}{4} (q(x,\mathsf{p}_{i}(x)) - q(x,\mathsf{h}_{i}(x)))^{2}$$
 (differentiating with respect to μ , h to optimize)
$$= \frac{1}{4} (p(x,\mathsf{p}_{i}(x)) - p(x,\mathsf{h}_{i}(x)))^{2}$$

Therefore, by Lemma 4, the conditional regret of the top-k loss can be upper bounded as follows:

$$\Delta \mathcal{C}_{\ell_k,\mathcal{H}}(h,x) = \sum_{i=1}^k (p(x,\mathsf{p}_i(x)) - p(x,\mathsf{h}_i(x))) \leq 2k \left(\Delta \mathcal{C}_{\ell_{\mathrm{sq-hinge}},\mathcal{H}}(h,x)\right)^{\frac{1}{2}}.$$

By the concavity, take expectations on both sides of the preceding equation, we obtain

$$\mathcal{E}_{\ell_k}(h) - \mathcal{E}_{\ell_k}^*(\mathcal{H}) + \mathcal{M}_{\ell_k}(\mathcal{H}) \le 2k \Big(\mathcal{E}_{\ell_{\text{sq-hinge}}}(h) - \mathcal{E}_{\ell_{\text{sq-hinge}}}^*(\mathcal{H}) + \mathcal{M}_{\ell_{\text{sq-hinge}}}(\mathcal{H})\Big)^{\frac{1}{2}}.$$

The second part follows from the fact that when the hypothesis set \mathcal{H} is sufficiently rich such that $\mathcal{A}_{\ell_{\operatorname{sq-hinge}}}(\mathcal{H}) = 0$, we have $\mathcal{M}_{\ell_{\operatorname{sq-hinge}}}(\mathcal{H}) = 0$.

D.3. Proof of Theorem 18

Similarly, we study the constrained hinge loss, defined as $\ell_{\text{hinge}}(h, x, y) = \sum_{y' \neq y} \max\{0, 1 + h(x, y')\}$. The following result shows that ℓ_{hinge} admits an \mathcal{H} -consistency bound with respect to ℓ_k . The second part follows from the fact that when the hypothesis set \mathcal{H} is sufficiently rich such that $\mathcal{A}_{\ell_{\text{hinge}}}(\mathcal{H}) = 0$, we have $\mathcal{M}_{\ell_{\text{hinge}}}(\mathcal{H}) = 0$. Different from the constrained squared hinge loss, the bound for ℓ_{hinge} is linear: $\mathcal{E}_{\ell_{\text{hinge}}}(h) - \mathcal{E}^*_{\ell_{\text{hinge}}}(\mathcal{H}) \leq \epsilon \Rightarrow \mathcal{E}_{\ell_k}(h) - \mathcal{E}^*_{\ell_k}(\mathcal{H}) \leq k \epsilon$. This also implies that ℓ_{hinge} is Bayes-consistent with respect to ℓ_k .

Theorem 18 Assume that \mathcal{H} is symmetric and complete. Then, for any $1 \le k \le n$, the following \mathcal{H} -consistency bound holds for the constrained hinge loss:

$$\mathcal{E}_{\ell_k}(h) - \mathcal{E}_{\ell_k}^*(\mathcal{H}) + \mathcal{M}_{\ell_k}(\mathcal{H}) \le k \Big(\mathcal{E}_{\ell_{\text{hinge}}}(h) - \mathcal{E}_{\ell_{\text{hinge}}}^*(\mathcal{H}) + \mathcal{M}_{\ell_{\text{hinge}}}(\mathcal{H}) \Big).$$

In the special case where $A_{\ell_{\text{hinge}}}(\mathfrak{H}) = 0$, *for any* $1 \leq k \leq n$, *the following bound holds:*

$$\mathcal{E}_{\ell_k}(h) - \mathcal{E}_{\ell_k}^*(\mathcal{H}) \le k \Big(\mathcal{E}_{\ell_{\text{hinge}}}(h) - \mathcal{E}_{\ell_{\text{hinge}}}^*(\mathcal{H}) \Big).$$

Proof For the constrained hinge loss ℓ_{hinge} , the conditional regret can be written as

$$\Delta \mathcal{C}_{\ell_{\text{hinge}},\mathcal{H}}(h,x) = \sum_{y=1}^{n} p(x,y)\ell_{\text{hinge}}(h,x,y) - \inf_{h \in \mathcal{H}} \sum_{y=1}^{n} p(x,y)\ell_{\text{hinge}}(h,x,y)$$

$$\geq \sum_{y=1}^{n} p(x,y)\ell_{\text{hinge}}(h,x,y) - \inf_{\mu \in \mathbb{R}} \sum_{y=1}^{n} p(x,y)\ell_{\text{hinge}}(h_{\mu,i},x,y),$$

where for any
$$i \in [k]$$
, $h_{\mu,i}(x,y) = \begin{cases} h(x,y), & y \notin \{\mathsf{p}_i(x),\mathsf{h}_i(x)\} \\ h(x,\mathsf{p}_i(x)) + \mu & y = \mathsf{h}_i(x) \end{cases}$ Note that such a choice $h(x,\mathsf{h}_i(x)) - \mu & y = \mathsf{p}_i(x).$

of $h_{\mu,i}$ leads to the following equality holds:

$$\sum_{y \notin \{\mathsf{h}_i(x), \mathsf{p}_i(x)\}} p(x,y) \ell_{\mathrm{hinge}}(h,x,y) = \sum_{y \notin \{\mathsf{h}_i(x), \mathsf{p}_i(x)\}} p(x,y) \ell_{\mathrm{hinge}}(h_{\mu,i},x,y).$$

Let $q(x, p_i(x)) = 1 - p(x, p_i(x))$ and $q(x, h_i(x)) = 1 - p(x, h_i(x))$. Therefore, for any $i \in [k]$, the conditional regret of the constrained hinge loss can be lower bounded as

$$\Delta \mathcal{C}_{\ell_{\text{hinge}},\mathcal{H}}(h,x) \geq \inf_{h \in \mathcal{H}} \sup_{\mu \in \mathbb{R}} \left\{ q(x,\mathsf{p}_i(x)) (\max\{0,1+h(x,\mathsf{p}_i(x))\} - \max\{0,1+h(x,\mathsf{h}_i(x))-\mu\}) \right.$$

$$\left. + q(x,\mathsf{h}_i(x)) (\max\{0,1+h(x,\mathsf{h}_i(x))\} - \max\{0,1+h(x,\mathsf{p}_i(x))+\mu\}) \right\}$$

$$\geq q(x,\mathsf{h}_i(x)) - q(x,\mathsf{p}_i(x)) \qquad \text{(differentiating with respect to } \mu,h \text{ to optimize)}$$

$$= p(x,\mathsf{p}_i(x)) - p(x,\mathsf{h}_i(x))$$

Therefore, by Lemma 4, the conditional regret of the top-k loss can be upper bounded as follows:

$$\Delta \mathcal{C}_{\ell_k,\mathcal{H}}(h,x) = \sum_{i=1}^k (p(x,\mathsf{p}_i(x)) - p(x,\mathsf{h}_i(x))) \le k \Delta \mathcal{C}_{\ell_{\mathrm{hinge}},\mathcal{H}}(h,x).$$

By the concavity, take expectations on both sides of the preceding equation, we obtain

$$\mathcal{E}_{\ell_k}(h) - \mathcal{E}_{\ell_k}^*(\mathcal{H}) + \mathcal{M}_{\ell_k}(\mathcal{H}) \leq k \Big(\mathcal{E}_{\ell_{\text{hinge}}}(h) - \mathcal{E}_{\ell_{\text{hinge}}}^*(\mathcal{H}) + \mathcal{M}_{\ell_{\text{hinge}}}(\mathcal{H}) \Big).$$

The second part follows from the fact that when the hypothesis set \mathcal{H} is sufficiently rich such that $\mathcal{A}_{\ell_{\text{hinge}}}(\mathcal{H}) = 0$, we have $\mathcal{M}_{\ell_{\text{hinge}}}(\mathcal{H}) = 0$.

