
Trading off Consistency and Dimensionality of Convex Surrogates for Multiclass Classification

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Abstract

1 In multiclass classification over n outcomes, we typically optimize some *surrogate*
2 *loss* $L : \mathbb{R}^d \times \mathcal{Y} \rightarrow \mathbb{R}$ assigning real-valued error to predictions in \mathbb{R}^d . In this
3 paradigm, outcomes must be embedded into the reals with dimension $d \approx n$ in
4 order to design a *consistent* surrogate loss. Consistent losses are well-motivated
5 theoretically, yet for large n , such as in information retrieval and structured pre-
6 diction tasks, their optimization may be computationally infeasible. In practice,
7 outcomes are typically embedded into some \mathbb{R}^d for $d \ll n$, with little known about
8 their suitability for multiclass classification. We investigate two approaches for
9 trading off consistency and dimensionality in multiclass classification while using
10 a convex surrogate loss. We first formalize *partial consistency* when the optimized
11 surrogate has dimension $d \ll n$. We then check if partial consistency holds under
12 a given embedding and low-noise assumption, providing insight into when to use a
13 particular embedding into \mathbb{R}^d . Finally, we present a new method to construct (fully)
14 consistent losses with $d \ll n$ out of multiple problem instances. Our practical
15 approach leverages parallelism to sidestep lower bounds on d .

16 1 Introduction

17 Multiclass classification, due to its combinatorial and discontinuous nature, is intractable to optimize
18 directly, which drives machine learners to optimize some nicer *surrogate loss*. To ensure these
19 surrogates properly “correspond” to the discrete classification task, we seek to design *consistent*
20 surrogates. If one uses a consistent surrogate loss, in the limit of infinite data and model expressivity,
21 one ends up with the same classifications as if one had solved the original intractable problem directly
22 with probability 1.

23 Surrogate losses form the backbone of gradient-based optimization for classification tasks. Optimizing
24 a surrogate is easier than direct optimization, but a large dimension d of the surrogate loss $L : \mathbb{R}^d \times \mathcal{Y} \rightarrow \mathbb{R}$
25 can make gradient-based optimization intractable. Therefore, previous literature has
26 operated under the premise that the prediction dimension d should be as low as possible, subject to
27 consistency for the classification task [Ramaswamy and Agarwal, 2016, Finocchi et al., 2024,
28 2020]. For multi-class classification, the lower bound on d is $n - 1$ [Ramaswamy and Agarwal,
29 2016].

30 These previous works implicitly focus on a binary approach to consistency: a surrogate is either
31 consistent for every possible label distribution, or it is not consistent. But there is a way out: lower
32 bounds on the surrogate dimension d rely on edge-cases that rarely show up in reality [Ramaswamy
33 and Agarwal, 2016]. As a result, practitioners are often willing to trade-off the guarantee of con-
34 sistency in order to improve the computational tractability of optimization. However, we currently
35 lack rigorous analysis tools to analyze many of the partially-consistent surrogates commonly used in
36 practice. Thus, *unlike previous works, our work focuses on this more realistic paradigm of partial*

37 *consistency*. We apply our unique approach to rigorously analyze a popular surrogate construction
 38 that encompasses methods such as one-hot and binary encoding. Our approach allows for fine-grained
 39 control of the trade-off between consistency and dimension.

40 Prior works have informally brushed upon the proposed partial-consistency paradigm, without
 41 rigorous study. For example, Agarwal and Agarwal [2015] impose a low-noise assumption to
 42 construct a surrogate for classification with $d = \log(n)$. However, their work does not provide any
 43 way to control the consistency-dimension trade-off. Similarly, Struminsky et al. [2018] characterize
 44 the excess risk bounds of inconsistent surrogates, which teaches us about the learning rates for
 45 inconsistent surrogates, but not *under which distributional assumptions* we can recover consistency
 46 guarantees.

47 Using different techniques than both of these approaches, we seek to understand the tradeoffs of
 48 consistency, surrogate prediction dimension, and number of problem instances through the use of
 49 polytope embeddings which are common in the literature [Wainwright et al., 2008, Blondel et al.,
 50 2020]. When embedding outcomes into $d \ll n$ dimensions, we first show there always exists a
 51 set of distributions where *hallucinations* occur: where the report minimizing the surrogate leads
 52 to a prediction \hat{y} such that the underlying true distribution has no weight on the prediction; that is,
 53 $\Pr[Y = \hat{y}] = 0$ (Theorem 3). Following this, we show that every polytope embedding is partially
 54 consistent under strong enough low-noise assumptions (Theorem 5). Finally, we demonstrate through
 55 leveraging the embedding structure and multiple problem instances that the mode (in particular, a
 56 full rank ordering) over n outcomes embedded into a $\frac{n}{2}$ dimensional surrogate space is elicitable
 57 over all distributions via $O(n^2)$ problem instances (Theorem 10). This alternative approach to
 58 recovering consistency is parallelizable, detangling the complexity of gradient computation of one
 59 high-dimensional surrogate.

60 2 Background and Notation

61 Let \mathcal{Y} be a finite label space, and throughout let $n = |\mathcal{Y}|$. Define $\mathbb{R}_+^{\mathcal{Y}}$ to be the nonnegative orthant.
 62 Let $\Delta_{\mathcal{Y}} = \{p \in \mathbb{R}_+^{\mathcal{Y}} \mid \|p\|_1 = 1\}$ be the set of probability distributions on \mathcal{Y} , represented as vectors.
 63 We denote the point mass distribution of an outcome $y \in \mathcal{Y}$ by $\delta_y \in \Delta_{\mathcal{Y}}$. Let $[d] := \{1, \dots, d\}$.
 64 In general, we denote a discrete loss by $\ell : \mathcal{Y} \times \mathcal{Y} \rightarrow \mathbb{R}_+$ with outcomes denoted by $y \in \mathcal{Y}$ and a
 65 surrogate loss by $L : \mathbb{R}^d \times \mathcal{Y} \rightarrow \mathbb{R}$ with surrogate reports $u \in \mathbb{R}^d$ and outcomes $y \in \mathcal{Y}$. The surrogate
 66 must be accompanied by a link $\psi : \mathbb{R}^d \rightarrow \mathcal{Y}$ mapping the convex surrogate model’s predictions back
 67 into the discrete target space, and we discuss consistency of a pair (L, ψ) with respect to the target ℓ .

68 For $\epsilon > 0$, we define an epsilon ball via $B_{\epsilon}(u) = \{u \in \mathbb{R}^d \mid \|u - x\|_2 < \epsilon\}$ and $B_{\epsilon} := B_{\epsilon}(\vec{0})$.
 69 Given a closed convex set $\mathcal{C} \subset \mathbb{R}^d$, we define a projection operation onto \mathcal{C} via $\text{Proj}_{\mathcal{C}}(u) :=$
 70 $\arg \min_{x \in \mathcal{C}} \|u - x\|_2$. Full tables of notation are found in Appendix A.

71 2.1 Property Elicitation, Consistency, and Prediction Dimension

72 Discrete label prediction requires optimization of a target loss function, ℓ , e.g. multi-class classifica-
 73 tion and 0-1 loss. When designing surrogate losses, consistency is the key notion of correspondence
 74 between surrogate and target loss. Intuitively, consistency implies that minimizing surrogate risk cor-
 75 responds to solving the target problem. Finocchiaro et al. [2021] show that surrogate loss consistency
 76 is a necessary precursor to excess risk bounds and convergence rates.

77 Consistency is generally a difficult condition to work with directly. Hence, we will use the notion
 78 of *calibration*, which is equivalent to consistency in our setting with finite outcomes. Our approach
 79 follows from the property elicitation literature, which allows us to abstract away from the feature space
 80 \mathcal{X} and focus on the conditional distributions over the labels, $p = \Pr[Y \mid X = x] \in \Delta_{\mathcal{Y}}$ [Bartlett
 81 et al., 2006, Zhang, 2004, Ramaswamy and Agarwal, 2016, Steinwart, 2007]. In this approach, the
 82 central object of study is a *property* which maps label distributions to reports that minimize the loss.

Definition 1 (Property, Elicits, Level Set). *Let \mathcal{R} be an arbitrary report set. For $\mathcal{P} \subseteq \Delta_{\mathcal{Y}}$, a property is a set-valued function $\Gamma : \mathcal{P} \rightarrow 2^{\mathcal{R}} \setminus \{\emptyset\}$, which we denote $\Gamma : \mathcal{P} \rightrightarrows \mathcal{R}$. A loss $L : \mathcal{Y} \times \mathcal{Y} \rightarrow \mathbb{R}$ elicits the property Γ on \mathcal{P} if*

$$\forall p \in \mathcal{P}, \Gamma(p) = \arg \min_{u \in \mathcal{R}} \mathbb{E}_{Y \sim p}[L(u, Y)].$$

83 If L elicits a property, it is unique and we denote it $\text{prop}[L]$. The level set of Γ for report r is the set
 84 $\Gamma_r := \{p \in \mathcal{P} \mid r = \Gamma(p)\}$. If $\text{prop}[L] = \Gamma$ and $|\Gamma(p)| = 1$ for all $p \in \mathcal{P}$, we say that L is strictly
 85 proper for Γ .

86 Once a model is optimized wrt. a surrogate L , it predicts reports in the surrogate space, \mathbb{R}^d . Then, to
 87 map surrogate reports to discrete labels, the surrogate loss must be paired with a link, $\psi : \mathbb{R}^d \rightarrow \mathcal{Y}$.
 88 Intuitively, a surrogate and link pair (L, ψ) are calibrated with respect to a target loss ℓ , if the optimal
 89 expected surrogate loss when making the *incorrect classification* (by ψ) is strictly greater than the
 90 optimal surrogate loss.

Definition 2 (ℓ -Calibrated Loss). Given discrete loss $\ell : \mathcal{Y} \times \mathcal{Y} \rightarrow \mathbb{R}_+$, surrogate loss $L : \mathbb{R}^d \times \mathcal{Y} \rightarrow \mathbb{R}$, and link function $\psi : \mathbb{R}^d \rightarrow \mathcal{Y}$. We say that (L, ψ) is ℓ -calibrated over $\mathcal{P} \subseteq \Delta_{\mathcal{Y}}$ if, for all $p \in \mathcal{P}$,

$$\inf_{u \in \mathbb{R}^d : \psi(u) \notin \text{prop}[\ell](p)} \mathbb{E}_{Y \sim p}[L(u, Y)] > \inf_{u \in \mathbb{R}^d} \mathbb{E}_{Y \sim p}[L(u, Y)].$$

91 If \mathcal{P} is not specified, then we are discussing calibration over $\Delta_{\mathcal{Y}}$.

92 Our analysis crucially relies on the ability to specify \mathcal{P} when invoking the definition of calibration.
 93 This is because the surrogates we analyze break the $d = n - 1$ lower bound on the dimension of any
 94 consistent surrogate loss. So the surrogates will not be calibrated over the whole simplex $\Delta_{\mathcal{Y}}$. To aid
 95 in our analysis, we use a condition that shows that converging to a property value implies calibration
 96 for the target loss itself [Agarwal and Agarwal, 2015].

