On Structured Prediction Theory with Calibrated Convex Surrogate Losses

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Abstract

We provide novel theoretical insights on structured prediction in the context of efficient convex surrogate loss minimization with consistency guarantees. For any task loss, we construct a convex surrogate that can be optimized via stochastic gradient descent and we prove tight bounds on the so-called “calibration function” relating the excess surrogate risk to the actual risk. In contrast to prior related work, we carefully monitor the effect of the exponential number of classes in the learning guarantees as well as on the optimization complexity. As an interesting consequence, we formalize the intuition that some task losses make learning harder than others, and that the classical 0-1 loss is ill-suited for structured prediction.

1 Introduction

Structured prediction is a subfield of machine learning aiming at making multiple interrelated predictions simultaneously. The desired outputs (labels) are typically organized in some structured object such as a sequence, a graph, an image, etc. Tasks of this type appear in many practical domains such as computer vision [31], natural language processing [38] and bioinformatics [17].

The structured prediction setup has at least two typical properties differentiating it from the classical binary classification problems extensively studied in learning theory:

1. Exponential number of classes: this brings both additional computational and statistical challenges. By exponential, we mean exponentially large in the size of the natural dimension of output, e.g., the number of all possible sequences is exponential w.r.t. the sequence length.

2. Cost-sensitive learning: in typical applications, prediction mistakes are not all equally costly. The prediction error is usually measured with a highly-structured task-specific loss function, e.g., Hamming distance between sequences of multi-label variables or mean average precision for ranking.

Despite many algorithmic advances to tackle structured prediction problems [3, 32], there have been relatively few papers devoted to its theoretical understanding. Notable recent exceptions that made significant progress include Cortes et al. [12] and London et al. [25] (see references therein) which proposed data-dependent generalization error bounds in terms of popular empirical convex surrogate losses such as the structured hinge loss [40, 41, 43]. A question not addressed by these works is whether their algorithms are consistent: does minimizing their convex bounds with infinite data lead to the minimization of the task loss as well? Alternatively, the structured probit and ramp losses are consistent [28, 27], but non-convex and thus it is hard to obtain computational guarantees for them. In this paper, we aim at getting the property of consistency for surrogate losses that can be efficiently minimized with guarantees, and thus we consider convex surrogate losses.

The consistency of convex surrogates is well understood in the case of binary classification [46, 4, 39] and there is significant progress in the case of multi-class 0-1 loss [45, 42] and general loss.
functions [2, 35, 44]. A large body of work specifically focuses on the related tasks of ranking [16, 8, 36] and ordinal regression [34].

Contributions. In this paper, we study consistent convex surrogate losses specifically in the context of an exponential number of classes. We argue that even while being consistent, a convex surrogate might not allow efficient learning. As a concrete example, Ciliberto et al. [9] recently proposed a consistent approach to structured prediction, but the constant in their generalization error bound can be exponentially large as we explain in our section on related works. There are two possible sources of difficulties from the optimization perspective: to reach adequate accuracy on the task loss, one might need to optimize a surrogate loss to exponentially small accuracy or an optimization method might need an exponential number of steps because of unfortunate properties of the objective. We propose a theoretical framework that jointly tackles these two aspects and allows to judge the feasibility of efficient learning. In particular, we construct a calibration function [39], i.e., a function setting the relationship between accuracy on the surrogate and task losses, and normalize it by the means of convergence rate of an optimization algorithm.

Aiming for the simplest possible application of our framework, we propose a family of convex surrogates that are consistent for any given task loss and can be optimized using stochastic gradient descent. For a special case of our family (quadratic surrogate), we provide a complete analysis including general lower and upper bounds on the calibration function for any task loss, with exact values for the 0-1, block 0-1 and Hamming losses. We observe that to have a tractable learning algorithm, one needs both a structured loss (not the 0-1 loss) and appropriate constraints on the predictor, e.g., in the form of linear constraints for the score vector functions. Our framework also indicates that in some cases it might be beneficial to use non-consistent surrogates. In particular, a non-consistent surrogate might allow optimization only up to specific accuracy, but exponentially faster than a consistent one.

This paper is organized as follows. In Sections 2 and 3, we introduce the structured prediction setting suitable for studying consistency. Section 4 introduces the surrogate losses we work with, presents our bounds on calibration functions, computes the exact calibration functions for some special cases. We review connections to some related works in Section 5 and conclude in Section 6.

2 Structured prediction setup

In structured prediction, the goal is to predict a structured output \( y \in \mathcal{Y} \) (such as a sequence, a graph, an image) given an input \( x \in \mathcal{X} \). The quality of prediction is measured by a task-dependent loss function \( L(\hat{y}, y \mid x) \geq 0 \) specifying the cost for predicting \( \hat{y} \) when the correct output is \( y \). In this paper, we consider the case when the number of possible predictions and the number of possible labels are both finite. For simplicity,\(^\text{1}\) we also assume that the sets of possible predictions and correct outputs always coincide and do not depend on \( x \). We refer to this set as the set of labels \( \mathcal{Y} \), denote its cardinality by \( k \), and map its elements to \( 1, \ldots, k \). In this setting, assuming that the loss function depends only on \( \hat{y} \) and \( y \), but not on \( x \) directly, the loss is defined by a loss matrix \( L \in \mathbb{R}^{k \times k} \).

We assume that all elements of matrix \( L \) are non-negative and will use \( L_{\text{max}} \) to denote the maximal element. Compared to multi-class classification, \( k \) is typically exponentially large in the size of the natural dimension of \( y \), e.g., contains all possible sequences of symbols from a finite alphabet.

Following standard practices in structured prediction [11, 40], we define the prediction model by a score function \( f : \mathcal{X} \rightarrow \mathbb{R}^k \) specifying a score \( f_y(x) \) for each possible output \( y \in \mathcal{Y} \). The final prediction is done by selecting a label with the maximal value of the score

\[
\text{pred}(\hat{f}(x)) := \underset{y \in \mathcal{Y}}{\text{Argmax}} \, f_y(x),
\]

with some fixed strategy to resolve ties. To simplify analysis, we assume that among the labels with maximal scores, the predictor always picks the one with the smallest index.

The goal of prediction-based machine learning consists in finding a predictor that works well on the unseen test set, i.e., data points coming from the same distribution \( D \) as the one generating training data. One way to formalize this is to minimize the generalization error, often referred to as the actual (or population) risk based on the loss \( L \),

\[
R_L(f) := E_{(x, y) \sim D} \, L(\text{pred}(\hat{f}(x)), y).
\]

\(\text{1} \)Our analysis is compatible with rectangular losses, e.g., ranking losses studied by Ramaswamy et al. [36].
Minimizing the actual risk (2) is often hard. The standard approach is to minimize a surrogate risk, which is a different objective easier to optimize, e.g., convex. We define a surrogate loss as a functional \( \Phi : \mathbb{R}^k \times \mathcal{Y} \rightarrow \mathbb{R} \) depending on a score vector \( f = f(x) \in \mathbb{R}^k \) and a label \( y \in \mathcal{Y} \) as input arguments. We denote the \( y \)-th component of \( f \) with \( f_y \). The surrogate risk (the \( \Phi \)-risk) is defined as

\[
\mathcal{R}_\Phi (f) := E_{(x, y) \sim D} \Phi(f(x), y),
\]

where the expectation is taken w.r.t. the data-generating distribution \( D \). To make minimization of (3) well-defined, we always assume that the surrogate loss \( \Phi \) is bounded from below and continuous.

Examples of common surrogate losses include the structured hinge-loss [40, 43] \( \Phi_{\text{SSVM}}(f, y) := \max_{y \in \mathcal{Y}} (f_y + L(y, y)) - f_y \), the log loss (maximum likelihood learning) used, e.g., in conditional random fields [22], \( \Phi_{\log}(f, y) := -f_y + \log \sum_{y' \in \mathcal{Y}} \exp f_{y'} \), and their hybrids [19, 37].

In terms of the task losses, we consider the unstructured 0-1 loss \( L_{01}(\hat{y}, y) := [\hat{y} \neq y] \), and the two structured losses: block 0-1 loss with \( b \) equal blocks of labels \( L_{01,b}(\hat{y}, y) := [\hat{y} \neq y] \) and their hybrids [19, 37].

We now formalize the connection between the actual risk (2) and the surrogate risk with the actual excess risk via the so-called calibration function, see Definition 1 [4, 45, 39, 16, 2]. As it is standard for this kind of analysis, the setup is non-parametric, i.e., it does not take into account the dependency of scores on input variables \( x \). For now, we assume that a family of score functions \( \Phi \) consists of all vector-valued Borel measurable functions \( f : \mathcal{X} \rightarrow \mathcal{F} \), where \( \mathcal{F} \subseteq \mathbb{R}^k \) is a subspace of all allowed score vectors that will play an important role in our analysis. This setting is equivalent to pointwise analysis, i.e., looking at data points individually. We bring the dependency on input back into the analysis in Section 3.3 where we assume a specific family of score functions.

Let \( \mathcal{D}_X \) represent the marginal distribution for \( D \) on \( x \) and \( P(\cdot | x) \) denote its conditional given \( x \). We can now rewrite the risk \( \mathcal{R}_L \) and the surrogate \( \Phi \)-risk \( \mathcal{R}_\Phi \) via the so-called calibration function, see Definition 1 [4, 45, 39, 16, 2].

\[
\mathcal{R}_L(f) = E_{x \sim \mathcal{D}_X} \ell(f(x), P(\cdot | x)), \quad \mathcal{R}_\Phi(f) = E_{x \sim \mathcal{D}_X} \phi(f(x), P(\cdot | x)),
\]

where the conditional risk \( \ell \) and the conditional \( \Phi \)-risk \( \phi \) depend on a vector of scores \( f \) and a conditional distribution on the set of output labels \( q \) as

\[
\ell(f, q) := \sum_{c=1}^k q_c L(\text{pred}(f), c), \quad \phi(f, q) := \sum_{c=1}^k q_c \Phi(f, c).
\]

The calibration function \( H_{\Phi, L, F} \) between the surrogate loss \( \Phi \) and the task loss \( L \) relates the excess surrogate risk with the actual excess risk via the excess risk bound:

\[
H_{\Phi, L, F}(\delta \ell(f, q)) \leq \delta \phi(f, q), \quad \forall f \in F, \forall q \in \Delta_k,
\]

(4)

where \( \delta \phi(f, q) = \phi(f, q) - \inf_{f' \in F} \phi(f', q) \), \( \delta \ell(f, q) = \ell(f, q) - \inf_{f \in F} \ell(f, q) \) are the excess risks and \( \Delta_k \) denotes the probability simplex of dimension \( k - 1 \).

In other words, to find a vector \( f \) that yields an excess risk smaller than \( \varepsilon \), we need to optimize the \( \Phi \)-risk up to \( H_{\Phi, L, F}(\varepsilon) \) accuracy (in the worst case). We make this statement precise in Theorem 2 below, and now proceed to the formal definition of the calibration function.

**Definition 1 (Calibration function).** For a task loss \( L \), a surrogate loss \( \Phi \), a set of feasible scores \( F \), the calibration function \( H_{\Phi, L, F}(\varepsilon) \), \( \varepsilon \geq 0 \), equals the smallest excess of the conditional surrogate risk when the excess of the conditional actual risk is larger than \( \varepsilon \),

\[
H_{\Phi, L, F}(\varepsilon) := \inf_{f \in F, q \in \Delta_k} \delta \phi(f, q) \quad \text{s.t.} \quad \delta \ell(f, q) \geq \varepsilon.
\]

(5)

(6)

We set \( H_{\Phi, L, F}(\varepsilon) \) to \( +\infty \) when the feasible set is empty.

By construction, \( H_{\Phi, L, F} \) is non-decreasing on \([0, +\infty)\), \( H_{\Phi, L, F}(\varepsilon) \geq 0 \), the inequality (4) holds, and \( H_{\Phi, L, F}(0) = 0 \). Note that \( H_{\Phi, L, F} \) can be non-convex and even non-continuous.

\[^{2}\text{Here we use the Iverson bracket notation, i.e., } [A] := 1 \text{ if a logical expression } A \text{ is true, and zero otherwise.}\]
3.2 Notion of consistency

We use the calibration function to set a connection between optimizing the surrogate and task losses by Theorem 2, which is similar to Theorem 3 of Zhang [45].

**Theorem 2** (Calibration connection). Let \( H_{\Phi,L,F} \) be the calibration function between the surrogate loss \( \Phi \) and the task loss \( L \) and \( \hat{H}_{\Phi,L,F} \) be a convex non-decreasing lower bound of the calibration function. Assume that \( \Phi \) is continuous and bounded from below and all the score vectors \( f(x) \) belong to a non-empty open set \( F \subseteq \mathbb{R}^k \). Then, for any \( \varepsilon > 0 \) with finite \( H_{\Phi,L,F}(\varepsilon) \) and any \( \hat{f} \in \hat{F} \), we have

\[
\mathcal{R}_\Phi(\hat{f}) < \mathcal{R}_F^\varepsilon + \hat{H}_{\Phi,L,F}(\varepsilon) \implies \mathcal{R}_L(\hat{f}) \leq \mathcal{R}_L^\varepsilon + \varepsilon,
\]

where \( \mathcal{R}_F^\varepsilon \) and \( \mathcal{R}_L^\varepsilon \) are the lowest achievable \( \Phi \)-risk and actual risk, respectively.

**Proof.** We take the expectation of (4) w.r.t. \( x \), where the second argument of \( \ell \) is set to the conditional distribution \( P(\cdot | x) \). Then, we apply the Jensen’s inequality (since \( \hat{H}_{\Phi,L,F} \) is convex) to get

\[
\hat{H}_{\Phi,L,F}(\mathcal{R}_L(\hat{f}) - \mathcal{R}_L^\varepsilon) \leq \mathcal{R}_\Phi(\hat{f}) - \mathcal{R}_F^\varepsilon < \hat{H}_{\Phi,L,F}(\varepsilon),
\]

which implies (7) by monotonicity of \( \hat{H}_{\Phi,L,F} \). \( \square \)

Theorem 2 depends on the existence of an appropriate convex non-decreasing lower bound \( \hat{H}_{\Phi,L,F}(\varepsilon) \). Zhang [45, Proposition 25] claims that \( \hat{H}_{\Phi,L,F} \) defined as the lower convex envelope of the calibration function \( H_{\Phi,L,F} \) satisfies \( \hat{H}_{\Phi,L,F}(\varepsilon) > 0 \), \( \forall \varepsilon > 0 \), if \( H_{\Phi,L,F}(\varepsilon) > 0 \), \( \forall \varepsilon > 0 \), and, e.g., the set of labels is finite. This statement implies that the appropriate \( \hat{H}_{\Phi,L,F} \) always exists and allows to characterize consistency through properties of the calibration function \( H_{\Phi,L,F} \).