D.4. Proof of Theorem 19

The constrained ρ -margin loss is defined as $\ell_{\rho}(h,x,y) = \sum_{y'\neq y} \min\{\max\{0,1+h(x,y')/\rho\},1\}$. Next, we show that that ℓ_{ρ} benefits form \mathcal{H} -consistency bounds as well. The second part follows from the fact that when the hypothesis set \mathcal{H} is sufficiently rich such that $\mathcal{A}_{\ell_{\rho}}(\mathcal{H}) = 0$, we have $\mathcal{M}_{\ell_{\rho}}(\mathcal{H}) = 0$. As with the constrained hinge loss, the bound for ℓ_{ρ} is linear: $\mathcal{E}_{\ell_{\rho}}(h) - \mathcal{E}_{\ell_{\rho}}^*(\mathcal{H}) \leq \epsilon \Rightarrow \mathcal{E}_{\ell_{k}}(h) - \mathcal{E}_{\ell_{k}}^*(\mathcal{H}) \leq k \epsilon$. As a by-product, ℓ_{ρ} is Bayes-consistent with respect to ℓ_{k} .

Theorem 19 Assume that \mathcal{H} is symmetric and complete. Then, for any $1 \le k \le n$, the following \mathcal{H} -consistency bound holds for the constrained ρ -margin loss:

$$\mathcal{E}_{\ell_k}(h) - \mathcal{E}_{\ell_k}^*(\mathcal{H}) + \mathcal{M}_{\ell_k}(\mathcal{H}) \le k \left(\mathcal{E}_{\ell_\rho}(h) - \mathcal{E}_{\ell_\rho}^*(\mathcal{H}) + \mathcal{M}_{\ell_\rho}(\mathcal{H}) \right).$$

In the special case where $A_{\ell_o}(\mathfrak{H}) = 0$, for any $1 \le k \le n$, the following bound holds:

$$\mathcal{E}_{\ell_k}(h) - \mathcal{E}_{\ell_k}^*(\mathcal{H}) \le k \left(\mathcal{E}_{\ell_\rho}(h) - \mathcal{E}_{\ell_\rho}^*(\mathcal{H}) \right).$$

Proof For the constrained ρ -margin loss ℓ_{ρ} , the conditional regret can be written as

$$\Delta C_{\ell_{\rho},\mathcal{H}}(h,x) = \sum_{y=1}^{n} p(x,y)\ell_{\rho}(h,x,y) - \inf_{h \in \mathcal{H}} \sum_{y=1}^{n} p(x,y)\ell_{\rho}(h,x,y)$$
$$\geq \sum_{y=1}^{n} p(x,y)\ell_{\rho}(h,x,y) - \inf_{\mu \in \mathbb{R}} \sum_{y=1}^{n} p(x,y)\ell_{\rho}(h_{\mu,i},x,y),$$

where for any $i \in [k]$, $h_{\mu,i}(x,y) = \begin{cases} h(x,y), & y \notin \{\mathsf{p}_i(x),\mathsf{h}_i(x)\} \\ h(x,\mathsf{p}_i(x)) + \mu & y = \mathsf{h}_i(x) \\ h(x,\mathsf{h}_i(x)) - \mu & y = \mathsf{p}_i(x). \end{cases}$ Note that such a choice

of $h_{\mu,i}$ leads to the following equality holds:

$$\sum_{y \notin \{h_i(x), p_i(x)\}} p(x, y) \ell_{\rho}(h, x, y) = \sum_{y \notin \{h_i(x), p_i(x)\}} p(x, y) \ell_{\rho}(h_{\mu, i}, x, y).$$

Let $q(x, p_i(x)) = 1 - p(x, p_i(x))$ and $q(x, h_i(x)) = 1 - p(x, h_i(x))$. Therefore, for any $i \in [k]$, the conditional regret of the constrained ρ -margin loss can be lower bounded as

$$\Delta \mathcal{C}_{\ell_{\rho},\mathcal{H}}(h,x)$$

$$\geq \inf_{h \in \mathcal{H}} \sup_{\mu \in \mathbb{R}} \left\{ q(x, \mathsf{p}_{i}(x)) \left(\min \left\{ \max \left\{ 0, 1 + \frac{h(x, \mathsf{p}_{i}(x))}{\rho} \right\}, 1 \right\} - \min \left\{ \max \left\{ 0, 1 + \frac{h(x, \mathsf{h}_{i}(x)) - \mu}{\rho} \right\}, 1 \right\} \right)$$

$$+ q(x, \mathsf{h}_{i}(x)) \left(\min \left\{ \max \left\{ 0, 1 + \frac{h(x, \mathsf{h}_{i}(x))}{\rho} \right\}, 1 \right\} - \min \left\{ \max \left\{ 0, 1 + \frac{h(x, \mathsf{p}_{i}(x)) + \mu}{\rho} \right\}, 1 \right\} \right) \right\}$$

$$\geq q(x, \mathsf{h}_{i}(x)) - q(x, \mathsf{p}_{i}(x))$$

$$= p(x, \mathsf{p}_{i}(x)) - p(x, \mathsf{h}_{i}(x))$$

$$(differentiating with respect to μ, h to optimize)$$

$$= p(x, \mathsf{p}_{i}(x)) - p(x, \mathsf{h}_{i}(x))$$

Therefore, by Lemma 4, the conditional regret of the top-k loss can be upper bounded as follows:

$$\Delta \mathcal{C}_{\ell_k,\mathcal{H}}(h,x) = \sum_{i=1}^k (p(x,\mathsf{p}_i(x)) - p(x,\mathsf{h}_i(x))) \le k\Delta \mathcal{C}_{\ell_\rho,\mathcal{H}}(h,x).$$

By the concavity, take expectations on both sides of the preceding equation, we obtain

$$\mathcal{E}_{\ell_k}(h) - \mathcal{E}_{\ell_k}^*(\mathcal{H}) + \mathcal{M}_{\ell_k}(\mathcal{H}) \le k \Big(\mathcal{E}_{\ell_\rho}(h) - \mathcal{E}_{\ell_\rho}^*(\mathcal{H}) + \mathcal{M}_{\ell_\rho}(\mathcal{H}) \Big).$$

The second part follows from the fact that when the hypothesis set \mathcal{H} is sufficiently rich such that $\mathcal{A}_{\ell_{\rho}}(\mathcal{H}) = 0$, we have $\mathcal{M}_{\ell_{\rho}}(\mathcal{H}) = 0$.

Appendix E. Proofs of \Re -consistency bounds for cost-sensitive losses

We first characterize the best-in class conditional error and the conditional regret of the target cardinality aware loss function (2), which will be used in the analysis of \Re -consistency bounds.

