On Statistical Learning of Simplices: Unmixing Problem Revisited

Amir Najafi * Saeed Ilchi * Amir H. Saberi † Abolfazl Motahari *
Babak H. Khalaj † Hamid R. Rabiee ‡

*Bioinformatics Research Laboratory (BRL), ‡Digital Media Laboratory (DML),
Department of Computer Engineering,
Sharif University of Technology, Tehran, Iran
†Department of Electrical Engineering,
Sharif University of Technology, Tehran, Iran

Abstract

Learning of a high-dimensional simplex from uniformly-sampled observations, generally known as the “unmixing problem”, is a long-studied task in computer science. More recently, a significant interest is focused on this problem from other areas, such as computational biology and remote sensing. In this paper, we have studied the Probably Approximately Correct (PAC)-learnability of simplices in terms of sample complexity. Our analysis shows that a sufficient sample size for reliable learning of a $K$-simplex is only $O(K^2 \log K)$, which yields a significant improvement over the current bound, i.e. $O(K^{22})$. In particular, we propose a continuous-relaxation for Maximum Likelihood estimator which comes with a certificate of PAC-learnability, and is also followed by a scalable algorithm whose performance is extensively tested on synthetic and real-world datasets. Experimental results show that not only being comparable to rival methods on noiseless samples, our framework is superior to the state-of-the-art in noisy cases.

1 Introduction

In many applications, any high-dimensional measurement from a physical system can be thought as a weighted average of a fixed number of unknown sources, where profiles associated to each source might not be easy to assess, separately. Moreover, combination weights for each measurement are assumed to be unknown as well. However, one can still attempt to infer the source profiles through careful analysis of a sufficiently large collection of samples. This computational problem arises in many areas, such as hyper-spectral remote sensing [1, 2], statistical mixture analysis, and recognition of tumor heterogeneity in cancer sciences and bioinformatics [3, 4, 5]. In all such cases, unmixing the data refers to the learning of all the unknown source profiles, as well as weights for all observed samples.

From a geometric point of view, this problem can be formulated as learning of a high-dimensional simplex. A $K$-dimensional simplex is defined as the set of all convex combinations of $K + 1$ fixed...
points in $\mathbb{R}^K$, also called vertices. For example, simplices with $K = 2$ and $K = 3$ correspond to triangles and tetrahedra, respectively. Learning of a simplex refers to inferring its vertices through observing randomly chosen points from its interior. This problem can also be viewed as solving the following set of equations:

$$\Theta p_i = X_i, \quad i = 1, \ldots, n,$$

where $X_i \in \mathbb{R}^K$ represents the $i$th observed points, each column of the $K \times (K+1)$ matrix $\Theta$ denotes a source profile, and $p_i \in [0,1]^{K+1}$ is the $i$th weight vector (with $1^T p_i = 1$) which generates $X_i$ from the source profiles. Note that matrix $\Theta$ and all the weight vectors $p_i$ are assumed to be unknown. For the sake of identifiability, we further assume that $\Theta$ has a bounded condition number, and $p_i$s are generated independently and distributed identically.

Some interesting questions in this setting would be: How many samples are required to reliably approximate the unknown simplex (sample complexity)? Or how well any algorithm can perform if observations become noisy? In this study, we have analyzed the sample complexity of learning simplices, and show that a sufficient sample size to ensure a total-variation error of at most $\epsilon$ with probability at least $1 - \zeta$ is

$$n \geq O \left( \frac{K^2 \log K}{\epsilon^2 \log \frac{1}{\zeta}} \right),$$

which is achievable by the Maximum Likelihood (ML) estimator. To the best of our knowledge, this result yields a significant improvement over the only existing bound, i.e. [6], where the sample complexity is $n \geq O(K^{22})$. However, ML algorithm is involved with combinatorial optimization and happens to be NP-hard for this particular problem. Motivated by this fact, we have proposed a (sub-optimal) continuously-relaxed scheme with a certificate of PAC-learnability, and the same sample complexity (order-wise) as that of ML. We do not provide a convexity guarantee for our relaxation, however, a heuristic Gradient Descent (GD)-based algorithm for the numerical optimization of our method is still derived and implemented. Experimental results demonstrate an acceptable performance for our method in the noiseless case, while they show a considerable superiority over rival strategies when data samples are noisy.

The paper is organized as follows: Section 1.1 reviews the related works. Section 2 explains the mathematical notation and also formally defines our problem. Our proposed method and theoretical results are presented in Section 3. Section 4 is devoted to experimental results on both synthetic and real-world datasets. Finally, conclusions are made in Section 5.

### 1.1 Related Works

Previous works in this domain can be divided into two separate categories: papers that follow a theoretical approach, and those trying to solve a real-world problem via heuristics.

From the theoretical side, authors of [7], a seminal work on learning linear transformations, proved the efficient PAC-learnability of hyper-cubes via $O(K^8)$ samples. They suggested a possibly similar result for simplices. However, authors in [6] have recently proved that simplices are efficiently PAC-learnable with a sample size of $n \geq O(K^{22})$, which seems far from the actual minimal sample complexity. From an algorithmic point of view, the ML estimator in the noiseless setting is equivalent to finding the minimum volume simplex that contains all the data points. This task is shown to be NP-hard, irrespective of the input representation which could be either via facets

---

1 In this paper, the term PAC-learnable refers to a learning task with a polynomial sample complexity w.r.t. $\epsilon$ and $\zeta$. This notation is consistent with that of [22]. Those cases which have a polynomial computational complexity as well, have been denoted as Efficiently PAC-learnable.
or vertices [8]. In this regard, [9] introduced an LP-relaxation that computes the determinant of a modified vertex matrix instead of the volume. Determinant can then be written as the sum of matrix co-factors and consequently optimized in a row-wise manner. However, authors do not provide any theoretical guarantees, while experiments are used for justification of their method. Authors of [10] studied a similar problem in lattice-based cryptography, where inputs are generated from a parallelepiped instead of a simplex. Our problem also shares some similarities to the Blind Source Separation (BSS) research, and in particular, the Independent Component Analysis (ICA) technique. However, assumptions on the statistical generation of weight vectors $p_i$ are crucially different in such cases. As a result, researchers in this area usually employ high-order statistical moments for capturing the source signals [11].

From a more applied perspective, learning of simplices is of practical interest in a variety of applications, including hyper-spectral imaging [12]. Hyper-spectral cameras capture electromagnetic energy scatters from a scene in multiple wavelengths, where the spectrum of each pixel is a combination of reflected (or radiated) patterns of its basic elements [2, 13]. Recently, this field has attracted an intensive research interest, which are mostly centered on analysis of the minimum volume simplex, c.f. [1, 2, 14, 15]. Another tightly related application to our paper is the recognition of common patterns in cancer tumors [4]. Tumors can have a high cell-type heterogeneity, and a sufficient knowledge of the genetic characteristics that correspond to each cell-type is vital for suggesting an effective treatment. However, biological datasets are mostly in bulk format which means each sample is an aggregation of cell populations from all the different cell-types. Again, the idea of finding the smallest inclusive simplex for capturing these hidden characteristics is exploited in several recent articles [3, 4, 5, 16].

2 Notation and Definitions

For $K \in \mathbb{N}$, let us denote the number of vertices in our model by $K+1$. Without loss of generality, the dimensionality of data points can be assumed to be $K$. Let us denote $\Phi$ as the set of all discrete $(K+1)$-dimensional probability mass functions, i.e. $\Phi \triangleq \{ p \in \mathbb{R}^{K+1} \mid \sum_k p_k = 1, p_k \geq 0 \}$. $\Phi$ is generally referred to as the standard simplex. Assume $\theta_0, \ldots, \theta_K \in \mathbb{R}^K$, and let $\Theta \triangleq [\theta_0 \mid \cdots \mid \theta_K]$ to denote the vertex matrix, where the $k$th column of $\Theta$ represents the $k$th vertex. We define $\mathcal{S}$ as a $K$-simplex with the vertex matrix $\Theta$ as

$$\mathcal{S} = \mathcal{S}(\Theta) \triangleq \left\{ x \in \mathbb{R}^K \mid x = \sum_k p_k \theta_k, \ p \in \Phi \right\}.$$  

Also, $\mathcal{S}_K$ represents the set of all $K$-simplices in $\mathbb{R}^K$. For a $K$-simplex $\mathcal{S} \in \mathcal{S}_K$, $\text{Vol}(\mathcal{S})$ denotes the Lebesgue measure (or volume) of $\mathcal{S}$. For $\mathcal{S} \in \mathcal{S}_K$, let $\mathcal{S}_{-k}$ be the $k$th polygonal facet of $\mathcal{S}$, or equivalently, the $(K-1)$-simplex obtained by removing the $k$th vertex of $\mathcal{S}$.

In Section 3 we argue that in continuously-relaxed regimes, learning of a simplex may heavily depend on its level of geometric regularity. In other words, simplices with more or less equally-sized facets are much easier to learn, compared to those which include very acute corners. Inspired by the isoperimetric inequality in geometry [17], let us define the $(\lambda, \bar{\lambda})$-isoperimetricity property for a $K$-simplex as follows:

---

$^2$Points within a $K$-simplex lie on a $K$-dimensional affine subspace, which is almost surely identifiable and efficiently learnable as long as $n \geq K+1$.  