We now define a notion of level-\( \eta \) consistency, which is more general than consistency.

**Definition 3** (level-\( \eta \) consistency). A surrogate loss \( \Phi \) is consistent up to level \( \eta, \eta \geq 0 \), w.r.t. a task loss \( L \) and a set of scores \( F \) if and only if the calibration function \( H_{\Phi,L,F}(\varepsilon) > 0 \) for all \( \varepsilon > \eta \) and there exists \( \hat{\varepsilon} > \eta \) such that \( \hat{H}_{\Phi,L,F}(\hat{\varepsilon}) \) is finite.

Looking at solely (level-0) consistency vs. inconsistency might be too coarse to capture practical properties related to optimization accuracy (see, e.g., [26]). For example, if \( H_{\Phi,L,F}(\varepsilon) = 0 \) only for very small values of \( \varepsilon \), then the method can still optimize the actual risk up to certain level which might be good enough in practice, especially if it means that it can be optimized faster. Examples of calibration functions for consistent and inconsistent surrogate losses are shown in Figure 1.

**Other notions of consistency.** Definition 3 with \( \eta = 0 \) through Theorem 2 implies Fisher consistency as formulated, e.g., by Pedregosa et al. [34] for general losses and Lin [24] for binary classification. Definition 3 is also closely related to many definitions of consistency used in the literature. For example, for a bounded from below and continuous surrogate, Definition 3 with \( \eta = 0 \) is equivalent to infinite-sample consistency [45], classification calibration [42], edge-consistency [16], \((L, \mathbb{R}^k)\)-calibration [35], prediction calibration [44]. See [45, Appendix A] for the detailed discussion.
3.3 Connection to optimization accuracy and statistical efficiency

The scale of a calibration function is not intrinsically well-defined: we could multiply the surrogate function by a scalar and it would multiply the calibration function by the same scalar, without changing the optimization problem. Intuitively, we would like the surrogate loss to be of order 1. If with this scale the transfer function is exponentially small (has a $1/k$ factor), then we have strong evidence that the stochastic optimization will be difficult (and thus learning will be slow).

To provide a formal treatment, we add to the picture the complexity of optimizing the surrogate loss with a stochastic approximation algorithm. By using a scale-invariant convergence rate, we provide a natural normalization of the calibration function. The following two observations are central to the theoretical insights provided in our work:

1. Scale. For a properly scaled surrogate loss, the scale of the calibration function is a good indication of whether a stochastic approximation algorithm will take a large number of iterations (in the worst case) to obtain guarantees of small excess of the actual risk (and vice-versa, a large coefficient indicates a small number of iterations). The actual verification requires computing the normalization quantities given in Theorem 6 below.

2. Statistics. The bound on the number of iterations directly relates to the number of training examples that would be needed to learn, if we see each iteration of the stochastic approximation algorithm as using one training example to optimize the expected surrogate.

To analyze the statistical convergence of surrogate risk optimization, we have to specify the set of score functions that we work with. We assume that the structure on input $x \in X$ is defined by a positive definite kernel $K : X \times X \to \mathbb{R}$. We denote the corresponding reproducing kernel Hilbert space (RKHS) by $\mathcal{H}$ and its explicit feature map by $\psi(x) \in \mathcal{H}$. By the reproducing property, we have $(f, \psi(x))_{\mathcal{H}} = f(x)$ for all $x \in X$, $f \in \mathcal{H}$ where $(\cdot, \cdot)_{\mathcal{H}}$ is the inner product in the RKHS. We define the subspace of allowed scores $\mathcal{F} \subseteq \mathbb{R}^k$ via the span of the columns of a matrix $F \in \mathbb{R}^{k \times n}$. The matrix $F$ explicitly defines the structure of the score function. With this notation, we will assume that the score function is of the form $f(x) = FW\psi(x)$ where $W : \mathcal{H} \to \mathbb{R}^r$ is a linear operator to be learned (a matrix if $\mathcal{H}$ is of finite dimension) that transforms a collection of $r$ feature maps in $\mathcal{H}$ to $\mathbb{R}^r$ by applying the RKHS inner product $\langle \cdot, \cdot \rangle$ $r$ times. Note that for structured losses, we usually have $r \ll k$. The set of all score functions is thus obtained by varying $W$ in this definition and is denoted by $\mathfrak{F}_{F, \mathcal{H}}$. As a concrete example of a score family $\mathfrak{F}_{F, \mathcal{H}}$ for structured prediction, consider the standard sequence model with unary and pairwise potentials. In this case, dimension $r$ equals $Ts + (T - 1)s^2$, where $T$ is the sequence length and $s$ is the number of labels of each variable. The columns of the matrix $F$ consist of $2T - 1$ groups (one for each unary and pairwise potential). Each row of $F$ has exactly one entry equal to one in each column group (with zeros elsewhere).

In this setting, we use the online projected averaged stochastic subgradient descent ASGD\(^3\) (stochastic w.r.t. $(x^{(n)}, y^{(n)}) \sim D$) to minimize directly the actual risk \([5]\). The $n$-th update consists in

$$W^{(n)} := P_D \left[ W^{(n-1)} - \gamma^{(n)} F^T \nabla \Phi(x)^T \right], \quad (8)$$

where $F^T \nabla \Phi(x)^T : \mathcal{H} \to \mathbb{R}^r$ is the stochastic functional gradient, $\gamma^{(n)}$ is the step size and $P_D$ is the projection on the ball of radius $D$ w.r.t. the Hilbert–Schmidt norm.\(^4\) The vector $\nabla \Phi(x) \in \mathbb{R}^k$ is a regular gradient of the sampled surrogate $\Phi(f(x), y)$ w.r.t. the scores, $\nabla \Phi = \nabla_f \Phi(f(x), y)_{f=f(x)}$. Note that one could apply SGD without having access to explicit feature maps by using the kernel trick, but the computational complexity of each update is linear in $n$ leading to overall quadratic complexity. The convergence properties of SGD in RKHS are analogous to the finite-dimensional SGD because they rely on dimension-free quantities. To use simple convergence analysis, we follow Ciliberto et al. [9] and make the following assumption:

**Assumption 4** (Well-specified optimization w.r.t. the function class $\mathfrak{F}_{F, \mathcal{H}}$). There exists a global minimum $f^* \in \mathcal{R}_\Phi(f)$ w.r.t. all measurable functions $f$ that belongs to $\mathfrak{F}_{F, \mathcal{H}}$.

Assumption 4 simply means that each row of $W^*$ defining $f^*$ belongs to the RKHS $\mathcal{H}$ implying a finite norm $\|W^*\|_{\mathcal{H}_S}$. Assumption 4 can be relaxed if the kernel $K$ is universal, but then the convergence analysis becomes much more complicated \([33]\).

\(^3\) See, e.g., \([33]\) for the formal setup of kernel SGD.

\(^4\) The Hilbert–Schmidt norm of a linear operator $A$ is defined as $\|A\|_{\mathcal{H}_S} = \sqrt{\text{tr} A^\dagger A}$ where $A^\dagger$ is the adjoint operator. In the case of finite dimension, the Hilbert–Schmidt norm coincides with the Frobenius matrix norm.
Theorem 5 (Convergence rate). Under Assumption 4 and assuming that (i) the functions $\Phi(f, y)$ are convex w.r.t. $f \in \mathbb{R}^k$ and bounded from below for all $y \in \mathcal{Y}$; (ii) the expected square of the norm of the stochastic gradient is bounded, $E_{(x,y) \sim D} \| F^T \nabla \psi(x)^T \|^2_{HS} \leq M^2$, ASGD with $N$ steps (8) and the constant step-size $\frac{2D}{\sqrt{MN}}$ admits the following rate on the averaged iterate:

$$E[\mathcal{R}_\Phi(\hat{f}(N))] - \mathcal{R}_\Phi^* \leq \frac{2DM}{\sqrt{N}} \quad \text{where} \quad \hat{f}(N) := \frac{1}{N} \sum_{n=1}^{N} F \psi(x)^T. \quad (9)$$

Theorem 5 is a straightforward extension of classical results [30, 33]. By combining the convergence rate of Thm. 5 with Thm. 2 that connects the surrogate and actual risks, we get Thm. 6 which explicitly gives the number of iterations required to achieve $\varepsilon$ accuracy on the population risk. Note that since SGD is applied in the online fashion, Thm. 6 also serves as the sample complexity bound, i.e., says how many samples are needed to achieve $\varepsilon$ target accuracy.

**Theorem 6 (Learning complexity).** Under the assumptions of Theorem 5 on the surrogate loss, ASGD finds a point $\hat{f}(N) \in \hat{\mathcal{F}}_{\mathcal{H}}$ satisfying $\mathcal{R}_L(\hat{f}(N)) \leq \mathcal{R}_L^* + \varepsilon$, in at most $N^*$ iterations with

$$N^* := \frac{AD^2 M^2}{H^2(\varepsilon)}. \quad (10)$$

**Proof.** By (9), $N^*$ steps of the algorithm, in expectation, result in $\overline{H}_{\Phi,L,.\mathcal{F}}(\varepsilon)$ accuracy on the surrogate risk, which by Theorem 2 implies $\varepsilon$-accuracy on the actual risk. \hfill \Box

4 Quadratic surrogate

The major obstacle in applying Theorem 6 is the computation of the calibration function $H_{\Phi,L,.\mathcal{F}}$. We focus on the special class of surrogates, quadratic surrogates, for which we can bound or even compute exactly the calibration functions. We define the quadratic surrogate as

$$\Phi_{quad}(f, y) = \frac{1}{2k} \| f + L(\cdot,y) \|_2^2, \quad L(\cdot, y) \text{ is the } y\text{-th column of the loss matrix } L. \quad (11)$$

The excess of the expected surrogate then takes a simple form:

$$\delta \phi_{quad}(F \theta, q) = \frac{1}{2k} \| F \theta + L q \|_2^2, \quad (12)$$

where a vector $\theta \in \mathbb{R}^r$ and a matrix $F \in \mathbb{R}^{k \times r}$ define the parameterization of the score subset $\mathcal{F}$, i.e., $\mathcal{F} = \text{span}(F) = \{ F \theta \mid \theta \in \mathbb{R}^r \}$. Equation (12) holds under the assumption that the subspace $\mathcal{F}$ contains the column space of the loss matrix $\text{span}(L)$, see Lemma 9 in Suppl. Mat. A. Importantly, the function $\delta \phi_{quad}(F \theta, q)$ is jointly convex in the conditional probability $q$ and parameters $\theta$.

One simple sufficient condition for the surrogate (11) being consistent is that $\mathcal{F} = \text{span}(F)$ fully contains $\text{span}(L)$. The detailed discussion on possible generalizations of (11) to other consistent surrogates is presented in Suppl. Mat. B.

**Lower bound on the calibration function.** The lower bound on the calibration function for an arbitrary task loss $L$, the corresponding quadratic surrogate $\Phi_{quad}(11)$ and some score subspace $\mathcal{F}$ characterizes the easiness of learning with this surrogate given the scaling intuition mentioned in Section 3.3. The proof of Theorem 7 is given in Suppl. Mat. C.1.

**Theorem 7 (Lower bound on $H_{\Phi_{quad}}$).** For any task loss $L$, its quadratic surrogate $\Phi_{quad}$ and a score subspace $\mathcal{F}$ containing the column space of $L$, the calibration function can be lower bounded:

$$H_{\Phi_{quad},L,.\mathcal{F}}(\varepsilon) \geq \frac{\varepsilon^2}{2k \max_{i,j} \| P_F \Delta_{ij} \|_2^2} \geq \varepsilon^2 \frac{1}{\mathcal{F}}, \quad (13)$$

where $P_F$ is the orthogonal projection on the subspace $\mathcal{F}$ and $\Delta_{ij} = e_i - e_j \in \mathbb{R}^k$ with $e_c$ being the $c$-th basis vector of the standard basis in $\mathbb{R}^k$.

**Lower bound for specific losses.** We now discuss the meaning of bound (13) for some specific losses (the detailed derivations are given in Suppl. Mat. C.3). For the 0-1, block 0-1 and Hamming losses ($L_{01}, L_{01,h}$ and $L_{Ham,T}$, respectively) with the smallest possible score subspaces $\mathcal{F}$ the bound (13) gives $\varepsilon^2 \frac{1}{4k}$ and $\varepsilon^2 \frac{1}{\mathcal{F}}$, respectively. All these bounds are tight (see Suppl. Mat. D). However, if $\mathcal{F} = \mathbb{R}^k$ the bound (13) is not tight for the block 0-1 and mixed losses (see also Suppl. Mat. D). In particular, the bound (13) cannot detect level-$\eta$ consistency for $\eta > 0$ (see Def. 3) and does not change when the loss changes, but the score subspace stays the same.

**Upper bound on the calibration function.** Theorem 8 gives an upper bound on the calibration function holding for unconstrained scores, i.e, $\mathcal{F} = \mathbb{R}^k$ (see the proof in Suppl. Mat. C.2).
Theorem 8 (Upper bound on $H_{\Phi_{quad}}$). If a loss matrix $L$ with $L_{\max} > 0$ defines a pseudometric on labels and there are no constraints on the scores, i.e., $F = \mathbb{R}^k$, then the calibration function for the quadratic surrogate $\Phi_{\text{quad}}$ can be upper bounded: $H_{\Phi_{quad}, L, \mathbb{R}^k}(\varepsilon) \leq \frac{\varepsilon^2}{2}$.

Theorem 8 shows that without some appropriate constraints on the scores, efficient learning is not guaranteed because of the $1/k$ scaling of the calibration function. From our lower bound in Theorem 7 (which guarantees consistency), the natural constraints on the score is $F = \text{span}(L)$, with the dimension of this space giving an indication of the intrinsic “difficulty” of a loss. By considering concrete examples of (tight) bounds in Suppl. Mat. C.3, we will see that the 0-1 loss is “hard” while the block 0-1 loss and the Hamming loss are “easy”.

Exact calibration functions. Note that the bounds proven in Theorems 7 and 8 imply that, in the case of no constraints on the scores $F = \mathbb{R}^k$, for the 0-1, block 0-1 and Hamming losses, we have

$$\frac{\varepsilon^2}{2} \leq H_{\Phi_{quad}, L, \mathbb{R}^k}(\varepsilon) \leq \frac{\varepsilon^2}{2k}, \quad (14)$$

where $L$ is the matrix defining a loss. For completeness, in Suppl. Mat. D, we compute the exact calibration functions for the 0-1 and block 0-1 losses. Note that the calibration function for the 0-1 loss equals the lower bound, illustrating the worst-case scenario.

