

Learning weakly convex sets in metric spaces

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Abstract

One of the central problems studied in the theory of machine learning is the question of whether, for a given class of hypotheses, it is possible to efficiently find a consistent hypothesis, i.e., which has zero training error. While problems involving *convex* hypotheses have been extensively studied, the question of whether efficient learning is possible for *non-convex* hypotheses composed of possibly several disconnected regions is still less understood. Although it has been shown quite a while ago that efficient learning of weakly convex hypotheses, a parameterized relaxation of convex hypotheses, is possible for the special case of Boolean functions, the question of whether this idea can be developed into a *generic paradigm* has not been studied yet. In this paper, we provide a positive answer and show that the consistent hypothesis finding problem can indeed be solved in polynomial time for a broad class of weakly convex hypotheses over metric spaces. To this end, we propose a general domain-independent algorithm for finding consistent weakly convex hypotheses and prove sufficient conditions for its efficiency that characterize the corresponding hypothesis classes. To illustrate our general algorithm and its properties, we discuss several non-trivial learning examples to demonstrate how it can be used to efficiently solve the corresponding consistent hypothesis finding problem. Without the weak convexity constraint, these problems are known to be computationally intractable. We then proceed to show that the general idea of our algorithm can even be extended to the case of *extensional* weakly convex hypotheses, as it naturally arise, e.g., when performing vertex classification in graphs. We prove that using our extended algorithm, the problem can be solved in polynomial time provided the distances in the domain can be computed efficiently.

Keywords: concept learning • consistent hypothesis finding • intersection-closed concept classes • convexity • closure systems

1 Introduction

One of the central problems of concept learning is the *consistent hypothesis finding* (CHF) problem defined as follows: Given a set of positive and negative

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examples of an unknown target concept, find a consistent hypothesis, i.e., which has zero training error, from the underlying hypothesis class if such a hypothesis exists. This problem has been extensively studied for *convex* hypothesis classes defined by geodesic convexity over metric spaces (Menger, 1928). Examples include axis-aligned hyperrectangles (Blumer et al., 1989), shortest-path convexity in graphs (Seiffarth et al., 2023), or conjunctions (Valiant, 1984). The CHF algorithms typically utilize that convex hypothesis classes can be characterized by a *convex hull* closure operator. A major weakness of convex hypotheses is that they are composed of a *single* contiguous block, which severely limits the expressive power of convex hypothesis classes. This limitation motivates the question of whether efficient learning is possible for *non-convex* hypotheses, i.e., those consisting of possibly several disconnected, not necessarily convex regions.

Ekin et al. (2000) give an affirmative answer to this question for the *special* case of Boolean functions by showing that the CHF problem can be solved efficiently for the class of functions satisfying k -convexity, a relaxed notion of convexity defined as follows: An n -ary Boolean function f is k -convex for some $k \geq 0$ if all points on all shortest paths between two true points of f with Hamming distance at most k are also true points of f . The true points of such a *weakly convex* Boolean function form a set of subcubes of the n -dimensional Boolean hypercube that have a pairwise distance greater than k . Accordingly, a k -convex Boolean function can be represented by a disjunctive normal form (DNF). It is a well-known result that, under widely believed complexity assumptions, finding a consistent DNF with the smallest number of terms, i.e., subcubes of the n -dimensional Boolean hypercube, is NP-hard, if there is no constraint on the relationship between the subcubes (Pitt and Valiant, 1988). Somewhat surprisingly, to the best of our knowledge, the question of whether the idea of k -convexity can be developed into a generic paradigm for solving the CHF problem for convex hypothesis classes over *other* metric spaces has not been studied yet.

In this work, we close this gap and provide a positive answer by adapting the above idea in (Ekin et al., 2000). We show that the CHF problem can indeed be solved efficiently for a broad class of *weakly convex* hypotheses over metric spaces, where a subset A of a metric space is weakly convex if it is (topologically) closed and for all $x, y \in A$ and z in the domain, z belongs to A whenever x and y are *close* to each other with respect to a threshold θ and the three points satisfy the triangle inequality with equality. To this end, we first prove that weakly convex sets give rise to a *unique* decomposition into a set of “connected” blocks that have a pairwise distance greater than θ and that the weakly convex hulls of a set grow monotonically with θ , while their number of “contiguous” blocks decreases. We also show that weakly convex hypothesis classes are intersection closed. Using these results, we provide a general *domain-independent* algorithm for solving the CHF problem for weakly convex hypothesis classes and prove sufficient conditions for the efficiency of this algorithm. Our CHF algorithm assumes that the hypotheses are given *intensionally*, i.e., by some property. Its solution is *optimal* in the sense that it computes the consistent weakly convex hull of the positive examples that has the *smallest* number of blocks.

To illustrate our general algorithm and its properties, we consider the CHF problem for unions of Boolean hypercubes, axis-aligned hyperrectangles, and convex polygons. While, for example, finding a consistent hypothesis with the smallest number of axis-aligned hyperrectangles is NP-hard in general (Bereg

et al., 2012), for weakly convex unions of axis-aligned hyperrectangles we show in a fairly simple way how our algorithm can be used to efficiently solve the CHF problem. Using this result, we then prove that weakly convex unions of axis-aligned hyperrectangles are polynomially PAC-learnable.

We also show that the general idea behind our algorithm can even be extended to the case that weakly convex hypotheses are given *extensionally*, i.e., by enumerating their elements, as it naturally arises, for example, in vertex classification in graphs. For this setting we show that our extended algorithm computes the consistent weakly convex hull of the positive examples with the *smallest* number of blocks in *polynomial* time, if the distance matrix for the domain can be computed efficiently.

Outline The rest of the paper is organized as follows. We overview the related work in Section 2 and collect the necessary notions in Section 3. In Section 4, we define weakly convex sets and prove some of their basic properties. Sections 5 and 6 are devoted to the algorithm learning weakly convex hypotheses in the intensional problem setting and to its extended version for the extensional case, respectively. Finally, we conclude in Section 7 and mention some problems for future work.

Remark A short version of this paper appeared in (Stadtländer et al., 2021).

2 Related Work

The CHF problem and its variants have been intensively studied also in other fields of computer science. For example, a closely related problem considered in discrete algorithms is the *red-blue set covering problem* (Carr et al., 2000) defined as follows: Given disjoint finite sets R and B of red and blue points and the trace¹ $\mathcal{S}|_{R \cup B}$ of a set system \mathcal{S} , find a family $\mathcal{S}' \subseteq \mathcal{S}$ such that \mathcal{S}' covers all blue points and as few red points as possible. Thus, in contrast to the CHF problem, the goal is to *minimize* the number of red points covered by \mathcal{S}' (i.e., which are “misclassified”), and not $|\mathcal{S}'|$. This problem is NP-hard even for the cases that $R, B \subseteq \mathbb{R}^2$ and \mathcal{S} is the family of axis-aligned unit squares (Chan and Hu, 2015) or that of axis-aligned rectangles (Abidha and Ashok, 2024). As another example, we mention computational geometry, where the CHF problem is called the *class cover problem* and defined as follows: Given disjoint finite sets R and B of red and blue points and a set system $\mathcal{S} \subseteq 2^{R \cup B}$, find a family $\mathcal{S}' \subseteq \mathcal{S}$ of the *smallest* cardinality that covers B and is disjoint with R (i.e., no misclassification is allowed). Various special cases of this problem have been studied in this research field. For example, this problem is NP-complete if \mathcal{S} is the trace of a set of balls centered at the blue points (Cannon and Cowen, 2004) or that of all axis-aligned rectangles of the plane (Bereg et al., 2012) on $R \cup B$. We also mention the *red-blue line separation* problem defined as follows: Given disjoint finite sets $R, B \subseteq \mathbb{R}^2$ of red and blue points and a positive integer k , decide if there is a set of at most k lines that separate the red and blue points. This problem is NP-complete (Megiddo, 1988) and remains NP-complete even for the case that the lines are required to be axis-parallel (Călinescu et al., 2005). The separating lines in this case define rectangular areas and the task is to cover all points with monochromatic axis-aligned rectangles.

¹The trace $\mathcal{F}|_Y$ of a set system $\mathcal{F} \subseteq 2^X$ on a set Y is the set system $\{S \cap Y : S \in \mathcal{F}\}$.

Our paper deals with the CHF problem for *intersection-closed* hypothesis classes. There are several results for this special case in machine learning (see, e.g., Auer and Cesa-Bianchi, 1998; Blumer et al., 1989; Helmbold et al., 1990; Natarajan, 1987; Pitt and Valiant, 1988). Such hypothesis classes are *closure systems* and their elements can be characterized by a *closure operator* (see, e.g., Davey and Priestley, 2002). We consider closure systems over *arbitrary* metric spaces defined by *geodesic convexity* (Menger, 1928; van de Vel, 1993). Recently, there has been an increasing interest in learning this kind of closure systems over *graphs*. Examples include vertex classification (de Araújo et al., 2019; Seiffarth et al., 2023; Thiessen and Gärtner, 2021; Thiessen and Gärtner, 2022) and recovering clusterings (Bressan et al., 2021). Unless otherwise specified, by convex sets we always mean geodesically convex sets over metric spaces.

Convex sets form *single* regions that are “connected”, i.e., contain all elements that lie “between” any two of their elements. However, this property can make them too restrictive for learning scenarios, raising the question whether efficient learning is possible for *non-convex* hypotheses that consist of possibly several well-separated, not necessarily convex regions. A natural step in this direction could be to consider the *generalized* CHF problem: Find k hypotheses for a given (or equivalently, for the smallest) k such that their union is consistent with the examples. However, this problem can be computationally intractable; examples include the infeasibility of deciding the existence of a consistent k -term-DNF for any $k \geq 2$ (Pitt and Valiant, 1988).

In the above approach, there is no restriction on convex sets. In contrast, our general purpose algorithm requires a minimum distance between the regions to guarantee efficiency. It is inspired by the definition of *k-convex* Boolean functions (Ekin et al., 2000), where the convexity condition must only hold for such points of the Hamming space that have a distance at most a threshold k . Ekin et al. (2000) show that the CHF problem can be solved *efficiently* for k -convex Boolean functions, which are strict extensions of single conjunctions. The same relaxation of convexity to k -convexity or to very similar notions have also been studied for various types of *discrete* metric spaces and for *fixed* values of k .² Examples include weakly modular graphs (Chepoi, 1989), Δ -matroids and basis graphs of matroids (Chepoi, 2007), ample classes (Chalopin et al., 2022), and hypercellular graphs (Chepoi et al., 2020). Similar to our work, these papers are all concerned with some “local to global convexity” results. However, they do *not* discuss their algorithmic and learnability aspects.

In the context of unsupervised learning, Bressan et al. (2021) introduce a distance-based notion of convexity for graphs, more precisely, for clusterings of the vertices of a graph. It differs, however, from our definition of weak convexity applied to graphs in at least two aspects: First, in a broad sense, they control the inter- and intra-cluster distances with *two* parameters instead of a single one. Second, their notion of “convex hull” is induced by a finite set of simple paths of bounded length that depends on the geodesic distance between their endpoints. In contrast, our notion of weak convexity is based on the set of all shortest paths of length bounded by a *static* threshold.

²Victor Chepoi, private communication, 2021.

3 Preliminaries

In this section, we collect the necessary notions and fix the notation. For any $n \in \mathbb{N}$ and $\tau \in \mathbb{R}$, $[n]$ and $\mathbb{R}_{\geq \tau}$ denote the sets $\{1, 2, \dots, n\}$ and $\{x \in \mathbb{R} : x \geq \tau\}$, respectively. The family of all finite subsets of a set X is denoted by $[X]^{<\infty}$. A *metric space* \mathcal{M} is a pair (X, D) , where X is a set and $D : X \times X \rightarrow \mathbb{R}_{\geq 0}$ is a metric on X . \mathcal{M} is complete if every Cauchy sequence in \mathcal{M} converges to an element of \mathcal{M} . It follows that finite metric spaces are complete. A subset $A \subseteq X$ is *closed* if it contains all of its limit points. For a subset A of a metric space \mathcal{M} , $\text{cl}(A)$ denotes the smallest closed subset of \mathcal{M} that contains A . The distance between two sets $A, B \subseteq X$ is defined by $D(A, B) = \inf\{D(a, b) : a \in A, b \in B\}$. The Manhattan and the Euclidean distances in \mathbb{R}^d are denoted by D_1 and D_2 , respectively.