Lemma 20 Assume that \Re is symmetric and complete. Then, for any $r \in \Re$ and $x \in \Re$, the best-in class conditional error and the conditional regret of the target cardinality aware loss function can be expressed as follows:

$$\begin{split} & \mathcal{C}^*_{\widetilde{\ell}}(\mathcal{R},x) = \min_{k \in \mathcal{K}} \sum_{y \in \mathcal{Y}} p(x,y) c(x,k,y) \\ & \Delta \mathcal{C}_{\ell_k,\mathcal{H}}(r,x) = \sum_{y \in \mathcal{Y}} p(x,y) c(x,\mathsf{r}(x),y) - \min_{k \in \mathcal{K}} \sum_{y \in \mathcal{Y}} p(x,y) c(x,k,y). \end{split}$$

Proof By definition, for any $r \in \mathbb{R}$ and $x \in \mathcal{X}$, the conditional error of the target cardinality aware loss function can be written as

$$C_{\widetilde{\ell}}(r,x) = \sum_{y \in \mathcal{Y}} p(x,y)c(x,\mathbf{r}(x),y).$$

Since \Re is symmetric and complete, we have

$$\mathcal{C}^{\star}_{\widetilde{\ell}}(r,x) = \inf_{r \in \mathcal{R}} \sum_{y \in \mathbb{Y}} p(x,y) c(x,\mathsf{r}(x),y) = \min_{k \in \mathcal{K}} \sum_{i=1}^k p(x,y) c(x,k,y).$$

Furthermore, the calibration gap can be expressed as

$$\Delta \mathfrak{C}_{\widetilde{\ell},\mathcal{H}}(r,x) = \mathfrak{C}_{\widetilde{\ell}}(r,x) - \mathfrak{C}_{\widetilde{\ell}}^{\star}(\mathcal{R},x) = \sum_{y \in \mathcal{Y}} p(x,y) c(x,\mathsf{r}(x),y) - \min_{k \in \mathcal{K}} \sum_{y \in \mathcal{Y}} p(x,y) c(x,k,y),$$

which completes the proof.

E.1. Proof of Theorem 15

For convenience, we let $\overline{c}(x,k,y) = 1 - c(x,k,y)$, $\overline{q}(x,k) = \sum_{y \in \mathcal{Y}} p(x,y) \overline{c}(x,k,y) \in [0,1]$ and $S(x,k) = \frac{e^{r(x,k)}}{\sum_{k' \in \mathcal{K}} e^{r(x,k')}}$. We also let $k_{\min}(x) = \operatorname{argmin}_{k \in \mathcal{K}} (1 - \overline{q}(x,k)) = \operatorname{argmin}_{k \in \mathcal{K}} \sum_{y \in \mathcal{Y}} p(x,y) c(x,k,y)$.

Theorem 15 Assume that \mathbb{R} is symmetric and complete. Then, the following \mathbb{R} -consistency bound holds for the cost-sensitive comp-sum loss:

$$\mathcal{E}_{\widetilde{\ell}}(r) - \mathcal{E}_{\widetilde{\ell}}^*(\mathcal{R}) + \mathcal{M}_{\widetilde{\ell}}(\mathcal{R}) \leq \gamma \Big(\mathcal{E}_{\widetilde{\ell}^{\mathrm{comp}}}(r) - \mathcal{E}_{\widetilde{\ell}^{\mathrm{comp}}}^*(\mathcal{R}) + \mathcal{M}_{\widetilde{\ell}^{\mathrm{comp}}}(\mathcal{R}) \Big);$$

In the special case where $\Re = \Re_{all}$, the following holds:

$$\mathcal{E}_{\widetilde{\ell}}(r) - \mathcal{E}_{\widetilde{\ell}}^*(\mathcal{R}_{\text{all}}) \leq \gamma \left(\mathcal{E}_{\widetilde{\ell}^{\text{comp}}}(r) - \mathcal{E}_{\widetilde{\ell}^{\text{comp}}}^*(\mathcal{R}_{\text{all}})\right)$$

where $\gamma(t) = 2\sqrt{t}$ when $\widetilde{\ell}^{comp}$ is either $\widetilde{\ell}_{log}$ or $\widetilde{\ell}^{comp}_{exp}$; $\gamma(t) = 2\sqrt{n^{\alpha}t}$ when $\widetilde{\ell}^{comp}$ is $\widetilde{\ell}_{gce}$; and $\gamma(t) = nt$ when $\widetilde{\ell}^{comp}$ is $\widetilde{\ell}_{mae}$.

Proof Case I: $\ell = \widetilde{\ell}_{\log}$. For the cost-sensitive logistic loss $\widetilde{\ell}_{\log}$, the conditional error can be written as

$$\mathcal{C}_{\widetilde{\ell}_{\log}}(r,x) = -\sum_{y \in \mathcal{Y}} p(x,y) \sum_{k \in \mathcal{K}} \overline{c}(x,k,y) \log \left(\frac{e^{r(x,k)}}{\sum_{k' \in \mathcal{K}} e^{r(x,k')}} \right) = -\sum_{k \in \mathcal{K}} \log(\mathcal{S}(x,k)) \overline{q}(x,k).$$

The conditional regret can be written as

$$\begin{split} \Delta \mathbb{C}_{\widetilde{\ell}_{\log}, \mathcal{R}}(r, x) &= -\sum_{k \in \mathcal{K}} \log(\mathbb{S}(x, k)) \overline{q}(x, k) - \inf_{r \in \mathcal{R}} \left(-\sum_{k \in \mathcal{K}} \log(\mathbb{S}(x, k)) \overline{q}(x, k) \right) \\ &\geq -\sum_{k \in \mathcal{K}} \log(\mathbb{S}(x, k)) \overline{q}(x, k) - \inf_{\mu \in [-\mathbb{S}(x, k_{\min}(x)), \mathbb{S}(x, \mathbf{r}(x))]} \left(-\sum_{k \in \mathcal{K}} \log(\mathbb{S}_{\mu}(x, k)) \overline{q}(x, k) \right), \end{split}$$

$$\text{where for any } x \in \mathfrak{X} \text{ and } k \in \mathfrak{K}, \, \mathbb{S}_{\mu}(x,k) = \begin{cases} \mathbb{S}(x,y), & y \notin \{k_{\min}(x),\mathsf{r}(x)\} \\ \mathbb{S}(x,k_{\min}(x)) + \mu & y = \mathsf{r}(x) \\ \mathbb{S}(x,\mathsf{r}(x)) - \mu & y = k_{\min}(x). \end{cases} \text{ Note that }$$

such a choice of S_{μ} leads to the following equality holds:

$$\sum_{k \notin \{\mathsf{r}(x),k_{\min}(x)\}} \log(\mathbb{S}(x,k)) \overline{q}(x,k) = \sum_{k \notin \{\mathsf{r}(x),k_{\min}(x)\}} \log(\mathbb{S}_{\mu}(x,k)) \overline{q}(x,k).$$

Therefore, the conditional regret of cost-sensitive logistic loss can be lower bounded as

$$\Delta \mathcal{C}_{\widetilde{\ell}_{\log},\mathcal{H}}(h,x) \geq \sup_{\mu \in [-\mathbb{S}(x,k_{\min}(x)),\mathbb{S}(x,\mathsf{r}(x))]} \left\{ \overline{q}(x,k_{\min}(x)) \left[-\log(\mathbb{S}(x,k_{\min}(x))) + \log(\mathbb{S}(x,\mathsf{r}(x)) - \mu) \right] + \overline{q}(x,\mathsf{r}(x)) \left[-\log(\mathbb{S}(x,\mathsf{r}(x))) + \log(\mathbb{S}(x,k_{\min}(x)) + \mu) \right] \right\}.$$

By the concavity of the function, differentiate with respect to μ , we obtain that the supremum is achieved by $\mu^* = \frac{\overline{q}(x, \mathbf{r}(x)) \delta(x, \mathbf{r}(x)) - \overline{q}(x, k_{\min}(x)) \delta(x, k_{\min}(x))}{\overline{q}(x, k_{\min}(x)) + \overline{q}(x, \mathbf{r}(x))}$. Plug in μ^* , we obtain