In what follows, we provide the calibration functions in the cases with constraints on the scores. For the block 0-1 loss with $b$ equal blocks and under constraints that the scores within blocks are equal, the calibration function equals (see Proposition 14 of Suppl. Mat. D.2)

$$H_{\Phi_{quad}, L_{01,b}, \mathcal{F}_{01,b}}(\varepsilon) = \frac{\varepsilon^2}{4b}, \quad 0 \leq \varepsilon \leq 1. \quad (15)$$

For the Hamming loss defined over $T$ binary variables and under constraints implying separable scores, the calibration function equals (see Proposition 15 in Suppl. Mat. D.3)

$$H_{\Phi_{quad}, L_{\text{Ham}, T}, \mathcal{F}_{\text{Ham}, T}}(\varepsilon) = \frac{\varepsilon^2}{8T}, \quad 0 \leq \varepsilon \leq 1. \quad (16)$$

The calibration functions (15) and (16) depend on the quantities representing the actual complexities of the loss (the number of blocks $b$ and the length of the sequence $T$) and can be exponentially larger than the upper bound for the unconstrained case.

In the case of mixed 0-1 and block 0-1 loss, if the scores $f$ are constrained to be equal inside the blocks, i.e., belong to the subspace $\mathcal{F}_{01,b} = \text{span}(L_{01,b}) \subseteq \mathbb{R}^k$, then the calibration function is equal to 0 for $\varepsilon \leq \frac{\varepsilon}{2}$, implying inconsistency. However, for $\varepsilon > \frac{\varepsilon}{2}$, the calibration function is of the order $\frac{1}{2}(\varepsilon - \frac{\varepsilon}{T})^2$. See Figure 1b for the illustration of this calibration function and Proposition 17 of Suppl. Mat. D.4 for the exact formulation and the proof. Note that, although being inconsistent, the calibration function under the constraints is exponentially larger than its unconstrained counterpart for $\varepsilon$ big enough and when the blocks are exponentially large (see Proposition 16).

Computation of the SGD constants. Applying Theorem 6 requires computation of the quantity $DM$ where $D$ bounds the norm of optimal solution and $M$ bounds the expected square of the norm of the stochastic gradient. In Suppl. Mat. E, we provide a way to bound this quantity for our quadratic surrogate (11) under Assumption 4. In particular, we show that we can have

$$DM = L_{\max}^2 \xi(\kappa(F)\sqrt{r}RQ_{\max}), \quad \xi(z) = z^2 + z, \quad (17)$$

where $\kappa(F)$ is the condition number of matrix $F$, $R$ is an upper bound on the RKHS norm of object feature map, $\|\psi(z)\|_H$, and $Q_{\max}$ is an upper bound on the sum $\sum_{c=1}^k \|q_c\|_H$, which can be seen as the generalization of inequality $\sum_{c=1}^k q_c \leq 1$ for probabilities. Constants $r$ and $Q_{\max}$ depend on the data, the constant $L_{\max}$ depends directly on the loss, constants $r$, $\kappa(F)$ depend on the choice of matrix $F$.

We compute constant $DM$ for specific losses we consider in Suppl. Mat. E.1. For the 0-1, block 0-1 and Hamming losses, we have $DM = O(k)$, $DM = O(b)$ and $DM = O(\log_2(b)k)$, respectively. These computation indicate that the quadratic surrogate allows efficient optimization for structured block 0-1 and Hamming losses, but for the 0-1 loss convergence can be very slow.

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\(^5\)A pseudometric is a function $d(a, b)$ satisfying the following axioms: $d(x, y) \geq 0$, $d(x, x) = 0$ (but possibly $d(x, y) = 0$ for some $x \neq y$), $d(x, y) = d(y, x)$, $d(x, z) \leq d(x, y) + d(y, z)$. 

7
5 Related works

Consistency for multi-class problems. Building on significant progress for the case of binary classification, see, e.g. [4], there has been a lot of interest in the multi-class case. Zhang [45], Tewari & Bartlett [42] analyze consistency of many existing surrogates for the 0-1 loss. Gao & Zhou [18] focus on multi-label classification. Narasimhan et al. [29] provide a consistent algorithm for arbitrary multi-class loss defined by a function of the confusion matrix.

The task of ranking has attracted a lot of attention and [16, 7, 8, 36] analyze different families of surrogate and task losses proving their (in-)consistency. In this line of work, Ramaswamy et al. [36] propose a quadratic surrogate for an arbitrary low rank loss which is related to our quadratic surrogate (11). They also prove that several important ranking losses, i.e., precision@q, expected rank utility, mean average precision, pairwise disagreement, are of low-rank. We conjecture that our approach is compatible with these losses and leave precise connections as future work.

Structured SVM (SSVM) and friends. SSVM [40, 41, 43] is one of the most used convex surrogates for the tasks with structured outputs, thus, its consistency has been a question of great interest. It is known that Crammer-Singer multi-class SVM [14], which SSVM is built on, is not consistent for 0-1 loss unless there is a majority class with probability at least $\frac{1}{2}$ [45, 28]. However, it is consistent for the “abstain” and ordinal losses in the case of 3 classes [35]. Structured ramp loss and probit surrogates are closely related to SSVM and are consistent [28, 15, 27, 20], but not convex.

Quadratic surrogates for structured prediction. Ciliberto et al. [9], Brouard et al. [6] consider minimizing $\sum_{i=0}^{n} \|g(x_i) - \psi_o(y_i)\|^2_k$ aiming to match the RKHS embedding of inputs $g : X \rightarrow H$ to the feature maps of outputs $\psi_o : Y \rightarrow H$. In their frameworks, the task loss is not considered at the learning stage, but only at the prediction stage. Our quadratic surrogate (11) depends on the loss directly. If analytically minimizing the empirical risk the two objectives can result in identical predictors, but when minimized with kernel SGD (population risk) they lead to different behavior.

Calibration functions. Bartlett et al. [4], Steinwart [39] provide calibration functions for most existing surrogates for binary classification. All these functions differ in term of shape, but are roughly similar in terms of constants. Pedregosa et al. [34] generalize these results to the case of ordinal regression. However, their calibration functions have at best $\frac{1}{2}$ factor, if the surrogate is normalized w.r.t. the number of classes. The task of ranking has been of significant interest. However, most of the literature [e.g., 10, 13, 21, 1], focuses on calibration functions (in the form of regret bounds) for bipartite ranking, which is related to cost-sensitive binary classification.

Ávila Pires et al. [2] generalize the theoretical framework developed by Steinwart [39] and present results for the multi-class SVM of Lee et al. [23] (the score vectors are constrained to sum to zero) that can be built for any task loss of interest. Their surrogate $\Phi$ is of the form $\sum_{c \in Y} L(c, y) a(f_c)$ where $\sum_{c \in Y} f_c = 0$ and $a(f)$ is some convex function with all subgradients at zero being positive.

Finally, Ciliberto et al. [9] provide the calibration function for their quadratic surrogate. Assuming that the loss can be represented as $L(y, \hat{y}) = (V \psi_o(y), \psi_o(y))_{H^2}$, $\hat{y}, y \in Y$ (this assumption can always be satisfied in the case of a finite number of labels, by taking $V$ as the loss matrix $L$ and $\psi_o(y) := e_y \in \mathbb{R}^k$ where $e_y$ is the $y$-th vector of the standard basis in $\mathbb{R}^k$). In their Theorem 2, they provide an excess risk bound leading to a lower bound on the corresponding calibration function $H_{\Phi, L, \mathbb{R}^k}(\epsilon) \geq \frac{\epsilon^2}{c_{\Delta}^2}$ where a constant $c_{\Delta} = \|V\|_2 \max_{y \in Y} \|\psi_o(y)\|$ simply equals the spectral norm of the loss matrix for the finite-dimensional construction provided above. However, the spectral norm of the loss matrix is exponentially large even for highly structured losses such as the block 0-1 and Hamming losses, i.e., $\|L_{01, b}\|_2 = k - \frac{k}{2}$, $\|L_{\text{Ham},T}\|_2 = \frac{k}{2}$. This conclusion puts the objective of Ciliberto et al. [9] on the same line with ours in the case without constraints on the scores.

6 Conclusion

In this paper, we studied consistency of convex surrogate losses specifically in the context of structured prediction. We analyzed calibration functions and proposed an optimization-based normalization aiming to connect consistency with the existence of efficient learning algorithms. Finally, we instantiated all components of our framework for several losses by computing the calibration functions and the constants coming from the normalization. By carefully monitoring exponential constants, we highlighted the difference between tractable and intractable task losses.
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Supplementary Material

On Structured Prediction Theory with Calibrated Convex Surrogate Losses

Outline

Section A: Technical lemmas useful for the proofs.
Section B: Discussion and consistency results on a family of surrogate losses.
Section C: Bounds on the calibration functions.
   Section C.1: Theorem 7 – a lower bound.
   Section C.2: Theorem 8 – an upper bound.
   Section C.3: Computation of the bounds for specific task losses.
Section D: Computations of the exact calibration functions for the quadratic surrogate.
   Section D.1: 0-1 loss.
   Section D.2: Block 0-1 loss.
   Section D.3: Hamming loss.
   Section D.4: Mixed 0-1 and block 0-1 loss.
Section E: Computing constants appearing in the SGD rate.
Section F: Properties of the basis of the Hamming loss.

A Technical lemmas

In this section, we prove two technical lemmas that will be used by the main theoretical claims of the paper.

Lemma 9. Consider the quadratic surrogate (11) defined for a task loss L. Let a subspace of scores $\mathcal{F} \subseteq \mathbb{R}^k$ be parametrized by $\theta \in \mathbb{R}^r$, i.e., $f = F\theta \in \mathcal{F}$ with $F \in \mathbb{R}^{k \times r}$, and assume that $\text{span}(L) \subseteq \mathcal{F}$. Then, the excess of the weighted surrogate loss can be expressed as

$$\delta_{\phi_{\text{quad}}}(F\theta, q) = \frac{1}{2k} \|F\theta + Lq\|_2^2.$$

Proof. By using the definition of the quadratic surrogate $\Phi_{\text{quad}}$ (11), we have

$$\phi(f(\theta), q) = \frac{1}{2k}(\theta^T F^T F \theta + 2 \theta^T F^T Lq) + r(q),$$

$$\theta^* := \arg\min_{\theta} \phi(f(\theta), q) = -(F^T F)^\dagger F^T Lq,$$

$$\delta\phi(f(\theta), q) = \frac{1}{2k}(\theta^T F^T F \theta + 2 \theta^T F^T Lq$$

$$+ q^T L^T F(F^T F)^\dagger F^T Lq),$$

where $r(q)$ denotes the quantity independent of parameters $\theta$. Note that $P_F := F(F^T F)^\dagger F^T$ is the orthogonal projection on the subspace $\text{span}(F)$, so if $\text{span}(L) \subseteq \text{span}(F)$ we have $P_F L = L$, which finishes the proof.

Lemma 10. In the case of a finite number of labels $k$, for any task loss $L$, surrogate loss $\Phi$, and set of scores $\mathcal{F}$, the calibration function can be written as

$$H_{\Phi, L, \mathcal{F}}(\epsilon) = \min_{i,j \in \text{pred}(\mathcal{F})} H_{ij}(\epsilon),$$

where $\text{pred}(\mathcal{F})$ denotes the set of predictions that can be made with the scores in $\mathcal{F}$. The function $H_{ij}(\epsilon)$ depends on the task loss $L$, surrogate loss $\Phi$, set of scores $\mathcal{F}$, and the differences $\epsilon_{ij}$ between the predictions $i$ and $j$.

Proof. By definition, the calibration function $H_{\Phi, L, \mathcal{F}}(\epsilon)$ is the minimum of the calibration functions $H_{ij}(\epsilon)$ over all possible predictions $i$ and $j$. Since $\text{pred}(\mathcal{F})$ is finite, there are finitely many $i$ and $j$ for which $H_{ij}(\epsilon)$ can be computed, and hence the minimum over $\text{pred}(\mathcal{F})$ can be found. This finishes the proof.

Theorem 7. Consider the quadratic surrogate (11) defined for a task loss $L$. Let a subspace of scores $\mathcal{F} \subseteq \mathbb{R}^k$ be parametrized by $\theta \in \mathbb{R}^r$, i.e., $f = F\theta \in \mathcal{F}$ with $F \in \mathbb{R}^{k \times r}$, and assume that $\text{span}(L) \subseteq \mathcal{F}$. Then, the excess of the weighted surrogate loss can be expressed as

$$\delta_{\phi_{\text{quad}}}(F\theta, q) = \frac{1}{2k} \|F\theta + Lq\|_2^2.$$

Theorem 8. Consider the quadratic surrogate (11) defined for a task loss $L$. Let a subspace of scores $\mathcal{F} \subseteq \mathbb{R}^k$ be parametrized by $\theta \in \mathbb{R}^r$, i.e., $f = F\theta \in \mathcal{F}$ with $F \in \mathbb{R}^{k \times r}$, and assume that $\text{span}(L) \subseteq \mathcal{F}$. Then, the excess of the weighted surrogate loss can be expressed as

$$\delta_{\phi_{\text{quad}}}(F\theta, q) = \frac{1}{2k} \|F\theta + Lq\|_2^2.$$

Theorem 9. Consider the quadratic surrogate (11) defined for a task loss $L$. Let a subspace of scores $\mathcal{F} \subseteq \mathbb{R}^k$ be parametrized by $\theta \in \mathbb{R}^r$, i.e., $f = F\theta \in \mathcal{F}$ with $F \in \mathbb{R}^{k \times r}$, and assume that $\text{span}(L) \subseteq \mathcal{F}$. Then, the excess of the weighted surrogate loss can be expressed as

$$\delta_{\phi_{\text{quad}}}(F\theta, q) = \frac{1}{2k} \|F\theta + Lq\|_2^2.$$
We finish the proof by noting that the constraint (6) in Definition 1 of the calibration function can be
f
Assumption 3 then implies that
a,b
An ideal surrogate should not only be consistent, but also allow efficient optimization, by, e.g., being
Analogously, the set of probability vectors
q
Theorem 11 (Sufficient conditions for consistency) Consider an arbitrary conditional probability vector
f
ℓ
1
the
1
we have
H
Now, we will prove by contradiction that
φ
Consideration 1 allows us to set the derivatives to zero and obtain
b
f
and
b
f
b
f
We finish the proof by noting that the constraint (6) in Definition 1 of the calibration function can be rewritten as \( \ell_j(q) - \ell_i(q) \geq \varepsilon \).