3
Definition 1. A $K$-simplex $S(\Theta) \in \mathbb{S}_K$ for $\Theta \triangleq [\theta_0] \cdots [\theta_K]$ is said to be $(\Delta, \bar{\lambda})$-isoperimetric for some $\Delta, \bar{\lambda} > 0$, if
\[ \max_{k,k'} \| \theta_k - \theta_{k'} \|_2 \leq \Delta \text{Vol}(S)^\frac{1}{K}, \quad \max_k \text{Vol}(S_k) \leq \bar{\lambda} \text{Vol}(S)^{\frac{K-1}{K}}. \]

The essence of $(\Delta, \bar{\lambda})$-isoperimetricity property is to ensure that a given $K$-simplex is comparably stretched along all the $K$ dimensions of $\mathbb{R}^K$. According to Lemma 6 (see Appendix D), for a perfectly regular simplex with equal side lines and all $K \in \mathbb{N}$, $\Delta$ and $\bar{\lambda}$ can be chosen to be as small as 1 and $e$, respectively. For a simplex $S \in \mathbb{S}_K$, $P_S$ denotes the probability distribution associated to $S$, i.e.
\[ P_S(X) \triangleq \frac{1_S(X)}{\text{Vol}(S)}, \quad \forall X \in \mathbb{R}^K, \quad (1) \]
where $1_S(X)$ is the indicator function of the $K$-simplex $S$ which returns 1 if $X \in S$, and zero otherwise. Also, $D_{\text{TV}}(\cdot, \cdot)$ represents the total-variation distance between two probability distributions.

2.1 Problem Definition
Assume $X_1, \ldots, X_n \in \mathbb{R}^K$ to be $n$ i.i.d. samples which are generated uniformly from $S_T \in \mathbb{S}_K$, i.e. $X_1, \ldots, X_n \sim P_{S_T}(X)$. The problem is to find an approximation of $S_T$, denoted by $S^*$, from the dataset $D \triangleq \{X_1, \ldots, X_n\}$ such that with probability at least $1 - \zeta$ the total variation between $P_{S^*}$ and $P_{S_T}$ is less than $\epsilon$.

3 Statistical Learning of Simplices: Main Results

In this section, we first derive the ML estimator for $S_T$, which we denote by $S_{\text{ML}}^*$, and then propose our continuous-relaxation as a softened version of ML. Maximum Likelihood (ML) estimation of $S_T$ works by finding the maximizer of the log-likelihood function $\log P_S(D)$ according to the following formulation:
\[ S_{\text{ML}}^* \triangleq \arg\max_{S \in \mathbb{S}_K} \left\{ \log P_S(D) = \log \prod_{i=1}^n P_S(X_i) = \sum_{i=1}^n \log 1_S(X_i) - n \log \text{Vol}(S) \right\}. \quad (2) \]
Solving for (2) is proved to be NP-hard, and thus impractical in real-world situations. A solution for the computational hardness of ML estimation is to replace its original objective function with a continuously-relaxed surrogate. In order to do so, first it should be noted that the program in (2) is equivalent to the following constrained minimization problem:
\[ S_{\text{ML}}^* = \arg\min_{S \in \mathbb{S}_K} \text{Vol}(S) \]
subject to $\min_{u \in S} \| X_i - u \|_2 = 0$, $\forall i$. \quad (3)
Motivated by the formulation in (3), one can employ the idea of Lagrangian relaxation and propose the following Continuously-Relaxed Risk (CRR) in order to approximate $S_T$.  

4
Definition 2 (Continuously-Relaxed Risk). Assume a dataset \( D = \{X_1, \ldots, X_n\} \) in \( \mathbb{R}^K \), parameter \( \gamma \geq 0 \), and an increasing and integrable function \( \ell : \mathbb{R} \to \mathbb{R} \). Then, the empirical Continuously-Relaxed Risk \( \hat{R}_{\text{CRR}} : \mathcal{S}_K \to \mathbb{R} \) is defined as:

\[
\hat{R}_{\text{CRR}} (\mathcal{S}; D, \gamma, \ell) \triangleq \frac{1}{\sqrt{n}} \sum_{i=1}^{n} \ell \left( \min_{u \in \mathcal{S}} \|X_i - u\|_2 \right) + \gamma \text{Vol} (\mathcal{S}).
\]

Also, let us define

\[
\mathcal{S}^* = \mathcal{S}^* (D, \gamma, \ell) \triangleq \arg\min_{\mathcal{S} \in \mathcal{S}_K} \hat{R}_{\text{CRR}} (\mathcal{S}; D, \gamma, \ell),
\]

as an approximation of \( \mathcal{S}_T \).

Parameter \( \gamma > 0 \) and \( \ell (\cdot) \) can be chosen by the user, where \( \ell (\cdot) \) must be increasing and integrable, but does not need to be strictly increasing or even continuous in general. However, choosing a differentiable \( \ell \) makes \( \hat{R}_{\text{CRR}} (\mathcal{S} (\Theta); D, \gamma, \ell) \) to be differentiable w.r.t. the vertex matrix \( \Theta \). In Section 3.2, we derive an efficient technique to numerically compute the derivatives of \( \hat{R}_{\text{CRR}} \) w.r.t. the vertex matrix \( \Theta \) which works for all differentiable functions \( \ell (\cdot) \).

3.1 PAC-Learnability and Sample Complexity

The following theorem gives an upper-bound on the information-theoretic sample complexity of learning \( \mathcal{S}_T \) via (5). Our results hold for any increasing and integrable function \( \ell : \mathbb{R} \to \mathbb{R} \).

Theorem 1 (PAC-Learnability for General \( \ell \)). Assume a \( K \)-simplex \( \mathcal{S}_T \) with Lebesgue measure \( V_T \triangleq \text{Vol} (\mathcal{S}_T) \), which is \((\lambda, \bar{\lambda})\)-isoperimetric for some \( \lambda, \bar{\lambda} \geq 0 \). Also, assume \( X_1, X_2, \ldots, X_n \) to be \( n \) i.i.d. samples uniformly drawn from \( \mathcal{S}_T \). Assume there exist \( \epsilon, \zeta > 0 \), such that

\[
n \geq \left( \frac{6 \ell (K V_T^{1/2})}{L \left( \frac{\epsilon V_T^{1/2}}{(K+1) \bar{\lambda}} \right)} \sqrt{2 \log \frac{mn}{K} + \log n + \sqrt{\log \frac{1}{\zeta}}} + \gamma V_T \epsilon \right)^2,
\]

where \( L (x) \triangleq \frac{1}{x} \int_{0}^{x} \ell (u) \, du - \ell (0) \). Then, with probability at least \( 1 - \zeta \) the optimizer of (5), denoted by \( \mathcal{S}^* \), satisfies the inequality \( \mathcal{D}_{\text{TV}} (\mathbb{P}_{\mathcal{S}_T}, \mathbb{P}_{\mathcal{S}^*}) \leq \epsilon \).

Proof of Theorem 1 is given in Appendix A. The proof includes mathematical techniques from high-dimensional geometry and calculus, as well as tools from Vapnik-Chervonenkis (VC) theory of statistical learning [22]. The general result of Theorem 1 for particular choices of the smoothing function \( \ell \) and/or under certain asymptotic regimes can be extended to several previously studied problems. The following corollaries are perhaps the two most notable consequences of Theorem 1.

Corollary 1 (Sample Complexity of ML). Assume a \( K \)-simplex \( \mathcal{S}_T \in \mathcal{S}_K \) and let \( X_1, \ldots, X_n \) to be \( n \) i.i.d. samples drawn uniformly from \( \mathcal{S}_T \). Assume there exist \( \epsilon, \zeta > 0 \), such that

\[
n \geq \frac{C \log K}{\epsilon^2} \log \frac{1}{\zeta},
\]

where \( C \) is a constant that does not depend on \( \epsilon, \zeta \) or \( K \). Then, with probability at least \( 1 - \zeta \) the maximum likelihood estimator of \( \mathcal{S}_T \), denoted by \( \mathcal{S}_{\text{ML}}^* \), satisfies \( \mathcal{D}_{\text{TV}} (\mathbb{P}_{\mathcal{S}_T}, \mathbb{P}_{\mathcal{S}_{\text{ML}}^*}) \leq \epsilon \).

The proof of Corollary 1 is given in Appendix B. Interestingly, for the case of ML estimation, one does not need to impose any geometric constraints on the shape of the simplex. On the other
hand, the particular function $\ell$ which corresponds to the result of Corollary 1 turns out to be non-smooth, which makes the optimization of (5) in this case to be combinatorial and consequently, NP-hard. This should not be surprising, since ML estimation of simplices has been already proved to be NP-hard by [8]. However, we show that for at least one class of differentiable functions $\ell$, the sample complexity for acquiring a reliable solution to (5) has the same orders of magnitude with that of ML, in terms of $\epsilon, \zeta$ and $K$.

**Corollary 2** (PAC-Learnability of Soft-ML). Assume a $K$-simplex $S_T \in S_K$ and let $X_1, \ldots, X_n$ to be $n$ i.i.d. samples drawn uniformly from $S_T$. Also, assume $S_T$ is $(\underline{\lambda}, \bar{\lambda})$-isoperimetric for some bounded $\underline{\lambda}, \bar{\lambda} > 0$. For any $\epsilon, \zeta > 0$ and parameter $\gamma \in \mathbb{R}^+$, let function $\ell : \mathbb{R} \rightarrow \mathbb{R}$ to be

$$\ell (u) \triangleq 1 - e^{-bu}, \quad \forall u \in \mathbb{R},$$

where $b \propto \frac{K}{\epsilon}$, and assume

$$n \geq \frac{C (\gamma) K^2 \log K}{\epsilon^2} \log \frac{1}{\zeta},$$

where $C (\gamma)$ does not depend on $\epsilon, \zeta$ or $K$. Then, with probability at least $1 - \zeta$, the minimizer of (5), denoted by $S^*$, satisfies the inequality $D_{TV} (\mathbb{P}_{S_T}, \mathbb{P}_{S^*}) \leq \epsilon$.

Proof of Corollary 2 is given in Appendix B. By using the Soft-ML setting of Corollary 2, the optimization problem of Definition 2 becomes differentiable w.r.t. $\Theta$ and many continuous optimization tools, such as GD, may apply. It should be noted that this result is not in contrast with the computational hardness of ML for two reasons: First, Corollary 2 does not say anything about the convexity of (4). Second, even if (4) happens to be convex with the above choice of $\ell (\cdot)$, we are still tackling a different problem compared to finding the smallest inclusive simplex which is pursued by ML.