A *closure system* over some ground set X is a pair (X, \mathcal{C}) with $\mathcal{C} \subseteq 2^X$ such that \mathcal{C} is closed under arbitrary intersection, where 2^X denotes the power set of X . We assume that $X \in \mathcal{C}$. One of the elementary properties of closure systems is that they can be characterized in terms of fixed points of closure operators (see, e.g., Davey and Priestley, 2002). More precisely, a function $\rho : 2^X \rightarrow 2^X$ is a *closure operator* if it satisfies the following properties for all $A, B \subseteq X$: (i) $A \subseteq \rho(A)$ (extensivity), (ii) $\rho(A) \subseteq \rho(B)$ if $A \subseteq B$ (monotonicity), and (iii) $\rho(\rho(A)) = \rho(A)$ (idempotency). If ρ is extensive and monotone, but not necessarily idempotent, then it is a *preclosure operator*. The fixed points of a closure operator ρ are called ρ -closed and the set system (X, \mathcal{C}_ρ) with $\mathcal{C}_\rho = \{A \subseteq X : \rho(A) = A\}$ is always a closure system. Conversely, for any closure system (X, \mathcal{C}) , the function $\rho : 2^X \rightarrow 2^X$ with $\rho(A) = \bigcap\{C \in \mathcal{C} : A \subseteq C\}$ for all $A \subseteq X$ is a closure operator satisfying $\mathcal{C} = \{\rho(A) : A \subseteq X\}$. One can easily check that the set operator cl defined above is a closure operator.

Our notion of *weak convexity* is inspired by that of *k-convexity* introduced by Ekin et al. (1999). More precisely, for the metric space $\mathcal{M}_H = (H_n, D_H)$, called the Hamming metric space, where $H_n = \{0, 1\}^n$ is the n -dimensional *Hamming* or *Boolean cube* and D_H is the L_1 or Hamming distance over H_n , a set $X \subseteq H_n$ is *k-convex* for some $k \geq 0$ integer if for all $x, y \in X$ with $D_H(x, y) \leq k$ and for all $z \in H_n$, $z \in X$ whenever $D_H(x, y) = D_H(x, z) + D_H(z, y)$.

An (*undirected*) *graph* is a pair $G = (V, E)$, where V is a finite set of vertices and $E \subseteq \{\{u, v\} \subseteq V\}$ is a set of edges; V , E , and an edge $\{x, y\} \in E$ will sometimes be denoted by $V(G)$, $E(G)$, and xy , respectively. A graph G' is a *subgraph* of G if $V(G') \subseteq V(G)$ and $E(G') \subseteq E(G)$. A *path* of length n for some $n \geq 0$ integer is a graph P with $V(P) = \{v_1, \dots, v_n\}$ and $E(P) = \{v_i v_{i+1} : i \in [n-1]\}$ if $n > 0$; $E(P) = \emptyset$ otherwise. The *length* of a path is the number of edges it contains. A graph is *connected* if all pairs of its vertices are connected by a path. If two vertices of a graph G are connected by a path, we define their *geodesic distance* by the length of a shortest path connecting them. Note that it is a metric on the set of vertices for connected graphs. A subset $X \subseteq V(G)$ for a graph G is *geodesically convex* (or simply, *convex*) if $V(P_{uv}) \subseteq X$ for all $u, v \in V(G)$ and for all shortest paths P_{uv} connecting u and v (see, e.g., Pelayo, 2013). For $\theta \in \mathbb{R}_{\geq 0}$ and a finite metric space (X, D) , the θ -*neighborhood graph* is the graph G with $V(G) = X$ and $E(G) = \{uv : u, v \in V(G) \text{ and } D(u, v) \leq \theta\}$.

For the standard definitions of *concepts*, *concept classes*, *VC-dimension*, and *polynomial PAC-learnability* from computational learning theory, the reader is referred to some standard text book (see, e.g., Kearns and Vazirani, 1994). Let

\mathcal{C} be a concept class over some domain X and $k \in \mathbb{N}$. The k -fold union of \mathcal{C} is defined by $\mathcal{C}_{\cup}^k = \{C_1 \cup \dots \cup C_k : C_i \in \mathcal{C} \text{ for all } i \in [k]\}$. Note that the definition does *not* require the C_i s to be pairwise distinct. The following problem is central to concept learning:

Problem 1 (The Consistent Hypothesis Finding (CHF) Problem). Given a concept class $\mathcal{C} \subseteq 2^X$ over some domain X and disjoint sets $E^+, E^- \subseteq X$ of positive and negative examples, return a concept $C \in \mathcal{C}$ that is consistent with E^+ and E^- , i.e., $E^+ \subseteq C$ and $E^- \cap C = \emptyset$ if such a concept exists; otherwise return the answer “No”.

In order to prove polynomial PAC-learnability, we will use the following basic results from computational learning theory (Blumer et al., 1989):

Theorem 2. Let $\mathcal{C} \subseteq 2^X$ be a concept class over some domain X with VC-dimension $d > 0$.

- (i) \mathcal{C} is polynomially PAC-learnable if d is bounded by a polynomial of its parameters and Problem 1 can be solved in time polynomial in the parameters and $|E^+ \cup E^-|$.
- (ii) For the VC-dimension of \mathcal{C}_{\cup}^k we have $\text{VC}_{\text{dim}}(\mathcal{C}_{\cup}^k) \leq 2dk \log(3k)$ for all $k \geq 1$.

4 Weak Convexity in Metric Spaces

In this section, we introduce the notion of *weak convexity* in metric spaces and establish some basic formal properties of weakly convex sets that will be utilized in the subsequent sections. By the most common definition, a set $A \subseteq \mathbb{R}^d$ is *convex* (Menger, 1928) if

$$D_2(x, z) + D_2(z, y) = D_2(x, y) \implies z \in A \quad (1)$$

for all $x, y \in A$ and $z \in \mathbb{R}^d$. Our notion of weak convexity generalizes (1). It is motivated by the fact that convex sets defined by (1) are always “contiguous” and cannot therefore capture well-separated regions of the domain that are “locally” convex.³ We address this problem by *adapting* the idea of k -convexity over Hamming metric spaces (Ekin et al., 1999) or that of g_k -convexity over graphs equipped with the geodesic distance (Farber and Jamison, 1986)⁴ to *arbitrary* finite and complete infinite metric spaces. In particular, analogously to Ekin et al. (1999) and Farber and Jamison (1986), we do *not* require (1) to hold for all points x and y , but only for such pairs which have a distance at most a user-specified threshold. In other words, while convexity is based on a *global* condition resulting in a single “contiguous” region, our notion of weak convexity relies on a *local* one, resulting in potentially several isolated regions, where the spread of locality is controlled by the above mentioned threshold. We will be interested in weakly convex hulls of finite sets. Since the convex hull of any

³The notion of local convexity in this paper is different from the one used in topology.

⁴The notion of g_k -convexity (Farber and Jamison, 1986) in graph theory has been used to study different graph classes for which global convexity can be characterized by weak (or local) geodesic convexity (see, e.g., Chalopin et al., 2022; Chepoi, 1989, 2007; Chepoi et al., 2020).

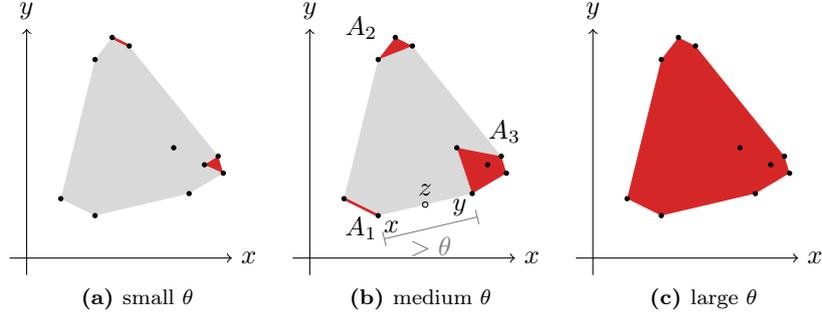


Figure 1. Examples of θ -convex sets in \mathbb{R}^2 for different values of θ .

bounded and closed, in particular, any finite subset of \mathbb{R}^d is closed, we require weakly convex sets to be closed. These considerations yield the following formal definition of *weak convexity*:

Definition 3. Let (X, D) be a complete metric space. A set $A \subseteq X$ is θ -convex (or simply, weakly convex) for some $\theta \in \mathbb{R}_{\geq 0}$ if A is closed (i.e., $\text{cl}(A) = A$) and for all $x, y \in A$ and $z \in X$ it holds that $z \in A$ whenever $D(x, y) \leq \theta$ and $z \in \mathcal{I}(x, y)$, where

$$\mathcal{I}(x, y) = \{z \in X : D(x, z) + D(z, y) = D(x, y)\} \quad (2)$$

denotes the interval of the points lying between x and y .

Notice that (2) implies $x, y \in \mathcal{I}(x, y)$. Furthermore, it does not require $x \neq y$. In particular, $\mathcal{I}(x, x) = \{x\}$ for all $x \in X$. The family of all weakly convex sets is denoted by $\mathcal{C}_{\theta, D}$; we omit D if it is clear from the context. The definitions imply $\mathcal{C}_{0, D} = 2^X$.

To illustrate the notion of weak convexity, consider the finite set of points $A \subseteq \mathbb{R}^2$ in Figure 1b. While the convex hull of A is indicated by the gray and red areas, the \subseteq -smallest θ -convex set containing A for some suitable $\theta \geq 0$ is drawn in red. The black points also belong to the θ -convex sets in 1a–1c. The most obvious difference is that there are three separated regions A_1, A_2 , and A_3 , instead of a single contiguous area. In other words, in contrast to convex sets in \mathbb{R}^2 , weakly convex sets need *not* be connected. This is a consequence of considering only point pairs with distance at most θ . For example, the points x and y in Figure 1b have a distance strictly greater than θ , implying that they do not generate z . Note that in the same way as convex sets, (parts of) weakly convex sets may be degenerated. For example, while A_2 and A_3 are regions with strictly positive area, A_1 is just a segment. We may even have isolated points (see Figure 1a). For sufficiently large θ , the \subseteq -smallest θ -convex set containing A becomes equal to the convex hull of A (cf. 1c).

Despite this unconventional behavior of weakly convex sets, $(X, \mathcal{C}_{\theta})$ forms a *closure system*. To see this, note that $\emptyset, X \in \mathcal{C}_{\theta}$. Let $\mathcal{F} \subseteq \mathcal{C}_{\theta}$ and $x, y \in \bigcap \mathcal{F}$ with $D(x, y) \leq \theta$. Then $\mathcal{I}(x, y) \subseteq F$ for all $F \in \mathcal{F}$ implying that $\bigcap \mathcal{F}$ is θ -convex. Thus, \mathcal{C}_{θ} has an associated *closure operator* $\rho_{\theta} : 2^X \rightarrow 2^X$ with $A \mapsto \bigcap \{C \in \mathcal{C}_{\theta} : A \subseteq C\}$ for all $A \subseteq X$. That is, ρ_{θ} maps a set A to the \subseteq -smallest θ -convex set containing A . It is called the *weakly convex hull operator* and its fixed points (i.e., the ρ_{θ} -closed sets) form exactly \mathcal{C}_{θ} .

4.1 Some Basic Properties of Weakly Convex Sets

We now present some basic properties of weakly convex sets that make them especially interesting for machine learning from a practical as well as from a theoretical viewpoint. As already mentioned, weakly convex sets need *not* be “contiguous” (cf. Figure 1), in contrast to, e.g., convex sets in Euclidean spaces. Instead, one can observe regions that are *separated* from each other, due to the fact that weak convexity utilizes a distance threshold θ . In Theorem 4 below we formally state this property of weakly convex sets. We note that this result generalizes that for the Hamming metric space (cf. Proposition 3.2 in Ekin et al., 2000) to complete metric spaces.

We first introduce some necessary notions. Let $\mathcal{M} = (X, D)$ be a metric space, $\theta \geq 0$, and $C \subseteq X$. Two points $a, b \in C$ are θ -connected in C , denoted $a \sim_{\theta, C} b$, if there is a finite sequence $a = p_1, p_2, \dots, p_r = b \in C$ such that $D(p_i, p_{i+1}) \leq \theta$ for all $i \in [r - 1]$. C is θ -connected if $a \sim_{\theta, C} b$ for all $a, b \in C$. Note that $\sim_{\theta, C}$ is an equivalence relation on C ; the equivalence class of a is denoted by $[a]_{\sim_{\theta, C}}$ (i.e., $[a]_{\sim_{\theta, C}} = \{b \in C : a \sim_{\theta, C} b\}$) for all $a \in C$.

Theorem 4. *Let (X, D) be a complete metric space, $\theta \geq 0$, and C be a subset of X that is finite if $\theta = 0$. Then C is θ -convex if and only if there is a unique family of non-empty sets $(B_i \subseteq C)_{i \in I}$ for some index set I that satisfies the following conditions:*

- (i) $C = \bigcup_{i \in I} B_i$,
- (ii) B_i is θ -convex for all $i \in I$,
- (iii) B_i is θ -connected for all $i \in I$,
- (iv) for all $i, j \in I$ with $i \neq j$, $D(a, b) > \theta$ for all $a \in B_i, b \in B_j$.