B Consistent surrogate losses
An ideal surrogate should not only be consistent, but also allow efficient optimization, by, e.g., being convex and allowing fast computation of stochastic gradients. In this paper, we study a generalization to arbitrary multi-class losses of a surrogate loss from Zhang [45, Section 4.4.2] that satisfies all these requirements:
\[
\Phi_{a,b}(f, y) = \frac{1}{k} \sum_{c=1}^{k} (L(c, y) a(f_c) + b(f_c)),
\]
where \( a, b : \mathbb{R} \to \mathbb{R} \) are convex functions. To minimize this surrogate, we can apply any version of the SGD algorithm, while computing the stochastic gradient by sampling \( y \) from the data generating distribution and a label \( c \) uniformly. Following Zhang [45], we show that the surrogates of the form \( 19 \) are consistent w.r.t. a task loss \( L \) under some sufficient assumptions formalized in Theorem 11.

Theorem 11 (Sufficient conditions for consistency). The surrogate loss \( \Phi_{a,b} \) is consistent w.r.t. a task loss \( L \), i.e., \( H_{\Phi_{a,b}, L, \mathbb{R}^k}(\varepsilon) > 0 \) for any \( \varepsilon > 0 \), under the following conditions on the functions \( a(f) \) and \( b(f) \):
1. The functions \( a \) and \( b \) are convex and differentiable.
2. The function \( ca(f) + b(f) \) is bounded from below and has a unique global minimizer (finite or infinite) for all \( c \in [0, L_{\max}] \).
3. The functions \( a(f) \) and \( \frac{b'(f)}{a'(f)} \) are strictly increasing.

Proof. Consider an arbitrary conditional probability vector \( q \in \Delta_k \). Assumption 2 then implies that the global minimizer \( f^* \) of the conditional surrogate risk \( \Phi(f, q) \) w.r.t. \( f \) is unique. Assumption 1 allows us to set the derivatives to zero and obtain \( \frac{b'(f)}{a'(f)} = -\ell_c(q) \) where \( \ell_c(q) := (Lq)_c \). Assumption 3 then implies that \( f^*_c \geq f^*_c \) holds if and only if \( \ell_c(q) \leq \ell_i(q) \).

Now, we will prove by contradiction that \( H(\varepsilon) := H_{\Phi_{a,b}, L, \mathbb{R}^k}(\varepsilon) > 0 \) for any \( \varepsilon > 0 \). Assume that for some \( \varepsilon > 0 \) we have \( H(\varepsilon) = 0 \). Lemma 10 then implies that for some \( i, j \in \mathcal{Y}, i \neq j \), we have

\footnote{Zhang [45] refers to this surrogate as “decoupled unconstrained background discriminative surrogate”. Note the \( \frac{1}{k} \) scaling to make \( \Phi_{a,b} \) of order 1.}
\( H_{ij}(\varepsilon) = 0 \). Note that the domain of (18) defining \( H_{ij} \) is separable w.r.t. \( q \) and \( f \). We can now rewrite (18) as

\[
H_{ij}(\varepsilon) = \inf_{q \in \Delta_{k,i}} \delta \phi^*(q), \quad \text{where} \quad \delta \phi^*(q) := \inf_{f \in F_j} \delta \phi(f, q).
\]

Lemma 27 of [45] implies that the function \( \delta \phi^*(q) \) is a continuous function of \( q \). Given that \( \Delta_{k,i} \) is a compact set, the infimum is achieved at some point \( q^* \in \Delta_{k,i} \). For this \( q^* \), the global minimum w.r.t. \( f \) exists (Assumption 2). The uniqueness of the global minimum implies that we have \( f^*_j = \max_{q \in Y} f_q^* \). The argument at the beginning of this proof then implies \( \ell_j(q^*) \leq \ell_j(q^*) - \varepsilon \) which contradicts the inequality \( \ell_i(q^*) \leq \ell_i(q^*) - \varepsilon \) in the definition of \( \Delta_{k,i} \).

Note that Theorem 11 actually proves that the surrogate \( \Phi_{a,b} \) is order-preserving [45], which is a stronger property than consistency.

Below, we give several examples of possible functions \( a(f), b(f) \) that satisfy the conditions in Theorem 11 and their corresponding \( f^*(\ell) \):

1. If \( a(f) = f, b(f) = f^2 \) then \( f^*(\ell) = -\ell \), leading to our quadratic surrogate (11).
2. If \( a(f) = \frac{1}{\Delta j} \exp(f) - \exp(-f), b(f) = \exp(-f) \) then \( f^*(\ell) = \frac{1}{2} \log(1 - \frac{1}{\Delta j} \exp(-f)) \).
3. If \( a(f) = \frac{1}{\Delta j} f, b(f) = \exp(1 + \exp(-f)) \) then \( f^*(\ell) = \log(1 - \frac{1}{\Delta j} \exp(-f)) \).

In the case of binary classification, these surrogates reduce to \( L_2 \), exponential, and logistic losses, respectively.

### C Bounds on the calibration function

#### C.1 Lower bound

**Theorem 7.** For any task loss \( L \), its quadratic surrogate \( \Phi_{\text{quad}} \), and a score subspace \( F \) containing the column space of \( L \), the calibration function can be lower bounded:

\[
H_{\Phi_{\text{quad}}, L,F}(\varepsilon) \geq \frac{\varepsilon^2}{2k \max_{ij} \| P_F \Delta_{ij} \|_2^2} \geq \frac{\varepsilon^2}{4k}.
\]

where \( P_F \) is the orthogonal projection on the subspace \( F \) and \( \Delta_{ij} = e_i - e_j \in \mathbb{R}^k \) with \( e_i \) being the \( i \)-th basis vector of the standard basis in \( \mathbb{R}^k \).

**Proof.** First, let us assume that the score subspace \( F \) is defined as the column space of a matrix \( F \in \mathbb{R}^{k \times r} \), i.e., \( f(\theta) = F \theta \). Lemma 9 gives us expression (12), which is jointly convex w.r.t. a conditional probability vector \( q \) and parameters \( \theta \).

The optimization problem (5)-(6) is non-convex because the constraint (6) on the excess risk depends of the predictor function \( \text{pred}(f) \), see Eq. (1), containing the Argmax operation. However, if we constrain the predictor to output label \( j \), i.e., \( f_j \geq f_c, \forall c \), and the label delivering the smallest possible expected loss to be \( i \), i.e., \( (Lq)_i \leq (Lq)_j, \forall c \), the problem becomes convex because all the constraints are linear and the objective is convex. Lemma 10 in Suppl. Mat. A allows to bound the calibration function with the minimization w.r.t. selected labels \( i \) and \( j \), \( H_{\Phi_{\text{quad}}, L,F}(\varepsilon) \geq \min_{i \neq j} H_{ij}(\varepsilon) \)

(we ignore constraints \( i, j \in \text{pred}(F) \) saying that we should consider only the labels that can be predicted with some feasible scores) where \( H_{ij}(\varepsilon) \) is defined as follows:

\[
H_{ij}(\varepsilon) = \min_{\theta, q} \frac{1}{2k} \| F\theta + Lq \|_2^2, \quad \text{s.t.} \quad (Lq)_i \leq (Lq)_j - \varepsilon, \\
(Lq)_i \leq (Lq)_c, \quad c \in \text{pred}(F) \\
(F\theta)_j \geq (F\theta)_c, \quad c \in \text{pred}(F) \\
q \in \Delta_k.
\]
We now explicitly solve the resulting constraint optimization problem via the KKT optimality conditions. The stationarity constraints give us

\[ \Delta_i^T L q = -\varepsilon, \]  

\[ \Delta_i^T F \theta = 0, \]  

where \( \Delta_i^T L q = (Lq)_i - (Lq)_j, \Delta_i^T F \theta = (F\theta)_i - (F\theta)_j, \) and \( \Delta_{ij} = e_i - e_j \in \mathbb{R}^k \) with \( e_c \in \mathbb{R}^k \) being a vector of all zeros with 1 at position \( c \).

The constraint (22) can be readily substituted with equality

\[ \Delta_i^T L q = -\varepsilon, \]  

because multiplication of both \( q \) and \( \theta \) by the constant \( \frac{\varepsilon}{\Delta_i^T L q} \in (0, 1) \) preserves feasibility and can only decrease the objective (21).

We now explicitly solve the resulting constraint optimization problem via the KKT optimality conditions. The stationarity constraints give us

\[ \frac{1}{k} F^T (F\theta + Lq) + \mu F^T \Delta_{ij} = 0, \]  

\[ \frac{1}{k} L^T (F\theta + Lq) + \nu L^T \Delta_{ij} = 0; \]  

the complementary slackness gives \( \nu \Delta_i^T F \theta = 0 \) and the feasibility constraints give (24), (23), and \( \nu \geq 0. \)

Equation (25) allows to compute

\[ \theta = -(F^T F)^\dagger (k\mu F^T \Delta_{ij} + F^T Lq). \]  

By substituting (27) into (26) and by using the identity

\[ P_F L = F(F^T F)^\dagger F^T L = L, \]

we get \( (\mu - \nu) L^T \Delta_{ij} = 0. \) If \( L^T \Delta_{ij} = 0, \) the problem (21), (23), (24) is infeasible for \( \varepsilon > 0 \) implying \( H_{ij}(\varepsilon) = +\infty. \) Otherwise, we have \( \mu = \nu. \)

By plugging (27) into the complementary slackness and combining with (24), we get

\[ \nu \mu k \| P_F \Delta_{ij} \|_2^2 = \nu \varepsilon \]

implying that either \( \nu = \mu = 0 \) or \( \mu k \| P_F \Delta_{ij} \|_2^2 = \varepsilon. \) In the first case, Eq. (27) implies \( F\theta = -Lq \) making satisfying both (24) and (23) impossible. Thus, the later is satisfied implying the objective (21) equal to

\[ \frac{1}{2k} \| F\theta + Lq \|_2^2 = \frac{\varepsilon^2}{2k \| P_F \Delta_{ij} \|_2^2}. \]

Finally, orthogonal projections contract the \( L_2 \)-norm, thus \( \| P_F \Delta_{ij} \|_2^2 \leq 2, \) which finishes the proof.

\[ \square \]

### C.2 Upper bound

**Theorem 8.** If a loss matrix \( L \) with \( L_{max} > 0 \) defines a pseudometric on labels and there are no constraints on the scores, i.e., \( F = \mathbb{R}^k, \) then the calibration function for the quadratic surrogate \( \Phi_{\text{quad}} \) can be upper bounded:

\[ H_{\Phi_{\text{quad}}, L, F}(\varepsilon) \leq \frac{\varepsilon^2}{2k}. \]

**Proof.** After applying Lemmas 9 and 10, we arrive at

\[ H_{ij}(\varepsilon) = \inf_{f, q} \frac{1}{2k} \| f + Lq \|_2^2, \]  

s.t. \( \ell_i(q) \leq \ell_j(q) - \varepsilon, \) \( \ell_i(q) \leq \ell_c(q), \) \( c \in Y, \) \( f_j \geq f_c, \) \( c \in Y, \) \( f \in \mathbb{R}^k, \) \( q \in \Delta_k. \)
We now consider labels \( i \) and \( j \) such that \( L_{ij} > 0 \) and the point \( q_i = \frac{1}{2} + \frac{\varepsilon}{2T^2}, q_j = \frac{1}{2} - \frac{\varepsilon}{2T^2}, \) \( q_c = 0 \) for \( c \not\in \{i, j\} \), \( f_j = f_i = -\ell_i(q), f_c = -\ell_c(q) \) for \( c \not\in \{i, j\} \). We have \( \ell_j(q) = q_i L_{ji} \) and \( \ell_i(q) = q_j L_{ij} \) and thus
\[
\ell_j(q) - \ell_i(q) = L_{ij} \frac{\varepsilon}{2T^2} = \varepsilon.
\]

We also have
\[
\ell_c(q) - \ell_i(q) = q_i L_{ci} + q_j L_{cj} - q_j L_{ij} \geq q_j (L_{ic} + L_{cj} - L_{ij}) \geq 0,
\]
because of the assumptions on the loss matrix \( L \) and the inequality \( q_i \geq q_j \). Finally, \( f_j - f_c = -\ell_i(q) + \ell_c(q) \geq 0 \).

Now, we have shown that the defined point is feasible so we compute the objective value. We have
\[
\frac{1}{2k} \| f + Lq \|^2 = \frac{1}{2k} (\ell_j(q) - \ell_i(q))^2 = \frac{\varepsilon^2}{2k},
\]
which completes the proof. \( \square \)

### C.3 Computation of the bounds for specific task losses

**0-1 loss.** Let \( L_{01} \) denote the loss matrix of the 0-1 loss, i.e., \( L_{01}(i, j) := [i \neq j]^2 \). It is convenient to rewrite it with a matrix notation \( L_{01} = 1_k 1_k^T - I_k \), where \( 1_k \in \mathbb{R}^k \) is the vector on all ones and \( I_k \) is the identity matrix. We have \( \text{rank}(L_{01}) = k - 1 \), which is almost the whole space. By putting no constraints on the scores, we can easily apply Theorem 7 and obtain the lower bound of \( \frac{\varepsilon^2}{2k} \), which is shown to be tight in Suppl. Mat. D.1, Proposition 12.

**Block 0-1 loss.** We use the symbol \( L_{01,b} \) to denote the loss matrix of the block 0-1 loss with \( b \) blocks, i.e., \( L_{01,b}(i, j) := [i \text{ and } j \text{ are not in the same block}] \). We use \( s_v \) to denote the size of block \( v \), \( v = 1, \ldots, b \), and then \( s_1 + \cdots + s_b = k \). In the case when all the blocks are of equal sizes, we denote their size by \( s \) and have \( k = bs \).

With a matrix notation, we have \( L_{01,b} = 1_k 1_k^T - U U^T \) where the columns of the matrix \( U \in \mathbb{R}^{k \times b} \) are indicators of the blocks. We have \( \text{rank}(L_{01,b}) = b \) and can simply define \( F_{01,b} := \text{span}(F_{01,b}) \) with \( F_{01,b} := U \). Then, we have \( U U^T = s I_b \) and \( \| P_{F_{01,b}} \Delta_{ij} \|_2^2 = \frac{s}{k} \) if labels \( i \) and \( j \) belong to different blocks, which leads to the bound \( \frac{\varepsilon^2}{4b} \), which is shown to be tight in Suppl. Mat. D.2, Proposition 14.