A thorough convexity analysis of our method goes beyond the scope of this paper. As a result, we make no claim regarding the computational complexity of the continuous-relaxation in Definition 2. Instead, we derive an efficient scheme to compute the gradient of (5) w.r.t. vertex matrix $\Theta$, and show that a simple heuristic approach, such as Gradient-Descent (GD), can achieve very good performances in practice.

### 3.2 Numerical Optimization

In this section, we first show how to compute gradient of (4), numerically, in order to employ it in a heuristic GD optimization as described in Algorithm 1. Later in Section 4, we have demonstrated the convergence and effectiveness of Algorithm 1 via several computer simulations.

According to (4), $\hat{R}_{CRR} (S)$ is naturally broken into two separate terms: one controls the distance of data points from $S$, and the second one is a regularization term on its volume. Gradient w.r.t. the second part, i.e. $\gamma \text{Vol} (S)$, is straightforward, since

$$\text{Vol} (S (\Theta)) = \frac{1}{K!} \left| \det \left[ \theta_1 - \theta_0 \right] \cdots \left| \theta_K - \theta_0 \right] \right|,$$

and for any $A \in \mathbb{R}^{K \times K}$ we simply have $\nabla_A \text{det} (A) = \text{adj}^T (A)$, where $\text{adj} (\cdot)$ denotes the adjugate function. To ensure that the gradient is well-defined, assume $\Theta$ to be non-degenerate, i.e. $S (\Theta)$ has a positive volume. This assumption only excludes a zero-measure subset of solutions from $S_K$.\(^3\)

\(^3\)According to the Lebesgue measure.
Algorithm 1 Learning of simplices via Gradient Descent

1: procedure Simplex Inference$(D = \{X_1, \ldots, X_n\}, K, \ell(\cdot), \gamma, T, \alpha)$
2: Select $\{i_0, i_1, \ldots, i_K\} \subset [n]$ uniformly at random.
3: Initialize $\Theta(0) = [X_{i_0} | \cdots | X_{i_K}]$
4: for $t = 0 : \cdots : T - 1$ do
5: $\Theta(t+1) \leftarrow \Theta(t) - \alpha \nabla_\Theta \hat{R}_{CRR}(S(\Theta) ; D, \ell, \gamma)$ $\triangleright$ According to (10) and Lemma 1
6: end for
7: end procedure

For the remaining term in (4), one needs to compute the gradient vectors

$$g_{ik} = \nabla_{\theta_k} \ell \left( \min_{u \in S} \|X_i - u\|_2 \right), \quad i \in [n], \; k \in [K],$$

or more generally, the gradient matrices $G_i \triangleq [g_{i0} | \cdots | g_{iK}]$, $i \in [n]$. The following lemma gives an straightforward procedure for numerical computation of $G_i$s.

Lemma 1 (Computation of $G_i$). For every $X \in \mathbb{R}^K$, $S(\Theta) \in S_K$, and differentiable function $\ell : \mathbb{R} \rightarrow \mathbb{R}$ the following relation holds:

$$\nabla_\Theta \ell \left( \min_{u \in S(\Theta)} \|X - u\|_2 \right) = -\ell' \left( \|X - \Theta p^*\|_2 \right) \frac{(X - \Theta p^*) p^{*T}}{\|X - \Theta p^*\|_2} \in \mathbb{R}^{K \times (K+1)},$$

where $\ell' (\cdot)$ denotes the derivative of $\ell (\cdot)$, and $p^*$ is defined as the solution of the following convex quadratic program:

$$p^* \triangleq \arg\min_{p \in \mathbb{R}^{K+1}} \|X - \Theta p\|_2^2$$

subject to $1^T p = 1$, $p \geq 0$.

It should be noted that gradient equals to zero if $X - \Theta p^* = 0$, which alternatively means $X \in S(\Theta)$.

Proof of Lemma 1 is given in Appendix C. In this regard, the overall gradient of the continuously-relaxed risk, $\hat{R}_{CRR}(S(\Theta) ; D, \ell, \gamma)$, w.r.t. vertex matrix $\Theta$ can be computed as

$$\nabla_\Theta \hat{R}_{CRR}(S(\Theta)) = \frac{1}{\sqrt{n}} \sum_{i=1}^n G_i + \gamma \left[ 0_K \left| \mathrm{adj}^T \left( \Theta_{1:K} - \theta_0 1_K^T \right) \right| \left( I_{(K+1)} - \frac{1}{K+1} 1_{(K+1)}^T 1_{(K+1)} \right) \right],$$

where for $m \in \mathbb{N}$, $0_m$ is an $m$-dimensional all-zero vector, $1_m$ is an $m$-dimensional all-one vector, and $I_m$ denotes an $m \times m$ identity matrix. $\Theta_{1:K}$ represents a $K \times K$ matrix $[\theta_1 | \cdots | \theta_K]$. Moreover, matrices $G_i$ are computed according to Lemma 1.

4 Experimental Results

This section is devoted to testing the performance of our method on synthetic and real-world datasets, and to compare it with some rival frameworks. Throughout this section, estimation error is measured in terms of the average Euclidean distance between the vertices of the ground truth.
Figure 1: Snapshots from running the method on a set of $n = 40$ noiseless samples in a two-dimensional simplex. As a reference, the original triangle is drawn in green.

$S_T$ and those of the estimated simplices, which for our algorithm is denoted as $\hat{S}^4$. For simplicity in notations, assume $\Theta = [\theta_0 | \cdots | \theta_K]$ and $\hat{\Theta} = [\hat{\theta}_0 | \cdots | \hat{\theta}_K]$ to be the vertex matrices of $S_T$ and $\hat{S}$, respectively. Then, error can be formulated as follows, mathematically:

$$error^2 \triangleq \min_{(i_0, \ldots, i_K)} \frac{1}{K + 1} \sum_{k=0}^{K} \| \theta_k - \hat{\theta}_{i_k} \|^2_2,$$

where minimization is taken over all permutations $(i_0, \ldots, i_K)$ of the numbers $[K] \triangleq \{0, 1, \ldots, K\}$.

All synthetic and real-world data points have been normalized in all dimensions to remove any scaling effect from error.

For the sake of simplicity, we have chosen $\ell(u) \triangleq u^2$ as our smoothing loss function in Definition 2. Additionally, we have empirically observed that in the absence of a proper initialization for Algorithm 1 mildly-increasing functions such as $\ell(u) = u$ or $u^2$ result into a considerably faster convergence when compared to bounded functions, e.g. $\ell(u) = 1 - e^{-bu}$ of Corollary 2. Parameters $\gamma$ and the learning rate $\alpha$ in Algorithm 1 are manually adjusted to improve the performance and convergence. Noticeably, we did not observe a considerable sensitivity to these parameters.

In the proceeding parts, we report the performance of our proposed method in three different tasks: on synthetic data, an important task in computational biology, and unmixing of hyperspectral data in remote sensing applications.

4.1 Synthetic Data

Figure 1 shows four snapshots of the output of Algorithm 1 while running on a set of $n = 40$ nominal synthetic noiseless data points in $\mathbb{R}^2$. Here, $K = 2$ is chosen to facilitate the visualization of the results. The “green” simplex denotes the true underlying one, i.e. $S_T$, while the “red” simplex is the output of Algorithm 1. As it can be seen, despite the fact that algorithm has started from an inappropriate initial point, it converges to an acceptable solution in a moderate number of iterations.

Figure 2 aims to analyze the sensitivity of our method to noise and also the dimension of the simplex, i.e. $K$. We have used synthetic datasets for this purpose. In particular, Figure 2a illustrates the performance of Algorithm 1 in the presence of noise. In this regard, $n = 100$ uniformly distributed samples have been generated from a two-dimensional simplex. Each sample has been added with a noise vector, which is drawn independently from a zero-mean Gaussian

---

4We use the notation $\hat{S}$ for the output of Algorithm 1 instead of $S^*$, since $S^*$ is already defined as the global optimizer of (5). However, Algorithm 1 may converge to a local minimizer which could be different from $S^*$. 
distribution $\mathcal{N}(0, \sigma^2 I)$, where $\sigma$ denotes the standard deviation of the noise components. Let us define the Signal to Noise Ratio (SNR) as $\text{SNR} \triangleq \lambda_{\text{min}}/\sigma$, where $\lambda_{\text{min}}$ is the smallest singular value of matrix $[\theta_1 - \theta_0] \cdots [\theta_K - \theta_0]$. Figure 2a depicts the error of our algorithm w.r.t. different values of SNR. It shows that our method has a small error in moderate and high SNR scenarios. However, the performance is degraded when the strength of noise becomes comparable to that of the underlying simplex. On the other hand, Figure 2b illustrates the error as a function of dimensionality $K$. For each point of the curve, dataset size has been increased proportionally to $K^2$, however due to the choice of $\ell(u) = u^2$ (instead of the one suggested in the proof of Corollary 2), error has been observed to increases smoothly w.r.t. $K$.

In Table 1 we have compared the error performance of our method with a number of well-known computational techniques for learning of simplices, namely MVSA [1], SISAL [18], VCA [19], and UNMIX [3]. We have used three datasets for the experiments which are i) Plain dataset: $n = 100$ data points generated from a simple two-dimensional simplex, ii) Noisy dataset: a noisy version of the Plain dataset with SNR = 1 (highly noisy), and iii) High-Dimensional (HD) dataset: $n = 1000$ data points generated uniformly from a noiseless simplex with $K = 9$. According to Table 1 our method has a comparable performance both in “Plain” and “HD” datasets, while it outperforms all the rival strategies in the case of Noisy dataset. The reason behind this result might be due to continuously-relaxed nature of our method which is in contrast to the majority of existing methods in this area. In fact, the flexibility of the objective function in Definition 2 gains more robustness to scenarios where data points happen to be out of the true simplex, e.g. in the presence of noise.

|        | Plain | Noisy | HD   |
|--------|-------|-------|------|
| Proposed | 0.22  | 0.48  | 0.79 |
| MVSA   | 0.14  | 1.84  | 0.76 |
| SISAL  | 0.16  | 1.65  | 0.77 |
| VCA    | 1.09  | 1.006 | 5.93 |
| UNMIX  | 0.14  | 1.83  | -    |

Table 1: Error comparison of the proposed methods with MVSA [1], SISAL [18], VCA [19], and UNMIX [3]. Methods have been tested on three different datasets. The values of error have been averaged over several runs, such that all relative standard deviations become less than 10%. UNMIX did not execute on “HD” dataset in a reasonable time.
4.2 Computational Biology

Unmixing cell-types from biological organs has turned into a highly attractive area in bioinformatics, and in particular, of cancer sciences. Recently, authors of [20] synthetically merged cells from three different tissues (namely brain, liver and kidney) for several rounds, where combination weights were known prior to each merging round. The aim of the whole experiment was to subsequently perform deconvolution on the merged samples (via micro-array gene-expression screens), and to check whether the initial gene-expression profiles are re-attainable or not. However, their dataset is still a potentially appropriate target for Algorithm 1. In fact, we can neglect the knowledge of the combination weights, and try to blindly infer both the unknown gene-expression profiles of tissues, as well as the combination weights, directly from the gene-expression levels of samples.

