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# 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, Finocchiaro 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  $(L, \psi)$  with respect to the target  $\ell$ .

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,  $\ell$ , 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  $\Gamma$  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  $\Gamma$  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  $\Gamma$ .

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  $(L, \psi)$  are calibrated with respect to a target loss  $\ell$ , if the optimal  
 89 expected surrogate loss when making the *incorrect classification* (by  $\psi$ ) is strictly greater than the  
 90 optimal surrogate loss.

**Definition 2** ( $\ell$ -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  $(L, \psi)$  is  $\ell$ -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** ( $\ell$ -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  
 link  $\psi : \mathbb{R}^d \rightarrow \mathcal{Y}$ . We will say  $(\Gamma, \psi)$  is  $\ell$ -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  $\Gamma$  is elicitable and  $(\Gamma, \psi)$  is an  $\ell$ -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  $\Gamma$  i.e.  $\text{prop}[L] = \Gamma$   
 100 and  $|\Gamma(p)| = 1$  for all  $p \in \mathcal{P}$ . Then,  $(L, \psi)$  is  $\ell$ -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 [Seger, 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  $L_{\varphi}^G$  defined by the embedding, any  $G$ -Bregman  
 111 Divergence, and a link function  $\psi^{\varphi}$ .

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  $\ell$ -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.

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

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

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

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

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

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

143 **Proposition 2.** *For a given induced loss  $L_{\varphi}^G$ , the unique report which minimizes the expected loss  
 144 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  
 145 minimizer of  $\mathbb{E}_{Y \sim \hat{p}}[L_{\varphi}^G(u, Y)]$  for some  $\hat{p} \in \Delta_{\mathcal{Y}}$ .*

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

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

### 153 3.2 Hallucination Regions

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

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

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

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

168 *Sketch.* Fix  $y \in \mathcal{Y}$ . We abuse notation and write  $\text{vert}(P_{-y}) := \text{vert}(P) \setminus \{v_y\}$ . Observe  
 169  $\text{conv}(\text{vert}(P_{-y})) \cap \psi_y^{\varphi} \subseteq \mathcal{H}$  since any point in this set can be expressed as a convex combina-  
 170 tion without needing vertex  $v_y$  implying there is a distribution embedded by  $\varphi$  to said point which  
 171 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  
 172  $u \notin \text{conv}(\text{vert}(P) \setminus v_y) \cap \psi_y^{\varphi}$  such that there exists some  $p \in \Delta_{\mathcal{Y}}$  where  $\varphi(p) = u$ ,  $p_y = 0$ ,  
 173 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

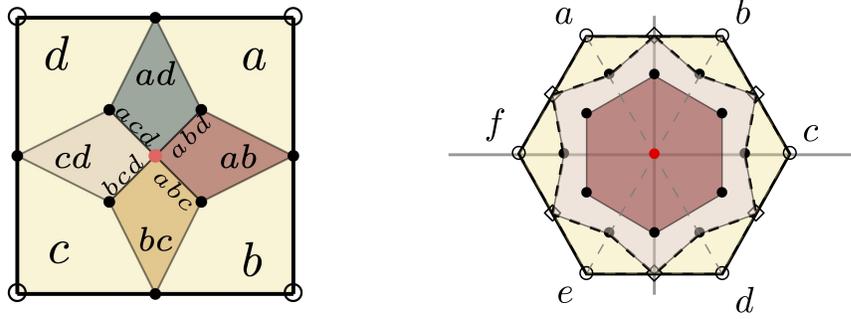


Figure 1: (Left) Mode level sets of  $\Delta_{\mathcal{Y}}$  where  $\mathcal{Y} = \{a, b, c, d\}$  embedded into a two dimensional unit cube. The center red point denotes the origin  $(0, 0)$  which is the hallucination region. (Right) An embedding of  $\Delta_{\mathcal{Y}}$  where  $\mathcal{Y} = \{a, b, c, d, e, f\}$  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  $\mathcal{H} \subseteq \bigcup_{y \in \mathcal{Y}} \text{conv}(\text{vert}(P_{-y})) \cap \psi_y^\varphi$ . 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  $\psi$  would be calibrated over the union if it mapped  $u$  to the mentioned  
 196 singleton. Given  $(L, \psi)$ ,  $\varphi$ , and a target loss  $\ell$ , 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  $(L, \psi)$ ,  $\varphi$ , and a target loss  $\ell$ . We*  
 199 *say  $R \subseteq P$  is a strict calibrated region via  $(L, \psi)$  with respect to  $\ell$  if  $(L, \psi)$  is  $\ell$ -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  $R_{\mathcal{Y}} := \bigcup_{y \in \mathcal{Y}} R_y$ .*