**Hamming loss.** Consider the (normalized) Hamming loss between tuples of \( T \) binary variables:

\[
L_{\text{Ham},T} (\hat{y}, y) := \frac{1}{T} \sum_{t=1}^{T} [\hat{y}_t \neq y_t] \tag{29}
\]
\[
= \frac{1}{T} \sum_{t=1}^{T} ([\hat{y}_t = 0][y_t = 1] + [\hat{y}_t = 1][y_t = 0])
\]
\[
= \alpha_0(y) + \sum_{t=1}^{T} \alpha_t(y)[\hat{y}_t = 1],
\]
where \( \hat{y}_t \) and \( y_t \) are the \( t \)-th variables of a prediction \( \hat{y} \) and a correct label \( y \), respectively. The vectors \( \alpha_t(\cdot) \) depend only on the column index of the loss matrix. The decomposition (29) implies that \( F_{\text{Ham},T} := \text{span}(F_{\text{Ham},T}) \) equals \( \text{span}(L_{\text{Ham},T}) \) for \( L_{\text{Ham},T} := \frac{1}{T} 1_T 1_T^T - H^{(T)}, \) \( H^{(T)} y := [y_t = 1], t = 1, \ldots, T. \) We also have that \( \text{rank}(L_{\text{Ham},T}) = \text{rank}(F_{\text{Ham},T}) = T + 1. \)

In Suppl. Mat. F, we show that \( \max_{i \neq j} \| P_{F_{\text{Ham},T}} \Delta_{ij} \|_2^2 = \frac{\varepsilon^2}{T^2}. \) By plugging this identity into the bound (13), we get \( H_{\text{Ham},T} \geq \frac{\varepsilon^2}{2T^2} \), which appears to be tight according to Proposition 15 of the Suppl. Mat. D.3.

**Non-tight cases.** In the cases of the block 0-1 loss and the mixed 0-1 and block 0-1 loss (Propositions 13 and 16, respectively), we observe gaps between the bound (13) and the exact calibration functions, which show the limitations of the bound. In particular, it cannot detect level-\( \eta \) consistency for \( \eta > 0 \) (see Def. 3) and does not change when the loss changes, but the score subspace stays the same.
D Exact calibration functions for quadratic surrogate

This section presents our derivations for the exact values of the calibration functions for different losses. While doing these derivations, we have used numerical simulations and symbolic derivations to check for correctness. Our numerical and symbolic tools are available online.\footnote{https://github.com/aosokin/consistentSurrogates_derivations}

D.1 0-1 loss

Proposition 12. Let \( L_{01} \) be the 0-1 loss, i.e., \( L_{01}(i, j) = |i \neq j| \). Then, the calibration function equals the following quadratic function w.r.t. \( \varepsilon \):

\[
H_{\text{quad}, L_{01}, \mathbb{R}^k}(\varepsilon) = \frac{\varepsilon^2}{4k}, \quad 0 \leq \varepsilon \leq 1.
\]

Note that, in the case of binary classification the function (12) is equal to the calibration functions for least squares and truncated least squares surrogates [4, 39].

Proof. First, Lemma 9 with \( F = \mathbb{R}^k \) and \( F = I_k \) gives us the expression

\[
\delta \phi_{\text{quad}}(F \theta, q) = \frac{1}{4k} \| f + Lq \|^2_2,
\]

with \( f = \theta \in \mathbb{R}^k \).

We now reduce the optimization problem (5)-(6) to a convex one by using Lemma 10 and by writing \( H_{\text{quad}, L_{01}, \mathbb{R}^k}(\cdot) = \min_{f, q} H_{ij}(f) \), which holds because \( \text{pred}(\mathbb{R}^k) = \mathbb{Y} \). Because of the symmetries of the 0-1 loss, all the choices of \( i \) and \( j \) give the same (up to a permutation of labels) optimization problem to compute \( H_{ij}(f) \). The definition of the 0-1 loss implies \( (Lq)_c = 1 - q_c \), which simplifies the excess of the expected task loss appearing in (6) to \( \delta \ell(f, q) = (Lq)_i - (Lq)_j = q_i - q_j \).

After putting all these together, we get

\[
H_{ij}(\varepsilon) = \min_{f, q} \frac{1}{4k} \sum_{c=1}^k (f_c + 1 - q_c)^2, \quad \text{s.t.} \quad q_i \geq q_j + \varepsilon, \quad q_i \geq q_c, \quad c = 1, \ldots, k, \quad f_j \geq f_c, \quad c = 1, \ldots, k,
\]

\[
\sum_{c=1}^k q_c = 1, \quad q_c \geq 0.
\]

We claim that there exists an optimal point of (31), \( f^*, q^* \), such that \( q_c^* = 0, c \notin \{i, j\} \), \( q_i^* = \frac{1}{2} + \frac{\delta}{2}, q_j^* = \frac{1}{2} - \frac{\delta}{2}; f_c^* = -1, c \notin \{i, j\} \), \( f_i^* := f_j^* \). After proving this we will minimize the objective w.r.t. remaining scores at this point.\footnote{Note that, without proving optimality of the assigned values \( q^* \) and \( f^* \), we obtain an upper bound on the calibration function. In the case of the 0-1 loss, this upper bound matches the lower bound provided by Theorem 7, so we do not need to prove optimality explicitly. However, we still give this proof as a simple illustration of the proof technique used also for the cases when the bound of Theorem 7 is not tight.}

First, if any \( q_c^* = \delta > 0, c \notin \{i, j\} \), we can safely move this probability mass to \( q_i \) and \( q_j \) with operation

\[
q_i^* := q_i^* - \delta = 0, \quad q_i^* := q_i^* + \frac{\delta}{2}, \quad q_j^* := q_j^* + \frac{\delta}{2},
\]

\[
f_c^* := f_c^* - \delta, \quad f_i^* := f_i^* + \frac{\delta}{2}, \quad f_j^* := f_j^* + \frac{\delta}{2},
\]

which keeps all the constraints of (31) feasible and does not change the objective value.

Second, all the scores \( f_c^* \) have to belong to the segment \([-1, 0]\) otherwise clipping them will decrease the objective. With this, setting \( f_c^* := -1, c \notin \{i, j\} \) can only decrease the objective and will not violate the constraints.
We now show that the equalities $q_i^* = q_j^* + \varepsilon$ and $f_i^* = f_j^*$ always hold at the optimum otherwise we can always decrease the objective. Indeed, if $q_i^* - q_j^* = \delta > \varepsilon$, the operation

$$
q_i^* := q_i^* - \frac{\delta - \varepsilon}{2}, \quad q_j^* := q_j^* + \frac{\delta - \varepsilon}{2},
$$

(32)

$$
f_i^* := f_i^* - \frac{\delta - \varepsilon}{2}, \quad f_j^* := f_j^* + \frac{\delta - \varepsilon}{2}.
$$

can only decrease the objective and cannot violate any constraints. If $f_i^* > f_j^*$ there is always a point $f^* \in [f_i^*, f_j^*]$ such that $2(f_i^* + 1 - q_i^*)^2 \leq (f_i^* + 1 - q_i^*)^2 + (f_j^* + 1 - q_i^*)^2$ because $q_i^* \geq q_j^*$.

At the optimal point defined above, it remains to find the value $f^*$ delivering the minimum of the objective. We can achieve this by computing

$$
H_{ij}(\varepsilon) = \frac{1}{2k} \min_{f \in [-1,0]} (f + \frac{1}{2} - \frac{\varepsilon}{2})^2 + (f + \frac{1}{2} + \frac{\varepsilon}{2})^2,
$$

which implies $f^* = -0.5$ and $H_{\text{quad}, L_{01}, \text{R}^k}(\varepsilon) = \frac{\varepsilon^2}{4k}$. \(\square\)

### D.2 Block 0-1 loss

Recall that $L_{01,b}$ is the block 0-1 loss, i.e., $L_{01,b}(i, j) = [i \text{ and } j \text{ are not in the same block}]$. We use $b$ to denote the total number of blocks and $s_v$ to denote the size of block $v$, $v = 1, \ldots, b$. In this section, we compute the calibration functions for the case of unconstrained scores (Proposition 13) and for the case of the scores belonging to the column span of the loss matrix (Proposition 14).

**Proposition 13.** Without constraints on the scores, the calibration function for the block 0-1 loss equals the following quadratic function w.r.t. $\varepsilon$:

$$
H_{\text{quad}, L_{01,b}, \text{R}^k}(\varepsilon) = \frac{\varepsilon^2}{4k} \min_{v=1, \ldots, b} \frac{2s_v}{s_v + 1} \leq \frac{\varepsilon^2}{4k}, \quad 0 \leq \varepsilon \leq 1.
$$

Note that when $s_v = 1$ we have $H_{\text{quad}, L_{01,b}, \text{R}^k}(\varepsilon)$ matching to the lower bound of Theorem 7. When $s_v \to \infty$ we have $H_{\text{quad}, L_{01,b}, \text{R}^k}(\varepsilon)$ matching to the upper bound of Theorem 8.

**Proof.** This proof is of the same structure as the proof of Proposition 12 above.

We use $b(i) \in 1, \ldots, b$ to denote the block to which label $i$ belongs and $\mathcal{Y}_v$ to denote the set of labels that belong to block $v$. We also use $Q_v, v \in 1, \ldots, b$, as a shortcut to $\sum_{i \in \mathcal{Y}_v} q_i$, which is the joint probability mass on block $v$.

We start by noting that the $i$-th component of the vector $L_{01,b}q$ equals $1 - Q_{b(i)}$. By applying Lemmas 9, 10, we get

$$
H_{ij}(\varepsilon) = \min_{f,q} \frac{1}{4k} \sum_{v=1}^b \sum_{i \in \mathcal{Y}_v} (f_c + 1 - Q_{b(i)})^2, \quad (33)
$$

$$
Q_{b(i)} - Q_{b(j)} \geq \varepsilon, \quad (34)
$$

$$
Q_{b(i)} \geq Q_u, \quad u = 1, \ldots, b,
$$

$$
f_j \geq f_c, \quad c = 1, \ldots, k,
$$

$$
\sum_{c=1}^k q_c = 1, \quad q_c \geq 0.
$$

Analogously to Proposition 12, we claim that there exists an optimal point of (33) such that $q_c = 0, c \notin \{i, j\}$; $q_i = 0.5 + \frac{\varepsilon}{2} = Q_{b(i)}$, $q_j = 0.5 - \frac{\varepsilon}{2} = Q_{b(j)}$; $f_c = -1, c \notin \mathcal{Y}_{ij}$; $\mathcal{Y}_{ij} := \mathcal{Y}_{b(i)} \cup \mathcal{Y}_{b(j)}$.

At first, note that if $b(i) = b(j)$, then the constraint (34) is never feasible, so we’ll assume that $b(i) \neq b(j)$.

We will now show that we can consider only configurations with all the probability mass on the two selected blocks. Consider some optimal point $f^*, q^*$ and denote with $\delta = \sum_{c \in \mathcal{Y}\setminus\mathcal{Y}_{ij}} q_c^*$ the probability mass on the unselected blocks. The operation

$$
f_c^* := f_c^* + \frac{\delta}{2}, \quad c \in \mathcal{Y}_{ij},
$$

$$
q_c^* := q_c^* + \frac{\delta}{2},
$$

$$
f_c^* := f_c^* + \frac{\delta}{2}, \quad c \notin \mathcal{Y}_{ij},
$$

$$
q_c^* := q_c^* + \frac{\delta}{2}.
$$

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can only decrease the objective of (33) because the summands corresponding to the unselected blocks are set to zero. All the constraints stay feasible and the summands corresponding to the selected blocks keep their values.

The probability mass within the block \( b(i) \) can be safely moved to \( q_i^* \) without changing the objective or violating any constraints. Analogously, the probability mass within the block \( b(j) \) can be safely moved to \( q_j^* \). By reusing the operation (32), we can now ensure that \( q_i^* = q_j^* + \varepsilon \).

At the point defined above, we now minimize the objective (33) w.r.t. \( f_c \), \( c \in \mathcal{Y}_{ij} \). At an optimal point, all values \( f_c^* = f_c + 1 \), \( c \in \mathcal{Y}_{ij} \), belong to the segment \([Q_{b(i)}^c - 1, Q_{b(i)}^c - 1]\), otherwise we can always truncate the values to the borders of the segment and get an improvement of the objective. For all the scores \( f_c^* = c \in \mathcal{Y}_{ij} \), the following identity holds

\[
\begin{align*}
    f_c^* &= \begin{cases} 
    Q_{b(c)}^c - 1, & \text{if } Q_{b(c)}^c - 1 < f_j^* \\
    f_j^*, & \text{otherwise}
    \end{cases},
\end{align*}
\]

(35)

It implies that, in the block of the label \( i \), we have \( f_c^* = f_j^* \), \( c \in \mathcal{Y}_{b(i)} \), and, in the block of the label \( j \), we have \( f_c^* = Q_{b(j)}^c - 1 \), \( c \in \mathcal{Y}_{b(j)} \). By plugging the obtained values of \( q_i^* \) and \( f_j^* \) into (33) and denoting the value \( f_j^* + 0.5 \) with \( \tilde{f} \), we get

\[
H_{ij}(\varepsilon) = \min_f \frac{1}{2\varepsilon} \left( s_{b(i)}(\tilde{f} - \frac{\varepsilon}{2})^2 + (\tilde{f} + \frac{\varepsilon}{2})^2 \right),
\]

s.t. \( \tilde{f} \in [-\frac{\varepsilon}{2}, \frac{\varepsilon}{2}] \).

(36)

By computing the gradient of the objective of (36), we get

\[
\tilde{f} = \frac{5}{12} s_{b(i)} - \frac{1}{12} s_{b(j)},
\]

which belongs to the segment \([-\frac{\varepsilon}{2}, \frac{\varepsilon}{2}] \). We compute the function value at this point:

\[
H_{ij}(\varepsilon) = \varepsilon^2 \frac{2 s_{b(i)}}{3 s_{b(i)} + s_{b(j)}},
\]

which finishes the proof.

\begin{proposition}
Let scores \( f \) be always consistent with the blocks of the loss, i.e. belong to subspace \( \mathcal{F}_{01,b} = \text{span}(L_{01,b}) \subseteq \mathbb{R}^k \). Then, the calibration function equals the following quadratic function w.r.t. \( \varepsilon \):

\[
H_{\Phi_{\text{quad}}, L_{01,b}, \mathcal{F}_{01,b}}(\varepsilon) = \frac{\varepsilon^2}{4k} \min_{v \neq u} \frac{2 s_v + s_u}{s_v + s_u}, \quad 0 \leq \varepsilon \leq 1.
\]

If all the blocks are of the same size we have \( H_{\Phi_{\text{quad}}, L_{01,b}, \mathcal{F}_{01,b}}(\varepsilon) = \varepsilon^2 \frac{b}{4b} \) where \( b \) is the number of blocks.