We have collected \( n = 42 \) samples from the above-mentioned dataset, where the initial dimensionality of data is \( K_{\text{init}} = 31100 \). Due to the presence of redundant information in the dataset\(^5\), samples have been linearly projected onto a corresponding 41-dimensional subspace via Principal Component Analysis (PCA), and then the proposed method has been applied. Figure 3 illustrates the final results. In particular, Figure 3a shows a qualitative two-dimensional visualization of the final simplex (via the first two principal components) which matches the ground truth gene-expression profiles of the tissues with a very high accuracy. From a more quantitative perspective, Figure 3b shows the decrease in the value of \( \text{error} \) between the estimated simplex and the ground truth as a function of iteration number. It can be clearly seen that \( \text{error} \) decreases uniformly until an acceptable result is achieved. Moreover, the obtained combination weights computed by our framework highly resemble the ground truth weights of [20].

4.3 Hyper-Spectral Remote Sensing

Another major application of the “unmixing problem” falls in the area of hyper-spectral remote sensing, where researchers aim to find the chemical composition of materials in remote areas via

\(^5\)Any \( n \) points in \( R^{K_{\text{init}}} \), for \( n \leq K_{\text{init}} \) lie on a \((n - 1)\)-dimensional linear subspace which is almost surely identifiable and can be simply learned via PCA. This way, the reduction of dimensionality in this case comes with no loss of information.
hyper-spectral imaging devices. Each pixel in a hyper-spectral image is a vector including radiation intensities (in different wave-lengths) from a relatively small region of a remote place. This way, pixels can be considered as weighted averages of a limited number of radiation profiles which correspond to the elements that are likely to be present in that region. The Cuprit dataset includes \( n = 47500 \) pixels, where each pixel has been measured in effectively \( m = 188 \) spectral intervals. Authors of \cite{21} have suggested the presence of \( K = 12 \) basic elements in the region that corresponds to the dataset, however, a smaller subset of them might be dominant.

We have randomly chosen \( n = 10000 \) points from this dataset and reduced the dimensionality of data to \( \text{dim} = 10 \) via PCA. The latter is due to eliminate the majority of linear dependencies. According to a simple eigen-analysis of the data matrix, we chose the number of vertices for the simplex as \( K + 1 = 3 \). Based on the above setting, Figure 4 illustrates the performance of the proposed method on the data compared to the ground truth profiles presented in the literature. Similar to the previous sub-section, Figure 4a depicts a two-dimensional visualization, obtained from the first two principal components, of the data samples and the estimated simplex via Algorithm 1 (shown in red). For the sake of comparison, the ground truth profiles have been shown by a green simplex. Evidently, our method finds the dominant elements with an acceptable accuracy. Figure 4b shows the approximation error vs. the number of iterations for Algorithm 1.

## 5 Conclusions

This paper aims to develop a computational framework for learning of simplices in arbitrary dimensions. In order to deal with the combinatorial structure of this problem, a continuously-relaxed optimization scheme has been proposed which enjoys from theoretical sample complexity bounds. In particular, we have shown that a sufficient sample complexity for both ML and our proposed Soft-ML surrogate are \( n \geq O(K^2) \), which is a significant improvement over existing bounds. In addition, a computationally tractable algorithm is proposed for numerical optimization of our scheme. Numerous experiments magnify the applicability of our method on synthetic and real-
world datasets. Our method has shown a comparable performance to a number of well-known rival strategies on noiseless data, while shows a considerable superiority in noisy regimes. For future works, one may attempt to provide similar sample complexity bounds for the noisy case, which has not been tackled yet.

References

[1] J. Li, A. Agathos, D. Zaharie, J. M. Bioucas-Dias, A. Plaza, and X. Li, “Minimum volume simplex analysis: A fast algorithm for linear hyperspectral unmixing,” IEEE Transactions on Geoscience and Remote Sensing, vol. 53, no. 9, pp. 5067–5082, 2015.

[2] A. Ambikapathi, T.-H. Chan, W.-K. Ma, and C.-Y. Chi, “Chance-constrained robust minimum-volume enclosing simplex algorithm for hyperspectral unmixing,” IEEE Transac-
tions on Geoscience and Remote Sensing, vol. 49, no. 11, pp. 4194–4209, 2011.

[3] D. Tolliver, C. Tsourakakis, A. Subramanian, S. Shackney, and R. Schwartz, “Robust unmixing of tumor states in array comparative genomic hybridization data,” Bioinformatics, vol. 26, no. 12, pp. i106–i114, 2010.

[4] G. Satas and B. J. Raphael, “Tumor phylogeny inference using tree-constrained importance sampling,” Bioinformatics, vol. 33, no. 14, pp. i152–i160, 2017.

[5] N. S. Zuckerman, Y. Noam, A. J. Goldsmith, and P. P. Lee, “A self-directed method for cell-type identification and separation of gene expression microarrays,” PLoS computational biology, vol. 9, no. 8, p. e1003189, 2013.

[6] J. Anderson, N. Goyal, and L. Rademacher, “Efficient learning of simplices,” in Conference on Learning Theory, 2013, pp. 1020–1045.

[7] A. Frieze, M. Jerrum, and R. Kannan, “Learning linear transformations,” in Foundations of Computer Science, 1996. Proceedings., 37th Annual Symposium on. IEEE, 1996, pp. 359–368.

[8] A. Packer, “Np-hardness of largest contained and smallest containing simplices for v-and h-polytopes,” Discrete and Computational Geometry, vol. 28, no. 3, pp. 349–377, 2002.

[9] T.-H. Chan, C.-Y. Chi, Y.-M. Huang, and W.-K. Ma, “A convex analysis-based minimum-volume enclosing simplex algorithm for hyperspectral unmixing,” IEEE Transactions on Signal Processing, vol. 57, no. 11, pp. 4418–4432, 2009.

[10] P. Q. Nguyen and O. Regev, “Learning a parallelepiped: Cryptanalysis of ggh and ntru signatures,” Journal of Cryptology, vol. 22, no. 2, pp. 139–160, 2009.

[11] A. Hyvärinen, J. Karhunen, and E. Oja, Independent component analysis. John Wiley & Sons, 2004, vol. 46.

[12] S. Zhang, A. Agathos, and J. Li, “Robust minimum volume simplex analysis for hyperspectral unmixing,” IEEE Transactions on Geoscience and Remote Sensing, vol. 55, no. 11, pp. 6431–6439, 2017.

[13] A. Agathos, J. Li, J. M. Bioucas-Dias, and A. Plaza, “Robust minimum volume simplex analysis for hyperspectral unmixing,” in Signal Processing Conference (EUSIPCO), 2014 Proceedings of the 22nd European. IEEE, 2014, pp. 1582–1586.
A Proof of Theorem 1

Recall that $S^*$ is obtained as

$$S^* \triangleq \operatorname{argmin}_{S \in \mathcal{S}_K} \left\{ \hat{R}_{\text{CRR}}(S) \triangleq \frac{1}{n} \sum_{i=1}^{n} \left\{ g(X_i, S) + \gamma \text{Vol}(S) \right\} \right\}, \quad (11)$$

where $g(X, S) \triangleq \sqrt{n} \ell \left( \min_{u \in S} \| X - u \|_2 \right)$. Instead of working directly with $S^*$ and obtaining an upper bound on $D_{TV}(\mathbb{P}_S, \mathbb{P}_{S^*})$, we define the following set

$$Q(\epsilon) \triangleq \left\{ S \in \mathcal{S}_K \mid \text{Vol}(S) \leq V_T, \text{Vol}(S \cap S_T) \geq (1 - \epsilon)V_T, S \cap S_T \neq \emptyset \right\},$$

and prove the following two claims:

Claim 1: For all $S \in Q(\epsilon)$, we have $D_{TV}(\mathbb{P}_S, \mathbb{P}_{S_T}) \leq \epsilon$. 


Claim 2: The probability that $S^* \in Q(\epsilon)$ is at least $1 - \zeta$, if the number of samples satisfies

$$n \geq \left( \frac{6\ell \left( K V_T^{1/2} \right) \left( \sqrt{K^2 \log \frac{n \epsilon}{K} + \log n} + \sqrt{\log n} \right) + \gamma V_T \epsilon}{L \left( \frac{V_T^{1/2}}{(K+1)^2} \right)} \right)^2.$$ 

In fact, combining the two claims yields a proof of the theorem. Next, we prove the claims separately.