Proof. The case $\theta = 0$ is trivial, so we assume $\theta > 0$. We first show the equivalence stated in the theorem. For the “if” direction, suppose conditions (i)–(iv) hold for a family $(B_i)_{i \in I}$. To show that C is θ -convex, let $x, y \in C$ with $D(x, y) \leq \theta$. Then, by (i) and (iv), $x, y \in B_i$ for some $i \in I$. Let $z \in \mathcal{I}(x, y)$. By (ii) we have $z \in B_i$ and thus $z \in C$ by (i). Any convergent sequence in C is almost completely contained in some B_i for $i \in I$; this follows from (iv) and $\theta > 0$. Since B_i is closed, its limit point is also contained in B_i and therefore in C by (i). Hence, C is θ -convex.

For the “only if” direction, assume that C is θ -convex. Let $(a_i \in C)_{i \in I}$ denote a complete set of representatives of $\sim_{\theta, C}$ for some index set I . Let $B_i = [a_i]_{\sim_{\theta, C}}$ for all $i \in I$. By construction, $(B_i)_{i \in I}$ satisfies (i), (iii), and (iv). In particular, (iv) follows from $\theta > 0$ and the fact that for all $a, b \in C$, $D(a, b) \leq \theta$ implies $[a]_{\sim_{\theta, C}} = [b]_{\sim_{\theta, C}}$. Thus, $D(a, b) > \theta$ for all $i \neq j, a \in B_i$, and $b \in B_j$. To see that B_i fulfills (ii), let $x, y \in B_i$ for some $i \in I$ such that $D(x, y) \leq \theta$, and let $z \in \mathcal{I}(x, y)$. Suppose for contradiction, that $z \notin B_i$. Then by the θ -convexity of C and (i) we have that $z \in B_j$ for some $j \neq i$ and by (iv) that $D(x, z), D(z, y) > \theta$. Therefore,

$$0 = D(x, z) + D(z, y) - D(x, y) > \theta ,$$

contradicting $\theta > 0$. Hence, $z \in B_i$. Finally, since C is closed, every convergent sequence in B_i has a limit point by (i), which lies in B_i by (iv) and $\theta > 0$. This completes the proof of (ii).

It remains to show that $(B_i)_{i \in I}$ is *unique* with respect to (i)–(iv). Let $(B'_j)_{j \in J}$ be a family of non-empty sets that satisfies (i)–(iv). Let $r \in J$, $x \in B'_r$, and $s \in I$ such that $x \in B_s$. We claim that $B'_r = B_s$. We only show $B'_r \subseteq B_s$; the proof of $B_s \subseteq B'_r$ is analogous. Suppose for contradiction that $B'_r \not\subseteq B_s$ and let $a \in B'_r \setminus B_s$. Then, by (iii), there is a finite sequence $x = p_1, \dots, p_t = a \in B'_r$ with $D(p_i, p_{i+1}) \leq \theta$ for all $i \in [t-1]$. It must be the case that there is an $i \in [t-1]$ such that $p_i \in B_s$ and $p_{i+1} \in B'_r \setminus B_s$. But then, since $p_{i+1} \notin B_s$, $D(p_i, p_{i+1}) > \theta$ because $(B_i)_{i \in I}$ satisfies (i) and (iv), which is a contradiction. Hence, $B'_r = B_s$. Thus, for all $j \in J$ there is an $i \in I$ such that $B'_j = B_i$, implying the uniqueness. \square

In what follows, the family $(B_i)_{i \in I}$ satisfying conditions (i)–(iv) in Theorem 4 will be referred to as the θ -decomposition of the θ -convex set C . Furthermore, the sets B_i in the θ -decomposition of C , denoted $\mathcal{B}_\theta(C)$, will be called θ -blocks or simply, *blocks*. We will omit θ from the notation and simply write $\mathcal{B}(C)$ if θ is clear from the context. In particular, we write $\mathcal{B}(\rho_\theta(A))$ instead of $\mathcal{B}_\theta(\rho_\theta(A))$ for any $A \subseteq X$. In Proposition 5 below we formulate a basic property of the blocks in a θ -decomposition.

Proposition 5. *Let $\mathcal{M} = (X, D)$ be a complete metric space, $\theta \geq 0$, and $A \in [X]^{<\infty}$. Then for all $B_1, B_2 \in \mathcal{B}(\rho_\theta(A))$, there are $a \in B_1$ and $b \in B_2$ such that*

$$D(B_1, B_2) = D(a, b) .$$

Proof. It follows from the property that all blocks are non-empty and θ -convex by Theorem 4 and hence closed. \square

Finally, we claim that the weakly convex hull operator is monotone with respect to θ and establish a connection between weak and ordinary convexity. For a metric space (X, D) and $A \subseteq X$, let $\rho(A)$ denote the closed convex hull of A .

Proposition 6. *Let (X, D) be a complete metric space, $0 \leq \theta \leq \theta' < \infty$, and let A be a subset of X that is finite if $\theta = 0$. Then*

$$(i) \quad \rho_\theta(A) \subseteq \rho_{\theta'}(A) \subseteq \rho(A),$$

(ii) *for all $x, y \in \rho_\theta(A)$, x, y are in the same block of $\rho_{\theta'}(A)$ if they are in the same block of $\rho_\theta(A)$.*

Proof. The claim is trivial if $\theta = 0$. Assume that $\theta > 0$. Regarding (i), the proof of the second containment is trivial. The first one follows from the fact that the family of θ' -convex sets containing A is a subfamily of that of θ -convex sets containing A . Indeed, any θ' -convex set C is θ -convex, as $\mathcal{I}(x, y) \subseteq C$ for all $x, y \in C$ with $D(x, y) \leq \theta \leq \theta'$. To prove (ii), let $x, y \in \rho_\theta(A)$ that belong to the same θ -block in $\rho_\theta(A)$. Then $\theta > 0$ and (iii) of Theorem 4 imply $x \sim_{\theta, \rho_\theta(A)} y$. By $\theta \leq \theta'$ and (i), we also have $x \sim_{\theta', \rho_{\theta'}(A)} y$. Hence, x, y lie in the same θ' -block of $\rho_{\theta'}(A)$. \square

Thus, for monotonically increasing θ s, the weakly convex hulls of a set A form a *monotone chain*, with a maximum element defined by the convex hull of A . In Figure 2 we present an example of this property for the case that the domain is the vertex set of a graph and the distance is the geodesic (or shortest-path)

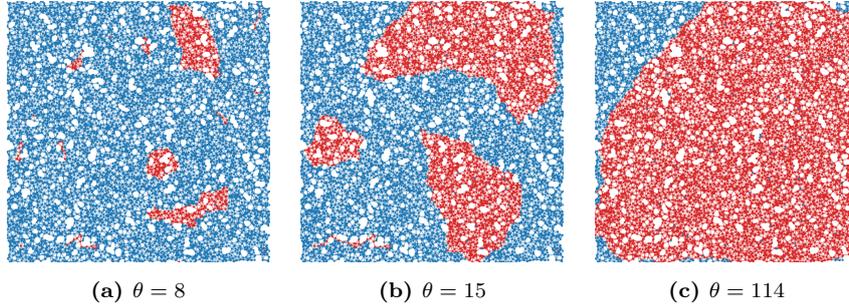


Figure 2. The geodesic θ -convex hulls (in red) of a set of 40 vertices for $\theta = 8, 15$, and 114 in a graph with 10,000 vertices.

distance. The graph in this example, used also in our experimental evaluation, has 10,000 vertices. We show three weakly convex subsets (color red) for $\theta = 8, 15$, and 114 (the diameter of the graph). They form the weak convex hulls of the same set of 40 vertices. A closer look at the figure shows that the weakly convex hull in (a) is a subset of that in (b), which, in turn, is a subset of the convex hull in (c), in accordance with Proposition 6. This property will be utilized in the next sections concerning learning weakly convex sets.

Remark 7. We note that a block of a weakly convex set is not necessarily convex. To see this, let $\theta \geq 2$ be an integer and consider the graph C consisting of a single cycle of length $2\theta + 3$ with the geodesic distance D as metric. Let $A = \{v_1, \dots, v_k\} \subseteq V(C)$ such that $D(v_i, v_{i+1}) \leq \theta$ for all $1 \leq i < k$, $D(v_1, v_k) = \theta + 1$, and the shortest path P_{v_1, v_k} connecting v_1 and v_k does not contain any vertices from $A \setminus \{v_1, v_k\}$. It follows that $\rho_\theta(A)$ consists of a single block. Furthermore, while $\rho(A) = V(C)$, $\rho_\theta(A)$ does not contain the interior points of P_{v_1, v_k} . Thus, $\rho_\theta(A)$ is not convex.

5 The Generic CHF Algorithm

In this section we present our general algorithm for solving the CHF problem for weakly convex hypothesis classes over a broad class of metric spaces. As long as θ is fixed, the CHF problem for a θ -convex hypothesis class \mathcal{C}_θ can be solved by computing the θ -convex hull of the positive examples. If, however, θ is not given in advance, which is a realistic scenario, we need to compute a solution from those of the CHF problems for \mathcal{C}_θ for all $\theta \geq 0$ that is *optimal* with respect to some criterion. Such an optimality criterion could be defined by the number of blocks in the weakly convex hull. This criterion leads, however, to solving a computationally intractable problem (see Section 7 for a discussion). We therefore restrict the set of feasible solutions to the θ -convex hulls of the positive examples for all $\theta \geq 0$ and return the *most general* consistent hypothesis (Mitchell, 1982) defined by the *largest* weakly convex hull of the positive examples for some θ that is disjoint with the negative examples. Out of the consistent weakly convex hulls, it is the closest approximation of the convex hull of the positive examples.

We consider the case that the hypotheses are given by some representation and refer to this scenario as the *intensional* problem setting. In order to formulate the CHF problem, we first define the notion of representation schemes. The definition below utilizes that weakly convex sets give rise to a unique block decomposition (cf. Theorem 4). More precisely, let $\mathcal{M} = (X, D)$ be a complete metric space and $\tau \geq 0$. A *representation scheme* for \mathcal{M} and τ is a function $\mu : \mathbb{R}_{\geq \tau} \times [X]^{<\infty} \rightarrow 2^{\{0,1\}^*}$ with

$$\mu(\theta, A) \mapsto \{\mu'(\theta, B \cap A) : B \in \mathcal{B}(\rho_\theta(A))\} \quad (3)$$

for all $\theta \geq \tau$ and $A \in [X]^{<\infty}$, where $\mu' : \mathbb{R}_{\geq \tau} \times [X]^{<\infty} \rightarrow \{0,1\}^* \cup \{\perp\}$ is a function such that for all $\theta', \theta'' \geq \tau$ and for all $A', A'' \in [X]^{<\infty}$ it satisfies

$$\mu'(\theta', A') \in \{0,1\}^* \iff |\mathcal{B}(\rho_{\theta'}(A'))| = 1 \quad (4)$$

and if $|\mathcal{B}(\rho_{\theta'}(A'))| = |\mathcal{B}(\rho_{\theta''}(A''))| = 1$ then

$$\rho_{\theta'}(A') = \rho_{\theta''}(A'') \iff \mu'(\theta', A') = \mu'(\theta'', A'') . \quad (5)$$

In other words, μ returns some *unique* representation of weakly convex hulls of *finite* subsets of the domain using some representation μ' of weakly convex blocks. The definition above is correct, as $\mu'(\theta, B \cap A) \in \{0,1\}^*$ for all blocks B in (3). For $R = \mu(\theta, A)$, the extension of R (i.e., $\rho_\theta(A)$) is denoted by $\text{ext}(R)$. For \mathcal{M} , τ , and μ , define the order \preceq on the set of representations of weakly convex sets as follows: For all $A, B \in [X]^{<\infty}$ and for all $\theta_1, \theta_2 \geq \tau$, $\mu(\theta_1, A) \preceq \mu(\theta_2, B)$ if and only if $\rho_{\theta_1}(A) \subseteq \rho_{\theta_2}(B)$. Clearly, \preceq is a partial order. Using the above notions, we are ready to define the CHF problem for the intensional setting. The supremum in the definition below is taken with respect to the relation \preceq .

Problem 8. *Given a complete metric space $\mathcal{M} = (X, D)$, a representation scheme μ for \mathcal{M} and some $\tau \geq 0$, and disjoint sets $E^+, E^- \in [X]^{<\infty}$ of labeled examples with $E^+ \neq \emptyset$, return*

$$\sup_{\theta \geq \tau} \{\mu(\theta, E^+) : \rho_\theta(E^+) \cap E^- = \emptyset\}$$

if such a θ exists; otherwise return “NO”.