\end{proposition}

\begin{proof}
The constraints on scores \( f \in \mathcal{F}_{01,b} \) simply imply that the scores within all the blocks are equal. Having this in mind, the proof exactly matches the proof of Proposition 13 until the argument around Eq. (35). Now we cannot set the scores of the block \( b(j) \) to different values, and, thus the all are equal to \( f^* \).

By plugging the obtained values of \( q_i^* \) and \( f_j^* \) into (33) and denoting the value \( f_j^* + 0.5 \) with \( \tilde{f} \), we get

\[
H_{ij}(\varepsilon) = \min_f \frac{1}{2\varepsilon} \left( s_{b(i)}(\tilde{f} - \frac{\varepsilon}{2})^2 + s_{b(j)}(\tilde{f} + \frac{\varepsilon}{2})^2 \right),
\]

s.t. \( \tilde{f} \in [-\frac{\varepsilon}{2}, \frac{\varepsilon}{2}] \).

(37)

By computing the gradient of the objective of (37), we get

\[
\tilde{f} = \frac{5}{12} s_{b(i)} - \frac{1}{12} s_{b(j)},
\]

which belongs to the segment \([-\frac{\varepsilon}{2}, \frac{\varepsilon}{2}] \). We now compute the function value at this point:

\[
H_{ij}(\varepsilon) = \varepsilon^2 \frac{2 s_{b(i)} s_{b(j)}}{3 s_{b(i)} + s_{b(j)}},
\]

which finishes the proof.

\end{proof}
D.3 Hamming loss

Recall that \( L_{\text{Ham},T} \) is the Hamming loss defined over \( T \) binary variables (see Eq. (29) for the precise definition). In this section, we compute the calibration function for the case of the scores belonging to the column span of the loss matrix (Proposition 15).

**Proposition 15.** Assume that scores \( f \) always belong to the column span of the Hamming loss matrix \( L_{\text{Ham},T} \), i.e., \( F_{\text{Ham},T} = \text{span}(L_{\text{Ham},T}) \subseteq \mathbb{R}^k \). Then, the calibration function can be computed as follows:

\[
H_{q, q_{\text{cal}}, L_{\text{Ham},T}, F_{\text{Ham},T}}(\varepsilon) = \frac{\varepsilon^2}{8T}.
\]

**Proof.** We start the proof by applying Lemma 10 and by elaborating on the vector of the expected losses \( L_{\text{Ham},T} q \). We note that the \( \hat{y} \)-th element \( \ell_\hat{y}(q) \), \( \hat{y} = (\hat{y}_t)_{t=1}^T, \hat{y} \in \{0, 1\} \), has a simple form of

\[
\ell_\hat{y}(q) = \sum_{y \in Y} \frac{q_y}{T} \sum_{t=1}^T [\hat{y}_t \neq y_t] = 1 - \frac{1}{T} \sum_{t=1}^T \sum_{y \in Y} q_y [\hat{y}_t = y_t].
\]

The quantity \( \sum_{y \in Y} q_y [\hat{y}_t = y_t] \) corresponds to the marginal probability of a variable \( t \) taking a label \( \hat{y}_t \). Note that the expected loss \( \ell_\hat{y}(q) \) only depends on \( q \) through marginal probabilities, thus two distributions \( q_1 \) and \( q_2 \) with the same marginals would be indistinguishable when plugged in (18). Having this in mind, we can consider only separable distributions, i.e., \( q_y = \prod_{t=1}^T (q_t | y_t = 1] + (1 - q_t) | y_t = 0) \), where \( q_t \in [0, 1], t = 1, \ldots, T \), are the parameters defining the distribution.

By combining the notation above with Lemmas 9 and 10, we arrive at the following optimization problem:

\[
H_{\hat{y}, \hat{y}}(\varepsilon) = \min_{f, q} \frac{1}{2T} \sum_{t=1}^T \left( f_t + 1 - \frac{1}{T} \sum_{t=1}^T q_t, y_t \right)^2,
\]

s.t. \( \frac{1}{T} \sum_{t=1}^T (q_t, \hat{y}_t - q_t, \hat{y}_t) \geq \varepsilon, \) \quad (39)

\( \frac{1}{T} \sum_{t=1}^T (q_t, \hat{y}_t - q_t, y_t) \geq 0, \quad y \in Y, \) \quad (40)

\( f_\hat{y} = f_y, \quad y \in Y, \) \quad (41)

\( 0 \leq q_t \leq 1, \quad t = 1, \ldots, T, \) \quad (42)

\( f \in F, \) \quad (43)

where \( q_t, y_t \) is a shortcut to \( q_t | y_t = 1] + (1 - q_t) | y_t = 0 \) and labels \( \hat{y} \) and \( \hat{y} \) serve as the selected labels \( i \) and \( j \), respectively.

The calibration function \( H_{q, q_{\text{cal}}, L_{\text{Ham},T}, F_{\text{Ham},T}}(\varepsilon) = \frac{\varepsilon^2}{8T} \) in the formulation of this proposition matches the lower bound provided by Theorem 7 in Sec. C.3. Thus, it suffices to construct a feasible w.r.t. (39)-(43) assignment of variables \( f, q \) and labels \( \hat{y}, \hat{y} \) such that the objective equals the lower bound.

It suffices to simply set \( \hat{y} \) to all zeros and \( \hat{y} \) to all ones. In this case, the constraints (39) and (40) take simplified form:

\[
\frac{1}{T} \sum_{t=1}^T (1 - 2q_t) \geq \varepsilon, \quad (44)
\]

\( q_t \leq \frac{1}{T}, \quad t = 1, \ldots, T. \quad (45)\)

We now set \( q_t := \frac{1}{2} - \frac{\varepsilon}{T}, t = 1, \ldots, T \), and \( f := -\frac{1}{2} 1_k \). This point is clearly feasible, so it remains to compute the value of the objective. We complete the proof by writing...
\[
\frac{1}{2k} \sum_{y \in Y} \left( f_y + 1 - \frac{1}{T} \sum_{t=1}^{T} q_t(y) \right)^2 = \\
\frac{1}{2k} \sum_{w=0}^{T} \left( \frac{T}{w} \left( \frac{1}{2} - \frac{1}{T} w \left( \frac{1}{2} - \frac{\varepsilon}{2} \right) + (T-w) \left( \frac{1}{2} + \frac{\varepsilon}{2} \right) \right) \right)^2 = \\
\frac{1}{2k} \sum_{w=0}^{T} \left( \frac{T}{w} \left( \frac{\varepsilon}{2} - \frac{w}{T} \right) \right)^2 = \frac{\varepsilon^2}{2k} \sum_{w=0}^{T} \left( \frac{1}{2} - \frac{w}{T} + \frac{w^2}{T^2} \right) = \\
\frac{\varepsilon^2}{2k} \left( \frac{1}{2} T^2 - \frac{1}{4} T^2 T^{-1} + \frac{1}{2} T (T+1) 2T^{-2} \right) = \frac{\varepsilon^2}{8k},
\]
where we use the equality \( k = 2T \) and the identities \( \sum_{i=0}^{T} (T_i) = 2T, \sum_{i=0}^{T} i (T_i) = T^2T -1, \sum_{i=0}^{T} i^2 (T_i) = T(T+1) 2T^{-2}. \)

**D.4 Mixed 0-1 and block 0-1 loss**

Recall that \( L_{01, b, \eta} \) is the convex combination of the 0-1 loss and the block 0-1 loss with \( b \) blocks, i.e.,
\[
L_{01, b, \eta} = \eta L_{01} + (1 - \eta) L_{01, b}, \quad 0 \leq \eta \leq 1.
\]
Let all the blocks be of the same size \( s = \frac{k}{b} \geq 2 \). In this section, we compute the calibration functions for the case of unconstrained scores (Proposition 16) and for the case when scores belong to the column span of the loss matrix (Proposition 17).

**Proposition 16.** If there are no constraints on scores \( f \) then the calibration function
\[
H_{\Phi_{\text{quad}}, L_{01, b, \eta}, \exists k}(\varepsilon) = \begin{cases} \\
\frac{\varepsilon^2}{2k}, & \varepsilon \leq \frac{n}{s - \eta}, \\
\frac{\varepsilon^2 s}{2k(s+1)} - \frac{n (s+1)(s-1)}{4k(s+1)} (2\varepsilon - \varepsilon \eta - \eta)
\end{cases}
\]
shows that the surrogate is consistent.

Note that when \( \eta = 0 \), we have \( H(\varepsilon) = \frac{\varepsilon^2}{4k} \frac{2s}{s+1} \) as in Proposition 13. When \( \eta \geq 0.5 \) we have \( H(\varepsilon) = \frac{\varepsilon^2}{4k} \), which matches Proposition 12.

**Proof.** This proof is very similar to the proof of Proposition 13, but technically more involved.

We start by noting that the \( i \)-th element of the vector \( L_{01, b, \eta} q \) equals
\[
\sum_{j: b(j) \neq b(i)} (1 - \eta) q_j + \sum_{j: j \neq i} \eta q_j = \eta(1 - q_i) + (1 - \eta)(1 - Q_{b(i)}),
\]
where for \( b(i) \) and \( Q_e \) we reuse the notation defined in the proof of Proposition 13. By combining this with Lemmas 9 and 10, we get
\[
H_{ij}(\varepsilon) = \min_{f, q} \frac{1}{2k} \sum_{v=1}^{b} \sum_{e \in \mathcal{E}_v} \left( f_e + 1 - \eta q_e - (1 - \eta) Q_{b(e)} \right)^2,
\]
s.t. \( \eta(q_i - q_j) + (1 - \eta)(Q_{b(i)} - Q_{b(j)}) \geq \varepsilon, \)
\( \eta(q_i - q_e) + (1 - \eta)(Q_{b(i)} - Q_{b(e)} \geq 0, \forall c \)
\( f_j \geq f_c, \forall c, \)
\( \sum_{c=1}^{k} q_e = 1, \quad q_e \geq 0, \forall c. \)

The blocks are all of the same size so we need to consider just the two cases: 1) the selected labels belong to the same block, i.e., \( b(i) = b(j) \); 2) the selected labels belong to the two different blocks, i.e., \( b(i) \neq b(j) \).

The first case can be proven by a straightforward generalization of the proof of Proposition 12. Given that the loss value is bounded by 1, the maximal possible value of \( \varepsilon \) when the constraints can be feasible equals \( \eta \). Thus, we have \( H(\varepsilon) = \frac{\varepsilon^2}{4k} \) for \( \varepsilon < \eta \) and \( +\infty \) otherwise.
We will now proceed to the second case. We show that
\[ H_{ij}(\varepsilon) = \begin{cases} \frac{\varepsilon^2}{4}, & \text{for } \varepsilon \leq \frac{n}{4}, \\ \frac{\varepsilon^2}{2} - \frac{n(n+1)(n+1)}{4(n+1)(n+1)}(2\varepsilon - \varepsilon\eta - \eta), & \text{otherwise}. \end{cases} \]

Similarly to the arguments used in Propositions 12 and 13, we claim that there is an optimal point of (47) such that \( q_c = 0, c \notin \{i, j\}; q_i = 0.5 + \frac{\varepsilon}{2}; q_j = 0.5 - \frac{\varepsilon}{2}; \) and \( f_i = -1 \) for \( c \notin \mathcal{Y}_{ij} := \mathcal{Y}_{b(i)} \cup \mathcal{Y}_{b(j)} \).

First, we will show that we can consider only configurations with all the probability mass on the two selected blocks \( b(i) \) and \( b(j) \). Given any optimal point \( f^* \) and \( q^* \), the operation (with \( \delta := \sum_{c \notin \mathcal{Y}_{ij}} q_c^* \))
\[
\begin{align*}
f_i^* &:= f_i^* + \frac{\delta}{2}, \\
f_j^* &:= f_j^* + \frac{\delta}{2}, \\
f_a^* &:= f_a^* + \frac{\delta}{2}(\eta - 3), \\
f_c^* &:= f_c^* - \frac{\delta}{2}(1 - \eta), \quad c \in \mathcal{Y}_i \setminus \{i, a\} \\
f_c^* &:= f_c^* + \frac{\delta}{2}(1 - \eta), \quad c \in \mathcal{Y}_j \setminus \{j\}
\end{align*}
\]
does not change the objective value of (47) because the quantities \( Q_{b(i)} + Q_{b(j)} \) change when we change \( q_i \) and \( q_j \). Adding \((1 - \eta)\frac{\delta}{2}\) to some scores compensates this and cannot violate the constraints because \( f_c^* \) goes up by \( \frac{\delta}{2} \geq (1 - \eta)\frac{\delta}{2} \).

Now we will show that it is possible to move all the mass to the two selected labels \( i \) and \( j \). We cannot simply move the mass within one block, but need to create some overflow and move it to another block in a specific way. Consider \( \delta := q_a^* \), which is some non-zero mass on a non-selected label of the block \( b(i) \). Then, the operation
\[
\begin{align*}
f_i^* &:= f_i^* + \delta \frac{\delta}{2}, \\
f_j^* &:= f_j^* + \delta \frac{\delta}{2}, \\
q_i^* &:= q_i^* + \delta (1 - \frac{\delta}{2}), \\
q_j^* &:= q_j^* + \delta \frac{\delta}{2}, \\
q_a^* &:= q_a^* - \delta = 0, \\
f_c^* &:= f_c^* - \delta \frac{\delta}{2}(1 - \eta), \quad c \in \mathcal{Y}_i \setminus \{i, a\} \\
f_c^* &:= f_c^* + \delta \frac{\delta}{2}(1 - \eta), \quad c \in \mathcal{Y}_j \setminus \{j\}
\end{align*}
\]
does not change the objective value of (47) because the quantities \( f_c + 1 - \eta q_c - (1 - \eta)Q_{b(c)} \), \( c \in \mathcal{Y}_{ij} \), stay constant and all the constraints of (47) stay feasible. We repeat this operation for all \( a \in \mathcal{Y}_{b(i)} \setminus \{i\} \) and, thus, move all the probability mass within the block \( b(i) \) to the label \( i \). In the block \( b(j) \), an analogous operation can move all the mass to the label \( j \).