Therefore, by Lemma 20, the conditional regret of the target cardinality aware loss function can be upper bounded as follows:

$$\Delta \mathcal{C}_{\widetilde{\ell},\mathcal{H}}(r,x) = \overline{q}(x,k_{\min}(x)) - \overline{q}(x,\mathsf{r}(x)) \le 2\left(\Delta \mathcal{C}_{\widetilde{\ell}_{\log},\mathcal{R}}(r,x)\right)^{\frac{1}{2}}.$$

By the concavity, take expectations on both sides of the preceding equation, we obtain

$$\mathcal{E}_{\widetilde{\ell}}(r) - \mathcal{E}_{\widetilde{\ell}}^{*}(\mathcal{R}) + \mathcal{M}_{\widetilde{\ell}}(\mathcal{R}) \leq 2 \left(\mathcal{E}_{\widetilde{\ell}_{\log}}(r) - \mathcal{E}_{\widetilde{\ell}_{\log}}^{*}(\mathcal{R}) + \mathcal{M}_{\widetilde{\ell}_{\log}}(\mathcal{R}) \right)^{\frac{1}{2}}.$$

The second part follows from the fact that $\mathcal{M}_{\widetilde{\ell}_{log}}(\mathcal{R}_{all}) = 0$.

Case II: $\ell = \widetilde{\ell}_{\exp}^{\mathrm{comp}}$. For the cost-sensitive sum exponential loss $\widetilde{\ell}_{\exp}^{\mathrm{comp}}$, the conditional error can be written as

$$\mathcal{C}_{\widetilde{\ell}_{\exp}^{\text{comp}}}(r,x) = \sum_{y \in \mathcal{Y}} p(x,y) \sum_{k \in \mathcal{K}} \overline{c}(x,k,y) \sum_{k' \neq k'} e^{r(x,k')-r(x,k)} = \sum_{k \in \mathcal{K}} \left(\frac{1}{\mathcal{S}(x,k)} - 1 \right) \overline{q}(x,k).$$

The conditional regret can be written as

$$\begin{split} \Delta \mathcal{C}_{\widetilde{\ell}_{\exp}^{\text{comp}}, \mathcal{R}}(r, x) &= \sum_{k \in \mathcal{K}} \left(\frac{1}{\mathbb{S}(x, k)} - 1 \right) \overline{q}(x, k) - \inf_{r \in \mathcal{R}} \left(\sum_{k \in \mathcal{K}} \left(\frac{1}{\mathbb{S}(x, k)} - 1 \right) \overline{q}(x, k) \right) \\ &\geq \sum_{k \in \mathcal{K}} \left(\frac{1}{\mathbb{S}(x, k)} - 1 \right) \overline{q}(x, k) - \inf_{\mu \in [-\mathbb{S}(x, k_{\min}(x)), \mathbb{S}(x, r(x))]} \left(\sum_{k \in \mathcal{K}} \left(\frac{1}{\mathbb{S}_{\mu}(x, k)} - 1 \right) \overline{q}(x, k) \right), \end{split}$$

$$\text{where for any } x \in \mathfrak{X} \text{ and } k \in \mathfrak{K}, \, \mathbb{S}_{\mu}(x,k) = \begin{cases} \mathbb{S}(x,y), & y \notin \{k_{\min}(x),\mathsf{r}(x)\} \\ \mathbb{S}(x,k_{\min}(x)) + \mu & y = \mathsf{r}(x) \\ \mathbb{S}(x,\mathsf{r}(x)) - \mu & y = k_{\min}(x). \end{cases} \text{ Note that }$$

such a choice of S_{μ} leads to the following equality holds:

$$\sum_{k \notin \{\mathsf{r}(x), k_{\min}(x)\}} \left(\frac{1}{\mathsf{S}(x,k)} - 1\right) \overline{q}(x,k) = \sum_{k \notin \{\mathsf{r}(x), k_{\min}(x)\}} \left(\frac{1}{\mathsf{S}_{\mu}(x,k)} - 1\right) \overline{q}(x,k).$$

Therefore, the conditional regret of cost-sensitive sum exponential loss can be lower bounded as

$$\Delta \mathcal{C}_{\widetilde{\ell}_{\exp}^{\text{comp}}, \mathcal{H}}(h, x) \ge \sup_{\mu \in [-S(x, k_{\min}(x)), S(x, \mathsf{r}(x))]} \left\{ \overline{q}(x, k_{\min}(x)) \left[\frac{1}{S(x, k_{\min}(x))} - \frac{1}{S(x, \mathsf{r}(x)) - \mu} \right] + \overline{q}(x, \mathsf{r}(x)) \left[\frac{1}{S(x, \mathsf{r}(x))} - \frac{1}{S(x, k_{\min}(x)) + \mu} \right] \right\}.$$

By the concavity of the function, differentiate with respect to μ , we obtain that the supremum is achieved by $\mu^* = \frac{\sqrt{\overline{q}(x, \mathbf{r}(x))} \mathbb{S}(x, \mathbf{r}(x)) - \sqrt{\overline{q}(x, k_{\min}(x))} \mathbb{S}(x, k_{\min}(x))}{\sqrt{\overline{q}(x, k_{\min}(x))} + \sqrt{\overline{q}(x, \mathbf{r}(x))}}$. Plug in μ^* , we obtain

Therefore, by Lemma 20, the conditional regret of the target cardinality aware loss function can be upper bounded as follows:

$$\Delta \mathcal{C}_{\widetilde{\ell},\mathcal{H}}(r,x) = \overline{q}(x,k_{\min}(x)) - \overline{q}(x,\mathsf{r}(x)) \leq 2\Big(\Delta \mathcal{C}_{\widetilde{\ell}_{\exp}^{\mathrm{comp}},\mathcal{R}}(r,x)\Big)^{\frac{1}{2}}.$$

By the concavity, take expectations on both sides of the preceding equation, we obtain

$$\mathcal{E}_{\widetilde{\ell}}(r) - \mathcal{E}_{\widetilde{\ell}}^{*}(\mathcal{R}) + \mathcal{M}_{\widetilde{\ell}}(\mathcal{R}) \leq 2 \left(\mathcal{E}_{\widetilde{\ell}_{\exp}^{\text{comp}}}(r) - \mathcal{E}_{\widetilde{\ell}_{\exp}^{\text{comp}}}^{*}(\mathcal{R}) + \mathcal{M}_{\widetilde{\ell}_{\exp}^{\text{comp}}}(\mathcal{R}) \right)^{\frac{1}{2}}.$$

The second part follows from the fact that $\mathcal{M}_{\widetilde{\ell}_{\exp}^{\mathrm{comp}}}(\mathcal{R}_{\mathrm{all}})$ = 0.