Proof of Claim 1. According to the definition and for all $S \in Q(\epsilon)$, we have

$$\text{Vol}(S) \leq V_T \quad \text{and} \quad \text{Vol}(S \cap S_T) \geq V_T (1 - \epsilon),$$

which results into the following three volume bounds: $\text{Vol}(S) \geq V_T (1 - \epsilon)$, $\text{Vol}(S - S_T) \leq \text{Vol}(S) - V_T (1 - \epsilon)$ and $\text{Vol}(S_T - S) \leq V_T \epsilon$. On the other hand, based on the definition of the total variation distance between $P_S$ and $P_{S_T}$, we have

$$D_{TV}(P_S, P_{S_T}) \triangleq \frac{1}{2} \left[ \int_{S - S_T} P_S + \int_{S_T - S} P_{S_T} + \int_{S \cap S_T} |P_S - P_{S_T}| \right] \leq \frac{1}{2} \left[ \frac{\text{Vol}(S) - V_T (1 - \epsilon)}{\text{Vol}(S)} + \epsilon \cdot \frac{V_T \epsilon}{V_T} + (1 - \epsilon) \left( \frac{V_T \epsilon}{V_T} - 1 \right) \right] = \epsilon.$$

This completes the proof.

Proof of Claim 2. Claim 2 can be shown by proving that the following three conditions are held with probability at least $1 - \zeta$:

C1: $V^* \triangleq \text{Vol}(S^*) \leq V_T$.

C2: $S^* \cap S_T \neq \emptyset$.

C3: $\text{Vol}(S^* \cap S_T) \geq (1 - \epsilon) V_T$.

In fact, the first two conditions do hold with certainty as the following lemma presents.

Lemma 2. We have $V^* \leq V_T$ and $S^* \cap S_T \neq \emptyset$, with certainty.

See Appendix D for the proof. From Lemma 2, one can deduce that $S^*$ belongs to either $Q(\epsilon)$ or $Q^c(\epsilon)$ which is defined as

$$Q^c(\epsilon) \triangleq \left\{ S \in \mathcal{S}_K \mid \text{Vol}(S) \leq V_T \, , \, \text{Vol}(S \cap S_T) < (1 - \epsilon)V_T \, , \, S \cap S_T \neq \emptyset \right\}.$$

For given $\epsilon$, we are interested in finding $n$ such that $S^* \in Q(\epsilon)$ with probability at least $1 - \zeta$. To this end, we seek an appropriate function $u(n, \epsilon)$ such that

$$\mathbb{P} \left\{ \inf_{S \in Q(\epsilon)} \hat{R}_{CRR}(S) - \hat{R}_{CRR}(S_T) > u(n, \epsilon) \right\} > 1 - \zeta.$$
Next, we find \( n \) such that \( u(n, \epsilon) \) is positive. In this way, one can deduce that \( S_T \) is preferable over all members of \( Q^c(\epsilon) \) with probability at least \( 1 - \zeta \). Since \( S^* \) is the optimal solution, it is in \( Q(\epsilon) \) with probability at least \( 1 - \zeta \).

To this aim, we obtain a candidate for \( u(n, \epsilon) \) by considering two facts for each \( S \in Q^c(\epsilon) \). First, \( \hat{R}_{CRR}(S) \) is very close to its statistical average \( \mathbb{E}_{S_T} \hat{R}_{CRR}(S) \). Second, \( \mathbb{E}_{S_T} \hat{R}_{CRR}(S) \) is sufficiently larger than \( \hat{R}_{CRR}(S_T) \). The main challenge is to show that these facts are held for all members in \( Q^c(\epsilon) \) with high probability. To prove the first fact, we define \( g_{\text{max}} \) as

\[
g_{\text{max}} \triangleq \sup_{X \in S_T} \sup_{S \in Q(\epsilon) \cup Q^c(\epsilon)} g(X, S),
\]

and use it to normalize the function \( g \) as

\[
\bar{g}(X, S) \triangleq \frac{\sqrt{n\ell}(\min_{u \in S} \|X - u\|_2)}{g_{\text{max}}}.
\]

It can be readily shown that

\[
g_{\text{max}} \leq \sqrt{n\ell} \left( \max_{u, u' \in S_T} \|u - u'\| \right) \leq \sqrt{n\ell} \left( 2KTV_T \right),
\]

which holds due to the \((\Delta, \lambda)\)-isoperimetricity assumption on \( S_T \) and the fact that \( S \cap S_T \neq \emptyset \). Defining the function set \( \mathcal{G}(\ell, \epsilon) \) as

\[
\mathcal{G}(\ell, \epsilon) \triangleq \{ \forall \bar{g}(X, S) : (X \in S_T) \times (S \in Q^c(\epsilon)) \rightarrow [0, 1] \},
\]

and using the fundamental theorem of Vapnik-Chervonenkis (VC) theory gives us the following bound, for all \( 0 < \zeta, \epsilon \leq 1 \):

\[
P \left\{ \sup_{S \in Q^c(\epsilon)} \left| \frac{\hat{R}_{CRR}(S) - \mathbb{E}_{S_T} \hat{R}_{CRR}(S)}{g_{\text{max}}} \right| \leq 2\mathcal{R}_n \{ \mathcal{G}(\ell, \epsilon) \} + \sqrt{\frac{\log \frac{2}{\zeta}}{2n}} \right\} \geq 1 - \zeta,
\]

where \( \mathcal{R}_n \{ \mathcal{G}(\ell, \epsilon) \} \) represents the Rademacher complexity of the function set \( \mathcal{G}(\ell, \epsilon) \), for sample size \( n \) and data distribution \( X_1, \ldots, X_n \sim \mathbb{P}_{S_T} \).

One of the main challenges is to find an appropriate upper bound on \( \mathcal{R}_n \{ \mathcal{G}(\ell, \delta) \} \). In the following lemma, we obtain an upper bound showing that both terms in the r.h.s. of inequality (a) in (13) are \( O(n^{-1/2}) \) neglecting all the logarithmic terms.

**Lemma 3.** The Rademacher complexity of the set function \( \mathcal{G}(\ell, \epsilon) \), for all \( 0 \leq \epsilon \leq 1 \) and increasing function \( \ell : \mathbb{R} \rightarrow \mathbb{R} \), can be bounded as

\[
\mathcal{R}_n \{ \mathcal{G}(\ell, \epsilon) \} \leq \sqrt{\frac{4}{n} \left( K^2 \log \frac{ne}{K} + \log n \right)}
\]

See Appendix D for the proof. The second fact, i.e. for all \( S \in Q^c(\epsilon) \) the value of \( \mathbb{E}_{S_T} \hat{R}_{CRR}(S) \) is sufficiently larger than \( \hat{R}_{CRR}(S_T) \), is formalized by the following lemma.
Lemma 4. Let $S_T \in S_K$ be $(\Delta, \bar{\lambda})$-isoperimetric and assume $D \triangleq \{X_1, \ldots, X_n\}$ are $n$ i.i.d. samples drawn uniformly from $S_T$. For any increasing and integrable function $\ell$, all $\gamma \geq 0$ and $0 < \epsilon \leq 1$, if

$$n \geq \left( \frac{\gamma V_T}{\ell \left( \frac{e^{V_T^{1/K}}}{(K+1)\bar{\lambda}} \right)} \right)^2,$$

then

$$\inf_{S \in Q^c(\epsilon)} \mathbb{E}_{S_T} \left\{ \hat{R}_{\text{CRR}} (S; D, \ell, \gamma) \right\} \geq \left( \sqrt{n} L \left( \frac{e^{V_T^{1/K}}}{(K+1)\bar{\lambda}} \right) - \gamma V_T \right) \epsilon + \hat{R}_{\text{CRR}} (S_T; D, \ell, \gamma),$$

where $L (x) \triangleq \int_0^x \ell (u) \, du - \ell (0)$.

See Appendix D for the proof. From (13) and Lemma 3, the following lower-bound holds for all $S \in Q^c(\epsilon)$ with probability at least $1 - \zeta$:

$$\hat{R}_{\text{CRR}} (S) \geq \mathbb{E}_{S_T} \hat{R}_{\text{CRR}} (S) - \ell \left( \frac{\Delta K V_T^{1/K}}{K+1} \right) \left( 4 \sqrt{K^2 \log \frac{ne}{K} + \log n + \sqrt{\log \frac{2}{\zeta}}} \right).$$

Substituting from Lemma 4 for all $S \in Q^c(\epsilon)$ and with probability at least $1 - \zeta$, we have

$$\hat{R}_{\text{CRR}} (S) - \hat{R}_{\text{CRR}} (S_T) \geq \left( \sqrt{n} L \left( \frac{e^{V_T^{1/K}}}{(K+1)\bar{\lambda}} \right) - \gamma V_T \right) \epsilon$$

$$- \ell \left( \frac{\Delta K V_T^{1/K}}{K+1} \right) \left( 4 \sqrt{K^2 \log \frac{ne}{K} + \log n + \sqrt{\log \frac{2}{\zeta}}} \right) \triangleq u(n, \epsilon),$$

subject to $n$ satisfies (14). In this way, we have obtained the desired $u(n, \epsilon)$. One can show that for

$$n \geq \left( 6 \ell \left( \frac{\Delta K V_T^{1/K}}{K+1} \right) \left( \sqrt{K^2 \log \frac{ne}{K} + \log n + \sqrt{\log \frac{1}{\zeta}}} \right) + \gamma V_T \epsilon \right)^2,$$

both (14) and $u(n, \epsilon) > 0$ are satisfied. Therefore,

$$\mathbb{P} \left\{ \inf_{S \in Q^c(\epsilon)} \hat{R}_{\text{CRR}} (S) - \hat{R}_{\text{CRR}} (S_T) > 0 \right\} > 1 - \zeta,$$

which implies $\mathbb{P} \{ S^* \in Q(\epsilon) \} > 1 - \zeta$.

This completes the proof of Claim 2.

\[ \Box \]

B Proof of Corollaries

Proof of Corollary 1. First, according to the result of Theorem 1, let us set the loss function $\ell (\cdot)$ as follows:

$$\ell^* (u) = \begin{cases} 
1 & u > 0 \\
0 & u \leq 0
\end{cases}.$$ 

This way, the corresponding integral function $L^* (\cdot)$ becomes the same as $\ell$. On the other hand, parameter $\gamma$ in our proposed Lagrangian-relaxation of Definition 2 works as the inverse of the Lagrangian multiplier, when one attempts to reformulate the Maximum-Likelihood (ML) optimization
of \((3)\). Thus, in the asymptotic regime of \(\gamma \to 0\) (equivalently, by increasing the Lagrangian multiplier to \(+\infty\)), the program in \((3)\) becomes equivalent to the ML estimation.