To present our solution to Problem 8, we need a restriction on complete metric spaces. Section 5.1 below is concerned with learning weakly convex Boolean functions in the Hamming metric space (H_n, D_H) . For $\theta = 1$, all subsets of H_n are 1-convex. Thus, to represent any of the 2^{2^n} 1-convex subsets, we need $\Omega(2^n)$ bits, implying that there is *no* compact representation of 1-convex sets. One of the problems is that the blocks of 1-convex subsets of H_n are not convex in general. To overcome this problem, we require, in addition to completeness, the metric space to satisfy the blockwise convexity property, defined as follows: A metric space $\mathcal{M} = (X, D)$ is *blockwise convex* for some $\tau \geq 0$, if it is complete and for all τ -convex sets $C \subseteq X$ with $C = \rho_\tau(A)$ for some $A \in [X]^{<\infty}$, C is *convex* whenever it is τ -connected. In other words, all blocks of the τ -convex hull of a finite set are convex. The definitions imply that if \mathcal{M} is blockwise convex for some $\tau \geq 0$, then it is blockwise convex for all $\tau' \geq \tau$. In the lemma below we first present some basic properties of weakly convex hulls in blockwise convex metric spaces.

Algorithm 1 INTENSIONAL CONSISTENT HYPOTHESIS FINDING

Require: blockwise convex metric space $\mathcal{M} = (X, D)$ for some $\tau \geq 0$ and representation scheme μ for \mathcal{M} and τ

Input: disjoint sets $E^+, E^- \in [X]^{<\infty}$ with $E^+ \neq \emptyset$

Output: $\mu(\theta, E^+)$ such that $\theta \geq \tau$, $\rho_\theta(E^+) \cap E^- = \emptyset$, and $\rho_{\theta'}(E^+) \cap E^- \neq \emptyset$ for all $\theta' > \theta$ satisfying $\rho_{\theta'}(E^+) \supseteq \rho_\theta(E^+)$ if such a θ exists; “No” otherwise

```

1:  $\mathcal{R}_0 \leftarrow \{\text{SINGLETON}(x) : x \in E^+\}$ ,  $i \leftarrow 0$  // cf. (6)
2: while  $|\mathcal{R}_i| > 1$  do
3:    $i \leftarrow i + 1$ 
4:    $\theta_i = \max\{\tau, \min\{\text{DISTANCE}(R_1, R_2) : R_1, R_2 \in \mathcal{R}_{i-1}, R_1 \neq R_2\}\}$  // cf. (7)
5:    $\mathcal{R} \leftarrow \mathcal{R}_{i-1}$ 
6:   while  $\exists R_1, R_2 \in \mathcal{R}$  with  $R_1 \neq R_2$  and  $\text{DISTANCE}(R_1, R_2) \leq \theta_i$  do
7:      $\mathcal{R} \leftarrow (\mathcal{R} \setminus \{R_1, R_2\}) \cup \{R\}$  with  $R = \text{JOIN}(\theta_i, R_1, R_2)$  // cf. (9)
8:    $\mathcal{R}_i \leftarrow \mathcal{R}$ 
9:   if  $\exists e \in E^-$  and  $R \in \mathcal{R}_i \setminus \mathcal{R}_{i-1}$  such that  $\text{MEMBERSHIP}(e, R) = \text{TRUE}$ 
     then
10:    if  $i = 1$  and  $\theta_i = \tau$  then return “No”
11:    else return  $\mathcal{R}_{i-1}$ 
12: return  $\mathcal{R}_i$ 

```

Lemma 9. Let $\mathcal{M} = (X, D)$ be a blockwise convex metric space for some $\tau \geq 0$, $A \in [X]^{<\infty}$ with $A \neq \emptyset$, $\theta_0 = 0$ and $\theta_i = \max\{\tau, \min\{D(B_1, B_2) > 0 : B_1, B_2 \in \mathcal{B}(\rho_{\theta_{i-1}}(A))\}\}$ for all $i \in [k]$, where k is the smallest integer satisfying $|\mathcal{B}(\rho_{\theta_k}(A))| = 1$. Then $k \leq |A|$ and for all $i \in [k-1]$,

(i) $\rho_{\theta_i}(A) \subseteq \rho_{\theta_{i+1}}(A)$,

(ii) $\rho_{\theta_i}(A) = \rho_{\theta'_i}(A)$ for all $\theta'_i \in [\theta_i, \theta_{i+1})$,

(iii) $\rho_{\theta_k}(A) = \rho_{\theta'_k}(A)$ for all $\theta'_k \geq \theta_k$.

Proof. We first prove that the θ_i s in the claim fulfill (i)–(iii) for all $i \in [k]$. Let $i \in [k-1]$. The proof of (i) follows directly from Proposition 6 because $\theta_i < \theta_{i+1}$. Regarding (ii), we claim that $\rho_{\theta_i}(A)$ satisfies all conditions of Theorem 4 for all $\theta'_i \in [\theta_i, \theta_{i+1})$, and hence, $\rho_{\theta_i}(A)$ is θ'_i -convex. This implies $\rho_{\theta_i}(A) \supseteq \rho_{\theta'_i}(A)$, from which we get (ii) by (i). To show this claim, note that (i) and (iii) of Theorem 4 hold trivially, (ii) by blockwise convexity, and (iv) by $\theta'_i < \theta_{i+1}$, together with the definition of θ_{i+1} . Finally, the proof of (iii) of the lemma is automatic, as $|\mathcal{B}(\rho_{\theta_k}(A))| = 1$ and hence, it is convex by blockwise convexity. The proof of $k \leq |A|$ follows from $|\mathcal{B}(\rho_{\theta_0}(A))| = |A|$ and from $|\mathcal{B}(\rho_{\theta_i}(A))| > |\mathcal{B}(\rho_{\theta_{i+1}}(A))|$ ($1 \leq i < k$). \square

We are ready to present our general domain-independent algorithm (see Algorithm 1) for solving Problem 8 for blockwise convex metric spaces. It utilizes the property that the θ -convex hulls of the positive examples form an ascending chain for increasing θ s and hence, the representations of any two weakly convex hulls are comparable with respect to \preceq defined above.

For disjoint finite sets $E^+, E^- \subseteq X$ of examples, Algorithm 1 first computes in \mathcal{R}_0 the set of representations of the singleton blocks containing x for all $x \in E^+$ (line 1), where function SINGLETON is defined by

$$\text{SINGLETON}(x) = \mu'(0, \{x\}) . \quad (6)$$

In each iteration i of the outer loop (lines 2–11), the algorithm computes in \mathcal{R}_i a new set of block representations from those in \mathcal{R}_{i-1} (lines 5–8). In particular, it takes the *smallest* pairwise distance θ_i between the blocks in \mathcal{R}_{i-1} if it is greater than τ ; otherwise τ (cf. line 4). More precisely, function DISTANCE called in line 4 with valid (block) representations $R_1, R_2 \in \{0, 1\}^*$ is defined by

$$\text{DISTANCE}(R_1, R_2) = D(\text{ext}(R_1), \text{ext}(R_2)) . \quad (7)$$

We note that (7) is the *semantic* definition of DISTANCE; it is assumed that the distance between $\text{ext}(R_1)$ and $\text{ext}(R_2)$ can be calculated *directly* from their representations R_1, R_2 .

The algorithm then sets \mathcal{R} to \mathcal{R}_{i-1} and in the inner loop (lines 6–7) it iteratively joins *all* pairs of block representations in \mathcal{R} that have distance at most θ_i , including also those that arise in the inner loop. In Lemma 12 we claim that $\mathcal{R}_i = \mu(\theta_i, E^+)$ for \mathcal{R}_i in line 8. To prove this, in Proposition 10 we first state that the θ -convex hull of two blocks with distance at most θ is always a single block.

Proposition 10. *Let $\mathcal{M} = (X, D)$ be a complete metric space and $B_1, B_2 \in \mathcal{B}(\rho_{\theta'}(A))$ for some $A \in [X]^{<\infty}$ and $\theta' \geq 0$. Let $\theta > 0$ such that $D(B_1, B_2) \leq \theta$. Then for $B = \rho_{\theta}(B_1 \cup B_2)$ it holds that*

- (i) $B = \rho_{\theta}(A \cap (B_1 \cup B_2))$ and
- (ii) B is a block (i.e., it is θ -connected).

Proof. The claim is trivial if $\theta \leq \theta'$, as $B_1 = B_2$ for this case by Theorem 4. Consider the case that $\theta > \theta'$. The proof of (i) is straightforward. Since B_1, B_2 are θ' -connected by Theorem 4, $B_1 \cup B_2$ is θ -connected, from which (ii) follows by noting that the θ -convex hull of a θ -connected set is θ -connected. \square

Using induction on i , Proposition 10 implies that if $D(\text{ext}(R_1), \text{ext}(R_2))$ for R_1, R_2 in line 7 is at most θ_i , then

$$\rho_{\theta_i}(\text{ext}(R_1) \cup \text{ext}(R_2)) = \rho_{\theta_i}(E^+ \cap (\text{ext}(R_1) \cup \text{ext}(R_2))) \quad (8)$$

consists of a *single* block, giving rise to the following definition of JOIN in line 7:

$$\text{JOIN}(\theta_i, R_1, R_2) = \mu'(\theta_i, E^+ \cap (\text{ext}(R_1) \cup \text{ext}(R_2))) . \quad (9)$$

Similarly to function DISTANCE, the algorithmic realization of JOIN is assumed to operate directly on R_1 and R_2 , and not on their extensions. In the proof of Lemma 12 below, we will use the following auxiliary result for R computed in line 7:

Lemma 11. *For all $i \geq 1$ and R computed in line 7 in iteration i of the outer loop, there exists $R' \in \mu(\theta_i, E^+)$ such that $\text{ext}(R) \subseteq \text{ext}(R')$.*

Proof. We prove the claim by induction on the generation order of R (cf. line 7). Suppose R has been generated in iteration i for some $R_1, R_2 \in \mathcal{R}$ and $i \geq 1$. The base case follows from (ii) of Proposition 10, as $R_1, R_2 \in \mathcal{R}_0$ and hence their extensions are singletons. Suppose the statement holds for all blocks generated before R . Let i_1, i_2 be the smallest indices such that $R_1 \in \mathcal{R}_{i_1}, R_2 \in \mathcal{R}_{i_2}$. Then, depending on i_1 , either the fact that $|\text{ext}(R_1)| = 1$ (for $i_1 = 0$) or the induction hypothesis (for $i_1 > 0$) together with Proposition 6 imply that there exists a block $R'_1 \in \mu(\theta_i, E^+)$ such that $\text{ext}(R_1) \subseteq \text{ext}(R'_1)$. Using a similar argument, there exists a block $R'_2 \in \mu(\theta_i, E^+)$ such that $\text{ext}(R_2) \subseteq \text{ext}(R'_2)$. Furthermore, by the choice of R_1, R_2 , there are $x \in \text{ext}(R_1)$ and $y \in \text{ext}(R_2)$ such that $D(x, y) \leq \theta_i$. Thus, the distance between $\text{ext}(R'_1)$ and $\text{ext}(R'_2)$ is at most θ_i and hence $R'_1 = R'_2$ by Theorem 4. The claim then follows from (8), (9), and the monotonicity of ρ_{θ_i} . \square

Defining $\theta_0 = 0$, below we claim that \mathcal{R}_i is a representation of $\rho_{\theta_i}(E^+)$ for all $i \geq 0$.

Lemma 12. *For all $i \geq 0$, $\mathcal{R}_i = \mu(\theta_i, E^+)$.*

Proof. The statement is trivial for $i = 0$. Regarding $i > 0$, we claim that the family of the extensions of the blocks in \mathcal{R}_i satisfies conditions (ii)–(iv) of Theorem 4. Indeed, (9) and Proposition 10 together imply (ii) and (iii), whereas (iv) follows by construction (cf. line 4). Thus, $C = \bigcup_{R \in \mathcal{R}_i} \text{ext}(R)$ and the family $(\text{ext}(R))_{R \in \mathcal{R}_i}$ fulfills the conditions of Theorem 4. Hence, C is θ_i -convex. But then, since $E^+ \subseteq C$, $\rho_{\theta_i}(E^+) \subseteq C$ holds by the monotonicity and idempotency of ρ_{θ_i} . Furthermore, we have $C \subseteq \rho_{\theta_i}(E^+)$ by Lemma 11. Thus, $C = \rho_{\theta_i}(E^+)$, completing the proof. \square

Finally, the algorithm checks whether each new block in \mathcal{R}_i is consistent with the negative examples by calling function MEMBERSHIP defined by

$$\text{MEMBERSHIP}(e, R) = \begin{cases} \text{TRUE} & \text{if } e \in \text{ext}(R) \\ \text{FALSE} & \text{o/w} \end{cases} \quad (10)$$

for all $e \in E^-$ and $R \in \mathcal{R}_i \setminus \mathcal{R}_{i-1}$. Similarly to DISTANCE and JOIN, the algorithmic realization of MEMBERSHIP is assumed to operate directly on R .