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.

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

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

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

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

## 218 4 Restoring Inconsistent Surrogates via Low-Noise Assumptions

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

### 223 4.1 Calibration via Low Noise Assumptions

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

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

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

240 We shall show that for some sufficiently small  $\alpha \in [0, .5)$ ,  $P_{\alpha}^y$  is a scaled down version of  $P$   
 241 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  
 242 all  $y \in \mathcal{Y}$ . Observe that by linearity of  $\varphi$ ,

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

243 and hence,  $P_{\alpha}^y$  is a scaled version of  $P$  positioned at  $v_y$ . Hence for some sufficiently small  $\alpha$ ,  
 244  $(1 - \alpha)v_y + \alpha v_{\hat{y}} \in B_{\epsilon''}(v_y)$  for all  $\hat{y}$  and hence  $P_{\alpha}^y \subseteq B_{\epsilon''}(v_y) \subseteq R_y$ . With said sufficiently small  
 245  $\alpha$ , define  $\psi_{\alpha}^P$  and the respective sets  $\text{conv}(\Psi_{\alpha}^y)$  for each  $y \in \mathcal{Y}$ . Using the previous  $\alpha$ , define the set  
 246  $\Theta_{\alpha}$  as well.

247  
 248 **Part 2 (Showing Calibration):** Recall, by Proposition 2, for any  $p \in \Delta_{\mathcal{Y}}$ ,  $u = \varphi(p)$  minimizes the  
 249 expected surrogate loss  $\mathbb{E}_{\mathcal{Y} \sim p}[L_{\varphi}^G(u, Y)]$ . For any fixed  $y \in \mathcal{Y}$ , observe that  $\text{conv}(\{(1 - \alpha)\delta_y + \alpha\delta_{\hat{y}} \mid$

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  $\Theta_{\alpha}$ . By our choice of  $\alpha$  and the construction of  $\psi_{\alpha}^P$ ,  
 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  $P_{\alpha}^y$  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  $\ell_{0-1}$ -calibrated  
 257 for  $\Theta_{\alpha}$ .  $\square$

## 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  $\Theta_{\alpha}$  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  $\Theta_{\alpha}$  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,  $\varphi$  be any polytope embedding, and  $L_{\varphi}^G$  be the loss  
 265 induced by  $(D_G, \varphi)$ . Fix  $\alpha \in [0, .5)$  and with it define  $\Theta_{\alpha}$ . 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  $\ell_{0-1}$ -calibrated for  $\Theta_{\alpha}$  where  $\psi_{\alpha}^{\varphi}(u) = \arg \min_{y \in \mathcal{Y}} \|u - P_{\alpha}^y\|_2$ .*

267 *Proof.* Pick an  $\alpha$  such that for all  $y, \hat{y} \in \mathcal{Y}$ ,  $P_{\alpha}^y \cap P_{\alpha}^{\hat{y}} = \emptyset$ . Define  $\Theta_{\alpha}$  and  $\psi_{\alpha}^P$  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  $P_{\alpha}^y$  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  $\psi_{\alpha}^{\varphi}$ , 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  $\ell_{0-1}$ -calibrated property with respect to  $\Theta_{\alpha}$ . Finally, since  $L_{\varphi}^G$  is strictly proper for  $\text{prop}[L_{\varphi}^G]$ , by  
 275 Theorem 1, we have that  $(L_{\varphi}^G, \psi_{\alpha}^{\varphi})$  is  $\ell_{0-1}$ -calibrated for  $\Theta_{\alpha}$ .  $\square$

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  $\Theta_{\alpha}$  when  $\alpha < .5$ .