In this regard, one just needs to apply the above setting to the sample complexity of Theorem 1, for any isoperimetricity assumption \((\lambda, \bar{\lambda})\), as

\[
\begin{align*}
\lim_{\gamma \to 0} \left( \frac{6\ell^* \left( \frac{\lambda K V_T}{\epsilon} \right) \left( \sqrt{K^2 \log \frac{n\epsilon}{K} + \log n + \sqrt{\log \frac{1}{\zeta}} \right) + \gamma V_T \epsilon}{L^* \left( \frac{\epsilon V_T^{1/K}}{(K+1)\bar{\lambda}} \right) \epsilon} \right)^2 \\
\geq \left( \frac{6 \left( \sqrt{K^2 \log \frac{n\epsilon}{K} + \log n + \sqrt{\log \frac{1}{\zeta}} \right)}{\epsilon} \right)^2.
\end{align*}
\]

It is straightforward to check that for moderately small \(\epsilon, \zeta > 0\), there exists constant \(C\) (which does not depend on \(\epsilon, \zeta, \) and \(K\)) such that the above lower-bound holds for \(n\) as long as

\[
n \geq CK^2 \log K \frac{1}{\epsilon^2} \log \frac{1}{\zeta}.
\]

As a result, the claim of Theorem 1 follows and the proof is complete.

\[\square\]

Proof of Corollary 2. Proof is similar to that of Corollary 1. First, let us compute the integral function \(L(\cdot)\):

\[
L(x) = \frac{1}{x} \int_0^x \left( 1 - e^{-bu} \right) du = 1 - \left( \frac{1 - e^{-bx}}{bx} \right), \quad x \triangleq \frac{\epsilon V_T^{1/K}}{(K+1)\bar{\lambda}}.
\]

Considering the fact that \(b = O(K/\epsilon)\), it can be easily verified that \(L(x)\) has a positive lower-bound which is independent of \(K, \epsilon\) and \(\zeta\). On the other hand, we have \(\ell(\cdot) \leq 1\) due to the particular choice of \(\ell\). Substituting the above results into the sample complexity of Theorem 1 and using the same techniques which we already used for the proof Corollary 1 completes the proof.

\[\square\]

C Proof of Lemma 1

Let \(Z \triangleq X - \Theta p^\star\), where \(p^\star\) denotes the solution of the convex quadratic program in \((9)\). By applying the chain rule, we have:

\[
\nabla_{\Theta} \ell \left( \min_{u \in S(\Theta)} \| X - u \|_2 \right) = \frac{\ell'(\|Z\|_2)}{2\|Z\|_2} \nabla_{\Theta} \left( \|Z\|_2^2 \right).
\]

Since \(p^\star\) could be found efficiently via a standard QP-solver, the only challenging part in computing r.h.s. of \((16)\) is to compute \(\nabla_{\Theta} \left( \|Z\|_2^2 \right)\). With a small abuse of notation, let \(p^\star(v)\) to be the solution of \((9)\), when \(X\) is replaced by \(v \in \mathbb{R}^K\). By assuming that \(S(\Theta)\) has a non-zero volume, the solution of \((9)\) is uniquely determined and as a result \(\mathbb{R}^K\) can be partitioned into \(2^K - 1\) non-overlapping subsets as follows:

\[
\forall \mathcal{U} \subseteq [K], \mathcal{U} \neq \varnothing, \quad \mathcal{T}_{\mathcal{U}} = \{v \in \mathbb{R}^K \mid \text{SUPP}(p^\star(v)) = \mathcal{U}\},
\]

17
where SUPP (v) = {i ∈ [K] | p∗ i (v) ≠ 0}. Figure 5 shows an example of the above-mentioned partitioning for K = 2. Let I ≜ SUPP (p∗ (X)), and assume X is in the interior of T I. It should be noted that for any fixed S (Θ), only a zero-measure subset of R K does not satisfy this assumption. Then,

∀k ∈ [K] \ I, \ ∇θ_k (∥Z∥_2^2) = 0,

(18)
since the vector Z is locally insensitive to any infinitesimal perturbation of θ_k, as long as k /∈ I. On the other hand, Z is the residual vector between X and its projection on the affine subspace spanned by Θ I. Considering the fact that X is in the interior of T I, the following holds:

∇Θ I (∥Z∥_2^2) = ∇Θ I (∥X - AFFPROJ{θ_i | i ∈ I} (X)∥_2^2),

(19)
where AFFPROJ_V (v) is the projection of v on the affine subspace spanned by the vectors in the set V. The r.h.s. of (19) has a closed form which results in the claimed formula of Lemma 1.

D Auxiliary Proofs

Proof of Lemma 2 First, we prove V* ≜ Vol (S*) ≤ V_T; The proof is by contradiction. Assume V* > V_T. Since min_u∈S_T ∥X_i - u∥_2 = 0 for i = 1, . . . , n, and the fact that ℓ is an increasing function, it can be readily seen that

̂R_CRR (S*) ≥ √nℓ (0) + γV* > √nℓ (0) + γV_T = ̂R_CRR (S_T),

which contradicts the fact that S* is the minimizer.

Next, it needs to be shown that having a non-empty intersection with S_T is necessary for each S* to be a minimizer of ̂R_CRR, regardless of the random sample set D. Again, let us proceed to the proof by contradiction. Assume S* and S_T do not intersect with each other. Since both simplices are convex bodies in a Euclidean space, then there must exist a hyper-plane w^T x + b, ∀x ∈ R^K, for some w ∈ R^K with ∥w∥_2 = 1 and b ∈ R, such that

w^T x + b > 0, \ ∀x ∈ S*

w^T x + b < 0, \ ∀x ∈ S_T.
The minimum distance between $S_T$ and $S^*$ with respect to the separating hyper-plane specified by $(w, b)$ can be defined as

$$ a \triangleq \min_{x \in S^*, y \in S_T} w^T (x - y), $$

where, according to the above assumptions, we have $a > 0$. Now consider the new solution $\hat{S}^* \triangleq S^* - \frac{a}{2} w$ (all points in $S^*$ are shifted with the vector $-\frac{a}{2} w$, toward the hyper-plane). Obviously, we have $\hat{S}^* \neq S^*$, even though they have the same volume. We now show that

$$ \hat{R}_{\text{CRR}} (\hat{S}^*) < \hat{R}_{\text{CRR}} (S^*), $$

which completes the proof, since $S^*$ was assumed to be a global minimizer of $\hat{R}_{\text{CRR}}$. To this aim, first let us define the set of points $\{Z_1, \ldots, Z_n\} \in S^*$ such that

$$ \hat{R}_{\text{CRR}} (S^*) = \frac{1}{\sqrt{n}} \sum_{i=1}^{n} \ell \left( \|X_i - Z_i\|_2^2 \right) + \gamma V^*. $$

Then, it can be easily verified that the following relations hold:

$$ \hat{R}_{\text{CRR}} (S^*) - \hat{R}_{\text{CRR}} (\hat{S}^*) = \frac{1}{\sqrt{n}} \sum_{i=1}^{n} \ell \left( \|X_i - Z_i\|_2^2 \right) - \frac{1}{\sqrt{n}} \sum_{i=1}^{n} \ell \left( \|X_i - Z_i + \frac{a}{2} w\|_2^2 \right) $$

$$ = \frac{1}{\sqrt{n}} \sum_{i=1}^{n} \left[ \ell \circ \sqrt{\gamma} \left( \|X_i - Z_i\|_2^2 \right) - \ell \circ \sqrt{\gamma} \left( \|X_i - Z_i + \frac{a}{2} w\|_2^2 \right) \right], $$

which by using the Mean theorem in calculus \[23\], can be alternatively written as

$$ \hat{R}_{\text{CRR}} (S^*) - \hat{R}_{\text{CRR}} (\hat{S}^*) = \frac{1}{\sqrt{n}} \sum_{i=1}^{n} \left[ a \|Z_i - X_i\|_2^2 - \|X_i - Z_i + \frac{a}{2} w\|_2^2 \right] \left( \ell \circ \sqrt{\gamma} \right)' (\rho_i) $$

$$ = \frac{1}{\sqrt{n}} \sum_{i=1}^{n} \left( \frac{a^2}{4} \right) \left( \ell \circ \sqrt{\gamma} \right)' (\rho_i) $$

$$ \geq \frac{1}{\sqrt{n}} \sum_{i=1}^{n} \left( \frac{a^2}{4} \right) \left( \ell \circ \sqrt{\gamma} \right)' (\rho_i) \geq 0, $$

where for a any function $f : \mathbb{R} \to \mathbb{R}$, $f'$ denotes the derivative, and $\rho_i$ is a real positive value between $\|X_i - Z_i\|_2^2$ and $\|X_i - Z_i + \frac{a}{2} w\|_2^2$. Note that since both $\ell (\cdot)$ and $\sqrt{\gamma}$ are strictly increasing functions, then $\left( \ell \circ \sqrt{\gamma} \right)' (\rho_i)$ is always positive.