Using the above definitions and considerations, we are ready to state our main result of this section concerning the correctness and complexity of Algorithm 1. We use the following notation in the theorem: T_S, T_D, T_J , and T_M denote the time complexity of functions SINGLETON, DISTANCE, JOIN, and MEMBERSHIP, respectively.

Theorem 13. *Let \mathcal{M} be a blockwise convex metric space for some $\tau \geq 0$ and μ a representation scheme for \mathcal{M} and τ . Then Algorithm 1 solves Problem 8 for \mathcal{M} correctly in time*

$$\mathcal{O}(m_{\oplus}^2 \log m_{\oplus} + m_{\oplus} T_S + m_{\oplus}^2 T_D + m_{\oplus} T_J + m_{\oplus} m_{\ominus} T_M) , \quad (11)$$

where $m_{\oplus} = |E^+|$ and $m_{\ominus} = |E^-|$.

Proof. It is easy to check that Algorithm 1 is correct if it returns “NO” or \mathcal{R}_0 . Otherwise, by (ii) and (iii) of Lemma 9, it suffices to consider the θ_i s

in Lemma 9 because those values already generate *all* weakly convex hulls of E^+ . Furthermore, (i) of Lemma 9 guarantees that if the θ_i -convex hull of E^+ is inconsistent with E^- for some i , then all θ_j -convex hulls of E^+ for $j \geq i$ are also inconsistent. These properties, together with Lemma 12, imply the correctness of Algorithm 1.

Regarding its time complexity, Algorithm 1 can be implemented by maintaining the sets

$$L_{BP} = \{(d, \{R_1, R_2\}) : R_1, R_2 \in \mathcal{R} \text{ with } 0 < \text{DISTANCE}(R_1, R_2) = d\}$$

and

$$L(R) = \{(d, \{R_1, R_2\}) \in L_{BP} : R \in \{R_1, R_2\}\}$$

for all $R \in \mathcal{R}$. L_{BP} (resp. $L(R)$) is used to quickly find two blocks with distance at most a threshold (resp. the nodes of L_{BP} that refer to R). They can be realized by a red-black (RB) tree and by doubly linked lists, respectively. Since insertion in RB trees (resp. in doubly linking lists) can be performed in logarithmic (resp. constant) time, the time complexity of the initialization (line 1) is

$$\mathcal{O}(m_{\oplus}^2 \log m_{\oplus} + m_{\oplus} T_S + m_{\oplus}^2 T_D) . \quad (12)$$

For the execution of line 7, one can select an *arbitrary* pair $R_1, R_2 \in \mathcal{R}$ that have distance at most θ_i (e.g., the pair in the root of the RB tree) and proceed as follows:

- (α) Delete all nodes N of the RB tree that contain R_1 or R_2 in their second entry as well as all occurrences of N in all doubly linking lists.
- (β) Compute the new block R by joining R_1 and R_2 and set $L(R) = \emptyset$.
- (γ) For all blocks $R' \in \mathcal{R} \setminus \{R_1, R_2, R\}$, compute the distance d between R and R' , insert $N = (d, \{R, R'\})$ into the RB tree, and add N to $L(R)$ and $L(R')$.

Suppose $|\mathcal{R}| = m$ before the execution of line 7. The algorithm carries out $\mathcal{O}(m)$ deletions in the RB tree and $\mathcal{O}(m)$ deletions in the doubly linked lists for (α), one join operation for (β), $\mathcal{O}(m)$ distance calculations and $\mathcal{O}(m)$ insertions for (γ). Line 7 is carried out at most $m_{\oplus} - 1$ times because $|\mathcal{R}| = m_{\oplus}$ initially and each execution of line 7 decreases the cardinality of \mathcal{R} by one. Together with (12), this implies (11) in the claim, by noting that the algorithm spends $\mathcal{O}(m_{\oplus} m_{\ominus} T_M)$ total time for checking the consistency in line 9 and that the insertion and deletion operation in RB trees (resp. doubly linking lists) can be carried out in logarithmic (resp. constant) time. \square

5.1 Some Illustrative Examples

In this section, we present some examples to illustrate the application of Algorithm 1 and Theorem 13 for three different domains.

Learning Weakly Convex Boolean Functions

As a first application of Theorem 13, we prove that the CHF problem for *weakly convex* Boolean functions can be solved in polynomial time. This result is not

new, it was shown with a *domain-specific* CHF algorithm in (Ekin et al., 2000). Nevertheless, we present this application example because it clearly demonstrates some nice properties of our *general purpose* algorithm. In particular, Algorithm 1 solves the related CHF problem in the *same* asymptotic time complexity as the domain-specific algorithm by Ekin et al. (2000) and this positive result can be obtained in a fairly *simple* way by using Algorithm 1 and Theorem 13.

More precisely, we consider the Hamming metric space $\mathcal{M}_H = (H_n, D_H)$ for some $n \in \mathbb{N}$ (cf. Section 3). A Boolean function $f : H_n \rightarrow \{0, 1\}$ is θ -convex for some $\theta \geq 0$ if its extension $\text{ext}(f) = \{x \in H_n : f(x) = 1\}$ is θ -convex in \mathcal{M}_H . In order to define a suitable representation scheme for θ -convex Boolean functions, we need some further notions. The set $\{x_1, \neg x_1, \dots, x_n, \neg x_n\}$ of Boolean *literals* is denoted by L_n . A *term* T is a conjunction of literals from L_n ; T is sometimes regarded as the set of literals it contains. A *conflict* between two terms T_i and T_j over L_n is an integer $p \in [n]$ such that $x_p \in T_i$ and $\neg x_p \in T_j$ or vice versa. We first claim some important properties of \mathcal{M}_H .

Proposition 14. *For all $n \geq 0$, $\mathcal{M}_H = (H_n, D_H)$ is blockwise convex for $\tau = 2$. In particular, for all $A \subseteq H_n$ that are 2-convex and 2-connected, A is a Boolean subcube of H_n .*

Proof. Since \mathcal{M}_H is finite, it is complete. We prove for A in the claim that $A = H_n[A]$, where $H_n[A]$ is the *smallest* Boolean subcube of H_n containing A . By definition, $A \subseteq H_n[A]$. To show $A \supseteq H_n[A]$, note that the conditions on A imply that A is connected (i.e., 1-connected), from which we have $A \supseteq H_n[A]$ by the result that a connected Boolean function is convex if and only if it is 2-convex (cf. Theorem 5.16 in Ekin et al. (1999)) and by the fact that a subset of H_n is convex if and only if it is a subcube of H_n . \square

We have the following result for the CHF problem for weakly convex Boolean functions:

Theorem 15. *For all $n \geq 0$, there is a representation scheme μ for $\mathcal{M}_H = (H_n, D_H)$ and $\tau = 2$. Furthermore, Algorithm 1 solves Problem 8 for \mathcal{M}_H , μ , and τ in time*

$$\mathcal{O}(nm_{\oplus}(m_{\oplus} + m_{\ominus})) . \quad (13)$$

Proof. Let $\theta \geq 2$. By Proposition 14 we have that \mathcal{M}_H is blockwise convex for θ and that the blocks of θ -convex sets are formed by (Boolean) subcubes of H_n . Utilizing the fact that any non-empty subcube of H_n can *uniquely* be represented by a term over L_n , we define $\mu'_H(\theta, A)$ for all subsets $A \subseteq H_n$ by the term representing $\rho_{\theta}(A)$, if $\rho_{\theta}(A)$ is a non-empty subcube of H_n ; otherwise by \perp . One can easily check that μ'_H satisfies (4) and (5). Theorem 4 then implies that $\mu_H : \mathbb{R}_{\geq 2} \times 2^{H_n} \rightarrow 2^{\{0,1\}^*}$ defined by

$$\mu_H(\theta, A) = \{\mu'_H(\theta, B) : B \in \mathcal{B}(\rho_{\theta}(A))\} \quad (14)$$

for all $A \subseteq H_n$ is a representation scheme for \mathcal{M}_H and $\tau = 2$. Note that $\mu_H(\theta, A)$ in (14) is a k -term-DNF with $k = |\mathcal{B}(\rho_{\theta}(A))|$.

Defining μ in Problem 8 by μ_H in (14), T_S, T_D, T_J, T_M in Theorem 13 are all in $\mathcal{O}(n)$ time for $\mathcal{M} = \mathcal{M}_H$. This is trivial for T_M and follows for T_S directly from $\mu'_H(\theta, \{x\}) = \bigwedge_{i=1}^n l_i$ with $l_i = x_i$, if $x_i = 1$; o/w $l_i = \neg x_i$, for all

$x = (x_1, \dots, x_n) \in H_n$. Regarding T_D and T_J , let T_i and T_j be terms over L_n . Then $D_H(\text{ext}(T_i), \text{ext}(T_j))$ is equal to the number of conflicts between T_i and T_j , and for all $\theta \geq 2$ and terms T_i, T_j with $D_H(\text{ext}(T_i), \text{ext}(T_j)) \leq \theta$, $\text{JOIN}(\theta, T_i, T_j)$ is the term with literals $T_i \cap T_j$. We get (13) from the general bound (11) in Theorem 13 by noting that $\log m_{\oplus} = \mathcal{O}(n)$. \square

A few remarks are in order. First, unless $R = NP$, it is NP-hard to find a consistent k -term-DNF, i.e., k subcubes of H_n such that their union is consistent with the examples, for the *smallest* k (Pitt and Valiant, 1988). While there is no restriction on the subcubes in this problem, weakly convex Boolean functions require a minimum distance between them. Although it is not guaranteed that the weakly convex hull returned by Algorithm 1 is optimal with respect to the number of blocks among *all* consistent weakly convex hypotheses, it is an *efficiently* computable alternative to the computationally *intractable* smallest consistent k -term-DNF. Second, the time complexity of the related domain-specific algorithm in (Ekin et al., 2000) is slower by a factor of $\log n$. However, that factor can be saved by applying the idea in our Algorithm 1 that linear search enables for an incremental calculation of the θ -convex hulls for increasing θ s. This is faster than binary search computing them *from scratch*. Third, Ekin et al. (2000) also prove that for all $\theta > n/2 - 1$, the concept class $\mathcal{F}_{n,\theta}$ is *polynomially* PAC-learnable, where $\mathcal{F}_{n,\theta}$ is defined as follows: For all $A \subseteq H_n$, $A \in \mathcal{F}_{n,\theta}$ if and only if A is θ -convex. Their proof is based on showing that the CHF problem can be solved in polynomial time for $\mathcal{F}_{n,\theta}$ (see, also, (i) of Theorem 2). This is trivial for $n < 6$; for $n \geq 6$, it can be shown by Theorem 15, a special case of Theorem 13, in a fairly *simple* way. Indeed, since $\theta > 2$, Theorem 15 guarantees that there exists a consistent hypothesis in $\mathcal{F}_{n,\theta}$ if and only if Algorithm 1 with \mathcal{M}_H , μ in (14) and for $E^+, E^- \subseteq H_n$ returns a solution \mathcal{R} of the CHF problem in polynomial time such that for all $R_1, R_2 \in \mathcal{R}$ with $R_1 \neq R_2$, $D_H(\text{ext}(R_1), \text{ext}(R_2)) > \theta$.

Learning Weakly Convex Unions of Axis-Aligned Hyperrectangles

As a second illustrative example for the application of Algorithm 1 and Theorem 13, we show that the CHF problem can be solved for *weakly convex* unions of axis-aligned hyperrectangles in polynomial time. The underlying metric space for this example is $\mathcal{M}_U = (U_d, D_1)$, where $U_d = [0, 1]^d$ denotes the *unit d -cube*. Note that \mathcal{M}_U can be regarded as a generalization of \mathcal{M}_H considered above. Before stating our result in Theorem 17, we first formulate some basic properties of \mathcal{M}_U .