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

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  $\alpha$  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  $\varphi$  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  $\ell_{0-1}$ -calibrated over  $\Theta_{\alpha}$ .*

295 The calibration region in Corollary 8 show that consistency in  $\Theta_{\alpha}$  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.

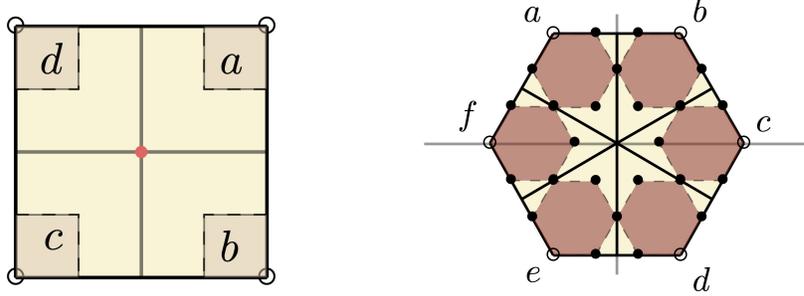


Figure 2: (Left) Corners represent the strict calibration regions for  $\Theta_\alpha$  where  $\mathcal{Y} = \{a, b, c, d\}$  is embedded into a two dimensional unit cube such that  $\alpha = .25$ . (Right) Auburn regions show that strict calibration holds for  $\Theta_\alpha$  where  $\mathcal{Y} =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

## 298 5 Elicitation in Low Dimensions with Multiple Problem Instances

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

306 **Definition 10.** Extending Definition 1, we say a loss and link pair  $(L, \psi)$ , where  $L : \mathbb{R}^d \times \mathcal{Y} \rightarrow \mathbb{R}$   
 307 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  $\forall p \in \mathcal{P}$ ,  $\Gamma(p) =$   
 308  $\psi(\arg \min_{u \in \mathbb{R}^d} \mathbb{E}_{Y \sim p} [L(u, Y)])$ .

309 **Definition 11** ( $(n, d, m)$ -Polytope Elicitable). Suppose we are given a property  $\gamma : \mathcal{P} \rightrightarrows \mathcal{Y}$  such that  
 310  $\mathcal{P} \subseteq \Delta_{\mathcal{Y}}$  and  $|\mathcal{Y}| = n$  finite outcomes. Say we have  $m$  unique polytope embeddings  $\{\varphi_j : \Delta_{\mathcal{Y}} \rightarrow$   
 311  $\mathbb{R}^d\}_{j=1}^m$  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  
 312 wrt.  $\varphi_j$ , 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  
 313 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  $p \in \Delta_{\mathcal{Y}}$   
 314 it holds that  $\Upsilon(\Gamma_1(p), \dots, \Gamma_m(p)) = \gamma(p)$ , we say that  $\gamma$  is  $(n, d, m)$ -Polytope Elicitable over  $\mathcal{P}$ .

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

317 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  
 318  $(\pm 1, 0, \dots, 0) \in \mathbb{R}^d$ . Observe that a  $d$ -cross polytope has  $2d$  vertices. For any vertex of a  $d$ -cross  
 319 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  $L_\varphi^G$ .  
 Let  $(v_{a_i}, v_{b_i})$ , be the  $i^{\text{th}}$  diagonal pair (i.e.  $\varphi(\delta_{a_i}) = v_{a_i}$ ). Define the property  $\Gamma^\varphi : \Delta_{2d} \rightarrow \mathcal{B}$   
 element-wise by