Definition 3 (ℓ -Calibrated Property). Let $\mathcal{P} \subseteq \Delta_{\mathcal{Y}}$, $\Gamma : \mathcal{P} \Rightarrow \mathbb{R}^d$, discrete loss $\ell : \mathcal{Y} \times \mathcal{Y} \rightarrow \mathbb{R}_+$, and
 $\psi : \mathbb{R}^d \rightarrow \mathcal{Y}$. We will say (Γ, ψ) is ℓ -calibrated for all $p \in \mathcal{P}$ and all sequences in $\{u_m\}$ in \mathbb{R}^d if,

$$u_m \rightarrow \Gamma(p) \Rightarrow \mathbb{E}_{Y \sim p}[\ell(\psi(u_m), Y)] \rightarrow \min_{r \in \mathcal{Y}} \mathbb{E}_{Y \sim p}[\ell(r, Y)].$$

97 **Theorem 1** ([Agarwal and Agarwal, 2015, Theorem 3]). Let $\ell : \mathcal{Y} \times \mathcal{Y} \rightarrow \mathbb{R}_+$ and $\mathcal{P} \subseteq \Delta_{\mathcal{Y}}$. Let
 98 $\Gamma : \mathcal{P} \Rightarrow \mathbb{R}^d$ and $\psi : \mathbb{R}^d \rightarrow \mathcal{Y}$ be such that Γ is elicitable and (Γ, ψ) is an ℓ -calibrated property over
 99 \mathcal{P} . Let $L : \mathbb{R}^d \times \mathcal{Y} \rightarrow \mathbb{R}$ be a convex function for all $y \in \mathcal{Y}$ and strictly proper for Γ i.e. $\text{prop}[L] = \Gamma$
 100 and $|\Gamma(p)| = 1$ for all $p \in \mathcal{P}$. Then, (L, ψ) is ℓ -calibrated over \mathcal{P} .

101 Finally, we present the 0-1 loss that we analyze, which is the target loss for multiclass classification.

102 **Definition 4** (0-1 Loss). We denote the 0-1 loss by $\ell_{0-1} : \mathcal{Y} \times \mathcal{Y} \rightarrow \{0, 1\}$ such that $\ell_{0-1}(y, \hat{y}) :=$
 103 $\mathbb{1}_{y \neq \hat{y}}$. Observe $\gamma^{\text{mode}}(p) := \text{prop}[\ell_{0-1}](p) = \{y \in \mathcal{Y} \mid y \in \arg \max_y p_y\}$.

104 3 Polytope Embedding and Existence of Calibrated Regions

105 Often, discrete outcomes are embedded in continuous space onto the vertices of the simplex via
 106 one-hot encoding, or the vertices of the unit cube via binary encoding [Seeger, 2018]. Generalizing,
 107 we introduce an approach to surrogate construction inspired by Wainwright et al. [2008] and Blondel
 108 et al. [2020] that encompasses the aforementioned embedding methods. This construction utilizes
 109 embeddings onto arbitrary low-dimensional polytopes $\varphi : \mathcal{Y} \rightarrow \mathbb{R}^d$. Then, an embedding scheme
 110 naturally induces a large class of loss functions L_{φ}^G defined by the embedding, any G -Bregman
 111 Divergence, and a link function ψ^{φ} .

112 Our analysis begins by defining a condition stronger than inconsistency that arises when embedding
 113 into $d < n - 1$ dimensions for multiclass classification. To this end, we introduce the notion of
 114 *hallucination* as a means to characterize the “worst case” behavior of a surrogate pair (§ 3.2). In a
 115 positive manner, we characterize the *calibration regions* of various embeddings (§ 3.3), which are
 116 sets $\mathcal{P} \subseteq \Delta_{\mathcal{Y}}$ such that our surrogate and link pair $(L_{\varphi}^G, \psi^{\varphi})$ are ℓ -calibrated over \mathcal{P} . We refer the
 117 reader to the Appendix B for omitted full proofs.

118 3.1 Polytope Embedding Construction

119 A Convex Polytope $P \subset \mathbb{R}^d$, or simply a polytope, is the convex hull of a finite number of points
 120 $u_1, \dots, u_n \in \mathbb{R}^d$. An extreme point of a convex set A , is a point $u \in A$ such that if $u = \lambda y + (1 - \lambda)z$
 121 with $y, z \in A$ and $\lambda \in [0, 1]$, then $y = u$ and/or $z = u$. We shall denote by $\text{vert}(P)$ a polytope’s
 122 set of extreme points. A polytope can be expressed by the convex hull of its extreme points, i.e.
 123 $P = \text{conv}(\text{vert}(P))$ [Brøndsted, 2012, Theorem 7.2]. Additional definitions pertaining to polytopes
 124 are used for proofs that are omitted to the appendix, we refer the reader to (§ B.1) for said definitions.

We propose the following embedding procedure that allows one to construct surrogate losses with almost any polytope, and any Bregman divergence.

Construction 1 (Polytope Embedding). *Given \mathcal{Y} outcomes, $|\mathcal{Y}| = n$, choose a polytope $P \subset \mathbb{R}^d$ such that $|\text{vert}(P)| = n$. Choose a bijection between \mathcal{Y} and $\text{vert}(P)$. According to this bijection, assign each vertex a unique outcome so that $\{v_y | y \in \mathcal{Y}\} = \text{vert}(P)$. Then the polytope embedding $\varphi : \Delta_{\mathcal{Y}} \rightarrow P$ is $\varphi(p) := \sum_{y \in \mathcal{Y}} p_y v_y$, which is the sum of p -scaled vectors*

Following the work of Blondel [2019] and their proposed Projection-based losses, we use the extremely general class of Bregman divergences (Definition 5) and a polytope embedding φ to define an induced loss L_{φ}^G (Definition 6).

Definition 5 (Bregman Divergence). *Given a strictly convex function $G : \mathbb{R}^d \rightarrow \mathbb{R}$, $D_G(u, v) := G(v) - [G(u) + \langle dG_v, u - v \rangle]$ is a Bregman divergence where dG_v denotes a subgradient of G at v . For this work, we shall always assume that $\text{dom}(G) = \mathbb{R}^d$.*

Definition 6 ((D_G, φ) Induced Loss). *Given a Bregman divergence D_G and a polytope embedding φ , we say (D_G, φ) induces a loss $L_{\varphi}^G : \mathbb{R}^d \times \mathcal{Y} \rightarrow \mathbb{R}$ defined as $L_{\varphi}^G(u, y) := D_G(u, v_y) = G(v_y) - [G(u) + \langle dG_{v_y}, u - v_y \rangle]$.*

We show that for any $p \in \Delta_{\mathcal{Y}}$, the report that uniquely minimizes the expectation of the loss L_{φ}^G is $\varphi(p)$, the embedding point of p . Furthermore, the polytope P contains all of, and only the minimizing reports in expectation under L_{φ}^G .

Proposition 2. *For a given induced loss L_{φ}^G , the unique report which minimizes the expected loss is $u^* := \arg \min_{u \in \mathbb{R}^d} \mathbb{E}_{Y \sim p} [L_{\varphi}^G(u, Y)] = \varphi(p)$ such that $u^* \in P$. Furthermore, every $\hat{u} \in P$ is a minimizer of $\mathbb{E}_{Y \sim \hat{p}} [L_{\varphi}^G(u, Y)]$ for some $\hat{p} \in \Delta_{\mathcal{Y}}$.*

We now define the maximum a posteriori (MAP) link, which will be used in conjunction with an induced loss L_{φ}^G to form a surrogate pair for the 0-1 loss. The MAP link projects surrogate predictions onto the polytope P , then links to the nearest vertex of P , and is commonly used in the literature [Tsochantaridis et al., 2005, Blondel, 2019, Xue et al., 2016].

Definition 7 (MAP Link). *Let φ be a polytope embedding. The MAP link $\psi^{\varphi} : \mathbb{R}^d \rightarrow \mathcal{Y}$ is defined as $\psi^{\varphi}(u) = \arg \min_{y \in \mathcal{Y}} \|\text{Proj}_P(u) - v_y\|_2$. The level set of the link for y is $\psi_y^{\varphi} = \{u \in \mathbb{R}^d | y = \psi^{\varphi}(u)\}$. We break ties arbitrarily but deterministically.*

3.2 Hallucination Regions

Since our polytope embedding violates surrogate dimension bounds, calibration for 0-1 loss will not hold for all distributions. In particular, we show there always exists some distribution p such that $p_y = 0$ yet $\mathbb{E}_{Y \sim p} L_{\varphi}^G(u, Y)$ is minimized at some u such that $\psi^P(u) = y$. This implies a “worst case” inconsistency where the reported outcome could never actually occur with respect to our embedding of n events via φ into $\text{vert}(P)$.

Definition 8 (Hallucination). *Given (L, ψ) such that $L : \mathbb{R}^d \times \mathcal{Y} \rightarrow \mathbb{R}_+$, $|\mathcal{Y}| = n$, $d < n$, and $\psi : \mathbb{R}^d \rightarrow \mathcal{Y}$, we say that a hallucination occurs at a surrogate report $u \in \mathbb{R}^d$ if, for some p , $u \in \arg \min_{\hat{u} \in \mathbb{R}^d} \mathbb{E}_{Y \sim p} [L(\hat{u}, Y)]$ and $\psi(u) := y$ but $p_y = 0$. We denote by $\mathcal{H} \subseteq P \subset \mathbb{R}^d$ as the hallucination region as the elements of P at which hallucinations can occur.*

We express the subspace of the surrogate space where hallucinations can occur as the hallucination region denoted by \mathcal{H} . In Theorem 3, we characterize the hallucination region for any polytope embedding while using the surrogate pair $(L_{\varphi}^G, \psi^{\varphi})$ and show that \mathcal{H} is never empty.