Case III: $\ell = \widetilde{\ell}_{gce}$. For the cost-sensitive generalized cross-entropy loss $\widetilde{\ell}_{gce}$, the conditional error can be written as

$$\mathfrak{C}_{\widetilde{\ell}_{gce}}(r,x) = \sum_{y \in \mathbb{Y}} p(x,y) \sum_{k \in \mathcal{K}} \overline{c}(x,k,y) \frac{1}{\alpha} \left(1 - \left(\frac{e^{r(x,k)}}{\sum_{k' \in \mathcal{K}} e^{r(x,k')}} \right)^{\alpha} \right) = \frac{1}{\alpha} \sum_{k \in \mathcal{K}} (1 - \mathbb{S}(x,k)^{\alpha}) \overline{q}(x,k).$$

The conditional regret can be written as

$$\Delta \mathcal{C}_{\widetilde{\ell}_{gce},\mathcal{R}}(r,x) = \frac{1}{\alpha} \sum_{k \in \mathcal{K}} (1 - \mathcal{S}(x,k)^{\alpha}) \overline{q}(x,k) - \inf_{r \in \mathcal{R}} \left(\frac{1}{\alpha} \sum_{k \in \mathcal{K}} (1 - \mathcal{S}(x,k)^{\alpha}) \overline{q}(x,k) \right)$$

$$\geq \frac{1}{\alpha} \sum_{k \in \mathcal{K}} (1 - \mathcal{S}(x,k)^{\alpha}) \overline{q}(x,k) - \inf_{\mu \in [-\mathcal{S}(x,k_{\min}(x)),\mathcal{S}(x,r(x))]} \left(\frac{1}{\alpha} \sum_{k \in \mathcal{K}} (1 - \mathcal{S}_{\mu}(x,k)^{\alpha}) \overline{q}(x,k) \right),$$

where for any $x \in \mathcal{X}$ and $k \in \mathcal{K}$, $\mathcal{S}_{\mu}(x,k) = \begin{cases} \mathcal{S}(x,y), & y \notin \{k_{\min}(x),\mathsf{r}(x)\} \\ \mathcal{S}(x,k_{\min}(x)) + \mu & y = \mathsf{r}(x) \\ \mathcal{S}(x,\mathsf{r}(x)) - \mu & y = k_{\min}(x). \end{cases}$ Note that

such a choice of S_{μ} leads to the following equality holds:

$$\sum_{k \notin \{r(x), k_{\min}(x)\}} \frac{1}{\alpha} \sum_{k \in \mathcal{K}} (1 - \mathcal{S}(x, k)^{\alpha}) \overline{q}(x, k) = \sum_{k \notin \{r(x), k_{\min}(x)\}} \frac{1}{\alpha} \sum_{k \in \mathcal{K}} (1 - \mathcal{S}_{\mu}(x, k)^{\alpha}) \overline{q}(x, k).$$

Therefore, the conditional regret of cost-sensitive generalized cross-entropy loss can be lower bounded as

$$\Delta \mathcal{C}_{\widetilde{\ell}_{gce},\mathcal{H}}(h,x) = \frac{1}{\alpha} \sup_{\mu \in [-S(x,k_{\min}(x)),S(x,\mathsf{r}(x))]} \left\{ \overline{q}(x,k_{\min}(x)) [-S(x,k_{\min}(x))^{\alpha} + (S(x,\mathsf{r}(x)) - \mu)^{\alpha}] + \overline{q}(x,\mathsf{r}(x)) [-S(x,\mathsf{r}(x))^{\alpha} + (S(x,k_{\min}(x)) + \mu)^{\alpha}] \right\}.$$

By the concavity of the function, differentiate with respect to μ , we obtain that the supremum is achieved by $\mu^* = \frac{\overline{q}(x, \mathbf{r}(x))^{\frac{1}{1-\alpha}} \S(x, \mathbf{r}(x)) - \overline{q}(x, k_{\min}(x))^{\frac{1}{1-\alpha}} \S(x, k_{\min}(x))}{\overline{q}(x, k_{\min}(x))^{\frac{1}{1-\alpha}} + \overline{q}(x, \mathbf{r}(x))^{\frac{1}{1-\alpha}}}$. Plug in μ^* , we obtain

Therefore, by Lemma 20, the conditional regret of the target cardinality aware loss function can be upper bounded as follows:

$$\Delta \mathcal{C}_{\widetilde{\ell},\mathcal{H}}(r,x) = \overline{q}(x,k_{\min}(x)) - \overline{q}(x,\mathsf{r}(x)) \leq 2n^{\frac{\alpha}{2}} \Big(\Delta \mathcal{C}_{\widetilde{\ell}_{\mathit{rec}},\mathcal{R}}(r,x)\Big)^{\frac{1}{2}}.$$

By the concavity, take expectations on both sides of the preceding equation, we obtain

$$\mathcal{E}_{\widetilde{\ell}}(r) - \mathcal{E}_{\widetilde{\ell}}^{*}(\mathcal{R}) + \mathcal{M}_{\widetilde{\ell}}(\mathcal{R}) \leq 2n^{\frac{\alpha}{2}} \Big(\mathcal{E}_{\widetilde{\ell}_{gce}}(r) - \mathcal{E}_{\widetilde{\ell}_{gce}}^{*}(\mathcal{R}) + \mathcal{M}_{\widetilde{\ell}_{gce}}(\mathcal{R}) \Big)^{\frac{1}{2}}.$$

The second part follows from the fact that $\mathfrak{M}_{\widetilde{\ell}_{\rm gce}}(\mathfrak{R}_{\rm all})$ = 0.

Case IV: $\ell = \widetilde{\ell}_{mae}$. For the cost-sensitive mean absolute error loss $\widetilde{\ell}_{mae}$, the conditional error can be written as

$$\mathfrak{C}_{\widetilde{\ell}_{\text{mae}}}(r,x) = \sum_{y \in \mathcal{Y}} p(x,y) \sum_{k \in \mathcal{K}} \overline{c}(x,k,y) \left(1 - \left(\frac{e^{r(x,k)}}{\sum_{k' \in \mathcal{K}} e^{r(x,k')}} \right) \right) = \sum_{k \in \mathcal{K}} (1 - \mathcal{S}(x,k)) \overline{q}(x,k).$$

The conditional regret can be written as

$$\Delta \mathcal{C}_{\widetilde{\ell}_{\text{mae}}, \mathcal{R}}(r, x) = \sum_{k \in \mathcal{K}} (1 - \mathcal{S}(x, k)) \overline{q}(x, k) - \inf_{r \in \mathcal{R}} \left(\sum_{k \in \mathcal{K}} (1 - \mathcal{S}(x, k)) \overline{q}(x, k) \right)$$

$$\geq \sum_{k \in \mathcal{K}} (1 - \mathcal{S}(x, k)) \overline{q}(x, k) - \inf_{\mu \in [-\mathcal{S}(x, k_{\min}(x)), \mathcal{S}(x, r(x))]} \left(\sum_{k \in \mathcal{K}} (1 - \mathcal{S}_{\mu}(x, k)) \overline{q}(x, k) \right),$$

where for any
$$x \in \mathcal{X}$$
 and $k \in \mathcal{K}$, $\mathcal{S}_{\mu}(x,k) = \begin{cases} \mathcal{S}(x,y), & y \notin \{k_{\min}(x),\mathsf{r}(x)\} \\ \mathcal{S}(x,k_{\min}(x)) + \mu & y = \mathsf{r}(x) \\ \mathcal{S}(x,\mathsf{r}(x)) - \mu & y = k_{\min}(x). \end{cases}$ Note that such a choice of \mathcal{S}_{μ} leads to the following equality holds:

such a choice of S_{μ} leads to the following equality hold

$$\sum_{k \in \mathcal{K}} (1 - \mathcal{S}(x, k)) \overline{q}(x, k) = \sum_{k \in \mathcal{K}} (1 - \mathcal{S}_{\mu}(x, k)) \overline{q}(x, k).$$

Therefore, the conditional regret of cost-sensitive mean absolute error can be lower bounded as

$$\Delta \mathcal{C}_{\widetilde{\ell}_{\text{mae}},\mathcal{H}}(h,x) \geq \sup_{\mu \in [-\mathcal{S}(x,k_{\min}(x)),\mathcal{S}(x,\mathsf{r}(x))]} \left\{ \overline{q}(x,k_{\min}(x))[-\mathcal{S}(x,k_{\min}(x)) + \mathcal{S}(x,\mathsf{r}(x)) - \mu] + \overline{q}(x,\mathsf{r}(x))[-\mathcal{S}(x,\mathsf{r}(x)) + \mathcal{S}(x,k_{\min}(x)) + \mu] \right\}.$$