Proposition 16. *For all $d \geq 0$ integer, \mathcal{M}_U satisfies the following properties:*

- (i) *It is blockwise convex for any $\tau > 0$. In particular, for all $A \in [U_d]^{<\infty}$ such that $\rho_\tau(A)$ is τ -connected, $\rho_\tau(A) = U_d[A]$, where $U_d[A]$ is the smallest axis-aligned subcube that contains A .*
- (ii) *For all $A \in [U_d]^{<\infty}$ and $\theta \geq 0$, $\rho_\theta(A)$ is a finite union of axis-aligned closed hyperrectangles.*

Proof. Regarding (i), the completeness holds by the definition of U_d . Let A be a subset of U_d satisfying the conditions in (i). One can easily check that if A is not τ -connected then there exists a τ -connected set $B \in [U_d]^{<\infty}$ such that

$A \subset B$ and $\rho_\tau(B) = \rho_\tau(A)$. Thus, it suffices to consider the case that A is τ -connected. We prove (i) by induction on $|A|$. The base case $|A| = 1$ is trivial. Suppose the claim holds for all τ -connected sets $A' \subset U_d$ with $|A'| \leq k$. Let $A = A' \cup \{a\}$ for some $A' \in [U_d]^{<\infty}$ and $a \in U_d$ such that $|A'| = k$ and A, A' are both τ -connected. The claim holds directly by the induction hypothesis if $\rho_\tau(A) = \rho_\tau(A')$. Suppose $a \notin \rho_\tau(A')$. Clearly, $\rho_\tau(A) \subseteq U_d[A]$. Conversely, let $x = (x_1, \dots, x_d) \in U_d[A]$, $\text{MIN}_i = \min_{y \in A'} y[i]$, and $\text{MAX}_i = \max_{y \in A'} y[i]$ for all $i \in [d]$. Let $a' = (a'_1, \dots, a'_d) \in U_d[A']$ be the point with the smallest D_1 distance to a . We show that $(x_1, a_2, \dots, a_n) \in \rho_\tau(A)$. The claim is automatic if $x_1 = a_1$. Otherwise, $a' \in \rho_\tau(A')$ holds by the induction hypothesis and hence, $D_1(a, a') \leq \tau$. Thus, for $\tau_1 = |a_1 - a'_1|$ we have $\tau_1 \leq \tau$. We prove the claim only for the case that $a_1 < a'_1$; the proof for $a_1 \geq a'_1$ can be shown with similar arguments. If $x_1 \in [a_1, a'_1]$, then $(x_1, a_2, \dots, a_n) \in \rho_\tau(\{a, a'\}) \subseteq \rho_\tau(A)$.

Otherwise (i.e., $x_1 \in (a'_1, \text{MAX}_1]$), let p_i (resp. p'_j) denote $(a_1 + i\tau_1, a_2, \dots, a_d) \in U_d[A]$ (resp. $(a'_1 + j\tau_1, a'_2, \dots, a'_d) \in U_d[A']$) for all $i = 0, \dots, \ell$ (resp. $j = 0, \dots, \ell - 1$), where $\ell = \lfloor (x_1 - a_1) / \tau_1 \rfloor$. By the induction hypothesis, $p'_j \in \rho_\tau(A') \subseteq \rho_\tau(A)$ for all j and hence, $p_i \in \rho_\tau(\{p_{i-1}, p'_{i-1}\}) \subseteq \rho_\tau(A)$ holds for all $i \in [\ell]$. Therefore,

$$(x_1, a_2, \dots, a_n) \in \rho_\tau(\{p_\ell, (\min\{a'_1 + \ell\tau_1, \text{MAX}_1\}, a'_2, \dots, a'_d)\}) \in \rho_\tau(A) .$$

Using the same arguments, we have

$$(x_1, \dots, x_i, a_{i+1}, \dots, a_d) \in \rho_\tau(A' \cup \{(x_1, \dots, x_{i-1}, a_i, \dots, a_d)\}) \subseteq \rho_\tau(A)$$

for $i = 2, \dots, d$, completing the proof of (i).

Regarding (ii), $\rho_\theta(A) = A$ for $\theta = 0$ and each block consists of a single point. It is closed as A is finite. For $\theta > 0$ the claim follows from Theorem 4 and (i). \square

We are ready to state the following result for Problem 8 for $\mathcal{M} = \mathcal{M}_U$:

Theorem 17. *For all $d \in \mathbb{N}$ and $\tau > 0$, there is a representation scheme μ_U for \mathcal{M}_U and τ . Furthermore, Algorithm 1 solves Problem 8 for \mathcal{M}_U , μ_U , and τ in time*

$$\mathcal{O}(m_\oplus^2 \log m_\oplus + m_\oplus^2 d + m_\oplus m_\ominus d) . \quad (15)$$

Proof. Let $\theta > 0$. By Proposition 16, \mathcal{M}_U is blockwise convex for θ . Furthermore, by (ii) of Proposition 16, for all $d \geq 0$ and $A \in [U_d]^{<\infty}$, $\rho_\theta(A)$ is the union of k axis-aligned hyperrectangles of U_d , where $k = |\mathcal{B}(\rho_\theta(A))| \leq |A|$. Utilizing the fact that an axis-aligned hyperrectangle can be represented by its minimum and maximum vertices, we define $\mu'_U(\theta, A)$ for all $A \subseteq U_d$ by (A_{\min}, A_{\max}) if $A = U_d[A]$; otherwise by \perp , where A_{\min} (resp. A_{\max}) denotes the component-wise minimum (resp. maximum) of the points in A .⁵ Clearly, μ'_U satisfies (4) and (5). Define $\mu_U : \mathbb{R}_{>0} \times [U_d]^{<\infty} \rightarrow 2^{\{0,1\}^*}$ by

$$\mu_U(\theta, A) = \{\mu'_U(B) : B \in \mathcal{B}(\rho_\theta(A))\}$$

for all $d \geq 0$ and $A \in [U_d]^{<\infty}$. It holds that μ_U is a representation scheme for \mathcal{M}_U and τ . Defining μ in Problem 8 by μ_U , (15) then follows by Theorem 13 by noting that T_S, T_D, T_J, T_M in Theorem 13 are all in $\mathcal{O}(d)$ time for $\mathcal{M} = \mathcal{M}_U$. \square

⁵We assume that real numbers are represented in $\mathcal{O}(1)$ space up to a certain precision.

A few comments on this result are in order. First, similar to Theorem 15, we obtained Theorem 17 in a fairly *simple* way by using our general result in Theorem 13. Second, the number of hyperrectangles returned by Algorithm 1 in polynomial time is *optimal* with respect to the set of weakly convex hulls of the positive examples. However, the hyperrectangles must be pairwise *non-overlapping*. In contrast, it is NP-hard to find the smallest number of possibly *overlapping* axis-aligned rectangles whose union is consistent with the examples, even for $d = 2$ (Bereg et al., 2012). Third, as we show below in Theorem 18 by using Theorem 17, the concept class formed by the θ -convex union of axis-aligned hyperrectangles is polynomially PAC-learnable. More precisely, we prove that for all $d > 0$, the concept class $\mathcal{HR}_{d,\theta} = \{\rho_\theta(A) : A \in [U_d]^{<\infty}\}$ is polynomially PAC-learnable for sufficiently large θ . We prove the claim for $d > 0$ by noting that it is straightforward for $d = 0$.

Theorem 18. *For any constant $c \geq 0$, $\mathcal{HR}_{d,\theta}$ is polynomially PAC-learnable for all $d \in \mathbb{N}$ and $\theta \geq \frac{2d}{e} \sqrt[d^{c-1}]{\frac{e}{d^{c-1}}}$.*

Proof. If $\theta \geq d$, then Proposition 16 implies that all concepts in $\mathcal{HR}_{d,\theta}$ consist of a single axis-aligned hyperrectangle of U_d ; this concept class is known to be efficiently PAC-learnable. For the case that $\frac{2d}{e} \sqrt[d^{c-1}]{\frac{e}{d^{c-1}}} \leq \theta < d$, by (i) of Theorem 2 it is sufficient to show that the CHF problem for $\mathcal{HR}_{d,\theta}$ can be solved in polynomial time and that the VC-dimension of $\mathcal{HR}_{d,\theta}$ is bounded by a polynomial of d . Setting $\tau = \frac{2d}{e} \sqrt[d^{c-1}]{\frac{e}{d^{c-1}}}$, we have $\theta > \tau = 0$ by $d > 0$. Proposition 16 and Theorem 17 imply that there exists a consistent hypothesis in $\mathcal{HR}_{d,\theta}$ if and only if Algorithm 1 with \mathcal{M}_U , τ , and μ defined above and for input $E^+, E^- \in [U_d]^{<\infty}$ returns a solution \mathcal{R} of the CHF problem such that for all $R_1, R_2 \in \mathcal{R}$ with $R_1 \neq R_2$, $D_1(R_1, R_2) > \theta$. Furthermore, Algorithm 1 runs in polynomial time. The proof then follows by Lemma 23 (see the Appendix), which states that

$$\text{VC}_{\dim}(\mathcal{HR}_{d,\theta}) = \mathcal{O}(d^{c+1} \log d) .$$

□

Learning Weakly Convex Unions of Polygons

In the previous example, the Manhattan distance D_1 induced axis-aligned hyperrectangles over \mathbb{R}^d . Our third example is concerned with the metric space $\mathcal{M}_2 = (\mathbb{R}^2, D_2)$. For this case, the Euclidean distance D_2 induces weakly convex unions of convex polygons. Using Algorithm 1 and Theorem 13, we show that the CHF problem can also be solved efficiently for this class of weakly convex hypotheses.

To present this result, we first recall some necessary notions. A point p of a convex set $C \subseteq \mathbb{R}^2$ is *extreme* if there are no $x, y \in C$ such that x, y, p are pairwise different and $p \in \mathcal{I}(x, y)$. Let $\text{extr}(C)$ denote the set of all extreme points of C . It is a well-known fact that if $A \in [\mathbb{R}^2]^{<\infty}$, then $\rho(A)$ is a convex polygon and $\text{extr}(\rho(A)) \subseteq A$ (see, e.g., Krein and Milman, 1940). A subset $A \subseteq \mathbb{R}^2$ is called *path-connected* if for all $x, y \in A$ there is a continuous function $f : [0, 1] \rightarrow A$ with $f(0) = x$ and $f(1) = y$. Moreover, A is called *locally convex* if for every $x \in A$ there exists $\delta_x > 0$ such that $B_{\delta_x}(x) \cap A$ is convex, where $B_r(x) = \{y \in X : D(x, y) < r\}$.

Proposition 19. *\mathcal{M}_2 satisfies the following properties:*

- (i) For all $\tau > 0$, \mathcal{M}_2 is blockwise convex for τ . In particular, if $\rho_\tau(A)$ is τ -connected for some $A \in [\mathbb{R}^2]^{<\infty}$ then $\rho_\tau(A) = \rho(A)$ is a convex polygon with $\text{extr}(\rho(A)) \subseteq A$.
- (ii) For all $A \in [\mathbb{R}^2]^{<\infty}$ and $\theta \geq 0$, $\rho_\theta(A)$ is the union of a finite set of convex polygons.

Proof. Regarding (i), clearly, \mathcal{M}_2 is complete. Let $\tau > 0$ and $A \in [\mathbb{R}^2]^{<\infty}$ such that $\rho_\tau(A)$ is τ -connected. We first show that $\rho_\tau(A)$ is (a) closed, (b) path-connected, and (c) locally convex. Property (a) is immediate from the definition of weakly convex sets. Since $\rho_\tau(A)$ is τ -connected and τ -convex, for any two of its points there is a polygonal chain and hence, a continuous path in $\rho_\tau(A)$ connecting them, implying (b). To show (c), let $x \in \rho_\tau(A)$, $\delta_x = \tau/2$, and $y, z \in B_{\delta_x}(x) \cap \rho_\tau(A)$. Then $D_2(y, z) \leq \tau$ and hence, $\mathcal{I}(y, z) \subseteq \rho_\tau(A) \cap B_{\delta_x}(x)$ because $\rho_\tau(A)$ is τ -closed and $B_{\delta_x}(x)$ is convex, implying (c). Applying the result shown independently by Tietze (1928) and Nakajima (1928) to \mathcal{M}_2 , any closed, path-connected⁶, and locally convex set in \mathcal{M}_2 is convex. Thus $\rho_\tau(A)$ is convex and hence $\rho(A) \subseteq \rho_\tau(A)$, which, together with (i) of Proposition 6, implies $\rho(A) = \rho_\tau(A)$. The proof of (i) is then completed by noting that the convex hull of any finite point set A in \mathcal{M}_2 forms a convex polygon whose extreme points lie in A (see, e.g., Krein and Milman, 1940). Finally, the proof of (ii) is immediate by (i) and Theorem 4. \square

We are ready to state the following result for Problem 8 for the case of $\mathcal{M} = \mathcal{M}_2$.