It remains to show that \( q_i^* - q_j^* = \varepsilon \). Indeed, if \( q_i^* - q_j^* = \delta' > \varepsilon \), the operation analogous to (32)
\[
\begin{align*}
f_i^* &:= f_i^* - \frac{\delta' - \varepsilon}{2}, \\
f_j^* &:= f_j^* + \frac{\delta' - \varepsilon}{2}, \\
q_i^* &:= q_i^* - \frac{\delta' - \varepsilon}{2}, \\
q_j^* &:= q_j^* + \frac{\delta' - \varepsilon}{2}, \\
f_c^* &:= f_c^* - (1 - \eta)\frac{\delta' - \varepsilon}{2}, \quad c \in \mathcal{Y}_{b(i)} \setminus \{i\}, \\
q_c^* &:= f_c^* + (1 - \eta)\frac{\delta' - \varepsilon}{2}, \quad c \in \mathcal{Y}_{b(j)} \setminus \{j\}
\end{align*}
\]
can always set \( q_i^* - q_j^* = \varepsilon \). After this operation, all the scores of the block \( b(i) \) go down and all the scores of the block \( b(j) \) go up at most as much as \( f_j^* \), so the constraints \( f_j \geq f_c \) cannot get violated.

We now proceed with the computation of \( H(\varepsilon) \). First, we note that convexity and symmetries of (47) implies that all the non-selected scores within each block are equal. Denote the scores of the non-selected labels of the block \( b(i) \) by \( f_i^* \), and the scores of the non-selected labels of the block \( b(j) \) by \( f_j^* \).

Analogous to all the previous propositions, the truncation argument gives us that all the values \( f^*_c \) belong to the segment \([-1, -0.5 + \frac{\varepsilon}{2}]\). For all the optimal values \( f^*_c, c \neq j \), the following identity holds:
\[
f^*_c = \begin{cases} f_j^*, & \text{if } \eta q_c^* + (1 - \eta)Q_{b(c)} - 1 \geq f_j^*, \\
\eta q_c^* + (1 - \eta)Q_{b(c)} - 1, & \text{otherwise}. \end{cases}
\]
Given that \( f^{*} \) wants to equal the maximal possible value \(-0.5 + \frac{\eta}{2}\), it implies that \( f^{*} = f^{*} \). Denote this value by \( f \).

By, plugging the values of \( q^{*} \) and \( f^{*} \) provided above into the objective of (47), we get

\[
\frac{1}{2k} \left[ (f + 0.5 - \frac{\eta}{2})^2 + (s - 1)(f' + 1 - (1 - \eta)(0.5 + \frac{\eta}{2}))^2 + (f + 0.5 + \frac{\eta}{2})^2 + (s - 1)(f' + 1 - (1 - \eta)(0.5 + \frac{\eta}{2}))^2 \right].
\]

By minimizing (48) without constraints, we get \( f^{*} = -0.5, f_i^{*} = \frac{1}{2}(1 + \varepsilon)(1 - \eta) - 1, f_j^{*} = \frac{1}{2}(1 - \varepsilon)(1 - \eta) - 1 \). We now need to compare \( f_i^{*} \) and \( f_j^{*} \) with \( f^{*} \) to satisfy the constraints \( f^{*} \geq f_i^{*} \) and \( f^{*} \geq f_j^{*} \). First, we have that

\[
f^{*} - f_j^{*} = \frac{1}{2}(\eta + \varepsilon - \eta \varepsilon) \geq 0, \quad \text{for } 0 \leq \varepsilon \leq 1 \text{ and } 0 \leq \eta \leq 1.
\]

Second, we have

\[
f^{*} - f_i^{*} = \frac{1}{2}(\eta - \varepsilon + \eta \varepsilon) \geq 0, \quad \text{for } 0 \leq \varepsilon \leq \frac{n}{1 - \eta} \text{ and } 0 \leq \eta \leq 1.
\]

We can now conclude that when \( \varepsilon \leq \frac{n}{1 - \eta} \) we have both \( f_i^{*} \) and \( f_j^{*} \) equal to their unconstrained minimum points leading to \( H(\varepsilon) = \varepsilon^2 \).

Now, consider the case \( \varepsilon > \frac{n}{1 - \eta} \). We have the constraint \( f \geq f_j^{*} \) violated, so at the minimum we have \( f_j^{*} = f \). The new unconstrained minimum w.r.t. \( f \) equals \( f^{*} = \frac{1}{s+1}(-1 - (s - 1)\eta - \frac{1}{2}(s - 1)(1 - \eta)(1 - \varepsilon)) \). We now show that the inequality \( f^{*} \geq f_i^{*} \) still holds. We have

\[
f^{*} - f_i^{*} = \frac{n + \varepsilon - \eta \varepsilon}{s+1} \geq 0, \quad \text{for } 0 \leq \varepsilon \leq 1 \text{ and } 0 \leq \eta \leq 1.
\]

Substitution of \( f^{*} \) and \( f_i^{*} \) into (48) gives us

\[
\frac{1}{k} \left( \frac{\epsilon^2 s}{2(s+1)} - \frac{\eta(\varepsilon + 1)(s - 1)}{4(s+1)}(2\varepsilon - \varepsilon \eta - \eta) \right),
\]

which equals \( H(\varepsilon) \) for \( \epsilon \leq \frac{n}{1 - \eta} \).

Comparing cases 1 and 2, we observe that \( H(\varepsilon) \) from case 2 is never larger than the one of case 1, thus case 2 provides the overall calibration function \( H(\varepsilon) \).

\[ \square \]

**Proposition 17.** If scores \( f \) are constrained to be equal inside the blocks, i.e. belong to the subspace \( F_{01,b} = \text{span}(L_{01,b}) \subseteq \mathbb{R}^k \), then the calibration function

\[ H_{\Phi_{\text{quad}}, F_{01,b}, \eta, F_{01,b}}(\varepsilon) = \begin{cases} 
\frac{(\varepsilon - \frac{n}{2})^2 \left( \frac{\eta}{k} + 1 - \eta \right)^2}{(1 - \frac{n}{2})^2}, & \frac{n}{2} < \varepsilon < 1, \\
0, & 0 \leq \varepsilon \leq \frac{n}{2}
\end{cases} \]

shows that the surrogate is consistent up to level \( \frac{n}{2} \).

When \( \eta = 0 \), we have \( H(\varepsilon) = \frac{\varepsilon^2}{2k} \) as in Proposition 14. When \( \eta = 1 \) we have \( H(\varepsilon) = 0 \), which corresponds to the case of fully inconsistent surrogate (0-1 loss and constrained scores).

**Proof.** This proof combines ideas from Proposition 16 and Proposition 14.

Note that, contrary to all the previous results, Lemma 9 is not applicable, because, for \( b < k \), we have that \( \text{span} L_{01,b,\eta} = \mathbb{R}^k \not= F_{01,b} = \text{span}(L_{01,b}) \).

We now derive an analog of Lemma 9 for this specific case. We define the subspace of scores \( F_{01,b} = \{ F\theta \mid \theta \in \mathbb{R}^b \} \) with a matrix \( F := F_{01,b} \in \mathbb{R}^{k \times b} \) with columns containing the indicator vectors of the blocks. We have \( F^T F = sI_b \) and thus \( (F^T F)^{-1} = \frac{1}{s}I_b \). We shortcut the loss matrix \( L_{01,b,\eta} \) to \( L \) and rewrite it as

\[
L = \eta L_{01} + (1 - \eta) L_{01,b} = 1_k 1_k^T - \eta I_k - (1 - \eta) F F^T.
\]
By redoing the derivation of Lemma 9, we arrive at a different excess surrogate:

$$
\phi(f(\theta), q) = \frac{1}{2\epsilon} (s\theta^T \theta + 2\theta^T F^T Lq) + r(q),
$$

$$\theta^* := \arg\min_\theta \phi(f(\theta), q) = -\frac{1}{s} F^T Lq,
$$

$$
\delta \phi(f(\theta), q) = \frac{1}{2\epsilon} (s\theta^T \theta + 2\theta^T F^T Lq + \frac{1}{s} q^T L^T F^T Lq)
= \frac{s}{2\epsilon} \| \theta + \frac{1}{s} F^T Lq \|^2
= \frac{s}{2\epsilon} \sum_{v=1}^b (\theta_v + 1 - (1 - \eta)Q_v - \frac{u}{s}Q_v)^2,
$$

where $$Q_v = \sum_{c \in \mathcal{Y}_v} q_c$$ is the total probability mass on block $$v$$ and $$\mathcal{Y}_v \subset \mathcal{Y}$$ denotes the set of labels of block $$v$$.

Analogously to Proposition 16 we can now apply Lemma 10 and obtain $$H_{ij}(\epsilon)$$.

$$H_{ij}(\epsilon) := \min_{\theta, q} \frac{s}{2\epsilon} \sum_{v=1}^b (\theta_v + 1 - (1 - \eta)Q_v - \frac{u}{s}Q_v)^2,
\text{s.t. } \eta(q_i - q_j) + (1 - \eta)(Q_{b(i)} - Q_{b(j)}) \geq \epsilon,
\eta(q_i - q_c) + (1 - \eta)(Q_{b(i)} - Q_{b(c)}) \geq 0, \forall c
\theta_{b(u)} \geq \theta_{u}, \forall u = 1, \ldots, b,
\sum_{c=1}^k q_c = 1, \quad q_c \geq 0, \quad \forall c.
$$

The main difference to (47) consists in the fact that we now minimize w.r.t. $$\theta$$ instead of $$f$$.

Note that, because of the way the predictor $$\text{pred}(f(\theta))$$ resolves ties (among the labels with maximal scores it always picks the label with the smallest index), not all labels can be ever predicted. Specifically, only one label from each block can be picked. This argument allows us to assume that $$b(i) \neq b(j)$$ in the remainder of this proof.

First, let us prove the case of $$\epsilon \leq \frac{u}{2}$$. We explicitly provide a feasible assignment of variables where the objective equals zero. We set $$q_i = \frac{1}{2}$$ and $$q_c = \frac{1}{2(s-1)}$$, $$c \in \mathcal{Y}_{b(j)} \setminus \{j\}$$. All the other labels (including $$j$$ and the unselected labels of the block $$b(i)$$) receive zero probability mass. This assignment of $$q$$ implies $$Q_{b(i)} = Q_{b(j)} = \frac{1}{2}$$ and the zero mass on the other blocks. We also set $$\theta_{b(i)}$$ and $$\theta_{b(j)}$$ to $$(1 - \eta)\frac{1}{2} + \frac{u}{2} - 1$$ to ensure zero objective value. Verifying other feasibility constraints we have $$\eta(q_i - q_j) + (1 - \eta)(Q_{b(i)} - Q_{b(j)}) = \frac{1}{s} \geq \epsilon$$ and $$\eta(q_i - q_c) + (1 - \eta)(Q_{b(i)} - Q_{b(c)}) = \eta(\frac{1}{s} - \frac{1}{2(s-1)}) \geq 0, c \in \mathcal{Y}_{b(j)} \setminus \{j\}$$. Other constraints are trivially satisfied.

Now, consider the case of $$\epsilon > \frac{u}{2}$$. As usual, we claim the following values of the variables $$f$$ and $$q$$ result in an optimal point. We have $$q^*_c = 0, c \notin \mathcal{Y}_{ij}; \theta^*_v = -1, v \notin \{b(i), b(j)\};$$ and $$q^*_c = Q^*_{b(i)} = \frac{1 + \epsilon - u}{2(1-\epsilon)}; q^*_c = 0, c \in \mathcal{Y}_{b(i)} \setminus \{i\}$$ (other labels in the block $$b(i)$$); $$q^*_j = 0, q^*_c = \frac{1 - \epsilon}{2 - (2 - \eta)(s-1)}, c \in \mathcal{Y}_{b(j)} \setminus \{j\}$$ (other labels in the block $$b(j)$$).

First, we will show that we can consider only configurations with all the probability mass on the two selected blocks $$b(i)$$ and $$b(j)$$. Given some optimal variables $$f^*$$ and $$q^*$$, the operation (with $$\delta = \sum_{c \in \mathcal{Y} \setminus \mathcal{Y}_{ij}} q^*_c$$)

$$q^*_c := 0, c \in \mathcal{Y} \setminus \mathcal{Y}_{ij},
q^*_i := q^*_i + \frac{\delta}{2},
q^*_j := q^*_j + \frac{\delta}{2},
$$

$$\theta^*_v := -1, v \notin \{b(i), b(j)\},
\theta^*_b(i) := \theta^*_b(i) + \frac{\delta}{2}(1 - \eta + \frac{u}{s}),
\theta^*_b(j) := \theta^*_b(j) + \frac{\delta}{2}(1 - \eta + \frac{u}{s})$$

can only decrease the objective of (49) because the summands corresponding to the unselected $$b - 2$$ blocks are set to zero. All the constraints stay feasible and the values corresponding to the blocks $$b(i)$$ and $$b(j)$$ do not change.
Now, we move the mass within the two selected blocks. To start with, moving the mass within one block does not change the objective, because it depends only on \(Q_{b(i)}\) and not on \(q\) directly. In the block \(b(j)\), it is safe to increase \(q_i\) and decrease the mass on the other labels, because \(q_i\) enters the constraints with the positive sign and all the rest with the negative sign.

In the block \(b(j)\), the situation is more complicated. When we move mass to some label \(c\) of this block we might violate constraints of (49) on \(q_i\):

\[
q_i \geq \varepsilon + q_j + (1 - \eta)(s - 1)\tilde{q}_j,
\]

\[
q_i \geq \tilde{q}_j + (1 - \eta)((s - 2)\tilde{q}_j + q_j),
\]

where \(\tilde{q}_j := \frac{1}{s-1}(Q_{b(j)} - q_j)\) stands for the mass on the non-selected label of the block \(b(j)\) (the masses of these labels can be always made equal because the problem is convex). We can safely set \(q_j\) to the value such that the constraints on \(q_i\) are as loose as possible. Searching for the point when the two constraints are as close as possible allows us to get the optimal value for \(q_j^*\):

\[
q_j^* = \max(0, \frac{Q_{b(i)}}{s} - \frac{\varepsilon(s-1)}{s}).
\]

If \(\frac{Q_{b(i)}}{s} - \frac{\varepsilon(s-1)}{s} > 0\) then \(Q_{b(i)} > \frac{s-1}{2}\) (because \(\varepsilon > \frac{q_j}{2}\)) and, in turn, \(Q_{b(i)} \geq q_i \geq e + (1 - \eta)Q_{b(i)} > \frac{q_j}{2} + \frac{s}{2}(1 - \eta)(s - 1) \geq \frac{q_j}{2} + \frac{s}{2}(1 - \eta) \geq \frac{q_j}{2}\). Since \(Q_{b(i)} + Q_{b(j)} = 1\), we have \(Q_{b(j)} < \frac{q_j}{2}\) and \(\frac{s-1}{s} > \frac{q_j}{2}\) leading to \(s < 2\), which contradicts the assumptions. We conclude that \(q_j^* = 0\).