Theorem 3. *For any given pair $(L_{\varphi}^G, \psi^{\varphi})$ and ℓ_{0-1} with embedding dimension $d < n - 1$; it holds that $\mathcal{H} = \cup_{y \in \mathcal{Y}} \text{conv}(\text{vert}(P) \setminus \{v_y\}) \cap \psi_y^{\varphi}$ and furthermore $\mathcal{H} \neq \emptyset$.*

Sketch. Fix $y \in \mathcal{Y}$. We abuse notation and write $\text{vert}(P_{-y}) := \text{vert}(P) \setminus \{v_y\}$. Observe $\text{conv}(\text{vert}(P_{-y})) \cap \psi_y^{\varphi} \subseteq \mathcal{H}$ since any point in this set can be expressed as a convex combination without needing vertex v_y implying there is a distribution embedded by φ to said point which has no weight on y . To show that $\mathcal{H} \subseteq \cup_{y \in \mathcal{Y}} \text{conv}(\text{vert}(P_{-y})) \cap \psi_y^{\varphi}$. Assume there exists a point $u \notin \text{conv}(\text{vert}(P) \setminus v_y) \cap \psi_y^{\varphi}$ such that there exists some $p \in \Delta_{\mathcal{Y}}$ where $\varphi(p) = u$, $p_y = 0$, and $\psi^{\varphi}(u) = y$. Since $\psi^{\varphi}(u) = y$ and $u \notin \text{conv}(\text{vert}(P_{-y})) \cap \psi_y^{\varphi}$, it must be the case that

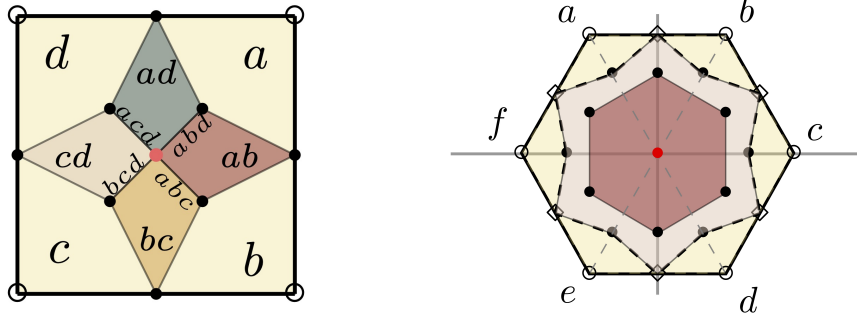


Figure 1: (Left) Mode level sets of Δ_Y where $\mathcal{Y} = \{a, b, c, d\}$ embedded into a two dimensional unit cube. The center red point denotes the origin $(0, 0)$ which is the hallucination region. (Right) An embedding of Δ_Y where $\mathcal{Y} = \{a, b, c, d, e, f\}$ into a three-dimensional permutahedron: the beige region expresses strict calibration regions, the light pink regions expresses regions with inconsistency, and the auburn region expresses regions with hallucinations. For example, consider the report $u = \vec{0}$. Since losses are convex, if $p = (0, \frac{1}{2}, 0, 0, \frac{1}{2}, 0)$, then $\text{conv}(\{b, e\})$ (dashed grey) is optimal, which includes u . However, $\vec{0}$ is also contained in $\text{conv}(\{a, d\})$ which is optimal for the distribution $p' = (\frac{1}{2}, 0, 0, \frac{1}{2}, 0, 0)$. Therefore, we cannot distinguish the optimal reports for a hallucination at $\vec{0}$.

174 $u \notin \text{conv}(\text{vert}(P_{-y}))$. However, that implies that u is strictly in the vertex figure and thus must
 175 have weight on the coefficient for y . Thus, forming a contradiction that $p_y = 0$ which implies that
 176 $\mathcal{H} \subseteq \cup_{y \in \mathcal{Y}} \text{conv}(\text{vert}(P_{-y})) \cap \psi_y^\varphi$. Finally, using Helly's Theorem [Rockafellar, 1997, Corollary
 177 21.3.2], we are able to show the non-emptiness of \mathcal{H} . \square

178 Theorem 3 suggests that using machine learning in high-risk settings such as medical and legal
 179 applications while violating the known $n - 1$ dimensional bound for surrogate losses in multiclass
 180 classification is inherently ill-advised without human intervention given the possibility for hallucina-
 181 tions. Furthermore, hallucinations may be forced by the target loss, as in the case of Hamming loss
 182 (see Appendix C). In these cases practitioners should carefully consider the choice of target loss. We
 183 conjecture that hallucinations are common for many structured prediction losses. However this is not
 184 a concern in our primary loss of study of multi-class classification.

185 3.3 Calibration Regions

186 Ideally, we would like calibration to hold over the entire simplex since that would imply minimizing
 187 surrogate risk would always correspond to solving the target problem regardless of the true underlying
 188 distribution. We observe that the mode's embedded level sets in the polytope overlap (see Figure 1L),
 189 which is unsurprising given that we are violating the lower bounds on surrogate prediction for the
 190 mode and hence calibration does not hold over the entire simplex. Since $|2^{\mathcal{Y}} \setminus \{\emptyset\}|$ is a finite set, we
 191 know that the number of unique mode level sets is finite. Although every point in the polytope is a
 192 minimizing report for some distribution, if multiple distributions with non-intersecting mode sets
 193 are embedded to the same point, there is no way to define a link function that is correct in all cases.
 194 However, if the union of mode sets for the p 's mapped to any $u \in P$ is a singleton, regardless of the
 195 underlying distribution*, a link ψ would be calibrated over the union if it mapped u to the mentioned
 196 singleton. Given (L, ψ) , φ , and a target loss ℓ , we define strict calibrated regions as the points for
 197 which calibration holds regardless of the actual distribution realized, which are possible at said points.

198 **Definition 9** (Strict Calibrated Region). Suppose we are given (L, ψ) , φ , and a target loss ℓ . We
 199 say $R \subseteq P$ is a strict calibrated region via (L, ψ) with respect to ℓ if (L, ψ) is ℓ -calibrated for all
 200 $p \in \varphi^{-1}(R) := \{p : \varphi(p) \in R\}$.

201 For any $y \in \mathcal{Y}$, we define $R_y := R \cap \psi_y$. We let $R_Y := \cup_{y \in \mathcal{Y}} R_y$.

202 By violating lower bounds, we are in a partially consistent paradigm where surrogate reports do not
 203 necessarily correspond to a unique distribution p . However, strict calibration regions allow us to

*We leave the more general case of linking u when $\bigcap_{p \in \varphi^{-1}(u)} \gamma(p) \neq \emptyset$ to future work.

check whether or not the loss is calibrated for the distribution p generating the data — even without explicit access to p . One simply has to check whether the report u is in $R_{\mathcal{Y}}$.

In Theorem 4, regardless of one’s chosen P , we show that there always exists a non-zero Lebesgue measurable strict calibration region and that $(L_{\varphi}^G, \psi^{\varphi})$ is calibrated for the 0-1 loss overall distributions embedded into the strict calibration region. This result shows that our surrogate and link construction for *any* d , always yields calibration regions in a robust sense — lending support to the practical use and study of these surrogates.

Theorem 4. *Let D_G be a Bregman divergence, φ be any polytope embedding, ψ^{φ} be the MAP link, and L_{φ}^G be the loss induced by (D_G, φ) . There exists a $\mathcal{P} \subseteq \Delta_{\mathcal{Y}}$ with non-zero Lebesgue measure and $\varphi(\mathcal{P}) \subseteq R_{\mathcal{Y}}$ via $(L_{\varphi}^G, \psi^{\varphi})$ with respect to ℓ_{0-1} .*

Although strict calibration regions R_y exist for each outcome $y \in \mathcal{Y}$ via the polytope embedding, tightly characterizing strict calibration regions is non-trivial. Since the level sets of elicitable properties are convex within the underlying simplex, characterizing the strict calibration regions becomes a collision detection problem, which is often computationally hard.

4 Restoring Inconsistent Surrogates via Low-Noise Assumptions

Looking towards application, we refine our results on the existence of strict calibration regions by examining a low-noise assumption, which provides an interpretable calibration region (§ 4.1). We show which low-noise assumptions imply calibration when embedding 2^d outcomes into d dimensions and $d!$ outcomes into d dimensions (§ 4.2). We refer the reader to Appendix B for omitted proofs.

4.1 Calibration via Low Noise Assumptions

We demonstrate that every polytope embedding leads to calibration under some low-noise assumption. Our results enable practitioners to choose the dimension d , unlike in previous works. Following previous work [Agarwal and Agarwal, 2015], we define a low noise assumption to be a subset of the probability simplex with low noise on the label distribution parameterized by $\hat{\alpha}$: $\Theta_{\hat{\alpha}} = \{p \in \Delta_{\mathcal{Y}} \mid \max_{y \in \mathcal{Y}} p_y \geq 1 - \hat{\alpha}\}$ where $\hat{\alpha} \in [0, 1]$. Given $\alpha \in (0, 1]$ and $y \in \mathcal{Y}$, we define the set $\Psi_{\alpha}^y = \{(1 - \alpha)\delta_{\hat{y}} + \alpha\delta_y \mid \hat{y} \in \mathcal{Y}\}$. With an embedding φ onto P , we define the set $P_{\alpha}^y := \varphi(\text{conv}(\Psi_{\alpha}^y))$, a scaled version of P anchored at v_y , that moves vertices $(1 - \alpha)$ towards y , (Figure 2R).

Theorem 5. *Let D_G be a Bregman divergence, φ be any polytope embedding, and L_{φ}^G be the loss induced by (D_G, φ) . There exists an $\alpha \in [0, .5)$ such that for the link $\psi_{\alpha}^{\varphi}(u) = \arg \min_{y \in \mathcal{Y}} \|u - P_{\alpha}^y\|_2$, $(L_{\varphi}^G, \psi_{\alpha}^{\varphi})$ is ℓ_{0-1} -calibrated over the distributions $\Theta_{\alpha} := \{p \in \Delta_{\mathcal{Y}} \mid \max_{y \in \mathcal{Y}} p_y \geq 1 - \alpha\}$.*

Proof. Part 1 (Choosing $\alpha \in [0, .5)$): By Theorem 4, there exists an $\epsilon > 0$ such that $B_{\epsilon}(v_y) \cap P \subseteq R_y$ for all $y \in \mathcal{Y}$. Given that $\text{vert}(P)$ are unique points, there exists a sufficiently small $\epsilon' > 0$ such that $B_{\epsilon'}(v) \cap B_{\epsilon'}(\hat{v}) = \emptyset$ for all $v, \hat{v} \in \text{vert}(P)$ where $v \neq \hat{v}$. Let $\epsilon'' = \min(\epsilon, \epsilon')$. For any $y \in \mathcal{Y}$, observe the set $\text{conv}(\Psi_{\alpha}^y)$, defined using any $\alpha \in [0, .5)$, is a scaled-down translated unit simplex and that for all $p \in \text{conv}(\Psi_{\alpha}^y) \subset \Delta_{\mathcal{Y}}$ it holds that $y = \text{mode}(p)$.

We shall show that for some sufficiently small $\alpha \in [0, .5)$, P_{α}^y is a scaled down version of P positioned at the respective vertex v_y . Furthermore, we shall show that $P_{\alpha}^y \subset B_{\epsilon''}(v_y) \cap P \subseteq R_y$ for all $y \in \mathcal{Y}$. Observe that by linearity of φ ,

$$P_{\alpha}^y := \varphi(\text{conv}(\Psi_{\alpha}^y)) = \text{conv}(\varphi(\{(1 - \alpha)\delta_{\hat{y}} + \alpha\delta_y \mid \hat{y} \in \mathcal{Y}\})) = \text{conv}(\{(1 - \alpha)v_y + \alpha v_{\hat{y}} \mid \hat{y} \in \mathcal{Y}\})$$

and hence, P_{α}^y is a scaled version of P positioned at v_y . Hence for some sufficiently small α , $(1 - \alpha)v_y + \alpha v_{\hat{y}} \in B_{\epsilon''}(v_y)$ for all \hat{y} and hence $P_{\alpha}^y \subseteq B_{\epsilon''}(v_y) \subseteq R_y$. With said sufficiently small α , define ψ_{α}^P and the respective sets $\text{conv}(\Psi_{\alpha}^y)$ for each $y \in \mathcal{Y}$. Using the previous α , define the set Θ_{α} as well.