Theorem 20. For all $\tau > 0$, there is a representation scheme μ_2 for $\mathcal{M}_2 = (\mathbb{R}^2, D_2)$ and τ . Furthermore, Algorithm 1 solves Problem 8 for \mathcal{M}_2 , μ_2 , and τ in time

$$\mathcal{O}(m_\oplus^2 \log m_\oplus + m_\oplus m_\ominus \log m_\oplus) . \quad (16)$$

Proof. By Proposition 19, \mathcal{M}_2 is complete and blockwise convex for any $\tau > 0$. Furthermore, (ii) of Proposition 19 implies that for all $A \in [\mathbb{R}^2]^{<\infty}$, $\rho_\theta(A)$ is the union of k convex polygons where $k = |\mathcal{B}(\rho_\theta(A))| \leq |A|$. Define $\mu_2 : \mathbb{R}_{>0} \times [\mathbb{R}^2]^{<\infty} \rightarrow \{0, 1\}^*$ by

$$\mu_2(\theta, A) = \{\text{extr}^\circ(B) : B \in \mathcal{B}(\rho_\theta(A))\}$$

for all $A \in [\mathbb{R}^2]^{<\infty}$, where $\text{extr}^\circ(B)$ is the sequence of the extreme points of the convex polygon B in counterclockwise order, starting with some canonical (e.g., the lexicographically smallest) extreme point. One can easily check that μ_2 is a representation scheme for \mathcal{M}_2 and τ with $\mu_2'(\theta, A)$ defined by $\text{extr}^\circ(\rho_\theta(A))$ for all $A \in [\mathbb{R}^2]^{<\infty}$ if $\rho_\theta(A)$ is a convex polygon in \mathcal{M}_2 ; otherwise by \perp . Defining μ in Problem 8 by μ_2 , for T_S, T_D, T_J, T_M in Theorem 13 we have that T_S can be carried out in $\mathcal{O}(1)$ time by noting $\mu_2'(\theta, \{x\}) = (x)$, T_D in $\mathcal{O}(\log m_\oplus)$ (Edelsbrunner, 1985), T_J in $\mathcal{O}(m_\oplus \log m_\oplus)$ using, e.g., Graham's scan (Graham, 1972) for computing the convex hull of the extreme points of two blocks, and

⁶In its general form, the Tietze-Nakajima theorem is stated for subsets of $\mathcal{M}_d = (\mathbb{R}^d, D_2)$ that are closed, connected, and locally convex. A subset $A \subseteq \mathbb{R}^d$ is *connected* if there are no open sets $A_1, A_2 \subseteq \mathbb{R}^d$ such that $A \cap A_1, A \cap A_2 \neq \emptyset$, $A_1 \cap A_2 \cap A = \emptyset$, and $A \subseteq A_1 \cup A_2$, where a set $B \subseteq \mathbb{R}^d$ is *open* if for all $x \in B$ there is $\epsilon > 0$ such that $B_\epsilon(x) = \{y \in \mathbb{R}^d : D_2(x, y) < \epsilon\} \subseteq B$. It is a well-known fact that path-connectedness implies connectedness even in general topological spaces.

T_M in $\mathcal{O}(\log m_\oplus)$ time by partitioning the plane into m_\oplus wedges (see Chapter 2 of Preparata and Shamos, 1985). We obtain (16) by substituting these time complexities into (11). \square

A few remarks on the algorithmic details are in order. All algorithms discussed in the proof of Theorem 20 work with a sequence of extreme points in counterclockwise order as a representation for the involved convex polygons. The algorithm of Edelsbrunner (1985) for computing the minimum distance of two polygons with m_1 and m_2 extreme points, respectively, has an asymptotic runtime of $\mathcal{O}(\log m_1 + \log m_2)$. It assumes, however, that the two convex polygons do not intersect. In our setting, it is easy to find examples where this does not hold during the execution of Algorithm 1. This is not a problem because, as Edelsbrunner (1985) also mentions, there are algorithms detecting the intersection of two convex polygons having the same time complexity (see, e.g., Dobkin and Kirkpatrick, 1983). Last but not least, the algorithm in (Preparata and Shamos, 1985) for deciding the membership problem in convex m -gons requires a $\mathcal{O}(m)$ time preprocessing step. It can be carried out directly after the join operation.

Finally, since the VC-dimension of convex polygons is unbounded, we cannot apply Theorem 2 to prove polynomial PAC-learnability for the concept class formed by weakly convex unions of polygons.

6 The Extensional Learning Setting

In this section, we present Algorithm 2, an adaptation of Algorithm 1 to the case of learning *extensional* weakly convex hypotheses, i.e., which are given by enumerating their elements. Accordingly, the domains are restricted to *finite* metric spaces. This learning setting naturally arise when weakly convex sets have no concise representation, e.g., in case of performing vertex classification in graphs. Similarly to Problem 8 in Section 5, we consider the case that θ is *not* given in advance and return the *largest* weakly convex hull of the positive examples that is consistent with the negative examples. Out of the consistent weakly convex hulls, it is the closest approximation of the convex hull of the positive examples. More precisely, we consider the following CHF problem:

Problem 21. Given a metric space $\mathcal{M} = (X, D)$ with $|X| = n$ for some positive integer n and disjoint sets $E^+, E^- \subseteq X$ of positive and negative examples, return

$$\max_{\theta \geq 0} \{ \rho_\theta(E^+) : \rho_\theta(E^+) \cap E^- = \emptyset \} .$$

Note that $E^+ \cap E^- = \emptyset$ and $\rho_0(E^+) = E^+$ together imply that Problem 21 always has a solution. Let $\theta_1 < \dots < \theta_k$ be the pairwise distances in X computed in line 1 of Algorithm 2 and define θ_0 by 0. The solution of Problem 21 can be obtained for some $\theta \in \{\theta_0, \theta_1, \dots, \theta_k\}$ because for all $A \subseteq X$, $\rho_{\theta_i}(A) = \rho_\theta(A)$ for all $\theta \in [\theta_i, \theta_{i+1})$, for every $i = 0, \dots, k-1$, and $\rho_{\theta'}(A) = \rho(A)$ for all $\theta' \geq \theta_k$. Algorithm 2 utilizes this fact and the monotonicity stated in Proposition 6. In particular, in iteration i of the outer loop, it calculates C_i from C_{i-1} by setting C to C_{i-1} (line 4) and adding the interval of x, y to C for all $x, y \in C$ with distance at most θ_i (cf. lines 5–6). It returns C_i for the largest i that is consistent

Algorithm 2 EXTENSIONAL CONSISTENT HYPOTHESIS FINDING

Require: finite metric space $\mathcal{M} = (X, D)$

Input: disjoint sets $E^+, E^- \subseteq X$ with $E^+ \neq \emptyset$

Output: $\rho_\theta(E^+)$ such that $\rho_\theta(E^+) \cap E^- = \emptyset$ and $\rho_{\theta'}(E^+) \cap E^- \neq \emptyset$ for all $\theta' > \theta$ satisfying $\rho_{\theta'}(E^+) \supseteq \rho_\theta(E^+)$

```
1: compute and sort all pairwise distances in  $X$ 
2:  $C_0 \leftarrow E^+$ 
3: for  $i = 1, \dots, k$  do
4:    $C \leftarrow C_{i-1}$ 
5:   while  $\exists x, y \in C$  with  $0 < D(x, y) \leq \theta_i$  do
6:     if  $\mathcal{I}(x, y) \cap E^- = \emptyset$  then  $C \leftarrow C \cup \mathcal{I}(x, y)$  // cf. (3) for the def. of
        $\mathcal{I}(x, y)$ 
7:     else return  $C_{i-1}$ 
8:    $C_i \leftarrow C$ 
9: return  $C_i$ 
```

with E^- . One can easily check that $C_i = \rho_{\theta_i}(E^+)$ for all $i \geq 0$, implying the correctness of Algorithm 2.

Regarding the time complexity of Algorithm 2, one can maintain the set of pairs x, y considered in line 5 in an RB tree with their distances as keys. Utilizing the fact that each pair of points in X is considered at most once, we need $\mathcal{O}(\log n)$ time for the insertion and for the deletion of a pair in the RB tree, where $n = |X|$. Furthermore, the interval $\mathcal{I}(x, y)$ can be calculated in $\mathcal{O}(n)$ time for all $x, y \in X$ from the pairwise distances computed in line 1. Thus, since the total number of pairs x, y considered in line 5 is $\mathcal{O}(n^2)$, the total time of the outer loop is $\mathcal{O}(n^3)$. Denoting the time complexity of computing all pairwise distances in line 1 by $T_P(\mathcal{M})$, we have the following result:

Theorem 22. *Algorithm 2 solves Problem 21 correctly in $\mathcal{O}(T_P(\mathcal{M}) + n^3)$ time and $\mathcal{O}(n^2)$ space.*

6.1 Learning Weakly Convex Sets in Graphs

In this section, we illustrate how Algorithm 2 works on vertex classification in graphs. More precisely, we experimentally demonstrate on different synthetic graph datasets that already for a relatively small set of training examples, Algorithm 2 is able to return a hypothesis that closely approximates the unknown target concept. For an undirected graph G , the underlying metric space is defined by $\mathcal{M} = (V(G), D_g)$, where D_g is the *geodesic* (or shortest-path) distance. For simplicity, G is assumed to be connected.

Datasets

For the experiments we generated two types of *synthetic* graph datasets: complete and incomplete grids, which are classical examples, e.g., in percolation theory (see, e.g., Kesten, 1982), as well as less regular graphs based on *Delaunay* triangulations (Delaunay, 1934). For each graph G , the target concept was defined by $\rho_\theta(A)$ for some $A \subseteq V(G)$ selected at random and θ defined below.

Type	Number of Vertices	Number of Graphs	Diameter Mean \pm SD		Density Mean \pm SD	
Grid	2500	845	100.77 \pm 22.88	1.037 \cdot 10 ⁻³ \pm 16.404 \cdot 10 ⁻⁵		
	5625	594	137.40 \pm 31.68	0.495 \cdot 10 ⁻³ \pm 8.784 \cdot 10 ⁻⁵		
	10000	400	173.63 \pm 41.01	0.308 \cdot 10 ⁻³ \pm 5.722 \cdot 10 ⁻⁵		
Delaunay	2500	130	56.10 \pm 1.16	2.274 \cdot 10 ⁻³ \pm 0.108 \cdot 10 ⁻⁵		
	5625	180	84.04 \pm 1.32	1.012 \cdot 10 ⁻³ \pm 0.023 \cdot 10 ⁻⁵		
	10000	178	112.45 \pm 1.52	0.570 \cdot 10 ⁻³ \pm 0.009 \cdot 10 ⁻⁵		

Table 1. Details of the balanced classification graph datasets. For each combination of graph type and size, the table shows the corresponding number of graphs and the mean and standard deviation of their diameters and edge densities.

All incomplete grids were generated from some complete non-periodic or periodic two-dimensional grid of size $\ell \times \ell$ by removing $t\%$ of the edges, where a periodic grid is obtained from a non-periodic one by connecting its corresponding boundary vertices horizontally and vertically. The edges for removal were selected uniformly at random, subject to the constraint that the resulting graph remained connected. For all $\ell \in \{50, 75, 100\}$, $t \in \{0, 20, 40\}$, $|A| \in \{10, 20, 30, 40\}$, and $\theta \in \{10, 15, 20, 25, 30\}$, we generated 25 periodic and 25 non-periodic grids with target concept $V^+ = \rho_\theta(A)$ and $V^- = V(G) \setminus V^+$. Note that $t = 0$ corresponds to complete grids. Our explorations clearly showed that extremely good classification results were obtained for strongly imbalanced graphs, either because V^+ formed an (almost) convex set (when $|V^+| \gg |V^-|$) or because most blocks of V^+ were singletons (when $|V^+| \ll |V^-|$). For our learning experiments we therefore used only those graphs that satisfied the constraint $|V^+|/|V| \in [0.25, 0.75]$ (see Table 1 for more details).

The synthetic graphs in the second type were generated by *Delaunay* triangulations (Delaunay, 1934). For each graph G we selected a finite set of points from the unit square $[0, 1]^2$ uniformly at random for $V(G)$ and connected two points $u, v \in V(G)$ by an undirected edge if and only if they co-occur in a triangle of the Delaunay triangulation. To increase the diameter of the generated graphs, we only kept the 95th percentile of edges with respect to the Euclidean length. To ensure connectivity, we deleted all isolated vertices after the edge removal. In this way, we generated 25 Delaunay graphs, each with a target concept, for all combinations of $|V(G)| \in \{2500, 5625, 10000\}$, $|A| \in \{10, 20, 30, 40\}$, $\theta \in \{10, 15, 20, 25, 30\}$, and set $V^+ = \rho_\theta(A)$ and $V^- = V(G) \setminus V^+$. For similar reasons discussed above for grids, we used only graphs satisfying $|V^+|/|V| \in [0.25, 0.75]$ for our experiments (see Table 1).