By the concavity of the function, differentiate with respect to μ , we obtain that the supremum is achieved by $\mu^* = -S(x, k_{\min}(x))$. Plug in μ^* , we obtain

$$\begin{split} &\Delta \mathcal{C}_{\widetilde{\ell}_{\mathrm{mae}},\mathcal{H}}(h,x) \\ &\geq \overline{q}(x,k_{\mathrm{min}}(x))\mathcal{S}(x,\mathsf{r}(x)) - \overline{q}(x,\mathsf{r}(x))\mathcal{S}(x,\mathsf{r}(x)) \\ &\geq \frac{1}{n}(\overline{q}(x,k_{\mathrm{min}}(x)) - \overline{q}(x,\mathsf{r}(x))). \end{split} \tag{minimum is achieved when } \mathcal{S}(x,\mathsf{r}(x)) = \frac{1}{n}) \end{split}$$

Therefore, by Lemma 20, the conditional regret of the target cardinality aware loss function can be upper bounded as follows:

$$\Delta \mathfrak{C}_{\widetilde{\ell},\mathcal{H}}(r,x) = \overline{q}(x,k_{\min}(x)) - \overline{q}(x,\mathsf{r}(x)) \leq n\Big(\Delta \mathfrak{C}_{\widetilde{\ell}_{\max},\mathcal{R}}(r,x)\Big).$$

By the concavity, take expectations on both sides of the preceding equation, we obtain

$$\mathcal{E}_{\widetilde{\ell}}(r) - \mathcal{E}_{\widetilde{\ell}}^{*}(\mathcal{R}) + \mathcal{M}_{\widetilde{\ell}}(\mathcal{R}) \leq n \Big(\mathcal{E}_{\widetilde{\ell}_{\text{mae}}}(r) - \mathcal{E}_{\widetilde{\ell}_{\text{mae}}}^{*}(\mathcal{R}) + \mathcal{M}_{\widetilde{\ell}_{\text{mae}}}(\mathcal{R}) \Big).$$

The second part follows from the fact that $\mathcal{M}_{\widetilde{\ell}_{max}}(\mathcal{R}_{all}) = 0$.

E.2. Proof of Theorem 16

The conditional error for the cost-sensitive constrained loss can be expressed as follows:

$$\begin{split} \mathcal{C}_{\widetilde{\ell}^{\text{cstnd}}}(r,x) &= \sum_{y \in \mathcal{Y}} p(x,y) \widetilde{\ell}^{\text{cstnd}}(r,x,y) \\ &= \sum_{y \in \mathcal{Y}} p(x,y) \sum_{k \in \mathcal{K}} c(x,k,y) \Phi(-r(x,k)) \\ &= \sum_{k \in \mathcal{K}} \widetilde{q}(x,k) \Phi(-r(x,k)), \end{split}$$

where $\widetilde{q}(x,k) = \sum_{y \in \mathbb{Y}} p(x,y) c(x,k,y) \in [0,1]$. Let $k_{\min}(x) = \operatorname{argmin}_{k \in \mathcal{K}} \widetilde{q}(x,k)$. We denote by $\Phi_{\exp}: t \mapsto e^{-t}$ the exponential loss function, $\Phi_{\operatorname{sq-hinge}}: t \mapsto \max\{0,1-t\}^2$ the squared hinge loss function, $\Phi_{\operatorname{hinge}}: t \mapsto \max\{0,1-t\}$ the hinge loss function, and $\Phi_{\rho}: t \mapsto \min\{\max\{0,1-t/\rho\},1\}$, $\rho > 0$ the ρ -margin loss function.

Theorem 16 Assume that \mathbb{R} is symmetric and complete. Then, the following \mathbb{R} -consistency bound holds for the cost-sensitive constrained loss:

$$\mathcal{E}_{\widetilde{\ell}}(r) - \mathcal{E}_{\widetilde{\ell}}^{*}(\mathcal{R}) + \mathcal{M}_{\widetilde{\ell}}(\mathcal{R}) \leq \gamma \left(\mathcal{E}_{\widetilde{\ell} \operatorname{cstnd}}(r) - \mathcal{E}_{\widetilde{\ell} \operatorname{cstnd}}^{*}(\mathcal{R}) + \mathcal{M}_{\widetilde{\ell} \operatorname{cstnd}}(\mathcal{R}) \right);$$

In the special case where $\Re = \Re_{all}$, the following holds:

$$\mathcal{E}_{\widetilde{\ell}}(r) - \mathcal{E}_{\widetilde{\ell}}^*(\mathcal{R}_{\rm all}) \leq \gamma \Big(\mathcal{E}_{\widetilde{\ell}^{\rm cstnd}}(r) - \mathcal{E}_{\widetilde{\ell}^{\rm cstnd}}^*(\mathcal{R}_{\rm all})\Big)$$

where $\gamma(t) = 2\sqrt{t}$ when $\widetilde{\ell}^{cstnd}$ is either $\widetilde{\ell}^{cstnd}_{exp}$ or $\widetilde{\ell}_{sq-hinge}$; $\gamma(t) = t$ when $\widetilde{\ell}^{cstnd}$ is either $\widetilde{\ell}_{hinge}$ or $\widetilde{\ell}_{\rho}$.

Proof Case I: $\ell = \widetilde{\ell}_{exp}^{cstnd}$. For the cost-sensitive constrained exponential loss $\widetilde{\ell}_{exp}^{cstnd}$, the conditional regret can be written as

$$\Delta \mathcal{C}_{\widetilde{\ell}_{\exp}^{\text{cstnd}}, \mathcal{R}}(r, x) = \sum_{k \in \mathcal{K}} \widetilde{q}(x, k \Phi_{\exp}(-r(x, k)) - \inf_{r \in \mathcal{R}} \sum_{k \in \mathcal{K}} \widetilde{q}(x, k) \Phi_{\exp}(-r(x, k))$$

$$\geq \sum_{k \in \mathcal{K}} \widetilde{q}(x, k) \Phi_{\exp}(-r(x, k)) - \inf_{\mu \in \mathbb{R}} \sum_{k \in \mathcal{K}} \widetilde{q}(x, k) \Phi_{\exp}(-r_{\mu}(x, k)),$$

 $\text{where for any } k \in \mathcal{K}, \, r_{\mu}(x,k) = \begin{cases} r(x,y), & y \notin \{k_{\min}(x), \mathsf{r}(x)\} \\ r(x,k_{\min}(x)) + \mu & y = \mathsf{r}(x) \\ r(x,\mathsf{r}(x)) - \mu & y = k_{\min}(x). \end{cases} \quad \text{Note that such a choice}$

of r_u leads to the following equality holds:

$$\sum_{k \notin \{r(x), k_{\min}(x)\}} \widetilde{q}(x, k) \Phi_{\exp}(-r(x, k)) = \sum_{k \notin \{r(x), k_{\min}(x)\}} \sum_{k \in \mathcal{K}} \widetilde{q}(x, k) \Phi_{\exp}(-r_{\mu}(x, k)).$$