Part 2 (Showing Calibration): Recall, by Proposition 2, for any $p \in \Delta_{\mathcal{Y}}$, $u = \varphi(p)$ minimizes the expected surrogate loss $\mathbb{E}_{Y \sim p}[L_{\varphi}^G(u, Y)]$. For any fixed $y \in \mathcal{Y}$, observe that $\text{conv}(\{(1 - \alpha)\delta_{\hat{y}} + \alpha\delta_y \mid$

250 $\hat{y} \in \mathcal{Y}\} = \{p : p_y \geq 1 - \alpha\} \subset \Delta_{\mathcal{Y}}$ and hence, by Proposition 2, $\cup_{y \in \mathcal{Y}} P_{\alpha}^y$ contains all of the
 251 minimizing surrogate reports with respect to Θ_{α} . By our choice of α and the construction of ψ_{α}^P ,
 252 every $u \in \cup_{y \in \mathcal{Y}} P_{\alpha}^y$ is linked to the proper unique mode outcome since $\cup_{y \in \mathcal{Y}} P_{\alpha}^y \subseteq R_{\mathcal{Y}}$. Assuming a
 253 low-noise condition where $p \in \Theta_{\alpha}$, any $u \notin \cup_{y \in \mathcal{Y}} P_{\alpha}^y$ is never optimal for any low-noise distribution.
 254 In such cases, we project the point to the nearest P_{α}^y as a matter of convention. Given that calibration
 255 is a result pertaining to minimizing reports, this design choice is non-influential. Finally, since every
 256 $\cup_{y \in \mathcal{Y}} P_{\alpha}^y \subseteq R_{\mathcal{Y}}$, by the definition of strict calibration region, it holds that $(L_{\varphi}^G, \psi_{\alpha}^{\varphi})$ is ℓ_{0-1} -calibrated
 257 for Θ_{α} . \square

258 4.2 Embedding into the Unit Cube and Permutahedron under Low-Noise

259 In this section, we demonstrate embedding onto the unit cube and the permutahedron [Blondel et al.,
 260 2020, Seger, 2018]. We show that by embedding 2^d outcomes into a d dimensional unit cube P^{\square} ,
 261 $(L_{\varphi}^G, \psi_{\alpha}^{P^{\square}})$ is calibrated over Θ_{α} for all $\alpha \in [0, \frac{1}{2})$. Furthermore, we found that by embedding $d!$
 262 outcomes into a d dimensional permutahedron P^w , $(L_{\varphi}^G, \psi_{\alpha}^{P^w})$ is calibrated for Θ_{α} for $\alpha \in (0, \frac{1}{d})$.
 263 Theorem 6 enables us to simultaneously study the aforementioned embeddings.

264 **Theorem 6.** *Let D_G be a Bregman divergence, φ be any polytope embedding, and L_{φ}^G be the loss
 265 induced by (D_G, φ) . Fix $\alpha \in [0, .5)$ and with it define Θ_{α} . If for all $y, \hat{y} \in \mathcal{Y}$ such that $y \neq \hat{y}$ it holds
 266 that $P_{\alpha}^y \cap P_{\alpha}^{\hat{y}} = \emptyset$, then $(L_{\varphi}^G, \psi_{\alpha}^{\varphi})$ is ℓ_{0-1} -calibrated for Θ_{α} where $\psi_{\alpha}^{\varphi}(u) = \arg \min_{y \in \mathcal{Y}} \|u - P_{\alpha}^y\|_2$.*

267 *Proof.* Pick an α such that for all $y, \hat{y} \in \mathcal{Y}$, $P_{\alpha}^y \cap P_{\alpha}^{\hat{y}} = \emptyset$. Define Θ_{α} and ψ_{α}^P accordingly. For
 268 $p \in \Theta_{\alpha}$ and some $y \in \mathcal{Y}$, say a sequence $\{u_m\}$ converges to $\text{prop}[L_{\varphi}^G](p) = \varphi(p) \in P_{\alpha}^y$, where the
 269 equality follows from Proposition 2. Given that each P_{α}^y is closed and pairwise disjoint, there exists
 270 some $\hat{\epsilon} > 0$ such that for all $y, \hat{y} \in \mathcal{Y}$ where $y \neq \hat{y}$, it also holds that $(P_{\alpha}^y + B_{\hat{\epsilon}}) \cap (P_{\alpha}^{\hat{y}} + B_{\hat{\epsilon}}) = \emptyset$
 271 where $+$ denotes the Minkowski sum. Since $\{u_m\}$ converges to $\varphi(p)$, there exists some $N \in \mathbb{N}$
 272 such that for all $n \geq N$, $\|u_n - \varphi(p)\|_2 < \hat{\epsilon}$. By the definition of ψ_{α}^{φ} , any u_n where $n \geq N$ will
 273 be mapped to y , the correct unique report given that $\text{prop}[L_{\varphi}^G](p) \in P_{\alpha}^y$. Hence, $(\text{prop}[L_{\varphi}^G], \psi_{\alpha}^{\varphi})$ is
 274 ℓ_{0-1} -calibrated property with respect to Θ_{α} . Finally, since L_{φ}^G is strictly proper for $\text{prop}[L_{\varphi}^G]$, by
 275 Theorem 1, we have that $(L_{\varphi}^G, \psi_{\alpha}^{\varphi})$ is ℓ_{0-1} -calibrated for Θ_{α} . \square

276 **Unit Cube** Define a unit cube in d -dimensions by $P^{\square} := \text{conv}(\{-1, 1\}^d)$. Binary encoding
 277 outcomes into the elements of $\{-1, 1\}^d$ (the vertices of a unit cube) is a commonly used method in
 278 practice (e.g., [Seger, 2018, Yu and Blaschko, 2018]). We show that calibration holds under a low
 279 noise assumption of Θ_{α} when $\alpha < .5$.

280 **Corollary 7.** *Let φ be an embedding from 2^d outcomes into the vertices of P^{\square} in d -dimensions and
 281 define an induced loss L_{φ}^G . Fix $\alpha \in [0, .5)$ and define Θ_{α} . $(L_{\varphi}^G, \psi_{\alpha}^{P^{\square}})$ is ℓ_{0-1} -calibrated for Θ_{α} .*

282 Corollary 7 suggests that binary encoding is an appropriate methodology when one has a prior over
 283 the data that the mode of the label distribution $\Pr[Y | X = x]$ is greater than half for all $x \in \mathcal{X}$.
 284 Interestingly, the bound of α is not dependent on the dimension of d . We now present a result for
 285 embedding outcomes into a factorially lower dimension via the permutahedron. Intuitively, ranking
 286 can be recast as a multiclass classification problem, in which case the outcomes are orderings of the d
 287 possible labels.

288 **Permutahedron** Let \mathcal{S}_d express the set of permutations on $[d]$. The permutahedron associated
 289 with a vector $w \in \mathbb{R}^d$ is defined to be the convex hull of the permutations of the indices of w , i.e.,
 290 $P^w := \text{conv}\{\pi(w) \mid \pi \in \mathcal{S}_d\} \subset \mathbb{R}^d$. The permutahedron may serve as an embedding from $d!$
 291 outcomes into d -dimensions; it is a natural choice for embedding full rankings over d items.

292 **Corollary 8.** *Let φ be an embedding from $d!$ outcomes into the vertices of P^w in d dimensions
 293 such that $w = (0, \frac{1}{\beta d}, \frac{2}{\beta d}, \dots, \frac{d-1}{\beta d}) \in \mathbb{R}^d$ where $\beta = \frac{d-1}{2}$. Fix $\alpha \in (0, \frac{1}{d})$. Then $(L_{\varphi}^G, \psi_{\alpha}^{P^w})$ is
 294 ℓ_{0-1} -calibrated over Θ_{α} .*

295 The calibration region in Corollary 8 show that consistency in Θ_{α} shrinks exponentially in d . Unless
 296 one has a prior that the data follows some form of a power distribution, Corollary 8 suggests not to
 297 factorially embed outcomes.

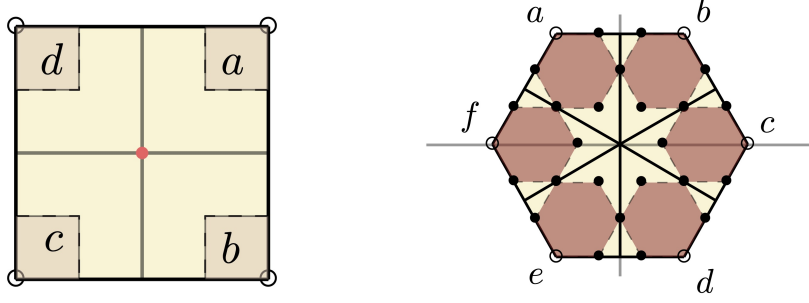


Figure 2: (Left) Corners represent the strict calibration regions for Θ_α where $\mathcal{Y} = \{a, b, c, d\}$ is embedded into a two dimensional unit cube such that $\alpha = .25$. (Right) Auburn regions show that strict calibration holds for Θ_α where $\mathcal{Y} = \{a, b, c, d, e, f\}$ is embedded into a three-dimensional permutahedron such that $\alpha = \frac{1}{3} - \epsilon$.

5 Elicitation in Low Dimensions with Multiple Problem Instances

The tools developed in previous sections now enable us to address the setting in which we require full consistency, $\mathcal{P} = \Delta_{\mathcal{Y}}$, but also desire surrogate prediction dimension $d \ll n - 1$. We side-step the $n - 1$ lower bound by utilizing multiple problem instances and aggregation of the outputs. Although cumulatively we have a larger surrogate prediction dimension than $n - 1$, each individual problem instance has a less than $n - 1$ surrogate prediction dimension. This approach is well-motivated since it allows for distributed computing of separate, smaller models which leads to faster convergence overall since in general optimization is at least $\text{poly}(d)$.

Definition 10. Extending Definition 1, we say a loss and link pair (L, ψ) , where $L : \mathbb{R}^d \times \mathcal{Y} \rightarrow \mathbb{R}$ and $\psi : \mathbb{R}^d \rightarrow \mathcal{Y}$, elicits a property $\Gamma : \mathcal{P} \rightrightarrows \mathcal{Y}$ on $\mathcal{P} \subseteq \Delta_{\mathcal{Y}}$ if $\forall p \in \mathcal{P}$, $\Gamma(p) = \psi(\arg \min_{u \in \mathbb{R}^d} \mathbb{E}_{Y \sim p}[L(u, Y)])$.