**Proof of Lemma** \[3\] Rademacher complexity of $\mathcal{G} (\ell, \epsilon)$ measures the capability of the hypothesis set to assign any randomly chosen binary labels to a set of $n$ generally positioned points in space. Mathematically speaking, it has the following definition:

$$ \mathcal{R}_n \{ \mathcal{G} (\ell, \epsilon) \} \triangleq \mathbb{E}_{X_1, \ldots, X_n, \epsilon, \mathcal{S} \sim \mathcal{P} \mathcal{S}_\epsilon} \left\{ \mathbb{E}_{\sigma} \left( \sup_{\mathcal{S} \in \mathcal{Q} (\epsilon)} \frac{1}{n} \sum_{i=1}^{n} \sigma_i \tilde{g} (X_i, \mathcal{S}) \right) \right\}, $$

where $\sigma \in \{-1, +1\}^n$ are i.i.d. Rademacher random variables, and $\tilde{g} (\cdot, \cdot)$ has already been defined in the lemma. We proceed to the proof by first showing that

$$ \mathcal{R}_n \{ \mathcal{G} (\ell, \epsilon) \} \leq \mathcal{R}_n \{ f \circ \mathcal{G} (\ell, \epsilon) \}, $$

(20)
where function \( f : \mathbb{R} \rightarrow \{0,1\} \) is defined as below:

\[
f(x) \triangleq \begin{cases} 
1 & x > 0 \\
0 & x \leq 0 
\end{cases}.
\]

The reason behind such approach is the fact that r.h.s. of (20) is easier to handle in terms of statistical complexity. Before proving (20), we need to make a number of new definitions. A soft version of the \( K \)-simplex \( S \in \mathbb{S}_K \) with a margin of \( \varepsilon \geq 0 \), denoted by \( S_{\varepsilon(\text{soft})} \), is defined as

\[
S_{\varepsilon(\text{soft})} \triangleq \left\{ \forall x \in \mathbb{R}^K \mid \min_{u \in S} \|x - u\|_2 \leq \varepsilon \right\}.
\]

In fact, \( S_{\varepsilon(\text{soft})} \) represents the union of the interior of \( S \) with all the outside points whose Euclidean distance from \( S \) is less than or equal to \( \varepsilon \). In this regard, let \( S_{K(\text{soft})} \) and \( Q_c(\varepsilon(\text{soft}) \right) \) represent the set of all simplices and all their softened versions (i.e. for all \( \varepsilon \geq 0 \)) in \( S_K \) and \( Q^c(\varepsilon) \), respectively.

We claim that for each \( \sigma \in \{-1,+1\}^n \), the following inequality holds:

\[
J \triangleq \sup_{S \in Q^c(\varepsilon)} \frac{1}{n} \sum_{i=1}^{n} \sigma_i \bar{g}(X_i, S) \leq \sup_{S \in Q_{\varepsilon(\text{soft})}} \frac{1}{n} \sum_{i=1}^{n} \sigma_i f(\bar{g}(X_i, S)) \triangleq J_{(\text{soft})}.
\] (21)

Since \( Q^c(\varepsilon) \) is closed and \( \bar{g} \) is continuous, there exists \( S_{\max} \in Q^c(\varepsilon) \) that maximizes the l.h.s. of (21). Without loss of generality, assume that:

\[
0 = \bar{g}(X_1, S_{\max}) = \cdots = \bar{g}(X_{n_0}, S_{\max}) < \bar{g}(X_{n_0+1}, S_{\max}) \leq \cdots \leq \bar{g}(X_n, S_{\max}),
\] (22)

where \( n_0 \) is defined as the number of data points in the dataset which make \( \bar{g}(X_1, S_{\max}) = 0 \). For the sake of simplicity, assume that for every \( i < j \), if \( \bar{g}(X_i, S_{\max}) = \bar{g}(X_j, S_{\max}) \), then \( \sigma_i \geq \sigma_j \). In this regard, to prove (21) one only needs to run the following procedure:

**Marking algorithm:** Assume all numbers \( n_0 \leq i \leq n \) are unmarked. Increase the index \( i \) from \( n_0 \) to \( n \). For each \( i \), if \( \sigma_i = +1 \) do nothing. If \( \sigma_i = -1 \), define \( j \) as the largest unmarked index such that \( n_0 \leq j < i \), and \( \sigma_j = +1 \). If there is no \( j \) satisfying these conditions, do nothing and just pass to the next \( i \). In the other case, match \( \sigma_i \) with \( \sigma_j \) and set both \( i \) and \( j \) as marked.

Note that according to the above algorithm, each matched pair contribute a negative value to \( J \). Let \( n^* \) be the largest index satisfying the conditions: \( n^* > n_0 \) and \( \sigma_{n^*} = -1 \). If there is no index with these conditions, set \( n^* = n_0 - 1 \). Then, the following facts hold for \( n^* \):

- For all matched pairs \( (\sigma_i, \sigma_j) \), either \( \min(i,j) < n^* \), or \( n^* < \max(i,j) \).
- For all unmarked \( i \leq n^* \), we have \( \sigma_i = -1 \).
- For all unmarked \( i > n^* \), we have \( \sigma_i = +1 \).

For the following arguments, define \( S_{\max}^{(\text{soft})} \) as

\[
S_{\max}^{(\text{soft})} \triangleq \left\{ \forall x \in \mathbb{R}^K \mid \min_{u \in S_{\max}} \|x - u\|_2 \leq \varepsilon = \min_{u \in S_{\max}} \|X_{n^*} - u\|_2 \right\} \subseteq Q_{\varepsilon(\text{soft})}(\varepsilon).
\]

Thanks to the above definition, we can now investigate the contribution of each data sample to both \( J \) and \( J_{(\text{soft})} \). It should be noted that each of the following cases apply to at least one member of \( Q_{\varepsilon(\text{soft})}(\varepsilon) \), and thus apply to the maximizer as well:
• Any unmatched data point \( X_i \) with \( n_0 \leq i \leq n^* \), contributes negatively to \( J \), while its contribution to \( J_{(\text{soft})} \) is at least zero.

• Any matched pair contribute to \( J \) non-positively, while their contribution to \( J_{(\text{soft})} \) is at least zero.

• For any unmatched data point \( X_i \) with \( i > n^* \), contribution to \( J \) is at most 1, while contribution to \( J_{(\text{soft})} \) is exactly 1.

In all the above-mentioned cases, contribution of each \( X_i \) to \( J \) is less than or equal to that of \( J_{(\text{soft})} \) which proves (21). A direct consequence of these arguments is the following:

\[
\mathcal{R}_n \left\{ \mathcal{G}(\ell, \epsilon) \right\} \leq \mathcal{R}_n \left\{ f \circ \mathcal{G}_{(\text{soft})}(\ell, \epsilon) \right\},
\]

where we define \( f \circ \mathcal{G}_{(\text{soft})}(\ell, \epsilon) \) as a hypothesis set for binary classification, where each data point inside the soft simplex is labeled as zero, while outside points are labeled as one. For such class of functions, we can bound the Rademacher complexity via a number of previously-established tools, e.g. growth functions. Alternatively, we need to bound the VC-dimension of \( f \circ \mathcal{G}_{(\text{soft})}(\ell, \epsilon) \), which is carried out in Lemma 5.

**Lemma 5.** For \( n \in \mathbb{N} \), let us denote \( \Pi_{S_{K_{(\text{soft})}}}(n) \) as the “growth function” of the function family \( S_{K_{(\text{soft})}} \), i.e. the set of all soft \( K \)-simplices in \( \mathbb{R}^K \). Then, the following upper-bound holds for all \( n \) and \( K \):

\[
\Pi_{S_{K_{(\text{soft})}}}(n) \leq (n + 1) \left( \frac{ne}{K + 1} \right)^{(K+1)^2}.
\]

See Appendix D for the proof. In this regard, according to Massart’s lemma in [22], and also using (21), we have

\[
\mathcal{R}_n \left\{ \mathcal{G}(\ell, \epsilon) \right\} \leq \sqrt{\frac{2 \log \Pi_{S_{K_{(\text{soft})}}}(n)}{n}},
\]

Substitution from Lemma 5 into the above inequality completes the proof.

**Proof of Lemma 4**. Lemma roughly states that when the overlap between a class of \( K \)-simplices and \( S_T \) are strictly smaller than \( 1 - \epsilon \), then with high probability “none” of them is able to cover all the training data points when \( n \) becomes sufficiently large. Thus, the expected value of cost function increases accordingly. First let us take a closer look at \( \mathbb{E}_{S_T} \hat{R}_{\text{CRR}}(S) \) and analyze its minimum over \( S \in \mathcal{Q}^c(\epsilon) \):

\[
\min_{S \in \mathcal{Q}^c(\epsilon)} \mathbb{E}_{S_T} \hat{R}_{\text{CRR}}(S) = \min_{S \in \mathcal{Q}^c(\epsilon)} \left\{ \sqrt{n} \mathbb{E}_{X \sim \mathcal{P}_{S_T}} \left[ \ell \left( \min_{u \in S} \|X - u\|_2 \right) \right] + \gamma \text{Vol}(S) \right\},
\]

where throughout the proof we refer to \( \text{Vol}(S) \) simply as \( V \) for the ease of notations.

The term \( \min_{u \in S} \|X - u\|_2 \) is zero for all \( X \in S \cap S_T \). Thus all the nonzero summands in the expectation correspond to the points in the differential set \( S_T - S \), which due to the minimization over \( S \in \mathcal{Q}^c(\epsilon) \), has a Lebesgue measure of at least \( \epsilon V_T \). In this regard, let us define the following sets:

\[
A_k = A_k(S, S_T) \triangleq \left\{ X \in S_T - S \left| \min_{u \in S} \|X - u\|_2 = \min_{u \in S_{-k}} \|X - u\|_2 \right. \right\}, \quad \forall k = 0, 1, \ldots, K,
\]
where \( S_{-k} \) represents the \( k \)th facet of \( S \). In other words, \( A_k \) shows the set of points inside \( S_T \) and outside of \( S \), which are closer to the \( k \)th facet of \( S \) than other facets. For each point that has an equal Euclidean distance from more than one facet, \( k \) can be chosen as any of those facets arbitrarily. In this regard, it is easy to see that

\[
A_k \cap A_l = \emptyset \iff k \neq l , \quad \bigcup_{k=0}^{K} A_k = S_T - S.
\]

Also, let

\[
\alpha_k \triangleq \frac{\text{Vol}(A_k)}{\sum_{i=0}^{K} \text{Vol}(A_i)} , \quad k = 0,1, \ldots, K,
\]

with \( \sum_k \alpha_k = 1 \). Consider the parameteric sets \( B_\delta , \epsilon \leq \delta \leq 1 \), defined as

\[
B_\delta \triangleq \left\{ S \in \mathcal{Q}^c (\epsilon) \left| \frac{\text{Vol}(S \cap S_T)}{V_T} = 1 - \delta \right. \right\}.
\]