Therefore, the conditional regret of cost-sensitive constrained exponential loss can be lower bounded as

$$\begin{split} &\Delta \mathcal{C}_{\widetilde{\ell}_{\exp}^{\text{cstnd}}, \mathcal{R}}(r, x) \\ &\geq \inf_{r \in \mathcal{R}} \sup_{\mu \in \mathbb{R}} \left\{ \widetilde{q}(x, k_{\min}(x)) \left(e^{r(x, k_{\min}(x))} - e^{r(x, \mathsf{r}(x)) - \mu} \right) + \widetilde{q}(x, \mathsf{r}(x)) \left(e^{r(x, \mathsf{r}(x))} - e^{r(x, k_{\min}(x)) + \mu} \right) \right\} \\ &= \left(\sqrt{\widetilde{q}(x, k_{\min}(x))} - \sqrt{\widetilde{q}(x, \mathsf{r}(x))} \right)^2 & \text{(differentiating with respect to } \mu, r \text{ to optimize)} \\ &= \left(\frac{\widetilde{q}(x, \mathsf{r}(x)) - \widetilde{q}(x, k_{\min}(x))}{\sqrt{\widetilde{q}(x, k_{\min}(x))} + \sqrt{\widetilde{q}(x, \mathsf{r}(x))}} \right)^2 \\ &\geq \frac{1}{4} (\widetilde{q}(x, \mathsf{r}(x)) - \widetilde{q}(x, k_{\min}(x)))^2. \end{split} \tag{0} \leq \widetilde{q}(x, k) \leq 1)$$

Therefore, by Lemma 20, the conditional regret of the target cardinality aware loss function can be upper bounded as follows:

$$\Delta \mathcal{C}_{\widetilde{\ell},\mathcal{H}}(r,x) = \widetilde{q}(x,\mathsf{r}(x)) - \widetilde{q}(x,k_{\min}(x)) \leq 2\Big(\Delta \mathcal{C}_{\widetilde{\ell}_{\exp}^{\mathrm{cstnd}},\mathcal{R}}(r,x)\Big)^{\frac{1}{2}}.$$

By the concavity, take expectations on both sides of the preceding equation, we obtain

$$\mathcal{E}_{\widetilde{\ell}}(r) - \mathcal{E}_{\widetilde{\ell}}^{*}(\mathcal{R}) + \mathcal{M}_{\widetilde{\ell}}(\mathcal{R}) \leq 2 \left(\mathcal{E}_{\widetilde{\ell}_{\exp}}^{\text{cstnd}}(r) - \mathcal{E}_{\widetilde{\ell}_{\exp}}^{*}(\mathcal{R}) + \mathcal{M}_{\widetilde{\ell}_{\exp}}^{\text{cstnd}}(\mathcal{R}) \right)^{\frac{1}{2}}.$$

The second part follows from the fact that $\mathcal{M}_{\widetilde{\ell}_{axm}^{cstnd}}(\mathcal{R}_{all}) = 0$.

Case II: $\ell = \widetilde{\ell}_{sq-hinge}$. For the cost-sensitive constrained squared hinge loss $\widetilde{\ell}_{sq-hinge}$, the conditional regret can be written as

$$\begin{split} \Delta \mathcal{C}_{\widetilde{\ell}_{\operatorname{sq-hinge}}, \mathcal{R}}(r, x) &= \sum_{k \in \mathcal{K}} \widetilde{q}(x, k) \Phi_{\operatorname{sq-hinge}}(-r(x, k)) - \inf_{r \in \mathcal{R}} \sum_{k \in \mathcal{K}} \widetilde{q}(x, k) \Phi_{\operatorname{sq-hinge}}(-r(x, k)) \\ &\geq \sum_{k \in \mathcal{K}} \widetilde{q}(x, k) \Phi_{\operatorname{sq-hinge}}(-r(x, k)) - \inf_{\mu \in \mathbb{R}} \sum_{k \in \mathcal{K}} \widetilde{q}(x, k) \Phi_{\operatorname{sq-hinge}}(-r_{\mu}(x, k)), \end{split}$$

$$\text{where for any } k \in \mathcal{K}, \, r_{\mu}(x,k) = \begin{cases} r(x,y), & y \notin \{k_{\min}(x), \mathsf{r}(x)\} \\ r(x,k_{\min}(x)) + \mu & y = \mathsf{r}(x) \\ r(x,\mathsf{r}(x)) - \mu & y = k_{\min}(x). \end{cases} \quad \text{Note that such a choice}$$

of r_{μ} leads to the following equality holds:

$$\sum_{k \notin \{r(x), k_{\min}(x)\}} \widetilde{q}(x, k) \Phi_{\text{sq-hinge}}(-r(x, k)) = \sum_{k \notin \{r(x), k_{\min}(x)\}} \sum_{k \in \mathcal{K}} \widetilde{q}(x, k) \Phi_{\text{sq-hinge}}(-r_{\mu}(x, k)).$$

Therefore, the conditional regret of cost-sensitive constrained squared hinge loss can be lower bounded as

$$\begin{split} &\Delta \mathfrak{C}_{\widetilde{\ell}_{\mathrm{sq-hinge}},\mathfrak{R}}(r,x) \\ &\geq \inf_{r \in \mathfrak{R}} \sup_{\mu \in \mathbb{R}} \left\{ \widetilde{q}(x,k_{\min}(x)) \left(\max\{0,1+r(x,k_{\min}(x))\}^2 - \max\{0,1+r(x,\mathsf{r}(x))-\mu\}^2 \right) \right. \\ &\left. + \widetilde{q}(x,\mathsf{r}(x)) \left(\max\{0,1+r(x,\mathsf{r}(x))\}^2 - \max\{0,1+r(x,k_{\min}(x))+\mu\}^2 \right) \right\} \\ &\geq \frac{1}{4} (\widetilde{q}(x,k_{\min}(x)) - \widetilde{q}(x,\mathsf{r}(x)))^2. \end{split} \tag{differentiating with respect to } \mu, r \text{ to optimize})$$

Therefore, by Lemma 20, the conditional regret of the target cardinality aware loss function can be upper bounded as follows:

$$\Delta \mathcal{C}_{\widetilde{\ell},\mathcal{H}}(r,x) = \widetilde{q}(x,\mathsf{r}(x)) - \widetilde{q}(x,k_{\min}(x)) \leq 2\Big(\Delta \mathcal{C}_{\widetilde{\ell}_{\mathrm{sq-hinge}},\mathcal{R}}(r,x)\Big)^{\frac{1}{2}}.$$

By the concavity, take expectations on both sides of the preceding equation, we obtain

$$\mathcal{E}_{\widetilde{\ell}}(r) - \mathcal{E}_{\widetilde{\ell}}^{*}(\mathcal{R}) + \mathcal{M}_{\widetilde{\ell}}(\mathcal{R}) \leq 2 \left(\mathcal{E}_{\widetilde{\ell}_{\operatorname{sq-hinge}}}(r) - \mathcal{E}_{\widetilde{\ell}_{\operatorname{sq-hinge}}}^{*}(\mathcal{R}) + \mathcal{M}_{\widetilde{\ell}_{\operatorname{sq-hinge}}}(\mathcal{R}) \right)^{\frac{1}{2}}.$$

The second part follows from the fact that $\mathfrak{M}_{\widetilde{\ell}_{sq-hinge}}(\mathfrak{R}_{all})$ = 0.