Definition 11 ((n, d, m) -Polytope Elicitable). Suppose we are given a property $\gamma : \mathcal{P} \rightrightarrows \mathcal{Y}$ such that $\mathcal{P} \subseteq \Delta_{\mathcal{Y}}$ and $|\mathcal{Y}| = n$ finite outcomes. Say we have m unique polytope embeddings $\{\varphi_j : \Delta_{\mathcal{Y}} \rightarrow \mathbb{R}^d\}_{j=1}^m$ where $d < n - 1$, and a set of induced losses $\{L_{\varphi_j}^G\}_{j=1}^m$ and links $\psi_j : \mathbb{R}^d \rightarrow \mathcal{B}_j$ defined wrt. φ_j , where \mathcal{B}_j is an arbitrary report set. For each $j \in [m]$, assume the pair $(L_{\varphi_j}^G, \psi_j)$ elicits the property $\Gamma_j : \mathcal{P} \rightrightarrows \mathcal{B}_j$. If there exists a function $\Upsilon : \mathcal{B}_1 \times \dots \times \mathcal{B}_m \rightrightarrows \mathcal{Y}$ such that for any $p \in \Delta_{\mathcal{Y}}$ it holds that $\Upsilon(\Gamma_1(p), \dots, \Gamma_m(p)) = \gamma(p)$, we say that γ is (n, d, m) -Polytope Elicitable over \mathcal{P} .

Equivalently, we will also say that the pair $(\{(L_{\varphi_j}^G, \psi_j)\}_{j=1}^m, \Upsilon)$ (n, d, m) -Polytope elicits the property γ with respect to \mathcal{P} .

We shall express a d -cross polytope by $P^\oplus := \text{conv}(\{\pi((\pm 1, 0, \dots, 0)) \mid \pi \in \mathcal{S}_d\})$ where $(\pm 1, 0, \dots, 0) \in \mathbb{R}^d$. Observe that a d -cross polytope has $2d$ vertices. For any vertex of a d -cross polytope $v \in \text{vert}(P^\oplus)$, we shall say that $(v, -v)$ forms a diagonal vertex pair.

Lemma 9. Say we are given a cross-polytope embedding $\varphi : \Delta_{2d} \rightarrow P^\oplus$ and induced loss L_φ^G . Let (v_{a_i}, v_{b_i}) , be the i^{th} diagonal pair (i.e. $\varphi(\delta_{a_i}) = v_{a_i}$). Define the property $\Gamma^\varphi : \Delta_{2d} \rightarrow \mathcal{B}$ element-wise by

$$\Gamma^\varphi(p)_i := \begin{cases} (<, a_i, b_i) & \text{if } p_{a_i} < p_{b_i} \\ (>, a_i, b_i) & \text{if } p_{a_i} > p_{b_i} \\ (=, a_i, b_i) & \text{if } p_{a_i} = p_{b_i}. \end{cases}$$

Furthermore define the link $\psi^{P^\oplus} : \mathbb{R}^d \rightarrow \mathcal{B}$ with respect to each diagonal pair as

$$\psi(u; v_{a_i}, v_{b_i})_i^{P^\oplus} := \begin{cases} (<, a_i, b_i) & \text{if } \|u - v_{a_i}\|_2 > \|u - v_{b_i}\|_2 \\ (>, a_i, b_i) & \text{if } \|u - v_{a_i}\|_2 < \|u - v_{b_i}\|_2 \\ (=, a_i, b_i) & \text{o.w.} \end{cases}$$

Then $(L_\varphi^G, \psi^{P^\oplus})$ elicits Γ^φ .

The following theorem states that by using multiple problem instances, based on Lemma 9, we can Polytope-elicite the mode. Algorithm 1 outlines how to aggregate the individual solutions to infer the mode. We defer the proof to Appendix B.

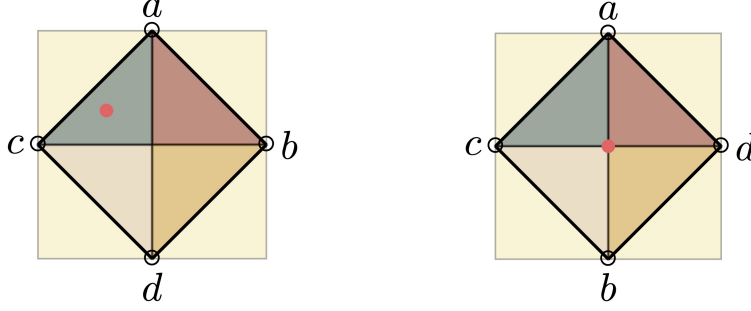


Figure 3: Four outcomes embedded in \mathbb{R}^2 in two different ways, with the minimizing reports \bullet for a distribution p ." (Left) Configuration φ_1 with \bullet at $(-.5, .3)$ implying $p_a > p_d$ and $p_b > p_c$. (Right) Configuration φ_2 with \bullet at $(0, 0)$ implying $p_a = p_b$ and $p_c = p_d$. This implies the true distribution is $p = (0.4, 0.4, 0.1, 0.1)$."

325 **Theorem 10.** *Let $d \geq 2$. The mode is $(2d, d, m)$ -Polytope Elicitable for some $m \in [2d-1, d(2d-1)]$.*

Algorithm 1 Elicit mode via comparisons and the d -Cross Polytopes

Require: $M = \{(L_{\varphi_j}^G, \psi_j^{P^\oplus})\}_{j=1}^m$
 Learn a model $h_j : \mathcal{X} \rightarrow \mathbb{R}^d$ for each instance $(L_{\varphi_j}^G, \psi_j^{P^\oplus}) \in M$
 For some fixed $x \in \mathcal{X}$, collect all $B_j \leftarrow \psi_j^{P^\oplus}(h_j(x))$ where $B_j \in \mathcal{B}_j$
 Report $R \leftarrow \text{FindMaxes}^\dagger(B_1, \dots, B_m)$

326 Although Theorem 10 states that the mode is $(2d, d, m)$ -Polytope Elicitable for some $m \in [2d -$
 327 $1, d(2d - 1)]$, it does not state how we select said $\{(L_{\varphi_j}^G, \psi_j^{P^\oplus})\}_{j=1}^m$ problem instances in an optimal
 328 manner. Unfortunately, selecting the min number of problem instances reduces to a minimum set
 329 cover problem which is computationally hard. Even so, through a greedy approach, one can choose
 330 problem instances that are log approximate optimal relative to the true best configuration. In practice
 331 using real data, given that these are asymptotic results, we may have conflicting logic for the provided
 332 individual reports. In Appendix D, we discuss an approach of how to address this in practice.

333 6 Discussion and Conclusion

334 This work examines various tradeoffs between surrogate loss dimension, restricting the region of
 335 consistency in the simplex when using the 0-1 loss, and number of problem instances. Since our
 336 analysis is based on an embedding approach commonly used in practice, our work provides theoretical
 337 guidance for practitioners choosing an embedding. We see several possible future directions. The
 338 first is a deeper investigation into hallucinations. Future work could investigate the size of the
 339 hallucination region in theory, and the frequency of reports in the hallucination region in practice.
 340 Another direction would be to construct a method that efficiently identifies the strict calibration
 341 regions and the distributions embedded into them. This would provide better guidance on whether or
 342 not a particular polytope embedding aligns with one's prior over the data. Finally, another direction
 343 is to identify other properties that can be elicited via multiple problem instances while also reducing
 344 the dimension of any one instance.

345 **Broader Impacts:** Our work broadly informs the selection of loss functions for machine learning.
 346 Thus our work may influence practitioners' choice of loss function. Of course, such loss functions
 347 can be used for ethical or unethical purposes. We do not know of particular risks of negative impacts
 348 of this work beyond risks of machine learning in general.

[†]Given all comparisons, a sorting algorithm can be used to compute the set of $r \in \mathcal{Y}$ such that p_r is maximum.

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Notation	Explanation
$r \in \mathcal{Y}$	Prediction space
$y \in \mathcal{Y}$	Label space
$\Delta_{\mathcal{Y}}$	Simplex over \mathcal{Y}
$[d] := \{1, \dots, d\}$	Index set
$\mathbb{1}_S \in \{0, 1\}^d$ s.t. $(\mathbb{1}_S)_i = 1 \Leftrightarrow i \in S$	0-1 Indicator on set $S \subseteq [d]$
$\mathcal{C} \subset \mathbb{R}^d$	Closed convex set
$u \in \mathbb{R}^d$	Surrogate prediction space
$\text{Proj}_{\mathcal{C}}(u) := \arg \min_{x \in \mathcal{C}} \ u - x\ _2$	Projection onto closed convex set
$\pi \in \mathcal{S}_d$	Permutations of $[d]$
$\ell : \mathcal{Y} \times \mathcal{Y} \rightarrow \mathbb{R}_+$	Discrete loss
$L : \mathbb{R}^d \times \mathcal{Y} \rightarrow \mathbb{R}$	Surrogate loss
$\mathbb{E}_{Y \sim p}[\ell(r, Y)]$	Expected discrete loss
$\mathbb{E}_{Y \sim p}[L(u, Y)]$	Expected surrogate loss

Table 1: Table of general notation

Notation	Explanation
$P \subset \mathbb{R}^d$	Polytope
$P^{\square} := \text{conv}(\{-1, 1\}^d)$	Unit cube
$P^w := \text{conv}\{\pi \cdot w \mid \pi \in \mathcal{S}_d\} \subset \mathbb{R}^d$ s.t. $w \in \mathbb{R}^d$	Permutahedron
$P^{\oplus} := \text{conv}(\{\pi((\pm 1, 0, \dots, 0)) \mid \pi \in \mathcal{S}_d\})$	Cross polytope

Table 2: Table of polytope notation

394 B Polytopes, Omitted Proofs, and Results

395 B.1 Polytopes

396 A Convex Polytope $P \subset \mathbb{R}^d$, or simply a polytope, is the convex hull of a finite number of points
 397 $u_1, \dots, u_n \in \mathbb{R}^d$. An extreme point of a convex set A , is a point $u \in A$ such that if $u = \lambda y + (1 - \lambda)z$
 398 with $y, z \in A$ and $\lambda \in [0, 1]$, then $y = u$ and/or $z = u$. We shall denote by $\text{vert}(P)$ a polytope's
 399 set of extreme points. A polytope can be expressed by the convex hull of its extreme points, i.e.
 400 $P = \text{conv}(\text{vert}(P))$ [Brondsted, 2012, Theorem 7.2].