In the learning problem over a particular graph, the target concept V^+ as well as θ are both unknown to the learning algorithm. About 64.4% of the selected target concepts consist of a single block. However, this does not necessarily imply that these target concepts are convex (see, e.g., the example in Remark 7). For each graph in the experiments, we constructed 10 learning tasks by sampling $|E^+| = |E^-| \in \{10, 20, 30, \dots, 100\}$ positive and negative examples independently and uniformly at random from V^+ and V^- , respectively. We note that the hypotheses computed by Algorithm 2 can have *two-sided* error. Besides false negatives, we can have also false positives. For example, the algorithm can

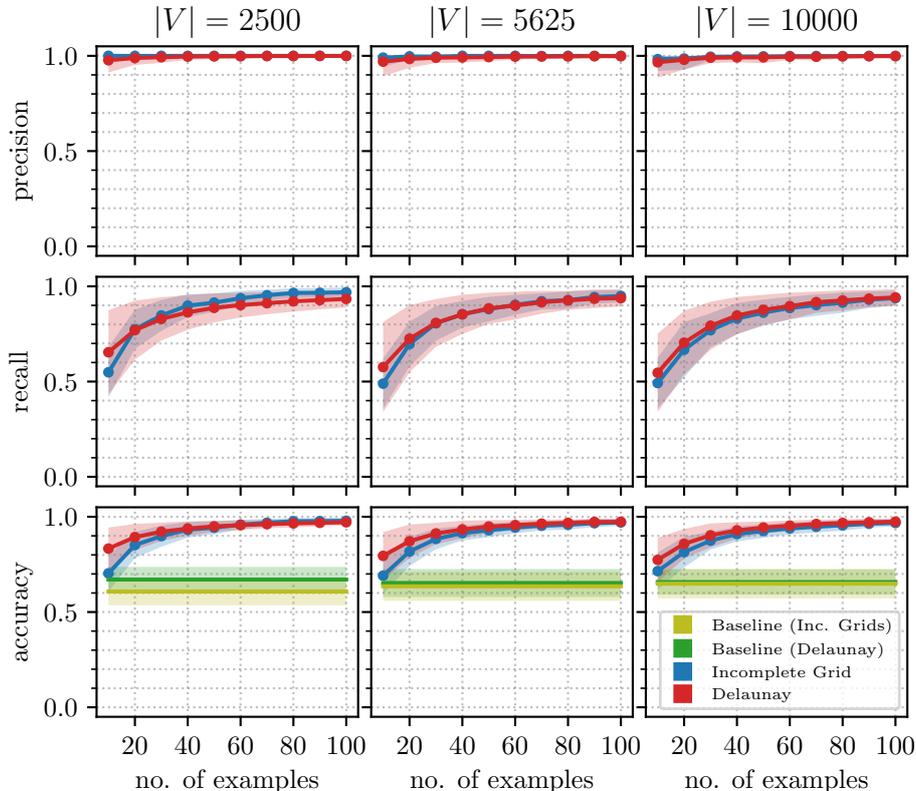


Figure 3. Precision, recall, and accuracy (y -axes) for various number of training examples (x -axes) for the balanced graphs with different graph sizes ($|V|$).

overestimate θ . Our early explorations of the experiments have, however, shown that this happened rarely. Thus, we expect a precision of 1.0 in most of the cases. Accordingly, the recall is the interesting performance indicator. Nonetheless, we also measure the accuracy in order to compare our learner to the naïve majority baseline classifier defined by $\max\{|V^+|/|V|, |V^-|/|V|\}$.

Results

The results are depicted in Figure 3. They are grouped vertically by the graphs’ size (i.e., $|V|$). We plot the *mean* precision, recall, and accuracy results (y -axes) obtained for different number of training examples (x -axes) with Algorithm 2 for grids (blue plots) and Delaunay graphs (red plots).⁷ In addition, we provide the mean baseline accuracy (green plots). For all plots, the shaded area indicates one standard deviation from the mean value of the respective performance measure. For $|E^+| = |E^-| \geq 20$, our learner outperforms the baseline significantly. It is remarkable that the learner does *not* require much more examples with increasing graph sizes to achieve the same performance. For example, on

⁷We note that in the case of Delaunay graphs, the experiments were carried out with weighted graphs as well, where the weight of an edge was defined by the Euclidean distance of its points. The predictive performance in the weighted case was slightly, but not substantially worse. The overall picture was the same as presented in Figure 3.

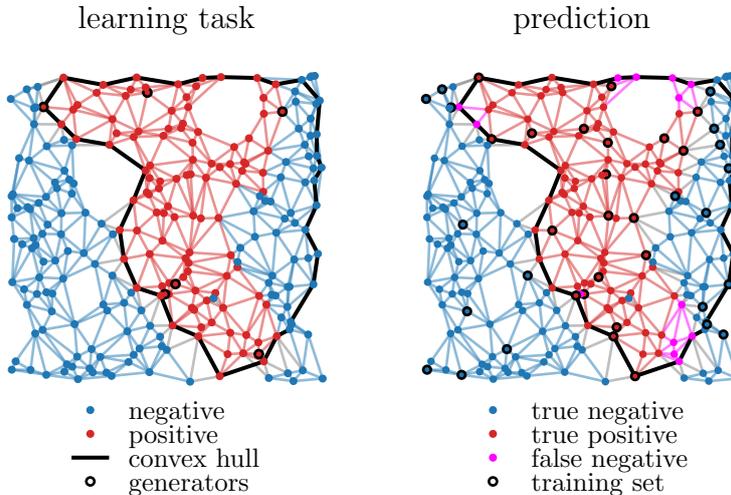


Figure 4. An exemplary Delaunay graph with 250 vertices. On the left, the unknown target concept (depicted in **red**). It is the θ -convex hull of the six generator vertices marked with black border for $\theta = 8$. The target concept is *not* convex; the convex hull of the generators contain the vertices enclosed by the black line. Notice that there is a negative point enclosed by three positive points in the lower part of the target concept. On the right, the figure shows the prediction of the hypothesis returned by our generic algorithm for the 40 training examples marked with a black border. The image depicts **true positives**, **true negatives**, and **false negatives**. In this case, there were no false positives. The convex hull of the positive examples contain the vertices enclosed by the black line. In this example it is the same as the convex hull on the left.

average 40 training examples are sufficient to achieve an accuracy of at least 0.9, regardless of the graph type. One can also observe that for all graph types and graph sizes, the baseline is between 0.6 and 0.7 on average with a standard deviation of less than 0.078. This is due to the fact that it is defined by majority.

In Figure 4 we give an illustrative example of a learning task for a Delaunay-based graph with $|V| = 250$, together with the node prediction using 40 trainings examples (20 positive and 20 negative examples). The training examples are marked with black outline and the predictions are encoded by colors. In particular, dark red corresponds to true positive, dark blue to true negative, and pink to false negative nodes. In this particular example we have no false positive node, which was the case for most graphs. Figure 2b in Section 4.1 depicts one of the actual Delaunay target concepts that were used in our experiments for 10,000 nodes. It consists of 3,518 nodes in 5 blocks. Notice the singleton block on the far bottom right.

In summary, our experimental results clearly show that using our *generic* Algorithm 2, a remarkable predictive accuracy can be obtained already with relatively small training sets, even though our approach does *not* utilize any domain-specific knowledge. We emphasize that the focus of this paper is on investigating different aspects of the CHF problem for hypotheses over arbitrary, and not for some specific metric spaces. The design and a systematic empirical evaluation of a domain-specific algorithm from our adaptation that, in addition,

utilizes some structural properties of the underlying graph goes beyond the scope of this paper (cf. Section 7 for a discussion).

7 Concluding Remarks

The illustrative examples in Sections 5.1 and 6.1 clearly demonstrate the usefulness and relevance of weakly convex sets for *machine learning*. While our focus in this work was solely on applications to *machine learning*, weakly convex sets seem to be useful for *data mining* applications (e.g., itemset mining, subgroup discovery) as well. Another potential application area could be *conceptual spaces* spanned by so-called *quality dimensions*, a general framework introduced by Gärdenfors (2000, 2014) for *geometric* representation of concepts. Gärdenfors’ underlying thesis for his theory is that *natural* concepts are *convex* regions of conceptual spaces. It is an interesting question whether *weak convexity* can be used effectively to *decompose* concepts into semantically *meaningful* “subconcepts”.

The inner loop of Algorithm 1 iteratively joining the blocks is very similar to *single linkage clustering*, raising the following question: Can the time complexity stated in Theorem 13 be further improved by using techniques (e.g., Sibson, 1973) that accelerate single linkage clustering algorithms?

The goal in Problems 8 and 21 is to return a θ -convex hull of the positive examples for the *largest* θ that does not contain any of the negative examples. This θ -convex hull is, however, *not* necessarily optimal with respect to the number of blocks.⁸ The number of blocks in a θ -convex set is bounded by the cardinality of the largest set S satisfying $D(x, y) > \theta$ for all $x, y \in S$. For graphs, this cardinality is precisely the θ -*independence number*, which is NP-hard to compute (Garey and Johnson, 1979). A related result of Bereg et al. (2012) states that the less restrictive problem of finding a consistent k -fold union of (possibly overlapping) axis-aligned hyperrectangles with *minimum* k is also NP-hard. In contrast, Problem 8 is computationally *tractable* because the solution can be found by searching in the monotone chain of θ -convex hypotheses that is uniquely defined by the training examples. The design and study of algorithms for the *approximation* of a consistent hypothesis with the *smallest* number of blocks is an interesting direction for future research.

The notion of weak convexity can be meaningless for certain metric spaces. For example, for metric spaces (X, D_2) with *finite* domains $X \subseteq \mathbb{R}^d$, $\mathcal{I}(x, y) = \{x, y\}$ holds almost surely for all $x, y \in X$. To overcome this problem, one can consider the following *relaxation* of weak convexity which allows the triangle inequality to hold up to some *tolerance* ε , instead of equality. More precisely, a subset $A \subseteq X$ of a metric space (X, D) is (θ, ε) -*convex* for some $\theta \geq 0$ and $\varepsilon \in [0, \theta]$, if for all $x, y \in A$ and $z \in X$ it holds that $z \in A$ whenever $D(x, y) \leq \theta$ and $D(x, z) + D(z, y) \leq D(x, y) + \varepsilon$. One can show that all results of Section 4 can naturally be generalized to this relaxed definition. Another interesting question

⁸In contrast to this long version, where the consistent hypothesis finding problems are to return a consistent weakly convex *hull* of the positive examples with the *smallest* number of blocks, in the short version of this paper it was *mistakenly* defined to return a weakly convex *set* with the *smallest* number of blocks that contains all positive and none of the negative examples, and stated *erroneously* that this latter problem can be solved in polynomial time for weakly convex Boolean functions and axis-aligned hyperrectangles (Stadtländer et al., 2021, Lemmas 20 and 22).

is whether this relaxed form of weak convexity can successfully be applied to *clustering* this kind of finite point sets.

Appendix

Lemma 23. *For any constant $c \geq 0$,*

$$\text{VC}_{\dim}(\mathcal{HR}_{d,\theta}) = \mathcal{O}(d^{c+1} \log d) \quad (17)$$

for all $d \in \mathbb{N}$ and $\theta \geq \frac{2d}{e} \sqrt{\frac{e}{d^{c-1}}}$.

Proof. Note first that all concepts in $\mathcal{HR}_{d,d}$ consist of a single block formed by an axis-aligned hyperrectangle in U_d , as $D_1(x,y) \leq d$ for all $x,y \in U_d$. Furthermore, they are θ -convex for any $\theta > 0$. We claim that for θ in the lemma,

$$\mathcal{HR}_{d,\theta} \subseteq (\mathcal{HR}_{d,d})_{\cup}^{\mathcal{O}(d^c)}, \quad (18)$$

i.e., each θ -convex set in $\mathcal{HR}_{d,\theta}$ is the union of at most $\mathcal{O}(d^c)$ axis-aligned hyperrectangles. Using that $\text{VC}_{\dim}(\mathcal{HR}_{d,d}) = 2d$, we get (17) by (18) and (ii) of Theorem 2.

It remains to prove (18). Note that for any $C \in \mathcal{HR}_{d,\theta}$, the number of blocks in C is bounded by the cardinality of a largest subset $S \subset U_d$ satisfying $D_1(x,y) > \theta$ for all $x,y \in S$. We show (18) by proving

$$|S| = \mathcal{O}(d^c). \quad (19)$$

To see (19), notice first that for all $v \in U_d$, for the volume of the intersection of U_d with the L_1 d -ball $\bar{B}_{d,r}^1(v) = \{u \in \mathbb{R}^d : D_1(v,u) \leq r\}$ we have

$$\text{vol}(\bar{B}_{d,r}^1(v) \cap U_d) \geq \frac{\text{vol}(\bar{B}_{d,r}^1(v))}{2^d}. \quad (20)$$

Thus, for all x,y above it holds that $\bar{B}_{d,\theta/2}^1(x) \cap \bar{B}_{d,\theta/2}^1(y) = \emptyset$, which, in turn, implies

$$|S| \leq \frac{2^d \text{vol}(U_d)}{\text{vol}(\bar{B}_{d,\theta/2}^1(v))} \quad (21)$$

by (20). Using $\text{vol}(\bar{B}_{d,r}^1(v)) = (2r)^d/d!$ and $d! \leq d^{d+1}/e^{d-1}$ (see, e.g., Knuth, 1997), from (21) we have

$$|S| \leq \frac{d^{d+1} 2^d}{e^{d-1} \theta^d} = \mathcal{O}(d^c) \quad (22)$$

for $\theta \geq \frac{2d}{e} \sqrt{\frac{e}{d^{c-1}}}$, completing the proof of (19). \square

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