Case III: $\ell = \widetilde{\ell}_{\text{hinge}}$. For the cost-sensitive constrained hinge loss $\widetilde{\ell}_{\text{hinge}}$, the conditional regret can be written as

$$\begin{split} \Delta \mathcal{C}_{\widetilde{\ell}_{\mathrm{hinge}}, \mathcal{R}}(r, x) &= \sum_{k \in \mathcal{K}} \widetilde{q}(x, k) \Phi_{\mathrm{hinge}}(-r(x, k)) - \inf_{r \in \mathcal{R}} \sum_{k \in \mathcal{K}} \widetilde{q}(x, k) \Phi_{\mathrm{hinge}}(-r(x, k)) \\ &\geq \sum_{k \in \mathcal{K}} \widetilde{q}(x, k) \Phi_{\mathrm{hinge}}(-r(x, k)) - \inf_{\mu \in \mathbb{R}} \sum_{k \in \mathcal{K}} \widetilde{q}(x, k) \Phi_{\mathrm{hinge}}(-r_{\mu}(x, k)), \end{split}$$

where for any
$$k \in \mathcal{K}$$
, $r_{\mu}(x,k) = \begin{cases} r(x,y), & y \notin \{k_{\min}(x), \mathsf{r}(x)\} \\ r(x,k_{\min}(x)) + \mu & y = \mathsf{r}(x) \\ r(x,\mathsf{r}(x)) - \mu & y = k_{\min}(x). \end{cases}$ Note that such a choice of r , leads to the following equality holds:

of r_{μ} leads to the following equality holds:

$$\sum_{k \notin \{\mathsf{r}(x), k_{\min}(x)\}} \widetilde{q}(x, k) \Phi_{\text{hinge}}(-r(x, k)) = \sum_{k \notin \{\mathsf{r}(x), k_{\min}(x)\}} \sum_{k \in \mathcal{K}} \widetilde{q}(x, k) \Phi_{\text{hinge}}(-r_{\mu}(x, k)).$$

Therefore, the conditional regret of cost-sensitive constrained hinge loss can be lower bounded as

$$\Delta \mathcal{C}_{\widetilde{\ell}_{\mathrm{hinge}},\mathcal{R}}(r,x) \geq \inf_{r \in \mathcal{R}} \sup_{\mu \in \mathbb{R}} \left\{ q(x,k_{\min}(x))(\max\{0,1+r(x,k_{\min}(x))\} - \max\{0,1+r(x,\mathsf{r}(x))-\mu\}) + q(x,\mathsf{r}(x))(\max\{0,1+r(x,\mathsf{r}(x))\} - \max\{0,1+r(x,k_{\min}(x))+\mu\}) \right\}$$

$$\geq q(x,\mathsf{r}(x)) - q(x,k_{\min}(x)). \quad \text{(differentiating with respect to } \mu,r \text{ to optimize)}$$

Therefore, by Lemma 20, the conditional regret of the target cardinality aware loss function can be upper bounded as follows:

$$\Delta \mathcal{C}_{\widetilde{\ell},\mathcal{H}}(r,x) = \widetilde{q}(x,\mathsf{r}(x)) - \widetilde{q}(x,k_{\min}(x)) \leq \Delta \mathcal{C}_{\widetilde{\ell}_{\operatorname{hinge}},\mathcal{R}}(r,x).$$

By the concavity, take expectations on both sides of the preceding equation, we obtain

$$\mathcal{E}_{\widetilde{\ell}}(r) - \mathcal{E}_{\widetilde{\ell}}^{\star}(\mathcal{R}) + \mathcal{M}_{\widetilde{\ell}}(\mathcal{R}) \leq \mathcal{E}_{\widetilde{\ell}_{\mathrm{hinge}}}(r) - \mathcal{E}_{\widetilde{\ell}_{\mathrm{hinge}}}^{\star}(\mathcal{R}) + \mathcal{M}_{\widetilde{\ell}_{\mathrm{hinge}}}(\mathcal{R}).$$

The second part follows from the fact that $\mathfrak{M}_{\widetilde{\ell}_{\mathrm{hinge}}}(\mathcal{R}_{\mathrm{all}})$ = 0.

Case IV: $\ell = \widetilde{\ell}_{\rho}$. For the cost-sensitive constrained ρ -margin loss $\widetilde{\ell}_{\rho}$, the conditional regret can be written as

$$\begin{split} \Delta \mathcal{C}_{\widetilde{\ell}_{\rho}, \mathcal{R}}(r, x) &= \sum_{k \in \mathcal{K}} \widetilde{q}(x, k) \Phi_{\rho}(-r(x, k)) - \inf_{r \in \mathcal{R}} \sum_{k \in \mathcal{K}} \widetilde{q}(x, k) \Phi_{\rho}(-r(x, k)) \\ &\geq \sum_{k \in \mathcal{K}} \widetilde{q}(x, k) \Phi_{\rho}(-r(x, k)) - \inf_{\mu \in \mathbb{R}} \sum_{k \in \mathcal{K}} \widetilde{q}(x, k) \Phi_{\rho}(-r_{\mu}(x, k)), \end{split}$$

where for any
$$k \in \mathcal{K}$$
, $r_{\mu}(x,k) = \begin{cases} r(x,y), & y \notin \{k_{\min}(x), \mathsf{r}(x)\} \\ r(x,k_{\min}(x)) + \mu & y = \mathsf{r}(x) \\ r(x,\mathsf{r}(x)) - \mu & y = k_{\min}(x). \end{cases}$ Note that such a choice of r_{μ} leads to the following equality holds:

$$\sum_{k \notin \{\mathsf{r}(x), k_{\min}(x)\}} \widetilde{q}(x, k) \Phi_{\rho}(-r(x, k)) = \sum_{k \notin \{\mathsf{r}(x), k_{\min}(x)\}} \sum_{k \in \mathcal{K}} \widetilde{q}(x, k) \Phi_{\rho}(-r_{\mu}(x, k)).$$

Therefore, the conditional regret of cost-sensitive constrained ρ -margin loss can be lower bounded as $\Delta \mathcal{C}_{\widetilde{\ell}_{\alpha},\mathcal{R}}(r,x)$

$$\geq \inf_{r \in \mathbb{R}} \sup_{\mu \in \mathbb{R}} \left\{ \widetilde{q}(x, k_{\min}(x)) \left(\min \left\{ \max \left\{ 0, 1 + \frac{r(x, k_{\min}(x))}{\rho} \right\}, 1 \right\} - \min \left\{ \max \left\{ 0, 1 + \frac{r(x, r(x)) - \mu}{\rho} \right\}, 1 \right\} \right) \right. \\ \left. + \widetilde{q}(x, r(x)) \left(\min \left\{ \max \left\{ 0, 1 + \frac{r(x, r(x))}{\rho} \right\}, 1 \right\} - \min \left\{ \max \left\{ 0, 1 + \frac{r(x, k_{\min}(x)) + \mu}{\rho} \right\}, 1 \right\} \right) \right\} \\ \geq \widetilde{q}(x, r(x)) - \widetilde{q}(x, k_{\min}(x)).$$
 (differentiating with respect to μ , r to optimize)

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Therefore, by Lemma 20, the conditional regret of the target cardinality aware loss function can be upper bounded as follows:

$$\Delta \mathfrak{C}_{\widetilde{\ell},\mathfrak{H}}(r,x) = \widetilde{q}(x,\mathsf{r}(x)) - \widetilde{q}(x,k_{\min}(x)) \leq \Delta \mathfrak{C}_{\widetilde{\ell}_{\rho},\mathfrak{R}}(r,x).$$

By the concavity, take expectations on both sides of the preceding equation, we obtain

$$\mathcal{E}_{\widetilde{\ell}}(r) - \mathcal{E}_{\widetilde{\ell}}^{*}(\mathcal{R}) + \mathcal{M}_{\widetilde{\ell}}(\mathcal{R}) \leq \mathcal{E}_{\widetilde{\ell}_{\rho}}(r) - \mathcal{E}_{\widetilde{\ell}_{\rho}}^{*}(\mathcal{R}) + \mathcal{M}_{\widetilde{\ell}_{\rho}}(\mathcal{R}).$$

The second part follows from the fact that $\mathfrak{M}_{\widetilde{\ell_{\rho}}}(\mathfrak{R}_{all})$ = 0.