401 We define the dimension of P via $\dim(P) := \dim(\text{affhull}(P))$ where $\text{affhull}(P)$ denotes the smallest
 402 affine set containing P . A set $F \subseteq P$ is a face of P if there exists a hyperplane $H(y, \alpha) := \{u \in$
 403 $\mathbb{R}^d \mid \langle u, y \rangle = \alpha\}$ such that $F = P \cap H$ and $P \subseteq H^+$ such that $H^+(y, \alpha) := \{u \in \mathbb{R}^d \mid \langle u, y \rangle \leq \alpha\}$.
 404 Let $F_i(P)$ where $i \in [d - 1]$ denote set of faces of dim i of a polytope P . A face of dimension
 405 zero is called a vertex and a face of dimension one is called an edge. We define the edge set of a
 406 polytope P by $E(P) := \{\text{conv}((v_i, v_j)) \mid (v_i, v_j) \subseteq \binom{\text{vert}(P)}{2}, \text{conv}((v_i, v_j)) \in F_1(P)\}$. We define
 407 the neighbors of a vertex v by $\text{ne}(v; P) := \{\hat{v} \in \text{vert}(P) \mid \text{conv}((v, \hat{v})) \in E(P)\}$. We will denote
 408 $\text{conv}((v, \hat{v})) \in E(P)$ by as $e_{v, \hat{v}}$ and $\text{ne}(v; P)$ by $\text{ne}(v)$ when clear from context.

409 B.2 Omitted Proofs from § 3

410 **Proposition 11.** For a given induced loss L_φ^G , the unique report which minimizes the expected loss
 411 is $u^* := \arg \min_{u \in \mathbb{R}^d} \mathbb{E}_{Y \sim p}[L_\varphi^G(u, Y)] = \varphi(p)$ such that $u^* \in P$. Furthermore, every $\hat{u} \in P$ is a
 412 minimizer of $\mathbb{E}_{Y \sim \hat{p}}[L_\varphi^G(u, Y)]$ for some $\hat{p} \in \Delta_Y$.

413 *Proof.* By [Banerjee et al., 2005, Theorem 1], the minimizer of $\mathbb{E}_{Y \sim p}[L_\varphi^G(u, Y)]$ is $\sum_{y \in \mathcal{Y}} p_y v_y =$
 414 $\varphi(p)$. Thus, by the construction of the polytope embedding, it holds that $u^* = \varphi(p)$. Since
 415 Bregman divergences are defined with respect to strictly convex functions, u^* uniquely minimizes
 416 $\mathbb{E}_{Y \sim p}[L_\varphi^G(u, Y)]$.

417 Conversely, every $\hat{u} \in P$ is expressible as a convex combination of vertices; hence, by the definition
 418 of φ , for some distribution, say $\hat{p} \in \Delta_Y$, it holds $\hat{u} = \varphi(\hat{p})$. Therefore, it holds that \hat{u} minimizes
 419 $\mathbb{E}_{Y \sim \hat{p}}[L_\varphi^G(u, Y)]$. \square

420 **Theorem 12.** For any given pair $(L_\varphi^G, \psi^\varphi)$ and ℓ_{0-1} with embedding dimension $d < n - 1$; it holds
 421 that $\mathcal{H} = \cup_{y \in \mathcal{Y}} \text{conv}(\text{vert}(P) \setminus \{v_y\}) \cap \psi_y^\varphi$ and furthermore $\mathcal{H} \neq \emptyset$.

422 *Proof.* Choose a $y \in \mathcal{Y}$. We abuse notation and write $\text{vert}(P) \setminus v_y := \text{vert}(P) \setminus \{v_y\}$. Observe all
 423 $u \in \text{conv}(\text{vert}(P) \setminus v_y) \cap \psi_y^\varphi$ can be expressed as a convex combination of vertices without needing
 424 vertex v_y . The coefficients of said convex combination express a $p \in \Delta_Y$ that is embedded to the point
 425 $u \in P$ where $p_y = 0$. Yet, by Proposition 2, said u is an expected minimizer of L_φ^G with respect to p .
 426 Given the intersection with ψ_y^φ and by Definition 8, it holds that $\cup_{y \in \mathcal{Y}} \text{conv}(\text{vert}(P) \setminus v_y) \cap \psi_y^\varphi \subseteq \mathcal{H}$.

427 We now shall show that $\mathcal{H} \subseteq \cup_{y \in \mathcal{Y}} \text{conv}(\text{vert}(P) \setminus v_y) \cap \psi_y^\varphi$. Fix $y \in \mathcal{Y}$. Assume there exists a
 428 point $u \notin \text{conv}(\text{vert}(P) \setminus v_y) \cap \psi_y^\varphi$ such that there exists some $p \in \Delta_Y$ where $\varphi(p) = u$, $p_y = 0$,
 429 and $\psi^\varphi(u) = y$. Since $\psi^\varphi(u) = y$ and $u \notin \text{conv}(\text{vert}(P) \setminus v_y) \cap \psi_y^\varphi$, it must be the case that
 430 $u \notin \text{conv}(\text{vert}(P) \setminus v_y)$. However, that implies that u is strictly in the vertex figure and thus must
 431 have weight on the coefficient for y . Thus, forming a contradiction that $p_y = 0$ which implies that
 432 $\mathcal{H} = \cup_{y \in \mathcal{Y}} \text{conv}(\text{vert}(P) \setminus v_y) \cap \psi_y^\varphi$.

433 To show non-emptiness of \mathcal{H} , we shall use Helly's Theorem (Rockafellar [1997], Corollary 21.3.2).
 434 W.l.o.g, assign an index such that $\mathcal{Y} = \{y_1, \dots, y_d, y_{d+1}, \dots, y_n\}$. Observe the elements of the set
 435 $\{\mathcal{Y} \setminus y_i\}_{i=1}^n$ each differ by one element. W.l.o.g, pick the first $d + 1$ elements of the previous set.
 436 Observe $|\cap_{i=1}^{d+1} \mathcal{Y} \setminus y_i| = |\mathcal{Y} \setminus \{y_1, \dots, y_d, y_{d+1}\}| = n - (d + 1) > 0$. Hence, by Helly's theorem
 437 and uniqueness of y_i 's, $\cap_{y \in \mathcal{Y}} \text{conv}(\text{vert}(P) \setminus v_y) \neq \emptyset$.

438 Pick a point $u' \in \cap_{y \in \mathcal{Y}} \text{conv}(\text{vert}(P) \setminus v_y)$. Since ψ^φ is well-defined, u' will be linked to some
 439 outcome $y' \in \mathcal{Y}$ and thus $u' \in \text{conv}(\text{vert}(P) \setminus v_{y'}) \cap \psi_{y'}^\varphi \subset \mathcal{H}$. Yet, u' can be expressed as a

convex combination which does not use $v_{y'}$ since it lies in $\cap_{y \in \mathcal{Y}} \text{conv}(\text{vert}(P) \setminus v_y)$. Thus, by using Proposition 2 and by the definition of Hallucination (Def. 8), we have that $\mathcal{H} \neq \emptyset$. \square

Lemma 1 (Proposition 1.2.4). [Hiriart-Urruty and Lemaréchal, 2004] If φ is an affine transformation of \mathbb{R}^n and $A \subset \mathbb{R}^n$ is convex, then the image $\varphi(A)$ is also convex. In particular, if the set A is a convex polytope, the image is also a convex polytope.

Lemma 2. Let D_G be a Bregman divergence, φ be any polytope embedding, ψ be the MAP link, and L_φ^G be the loss induced by (D_G, φ) . Assume the target loss is ℓ_{0-1} . If a point is in a strict calibrated region such that $u \in R_y$ for some $y \in \mathcal{Y}$, it is necessary that $u \in \text{conv}(\{v_y\} \cup \text{ne}(v_y)) \setminus \text{conv}(\text{ne}(v_y))$.

Proof. If $u \in R_y$ and $u \in P \setminus (\text{conv}(\{v_y\} \cup \text{ne}(v_y)) \setminus \text{conv}(\text{ne}(v_y)))$, then u can be expressed as a convex combination which has no weight on the coefficient for v_y . Hence, there exists a distribution embedded into u where y would not be the mode, thus violating the initial claim that $u \in R_y$. \square

Lemma 3. Let D_G be a Bregman divergence, φ be any polytope embedding, ψ be the MAP link, and L_φ^G be the loss induced by (D_G, φ) . For any $u \in e_{(v_i, v_j)} \in E(P)$, it holds that $|\varphi^{-1}(u)| = 1$.

Proof. Observe, the two vertices of an edge define the convex hull making up the edge and hence, by (Gruber [2007], Theorem 2.3) the two vertices are affinely independent. Therefore, all elements of the edge have a unique convex combination which are expressed by the convex combinations of the edge's vertices. Given the relation of the embedding φ and convex combinations of vertices expressing distributions, it holds that $|\varphi^{-1}(u)| = 1$. \square

Lemma 4. Let D_G be a bregman divergence, φ be a polytope embedding, and L_φ^G be the induced loss by (D_G, φ) . For all $y \in \mathcal{Y}$, it holds that $\dim(\varphi(\text{mode}_y)) = \dim(P) \geq 2$.

Proof. By the construction of φ , we know that $\dim(P) \geq 2$. Fix $y \in \mathcal{Y}$. By Lemma 3, we know that any edge connected from v_y and $\hat{v} \in \text{ne}(v_y)$, the distributions embedded into the half of the line segment closer to v_y , y is in the mode. By Lemma 1, we know that $\varphi(\gamma_y^{\text{mode}})$ is a convex set. Thus, the convex hull of the half line segments is part of $\varphi(\gamma_y^{\text{mode}})$. Since each vertex has at least $\dim(P)$ neighbors, it holds that $\dim(\varphi(\gamma_y^{\text{mode}})) = \dim(P)$. \square

Theorem 13. Let D_G be a Bregman divergence, φ be any polytope embedding, ψ^φ be the MAP link, and L_φ^G be the loss induced by (D_G, φ) . There exists a $\mathcal{P} \subseteq \Delta_{\mathcal{Y}}$ with non-zero Lebesgue measure and $\varphi(\mathcal{P}) \subseteq R_{\mathcal{Y}}$ via $(L_\varphi^G, \psi^\varphi)$ with respect to ℓ_{0-1} .

Proof. Recall that $\gamma^{\text{mode}}(p) := \text{prop}[\ell_{0-1}](p) = \text{mode}(p)$. Fix $y \in \mathcal{Y}$. For contradiction, assume for any $\hat{y} \in \mathcal{Y}$ where $y \neq \hat{y}$, it holds that $B_\epsilon(v_y) \cap \varphi(\gamma_{\hat{y}}^{\text{mode}}) \neq \emptyset$ for all $\epsilon > 0$. By Lemma 3, it holds that $\text{conv}(\{v_y\} \cup m_{v_y, \alpha}) \subseteq \varphi(\gamma_y^{\text{mode}})$ where $m_{v_y, \alpha} := \{(1 - \alpha)v_y + \alpha \bar{v} \mid \bar{v} \in \text{ne}(v_y)\}$ defined by any $\alpha \in (0, .5)$. Furthermore, the elements of $\cup_{m \in m_{v_y, \alpha}} \text{conv}(\{v_y\} \cup \{m\})$ have one distribution embedded onto it where y is the only valid mode thus, we know that $\varphi(\text{mode}_{\hat{y}}) \cap \cup_{m \in m_{v_y, \alpha}} \text{conv}(\{v_y\} \cup \{m\}) = \emptyset$. Since $\varphi(\gamma_{\hat{y}}^{\text{mode}}) \subset P$ is closed and convex, there must exist some non-negative min distance between $\varphi(\gamma_{\hat{y}}^{\text{mode}})$ and v_y which we shall denote by d_v . For any $\epsilon \in (0, d_{v_y})$, we can define $B_\epsilon(v_y)$ such that $B_\epsilon(v_y) \cap \varphi(\gamma_{\hat{y}}^{\text{mode}}) = \emptyset$, forming a contradiction.