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

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

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

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

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

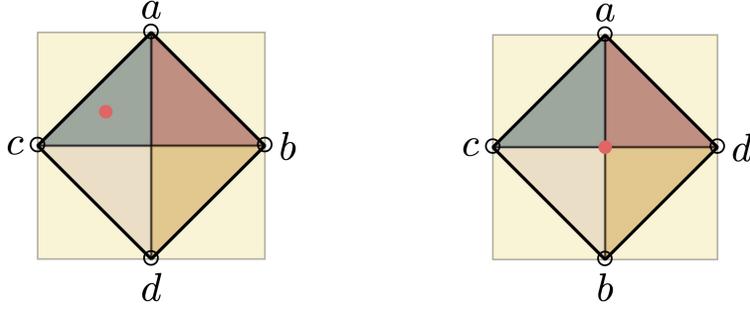


Figure 3: Four outcomes embedded in  $\mathbb{R}^2$  in two different ways, with the minimizing reports  $\bullet$  for a distribution  $p$ ." (Left) Configuration  $\varphi_1$  with  $\bullet$  at  $(-.5, .3)$  implying  $p_a > p_d$  and  $p_b > p_c$ . (Right) Configuration  $\varphi_2$  with  $\bullet$  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

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**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.

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<sup>†</sup>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  $L_\varphi^G$ , 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  $\hat{p} \in \Delta_{\mathcal{Y}}$ .

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  $\varphi$ , for some distribution, say  $\hat{p} \in \Delta_{\mathcal{Y}}$ , 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  $\ell_{0-1}$  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  $p \in \Delta_{\mathcal{Y}}$  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  $L_\varphi^G$  with respect to  $p$ .  
 426 Given the intersection with  $\psi_y^\varphi$  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  $p \in \Delta_{\mathcal{Y}}$  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  $\psi^\varphi$  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

440 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  
 441 Proposition 2 and by the definition of Hallucination (Def. 8), we have that  $\mathcal{H} \neq \emptyset$ .  $\square$

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

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

449 *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  
 450 a convex combination which has no weight on the coefficient for  $v_y$ . Hence, there exists a distribution  
 451 embedded into  $u$  where  $y$  would not be the mode, thus violating the initial claim that  $u \in R_y$ .  $\square$

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

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

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

461 *Proof.* By the construction of  $\varphi$ , we know that  $\dim(P) \geq 2$ . Fix  $y \in \mathcal{Y}$ . By Lemma 3, we know  
 462 that any edge connected from  $v_y$  and  $\hat{v} \in \text{ne}(v_y)$ , the distributions embedded into the half of the line  
 463 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,  
 464 the convex hull of the half line segments is part of  $\varphi(\gamma_y^{\text{mode}})$ . Since each vertex has at least  $\dim(P)$   
 465 neighbors, it holds that  $\dim(\varphi(\gamma_y^{\text{mode}})) = \dim(P)$ .  $\square$

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

469 *Proof.* Recall that  $\gamma^{\text{mode}}(p) := \text{prop}[\ell_{0-1}](p) = \text{mode}(p)$ . Fix  $y \in \mathcal{Y}$ . For contradiction, assume  
 470 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,  
 471 it holds that  $\text{conv}(\{v_y\} \cup m_{v_y, \alpha}) \subseteq \varphi(\gamma_y^{\text{mode}})$  where  $m_{v_y, \alpha} := \{(1 - \alpha)v_y + \alpha \bar{v} \mid \bar{v} \in \text{ne}(v_y)\}$   
 472 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  
 473 distribution embedded onto it where  $y$  is the only valid mode thus, we know that  $\varphi(\text{mode}_{\hat{y}}) \cap$   
 474  $\cup_{m \in m_{v_y, \alpha}} \text{conv}(\{v_y\} \cup \{m\}) = \emptyset$ . Since  $\varphi(\gamma_{\hat{y}}^{\text{mode}}) \subset P$  is closed and convex, there must exist  
 475 some non-negative min distance between  $\varphi(\gamma_{\hat{y}}^{\text{mode}})$  and  $v_y$  which we shall denote by  $d_v$ . For any  
 476  $\epsilon \in (0, d_v)$ , we can define  $B_\epsilon(v_y)$  such that  $B_\epsilon(v_y) \cap \varphi(\gamma_{\hat{y}}^{\text{mode}}) = \emptyset$ , forming a contradiction.