So, at this point, we have \(\tilde{q}_i = \frac{1}{s}Q_2\) or \(\tilde{q}_i = \frac{s}{2}Q_2 + \frac{q_j}{2}\), which are both positive.

We now have that \(q_j^* = 0\); \(q_i^* > 0\); \(i \in \mathcal{Y}_{b(i)} \setminus \{j\}\); \(q_i^* > 0\), \(\mathcal{Y}_{b(i)} \neq \{b(i), b(j)\}\). It remains to find the exact values of \(q_i^*\) and \(\tilde{q}_i\), \(i \in \mathcal{Y}_{b(j)} \setminus \{j\}\). The equalities \(\eta(q_i - q_j) + (1 - \eta)(Q_{b(i)} - Q_{b(j)}) = \varepsilon\) and \(Q_{b(i)} + Q_{b(j)} = 1\) give us \(q_i^* = \frac{1+\varepsilon-\eta}{1-\eta}\) and \(\tilde{q}_i^* = \frac{1+\varepsilon-\eta}{(2-\eta)(s-1)}\). The first equality is true because the quadratic objective pushes the values of \(Q\) to be equal.

We now finish the computation of \(H(\varepsilon)\). First, we note that, due to the truncation argument similar to (32), we have both \(\theta_i^*\) and \(\theta_j^*\) in the segment \([1 - \eta)Q_{b(j)} + \frac{2}{s}Q_{b(i)} - 1, (1 - \eta)Q_{b(i)} + \frac{2}{s}Q_{b(j)} - 1]\) and

\[
\theta_i^* = \begin{cases} 
\theta_i^*, & \text{if } (1 - \eta)Q_{b(j)} + \frac{2}{s}Q_{b(i)} - 1 \geq \theta_j^*, \\
(1 - p)Q_{b(i)} + \frac{2}{s}Q_{b(j)} - 1, & \text{otherwise},
\end{cases}
\]

which implies that \(\theta_i^* = \theta_j^* = \theta\).

Substituting the values \(Q_{b(i)}^*\) and \(Q_{b(j)}^*\) provided above into the objective of (49) and performing unconstrained minimization w.r.t. \(\theta\) (we use the help of MATLAB symbolic toolbox) we get

\[
\theta^* = \frac{s - \eta + \eta s}{2s}
\]

and, consequently,

\[
H_{ij}(\varepsilon) = \frac{s(1 - \eta)^2(1 + \eta)^2}{(1 - \eta)(s - 1)}
\]

which finishes the proof.

\(\square\)

## E  Constants in the SGD rate

To formalize the learning difficulty by bounding the required number of iterations to get a good value of the risk (Theorem 6), we need to bound the constants \(D\) and \(M\). In this section, we provide a way to bound these constants for the quadratic surrogate (11) under Assumption 4.

Consider the family of score functions \(\tilde{F}_{f, \mathcal{H}}\) defined via an explicit feature map \(\psi(x) \in \mathcal{H}\), i.e.,

\[
f(x) = FW\psi(x), W : \mathcal{H} \rightarrow \mathbb{R}^r, F \in \mathbb{R}^k \times \mathbb{R}.
\]

Then the surrogate risk can be written as

\[
\mathcal{R}_{\psi}(f(x)) = \mathbb{E}_{(x, y) \sim D} \frac{1}{2} \|FW\psi(x) + L(:, y)\|^2_{\mathbb{R}^r}
\]

and its stochastic w.r.t. \((x, y)\) gradient as

\[
g_{x, y}(W) = \frac{1}{k} F^T(FW\psi(x) + L(:, y))\psi(x)^T
\]
where $L(\cdot, y)$ denotes the column of the loss matrix corresponding to the correct label $y$. Note that computing the stochastic gradient requires performing products $F^T F$ and $F^T L(\cdot, y)$ for which direct computation is expensive when $k$ is large, but which can be done in closed form for the structured losses we consider (the Hamming and block 0-1 loss). More generally, these operations require suitable inference algorithms.

Assumption 4 implies that each marginal posterior distribution $q_c(x)$ belongs to RKHS, $q_c \in \mathcal{H}$, $c = 1, \ldots, k$. To derive the bound, we also assume that $\sum_{c=1}^k \|q_c\|_{\mathcal{H}} \leq Q_{\text{max}}$, which implies that for each $x$ there exists $v_c \in \mathcal{H}$ such that $q_c(x) = \langle v_c, \psi(x) \rangle_{\mathcal{H}}$. Concatenating all $v_c$, we get an operator $V : \mathcal{H} \to \mathbb{R}^k$. We also assume that $\|\psi(x)\|_{\mathcal{H}} \leq R$ for all $x \in \mathcal{X}$.

Under this assumption, we can write the theoretical minimum of the surrogate risk. The expected gradient equals

$$k \nabla_W R_{\Phi}(f(x)) = F^T F W E_{x \sim D_X} (\psi(x) \psi(x)^T) + F^T L E_{x \sim D_X} (q_x \psi(x)^T)$$

$$= F^T F W E_{x \sim D_X} (\psi(x) \psi(x)^T) + F^T LV E_{x \sim D_X} (\psi(x) \psi(x)^T)$$

giving $W^* = -(F^T F)^{-1} F^T LV$ as a solution of equation $\nabla_W R_{\Phi}(f(x)) = 0$.

We can now bound the Hilbert-Schmidt norm of optimal parameters $W^*$ as

$$\|W^*\|_{HS} = \|((F^T F)^{-1}) F^T LV\|_{HS} \leq \sqrt{\|F^T F\|_2} \|LV\|_{HS} \leq \sqrt{\sigma_{\min}^{-1}(F)} \sqrt{\kappa L_{\text{max}} Q_{\text{max}}} =: D$$

where $\| \cdot \|_{HS}$ and $\| \cdot \|_2$ denote the Hilbert-Schmidt and spectral norms, respectively, and $\sigma_{\min}^{-1}(F)$ stands for the smallest singular value of the matrix $F$. Here, we use the standard connection of the Frobenius and spectral norms, since the rank of the matrix is at most $r$. The remaining two inequalities come from submultiplicativity and rotation-invariance of the spectral norm.

We now bound the Hilbert-Schmidt norm of the stochastic gradient $g_{x,y}(W)$.

$$\|g_{x,y}(W)\|_{HS} \leq \frac{1}{k} \|F^T F W \psi(x) + F^T L (\cdot, y)\|_2 \|\psi(x)\|_{\mathcal{H}}$$

$$\leq \frac{1}{k} \left( \|F^T F W \psi(x)\|_2 + \|F^T L (\cdot, y)\|_2 \right) \|\psi(x)\|_{\mathcal{H}}$$

$$\leq \frac{1}{k} \left( \|F^T F\|_2 \|W\|_{HS} \|\psi(x)\|_{\mathcal{H}} + \|F\|_2 \|L (\cdot, y)\|_2 \right) \|\psi(x)\|_{\mathcal{H}}$$

$$\leq \frac{1}{k} \sigma_{\max}^2(F) D R^2 + \frac{1}{k} \sigma_{\max}(F) \sqrt{\kappa L_{\text{max}} R} =: M$$

where $R$ is an upper bound on $\|\psi(x)\|_{\mathcal{H}}$ and $\sigma_{\max}(F)$ is a maximal singular value of $F$.

The bound of Theorem 5 contains the quantity $DM$ and the step size of SGD depends on $\frac{D}{M}$, so, to be practical, both quantities cannot be exponential (for numerical stability; but the important quantity is the number of iterations from Theorem 6). We have

$$DM = \kappa^2(F) R^2 T L_{\text{max}}^2 Q_{\text{max}}^2 + \kappa(F) R \sqrt{T} L_{\text{max}}^2 Q_{\text{max}} = L_{\text{max}}^2 \kappa(F) \sqrt{T} R Q_{\text{max}}$$

$$= \frac{\sigma_{\max}(F) \sigma_{\min}(F) R}{\kappa(F) \sqrt{T}} \frac{R}{\rho_{\min}^{\frac{1}{2}}}$$

where $\kappa(F) = \frac{\sigma_{\max}}{\sigma_{\min}}$ is the condition number of $F$. Note that the quantity $DM$ is invariant to the scaling of matrix $F$ The quantity $\frac{D}{M}$ scales proportionally of the square of $F$ and thus rescaling $F$ can always bring it to $O(1)$.

### E.1 Constants for specific losses

We now estimate constants $D$ and $M$ for 0-1, block 0-1 and Hamming losses. For the definition of the losses and the corresponding matrices $F$, we refer to Section C.3.

**0-1 loss.** For the 0-1 loss $L_{01}$ and $F = I_k$, we have $L_{\text{max}} = 1$, $r = k$, $\sigma_{\min} = \sigma_{\max} = 1$, thus $DM = O(k)$ is very large leading to very slow convergence of ASGD.

**Block 0-1 loss.** For the block 0-1 loss $L_{01,b}$ and matrix $F_{01,b}$, we have $L_{\text{max}} = 1$, $r = b$, $\sigma_{\min} = \sigma_{\max} = \sqrt{s}$, thus $DM = O(b)$.

**Hamming loss.** For the Hamming loss, we have $L_{\text{max}} = 1$, $r = \log_2 k + 1$, $\kappa(F_{\text{Ham},T}) \leq \log_2 k + 2$ (see the derivation in Section F). Finally, we have $DM = O(\log^3 k)$. 

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F Properties of the basis of the Hamming loss

As defined in (29), the matrix \( L_{\text{Ham},T} \in \mathbb{R}^{k \times k} \) is the matrix of the Hamming loss between tuples of \( T \) binary variables, and the number of labels equals \( k = 2^T \). Also recall that \( F_{\text{Ham},T} := [\frac{1}{2}1_{2T}, h^{(1)}, \ldots, h^{(T)}], (h^{(t)})_y := [y_1 = 1], t = 1, \ldots, T \). We have \( F_{\text{Ham},T} = \text{span}(F_{\text{Ham},T}) = \text{span}(L_{\text{Ham},T}) \) and \( \text{rank}(L_{\text{Ham},T}) = \text{rank}(F_{\text{Ham},T}) = T + 1 \).

We now explicitly compute \( \max_{i \neq j} \| P_{\text{Ham},T} \Delta_{ij} \|_2^2 \). We shortcut \( F_{\text{Ham},T} \) by \( F \) and compute:

\[
F^T F = 2T^2 - \begin{bmatrix} 1 & 1 & \cdots & 1 \\ 1 & 2 & 1 & \cdots \\ 1 & 1 & 2 & \cdots \\ \cdots & \cdots & \cdots & 1 \\ 1 & 1 & 1 & 2 \end{bmatrix}. \tag{51}
\]

We can compute the inverse matrix explicitly as well:

\[
(F^T F)^{-1} = 2^{2T} - \begin{bmatrix} 1 + T & -1 & \cdots & -1 \\ -1 & 1 & 0 & \cdots \\ -1 & 0 & 1 & \cdots \\ \cdots & \cdots & \cdots & 0 \\ -1 & \cdots & 0 & 1 \end{bmatrix}. \tag{52}
\]

The vector \( F^T \Delta_{ij} \) equals the difference of the two rows of \( F \), i.e., \( [0, c_1, \ldots, c_T]^T \in \mathbb{R}^{T+1} \) with each \( c_t \in \{-1, 0, +1\} \). Let this vector have \( T_+ \) ones and \( T - T_+ \) minus ones. The vector \( (F^T F)^{-1} F^T \Delta_{ij} \) then equals \( 2^{2T} [ -\sum c_t; c_1; \ldots; c_T ] \). Since all the columns of \( F \) are linearly independent, the maximal norm of \( F(F^T F)^{-1} F^T \Delta_{ij} \) is reached when all \( c_t \) equal +1 or all equal −1. In this case, we have \( \hat{h} := P_{\text{Ham},T} \Delta_{ij} = 2^{2T} (-\frac{T}{2} 1_{2T} + \sum_t h^{(t)}) \). The \( L_2 \)-norm is also easy to compute:

\[
\| \hat{h} \|_2^2 = 2^{4-2T} \sum_{i=0}^T (t - \frac{T}{2})^2 \binom{T}{i}^2
= 2^{4-2T} \frac{T^2}{4} 2^T - T^2 2^{T-1} + T(T + 1) 2^{T-2}
= 2^{2-T}T = \frac{4^T}{T^2},
\]

where we use the identities \( \sum_{i=0}^T \binom{T}{i} = 2^T \), \( \sum_{i=0}^T i \binom{T}{i} = T 2^{T-1} \), \( \sum_{i=0}^T i^2 \binom{T}{i} = T(T + 1) 2^{T-2} \).

We now compute the smallest and largest eigen values of the Gram matrix (51) for \( F_{\text{Ham},T} \). Ignoring the scaling factor \( 2^{T-2} \), we see by Gaussian elimination that the determinant and thus the product of all eigen values equals 1. If we subtract \( I_{T+1} \) the matrix becomes of rank 2, meaning that \( T - 1 \) eigen values equal 1. The trace, i.e., the sum of the eigen values of (51), without the scaling factor \( 2^{T-2} \) equals \( 2T + 1 \). Summing up, we have \( \lambda_{\text{min}} = 1 \) and \( \lambda_{\text{max}} = \lambda_{\text{min}} + 2 = 2^T \). We can now compute \( \lambda_{\text{min}} = \frac{1}{2}(T + 2 - \sqrt{T^2 + 4T}) \in [\frac{1}{T+2}, \frac{1}{T}] \) and \( \lambda_{\text{max}} = \frac{1}{2}(T + 2 + \sqrt{T^2 + 4T}) \in [T + 1, T + 2] \). By putting back the multiplicative factor, we get \( \sigma_{\text{min}} = \sqrt{\lambda_{\text{min}}} \geq \frac{\sqrt{T}}{2\sqrt{\log_2 k + 2}} \) and \( \sigma_{\text{max}} = \sqrt{\lambda_{\text{max}}} \leq \frac{\sqrt{T}}{2\sqrt{\log_2 k + 2}} \) thus condition number \( \kappa \leq \log_2 k + 2 \).