For each $v_y \in \text{vert}(P)$ define a d_{v_y} and let $\epsilon' \in \cap_{v_y \in \text{vert}(P)} (0, d_{v_y})$. By the construction of P and the definition of ψ^φ , there exists a $\epsilon'' > 0$ such that for all $u \in B_{\epsilon''}(v_y)$ it holds that $\psi(u) = y$ and $B_{\epsilon''}(v_y) \subset \psi^\varphi$. For any $y \in \mathcal{Y}$, we know that $B_{\min\{\epsilon', \epsilon''\}}(v_y) \cap P \subseteq R_y$ by the construction of our epsilon ball. We claim $\varphi^{-1}(B_{\min\{\epsilon', \epsilon''\}}(v_y) \cap P)$ is a set of distributions for which calibration holds.

For $p \in \Delta_{\mathcal{Y}}$ such that $\varphi(p) \in B_{\min\{\epsilon', \epsilon''\}}(v_y) \cap P$ for some $v_y \in \text{vert}(P)$, suppose a sequence $\{u_m\}$ converges to $\text{prop}[L_\varphi^G](p) = \varphi(p)$ (equality by Proposition 2). By construction of $B_{\min\{\epsilon', \epsilon''\}}(v_y) \cap P$, $\psi^\varphi(\varphi(p)) = y \in \text{mode}(p)$ and hence, a minimizing report for $\ell_{0-1}(y; p)$. Furthermore, since $B_{\min\{\epsilon', \epsilon''\}}(v_y) \subset \psi_{\varphi^{-1}(v_y)}^\varphi$, all elements within $B_{\min\{\epsilon', \epsilon''\}}(v_y)$ link to y . Since $\{u_m\}$ converges to $\text{prop}[L_\varphi^G](p)$, there exists some $N \in \mathbb{N}$ and $n \geq N$, such that $\|u_n - \varphi(p)\|_2 < \min\{\epsilon', \epsilon''\}$,

487 meaning that $\mathbb{E}_{\mathcal{Y} \sim P}[\ell_{0-1}(\psi^\varphi(u_m), Y)] \rightarrow \min_{y \in \mathcal{Y}} \mathbb{E}_{\mathcal{Y} \sim P}[\ell_{0-1}(y, Y)]$. Hence, for any $v_y \in \text{vert}(P)$,
 488 $(\text{prop}[L_\varphi^G], \psi^\varphi)$ is ℓ_{0-1} -calibrated property with respect to $\varphi^{-1}(B_{\min\{\epsilon', \epsilon''\}}(v_y) \cap P)$. Further-
 489 more, by the construction of $B_{\min\{\epsilon', \epsilon''\}}(v_y)$ for each $v_y \in \text{vert}(P)$, we have that L_φ^G is strictly
 490 for $\text{prop}[L_\varphi^G]$. Thus, by Theorem 1, $(L_\varphi^G, \psi^\varphi)$ is ℓ_{0-1} -calibrated for at least the distributions
 491 $\mathcal{P} = \cup_{v_y \in \text{vert}(P)} \varphi^{-1}(B_{\min\{\epsilon', \epsilon''\}}(v_y) \cap P)$ as well as $\varphi(\mathcal{P}) \subseteq R_{\mathcal{Y}}$. Furthermore, since $B_{\min\{\epsilon', \epsilon''\}}$
 492 for each $v_y \in \text{vert}(P)$ is non-empty, we have that $\mathcal{P} \neq \emptyset$. \square

493 B.3 Omitted Proofs from § 4

494 **Corollary 14.** *Let φ be an embedding from 2^d outcomes into the vertices of P^\square in d -dimensions and*
 495 *define an induced loss L_φ^G . Fix $\alpha \in [0, .5]$ and define Θ_α . $(L_\varphi^G, \psi_\alpha^{P^\square})$ is ℓ_{0-1} -calibrated for Θ_α .*

496 *Proof.* W.l.o.g, say the outcome $y_1 \in \mathcal{Y}$ is embedded into $\mathbb{1}_{[d]} \in \text{vert}(P^\square)$. Say $\alpha = .5$. Observe
 497 that

$$\Psi_\alpha^{y_1} = \left\{ \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 1-\alpha \\ \alpha \\ \vdots \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 1-\alpha \\ 0 \\ \alpha \\ \vdots \\ 0 \end{pmatrix}, \dots, \begin{pmatrix} 1-\alpha \\ 0 \\ \vdots \\ \alpha \\ 0 \end{pmatrix}, \begin{pmatrix} 1-\alpha \\ 0 \\ \vdots \\ 0 \\ \alpha \end{pmatrix} \right\}$$

498 and that $1 \geq (1-\alpha) \pm \alpha \geq 0$ for any $\alpha \in (0, .5)$. Hence, for any $\alpha \in (0, .5)$ it holds that
 499 $P_{0.5}^{y_1} = \text{conv}(\{0, 1\}^d)$ and furthermore $P_\alpha^{y_1} \subset P_{0.5}^{y_1} \subset \mathbb{R}_{>0}^d$. By symmetry of P^\square and the linearity
 500 of φ , for any $\alpha \in (0, .5)$ and $y \in \mathcal{Y}$, we have that P_α^y is a strict subset of the orthant that contains v_y .
 501 Hence, for all $y, \hat{y} \in \mathcal{Y}$ such that $y \neq \hat{y}$, it holds that $P_\alpha^y \cap P_\alpha^{\hat{y}} = \emptyset$. Thus by Theorem 6, $(L_\varphi^G, \psi_\alpha^{P^\square})$
 502 is ℓ_{0-1} -calibrated for Θ_α where $\alpha \in (0, .5)$. \square

503 **Corollary 15.** *Let φ be an embedding from $d!$ outcomes into the vertices of P^w in d dimensions*
 504 *such that $w = (0, \frac{1}{\beta d}, \frac{2}{\beta d}, \dots, \frac{d-1}{\beta d}) \in \mathbb{R}^d$ where $\beta = \frac{d-1}{2}$. Fix $\alpha \in (0, \frac{1}{d})$. Then $(L_\varphi^G, \psi_\alpha^{P^w})$ is*
 505 *ℓ_{0-1} -calibrated over Θ_α .*

Proof. Let $\Delta_d := \text{conv}(\{\mathbb{1}_i \in \mathbb{R}^d \mid i \in [d]\})$ and observe $P^w \subset \Delta_d$ since for all π , $\|\pi \cdot w\|_1 =$
 $\|w\|_1 = 1$. Observe that P^w can be symmetrically partitioned into $d!$ regions with disjoint interiors,
 one for each permutation $\pi \in \mathcal{S}_d$ via $\Delta_d^\pi := \{u \in \Delta_d \mid u_1 \leq \dots \leq u_d\}$. Fix $\pi \in \mathcal{S}_d$ and
 w.l.o.g assume π is associated with the constraints $\Delta_w^\pi := \{u \in \Delta_w \mid u_1 \leq \dots \leq u_d\}$ implying that
 $\pi(w) = (\frac{0}{\beta d}, \frac{1}{\beta d}, \dots, \frac{d-1}{\beta d})$. Let $\alpha = \frac{1}{d}$ and define Θ_α . With respect to Θ_α , let $y := \varphi^{-1}(\pi(w)) \in \mathcal{Y}$
 and $\hat{y} := \varphi^{-1}(\hat{\pi}(w)) \in \mathcal{Y}$ such that $\hat{\pi} \in \mathcal{S}_d$. Thus the set $\Psi_\alpha^y := \{(1 - \frac{1}{d})\delta_y + (\frac{1}{d})\delta_{\hat{y}} \mid y, \hat{y} \in \mathcal{Y}\}$ is
 mapped via φ to the following points

$$\varphi(\Psi_\alpha^y) = \{(1 - \frac{1}{d})(\pi(w)) + (\frac{1}{d})(\hat{\pi}(w)) \mid \hat{\pi} \in \mathcal{S}_d\}$$

506 within the permutahedron.

507 We shall show that $P_\alpha^y \subseteq \Delta_d^\pi$. If this were not true, there would exists an element of $w^{\pi, \hat{\pi}} \in \varphi(\Psi_\alpha^y)$
 508 such such that for some pair of adjacent indices, say $i, i+1 \in [d-1]$, $w_i^{\pi, \hat{\pi}} > w_{i+1}^{\pi, \hat{\pi}}$. For sake of
 509 contradiction, fix $i \in [d-1]$ and assume there exists a $\hat{\pi} \in \mathcal{S}_d$ such that $w_i^{\pi, \hat{\pi}} > w_{i+1}^{\pi, \hat{\pi}}$. Observe that

any element of $\hat{\pi}(w)$ can be expressed by $\frac{j}{\beta d}$ using some $j \in \{0, 1, \dots, d-1\}$. Thus,

$$\begin{aligned}
w_i^{\pi, \hat{\pi}} &> w_{i+1}^{\pi, \hat{\pi}} \\
\Leftrightarrow (1 - \frac{1}{d})(\frac{i-1}{\beta d}) + (\frac{1}{d})(\hat{\pi}(w))_j &> (1 - \frac{1}{d})(\frac{i}{\beta d}) + (\frac{1}{d})(\hat{\pi}(w))_{\hat{j}} \\
\Rightarrow (1 - \frac{1}{d})(\frac{i-1}{\beta d}) + (\frac{1}{d})(\frac{j}{\beta d}) &> (1 - \frac{1}{d})(\frac{i}{\beta d}) + (\frac{1}{d})(\frac{\hat{j}}{\beta d}) && \text{Multiply by } \beta d \\
\Rightarrow (i-1)(1 - \frac{1}{d}) + j(\frac{1}{d}) &> i(1 - \frac{1}{d}) + \hat{j}(\frac{1}{d}) \\
\Rightarrow 1 - d > \hat{j} - j
\end{aligned}$$

for some $j, \hat{j} \in \{0, 1, \dots, d-1\}$ where $j \neq \hat{j}$.

Case 1: ($j < \hat{j}$): The smallest value possible for $\hat{j} - j$ is $0 - (d-1)$ however, $1 - d \not> 1 - d$.

Case 2: ($j > \hat{j}$): The smallest value possible for $\hat{j} - j$ is 1 however, $1 - d \not> 1$.