477 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  
 478 the definition of  $\psi^\varphi$ , there exists a  $\epsilon'' > 0$  such that for all  $u \in B_{\epsilon''}(v_y)$  it holds that  $\psi(u) = y$  and  
 479  $B_{\epsilon''}(v_y) \subset \psi_\varphi^\varphi$ . For any  $y \in \mathcal{Y}$ , we know that  $B_{\min\{\epsilon', \epsilon''\}}(v_y) \cap P \subseteq R_y$  by the construction of  
 480 our epsilon ball. We claim  $\varphi^{-1}(B_{\min\{\epsilon', \epsilon''\}}(v_y) \cap P)$  is a set of distributions for which calibration  
 481 holds.

482 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  $\{u_m\}$   
 483 converges to  $\text{prop}[L_\varphi^G](p) = \varphi(p)$  (equality by Proposition 2). By construction of  $B_{\min\{\epsilon', \epsilon''\}}(v_y) \cap P$ ,  
 484  $\psi^\varphi(\varphi(p)) = y \in \text{mode}(p)$  and hence, a minimizing report for  $\ell_{0-1}(y; p)$ . Furthermore, since  
 485  $B_{\min\{\epsilon', \epsilon''\}}(v_y) \subset \psi_\varphi^{\varphi^{-1}(v_y)}$ , all elements within  $B_{\min\{\epsilon', \epsilon''\}}(v_y)$  link to  $y$ . Since  $\{u_m\}$  converges  
 486 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  $\ell_{0-1}$ -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  $L_\varphi^G$  is strictly  
 490 for  $\text{prop}[L_\varphi^G]$ . Thus, by Theorem 1,  $(L_\varphi^G, \psi^\varphi)$  is  $\ell_{0-1}$ -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  $\varphi$  be an embedding from  $2^d$  outcomes into the vertices of  $P^\square$  in  $d$ -dimensions and*  
 495 *define an induced loss  $L_\varphi^G$ . Fix  $\alpha \in [0, .5)$  and define  $\Theta_\alpha$ .  $(L_\varphi^G, \psi_\alpha^{P^\square})$  is  $\ell_{0-1}$ -calibrated for  $\Theta_\alpha$ .*

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  $\varphi$ , for any  $\alpha \in (0, .5)$  and  $y \in \mathcal{Y}$ , we have that  $P_\alpha^y$  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  $\ell_{0-1}$ -calibrated for  $\Theta_\alpha$  where  $\alpha \in (0, .5)$ .  $\square$

503 **Corollary 15.** *Let  $\varphi$  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  *$\ell_{0-1}$ -calibrated over  $\Theta_\alpha$ .*

*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  $\pi$ ,  $\|\pi \cdot w\|_1 =$   
 $\|w\|_1 = 1$ . 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  $\pi$  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  $\Theta_\alpha$ . With respect to  $\Theta_\alpha$ , 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  $\varphi$  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 exist 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

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

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

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

512

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

514

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

516

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

#### 523 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  $L_\varphi^G$ .  
Let  $(v_{a_i}, v_{b_i})$ , be the  $i^{\text{th}}$  diagonal pair (i.e.  $\varphi(\delta_{a_i}) = v_{a_i}$ ). Define the property  $\Gamma^\varphi : \Delta_{2d} \rightarrow \mathcal{B}$   
element-wise by

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

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

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

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

526 *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  $\varphi$   
527 accordingly. We will show that the following is true for all distributions mapped via  $\varphi$  to  $u \in P^\oplus$ .

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

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

531

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

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

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  $\varphi$ , 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  $\Gamma^\varphi$ .

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,  $\Gamma^{\varphi_j}$ , defined in Lemma 9. First we  
 547 construct a set of embeddings so that we guarantee that all the  $\varphi_j$ '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  $\Gamma^\varphi$ , minimizing each  $L_{\varphi_j}^G$  with a separate model yields us comparisons  
 551 via the link  $\psi^{P^\oplus}$ . 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  $\Upsilon$  as Algorithm 1, we have that  
 553  $\Upsilon(\{L_{\varphi_j}^G, \psi^{P^\oplus}\}) = \text{mode}(p)$ .

554 Assuming there exist  $\varphi_j$ s such that there is no redundancy in comparison pairs between each  $\Gamma^{\varphi_j}$ , 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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