Hence, $P_\alpha^y \subseteq \Delta_d^\pi$ and specifically, there can exist an extreme point of P_α^y that lies on the boundary of Δ_d^π as shown in **Case 1**. However, if $\alpha \in (0, \frac{1}{d})$, every extreme point of P_α^y moves closer to $\pi(w)$ (besides the extreme point itself already on $\pi(w)$) and therefore P_α^y lies strictly within Δ_d^π . By symmetry of P^w and the linearity of φ , this would imply that for all $y', y'' \in \mathcal{Y}$ such that $y' \neq y''$ it holds that $P_\alpha^{y'} \cap P_\alpha^{y''} = \emptyset$. Thus by Corollary 6, $(L_\varphi^G, \psi_\alpha^{P^w})$ is ℓ_{0-1} -calibrated for Θ_α where $\alpha \in (0, \frac{1}{d})$. \square

B.4 Omitted Proofs from § 5

Lemma 16. Say we are given a cross-polytope embedding $\varphi : \Delta_{2d} \rightarrow P^\oplus$ and induced loss L_φ^G . Let (v_{a_i}, v_{b_i}) , be the i^{th} diagonal pair (i.e. $\varphi(\delta_{a_i}) = v_{a_i}$). Define the property $\Gamma^\varphi : \Delta_{2d} \rightarrow \mathcal{B}$ element-wise by

$$\Gamma^\varphi(p)_i := \begin{cases} (<, a_i, b_i) & \text{if } p_{a_i} < p_{b_i} \\ (>, a_i, b_i) & \text{if } p_{a_i} > p_{b_i} \\ (=, a_i, b_i) & \text{if } p_{a_i} = p_{b_i}. \end{cases}$$

Furthermore define the link $\psi^{P^\oplus} : \mathbb{R}^d \rightarrow \mathcal{B}$ with respect to each diagonal pair as

$$\psi(u; v_{a_i}, v_{b_i})_i^{P^\oplus} := \begin{cases} (<, a_i, b_i) & \text{if } \|u - v_{a_i}\|_2 > \|u - v_{b_i}\|_2 \\ (>, a_i, b_i) & \text{if } \|u - v_{a_i}\|_2 < \|u - v_{b_i}\|_2 \\ (=, a_i, b_i) & \text{o.w.} \end{cases}$$

Then $(L_\varphi^G, \psi^{P^\oplus})$ elicits Γ^φ .

Proof. W.l.o.g, fix a diagonal pair (v_a, v_b) and let $v_a := \mathbb{1}_1$ and $v_b := -\mathbb{1}_1$. Define the embedding φ accordingly. We will show that the following is true for all distributions mapped via φ to $u \in P^\oplus$.

$$\begin{aligned}
\|u - v_a\|_2 > \|u - v_b\|_2 &\iff p_a < p_b \\
\text{OR } \|u - v_a\|_2 < \|u - v_b\|_2 &\iff p_a > p_b \\
\text{OR } \|u - v_a\|_2 = \|u - v_b\|_2 &\iff p_a = p_b.
\end{aligned}$$

First, fix $p \in \Delta_{2d}$. Recall, by Proposition 2, the minimizing report for L_φ^G in expectation is $u = \varphi(p) \in P \subset \mathbb{R}^d$. We will prove the forward direction of the first and second lines. Then the reverse directions follow from the contrapositives.

532 **Case 1, \implies :** Assume for contradiction that $p_a < p_b$ and $\|\varphi(p) - v_a\|_2 < \|\varphi(p) - v_b\|_2$. Then

$$\begin{aligned} \langle \varphi(p) - \mathbb{1}_1, \varphi(p) - \mathbb{1}_1 \rangle &< \langle \varphi(p) + \mathbb{1}_1, \varphi(p) + \mathbb{1}_1 \rangle \\ (u_1 - 1)^2 + \sum_{i=1} u_i^2 &< (u_1 + 1)^2 + \sum_{i=1} u_i^2 \\ &\implies -u_1 < u_1. \end{aligned}$$

533 By the definition of a d -cross polytope $P^\oplus := \text{conv}(\{\pi((\pm 1, 0, \dots, 0)) \mid \pi \in \mathcal{S}_d\})$ and the
 534 orthogonal relation between vertices, to express a $u \in P^\oplus$ as a convex combination of vertices, each
 535 diagonal pair of vertices coefficients solely influence the position along a single unit basis vector.
 536 Hence, due to the definition of φ , we have $u_1 = \mathbb{1}_1 \cdot p_a - \mathbb{1}_1 \cdot p_b < 0$ since we have assumed that
 537 $p_a < p_b$. Hence $-u_1 < u_1 < 0$, a contradiction.

538

539 **Case 2, \implies :** Assume $p_a > p_b$ and $\|\varphi(p) - v_a\|_2 < \|\varphi(p) - v_b\|_2$. By symmetry with case 1, all
 540 the inequalities are reversed, leading to the contradiction that $-u_1 > u_1 > 0$.

541

542 **Case 3:** ($p_a = p_b$): Follows from the if and only ifs of cases 1 and 2.

543 Hence $(L_\varphi^G, \psi_\varphi)$ elicits Γ^φ .

544

□

545 **Theorem 10.** Let $d \geq 2$. The mode is $(2d, d, m)$ -Polytope Elicitable for some $m \in [2d-1, d(2d-1)]$.

546 *Proof.* We will elicit the mode via the intermediate properties, Γ^{φ_j} , defined in Lemma 9. First we
 547 construct a set of embeddings so that we guarantee that all the φ_j 's allow comparison between any
 548 pair of outcome probabilities. For example, for each unique pair $(a, b)_j \in \binom{\mathcal{Y}}{2}$ define an embedding:
 549 $\varphi_j(\delta_a) = \mathbb{1}_1$ and $\varphi_j(\delta_b) = -\mathbb{1}_1$, and embed every other remaining report $r \in \mathcal{Y} \setminus \{a, b\}$ arbitrarily.
 550 Since $(L_\varphi^G, \psi^{P^\oplus})$ elicits Γ^φ , minimizing each $L_{\varphi_j}^G$ with a separate model yields us comparisons
 551 via the link ψ^{P^\oplus} . To find the set $r \in \mathcal{Y}$ such that p_r is maximum, we use a sorting algorithm
 552 that uses pairwise comparisons, such as bubble sort. Hence with Υ as Algorithm 1, we have that
 553 $\Upsilon(\{L_{\varphi_j}^G, \psi^{P^\oplus}\}) = \text{mode}(p)$.

554 Assuming there exist φ_j 's such that there is no redundancy in comparison pairs between each Γ^{φ_j} , we
 555 would need only $\frac{d(2d-1)}{d} = 2d-1$ problem instances. Hence, we establish our lower bound on the
 556 needed number of problem instances. □

557 C Hamming Loss Hallucination Example

558 Hamming loss $\ell : \mathcal{Y} \times \mathcal{Y} \rightarrow \mathbb{R}_+$ is defined by $\ell(y, \hat{y}) = \sum_{i=1}^d \mathbb{1}_{y_i \neq \hat{y}_i}$ where $\mathcal{Y} = \{-1, 1\}^d$.
 559 Suppose $d = 3$ and we have the following indexing over outcomes

$$\begin{aligned} \mathcal{Y} := \{y_1 \equiv (1, 1, 1), y_2 \equiv (1, 1, -1), y_3 \equiv (1, -1, 1), y_4 \equiv (-1, 1, 1), \\ y_5 \equiv (-1, -1, 1), y_6 \equiv (1, -1, -1), y_7 \equiv (-1, 1, -1), y_8 \equiv (-1, -1, -1)\}. \end{aligned}$$

Let us define the following distribution

$$p_\epsilon = (0, \frac{1}{3} - \epsilon, \frac{1}{3} - \epsilon, \frac{1}{3} - \epsilon, 0, 0, 0, 3\epsilon) \in \Delta_{\mathcal{Y}}$$

560 such that $\epsilon > 0$.

- 561 • $\mathbb{E}_{Y \sim p_\epsilon}[\ell(y_1, Y)] = 1 + 6\epsilon$
- 562 • $\mathbb{E}_{Y \sim p_\epsilon}[\ell(y_2, Y)] = \mathbb{E}_{Y \sim p_\epsilon}[\ell(y_3, Y)] = \mathbb{E}_{Y \sim p_\epsilon}[\ell(y_4, Y)] = \frac{4}{3} + 2\epsilon$
- 563 • $\mathbb{E}_{Y \sim p_\epsilon}[\ell(y_5, Y)] = \mathbb{E}_{Y \sim p_\epsilon}[\ell(y_6, Y)] = \mathbb{E}_{Y \sim p_\epsilon}[\ell(y_7, Y)] = \frac{7}{3} - 4\epsilon$
- 564 • $\mathbb{E}_{Y \sim p_\epsilon}[\ell(y_8, Y)] = 2 - 6\epsilon$

565 For all $\epsilon \in [0, \frac{1}{12})$, the minimizing report in expectation is $y_1 = (1, 1, 1)$. However, $p_{\epsilon,1} = 0$ and
 566 thus, a hallucination would occur under a calibrated surrogate and link pair.

567 D Linking under Multiple Problem Instances

568 As stated in § 5, when using real data, given that these are asymptotic results, we may have conflicting
 569 logic for the provided individual reports. In this section, we provide an approach such that the
 570 algorithm still reports information in the aforementioned scenario and will reduce to Algorithm 1
 571 asymptotically. We build a binary relation table $M \in \{0, 1\}^{n \times n}$ with the provided reports. Based
 572 on M , we select a largest subset of $S \subseteq \mathcal{Y}$ such that when M is restricted to rows and columns
 573 corresponding to the elements of S , denoted by M_S , we have that M_S is reflexive, antisymmetric,
 574 transitive, and strongly connected implying M_S has a total-order relation defined over its elements.
 575 Having a total-order relation infers the mode can be found via comparisons. The algorithm returns
 576 (R, S) , where R is the mode set with respect to the elements of S .

Algorithm 2 Elicit mode via comparisons and the d-Cross Polytopes over well-defined partial orderings

Require: $M = \{(L_{\varphi_j}^G, \psi_j^{P^\oplus})\}_{j=1}^m$

Learn a model $h_j : \mathcal{X} \rightarrow \mathbb{R}^d$ for each instance $(L_{\varphi_j}^G, \psi_j^{P^\oplus}) \in M$

For some fixed $x \in \mathcal{X}$, collect all $B_j \leftarrow \psi_j^{P^\oplus}(h_j(x))$ where $B_j \in \mathcal{B}_j$

Build $M \in \{0, 1\}^{n \times n}$ binary relation table with provided $\{B_j\}_{j=1}^m$ as such

- Label rows top to bottom by y_1, \dots, y_n and columns left to right by y_1, \dots, y_n .
- For all $(\cdot, p_{y_i}, p_{y_k}) \in B_j$, if $p_{y_i} \leq p_{y_k}$ set $M[i, k] = 1$ and 0 otherwise.

Select largest subset $S \subseteq \mathcal{Y}$ such that M_S is reflexive, antisymmetric, transitive, and strongly connected.

Report $(R, S) \leftarrow \text{FindMaxElements-of-}S(M; S)$

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