Obviously, we have \( \bigcup_{\epsilon \leq \delta \leq 1} B_\delta = \mathcal{Q}^c (\epsilon) \). Now we are ready to propose the following useful inequality for all \( \epsilon \leq \delta \leq 1 \):

\[
\min_{S \in B_\delta} \left\{ \mathbb{E}_{S_T} \hat{R}_{\text{CRR}} (S) - \gamma V \right\} = \sqrt{n} \min_{S \in B_\delta} \mathbb{E}_{S_T} \left[ \ell \left( \min_{u \in S} \| X - u \|_2 \right) \right] \\
\geq \delta \sqrt{n} \min_{S \in B_\delta} \sum_{k=0}^{K} \alpha_k \mathbb{E}_{A_k} \left[ \ell \left( \min_{u \in A_k} \| X - u \|_2 \right) \right] + (1 - \delta) \sqrt{n} \ell (0) \\
\geq \delta \sqrt{n} \min_{\alpha \in \Phi} \sum_{k=0}^{K} \alpha_k L(\Delta_k) + \sqrt{n} \ell (0) ,
\]

where \( \Phi \) denotes the standard simplex, or the set of all \((K+1)\)-dimensional discrete probability mass functions. \( L(x) \triangleq \frac{1}{x} \int_0^x \left( \ell (u) - \ell (0) \right) du \) for \( x \geq 0 \), \( \Delta_k \triangleq \text{Vol}(A_k) / (\max_k \text{Vol}(S_{-k})) \). The main intuition behind the above inequalities is the fact that the term

\[
\mathbb{E}_{A_k} \left[ \ell \left( \min_{u \in A_k} \| X - u \|_2 \right) \right]
\]

is minimized when \( A_k \) is concentrated in the form of a thin cylindrical structure above the largest facet of \( S \). The volume of the largest facet is \( \max_k \text{Vol}(S_{-k}) \), which makes \( \Delta_k \) to be the height of this imaginary cylinder. We have also taken advantage of the fact that \( \ell \) is increasing and integrable. Based on the definition, we have \( \text{Vol}(A_k) = \delta \alpha_k V_T \). Also, due to the \((\lambda, \bar{\lambda})\)-isoperimetricity of \( S_T \), we have

\[
\max_k \text{Vol}(S_{-k}) \leq \bar{\lambda} K V_T^\frac{K-1}{K} \quad \text{which implies} \quad \Delta_k \geq \left( \frac{\delta \alpha_k}{\bar{\lambda}} \right) V_T^{1/K} .
\]

Also, note that since \( \ell (\cdot) \) is assumed to be increasing, \( L(\cdot) \) is both increasing and convex. Therefore, the minimization over \( \alpha \in \Phi \) in (23) results in \( \alpha^* = \left( \frac{1}{K+1}, \ldots, \frac{1}{K+1} \right) \). Substitution into (23) yields
the following lower-bound for the expected risk minimized over $\mathcal{B}_i$:

\[
\min_{\mathcal{S} \in \mathcal{B}_i} \left\{ \mathbb{E}_{\mathcal{S}_T} \hat{R}_{\text{CRR}} (\mathcal{S}) \right\} \geq \delta \sqrt{n} L \left( \frac{\delta V_T^{1/K}}{(K + 1) \lambda} \right) + \gamma \min_{\mathcal{S} \in \mathcal{B}_i} \ Vol (\mathcal{S}) + \sqrt{n} \ell (0) \\
\geq \delta \sqrt{n} L \left( \frac{\delta V_T^{1/K}}{(K + 1) \lambda} \right) - \gamma V_T \delta + \hat{R}_{\text{CRR}} (\mathcal{S}_T),
\]

(24)

where we have used the facts that $\min_{\mathcal{S} \in \mathcal{B}_i} \ Vol (\mathcal{S}) = V_T (1 - \delta)$ and $\hat{R}_{\text{CRR}} (\mathcal{S}_T) = \sqrt{n} \ell (0) + \gamma V_T$. The rest of the proof is straightforward. Finding a lower-bound for $\mathbb{E}_{\mathcal{S}_T} \hat{R}_{\text{CRR}} (\mathcal{S})$ when $\mathcal{S} \in \mathcal{Q}^c (\epsilon)$ can be accomplished through the following set of relations and inequalities:

\[
\min_{\mathcal{S} \in \mathcal{Q}^c (\epsilon)} \left\{ \mathbb{E}_{\mathcal{S}_T} \hat{R}_{\text{CRR}} (\mathcal{S}) \right\} = \min_{\epsilon \leq \delta \leq 1} \min_{\mathcal{S} \in \mathcal{B}_i} \mathbb{E}_{\mathcal{S}_T} \hat{R}_{\text{CRR}} (\mathcal{S}) \\
\geq \min_{\epsilon \leq \delta \leq 1} \left( \delta \sqrt{n} L \left( \frac{\delta V_T^{1/K}}{(K + 1) \lambda} \right) - \gamma V_T \delta \right) + \hat{R}_{\text{CRR}} (\mathcal{S}_T). 
\]

Again, remember that $L (\cdot)$ is an increasing function. Therefore, given that the derivative of the r.h.s. of the above inequality remains positive w.r.t. $\delta$, and for all $\epsilon \leq \delta \leq 1$, then the minimum occurs at $\delta^* = \epsilon$. It can be easily verified that given the condition on $n$ in the lemma, the derivative remains positive and thus the proof is complete. \qed

Proof of Lemma 5 The proof is motivated by the fact that any $K$-simplex $\mathcal{S} \in \mathcal{S}_K$ can be viewed as a set of points in $\mathbb{R}^K$ satisfying the following set of constraints:

\[
\mathcal{S} = \left\{ \mathbf{u} \in \mathbb{R}^K \mid w_k^T \mathbf{u} + b_k \geq 0, \ \forall k = 0, 1, \ldots, K \right\},
\]

where for each $k$, the couple $H_k \triangleq (w_k, b_k) \in \mathbb{R}^K \times \mathbb{R}$ represent a $(K - 1)$-dimensional linear hyper-plane that includes the $k$th facet of $\mathcal{S}$. Not to mention that $w_k$ are considered to be inwards w.r.t. $\mathcal{S}$. We can then write $\mathcal{S} = \mathcal{S} (H_0, \ldots, H_K)$.\footnote{This is an alternative definition of a simplex which conflicts with the previous notations in the paper. However, the current way of defining $K$-simplices is specific to this lemma and solely for the sake of simplicity in notations.} Accordingly, one can think of a soft $K$-simplex as

\[
\mathcal{S}_{\epsilon (\text{soft})} (H_0, \ldots, H_K) = \left\{ \forall \mathbf{x} \in \mathbb{R}^K \mid \min_{\mathbf{u} \in \mathcal{S} (H_0, \ldots, H_K)} \| \mathbf{x} - \mathbf{u} \|_2 \leq \epsilon \right\}.
\]

Assume one aims to use $K$-simplices as binary classifiers, where for any $\mathcal{S} \in \mathcal{S}_K$ and $\mathbf{x} \in \mathbb{R}^K$, $\mathbf{x}$ is labeled as $+1$ if $\mathbf{x} \in \mathcal{S}$ while it is labeled $-1$ otherwise. Then, we are interested to bound the maximum number of ways that a set of $n$ generally-positioned points in $\mathbb{R}^K$ can be labeled via simplices in $\mathcal{S}_K$, i.e. the growth function of $\mathcal{S}_K$ or $\Pi_{\mathcal{S}_K} (n)$. Fortunately, this goal can be achieved by using the growth function of hyper-planes in $\mathbb{R}^K$, which is already solved.

Let us define $\mathcal{L}_{K+1} \triangleq \{-1, +1\}^{K+1}$ as the set of all binary super labels of dimension $K + 1$ and the function family $\mathcal{H}$, such that for $h = h (w_0, \ldots, w_K, b_0, \ldots, b_K) \in \mathcal{H} : \mathbb{R}^K \rightarrow \mathcal{L}_{K+1}$ is defined as:

\[
\forall \mathbf{x} \in \mathbb{R}^K, \ h (\mathbf{x}) \triangleq \left[ \text{sign} (w_0^T \mathbf{x} + b_0), \ldots, \text{sign} (w_K^T \mathbf{x} + b_K) \right]^T,
\]

where we define $\text{sign} (0) = 1$. Then, by letting $\mathcal{I}_K$ to be the set of all hyper-plane binary classifiers in $\mathbb{R}^K$ and according to the rule of product, the growth function of $\mathcal{H}$ can be computed as

\[
\Pi_{\mathcal{H}} (n) = \Pi_{\mathcal{I}_K} (n) \times \ldots \times \Pi_{\mathcal{I}_K} (n).
\]

\text{\textit{K+1 times}}
It is easy to see that $\Pi_{S_K}(n) \leq \Pi_{\mathcal{H}}(n)$. In fact, for any $S = (H_0, \ldots, H_K) \in S_K$, the hyper-plane parameter sets $H_0, \ldots, H_K$ uniquely identify a function in $\mathcal{H}$ that can assign super labels to $\mathbb{R}^K$, while only a subset of them can be generated by $S$. On the other hand, considering the fact that VC dimension of hyper-planes in $\mathbb{R}^K$ is exactly $K + 1$, and using the Sauer-Shelah lemma \cite{22}, we have the following bound for $\Pi_{I_K}(n)$:

$$
\Pi_{I_K}(n) \leq \sum_{i=0}^{K+1} \binom{n}{i} \leq \left(\frac{ne}{K+1}\right)^{K+1},
$$

which, according to the previous inequality means: $\Pi_{S_K}(n) \leq \left(\frac{ne}{K+1}\right)^{(K+1)^2}$.

However, the hypothesis set $S_{K(soft)}$ has one more degree of freedom comparing to $S_K$, which is the choice of $\varepsilon \geq 0$ or maximum Euclidean distance from the $K$-simplex. Intuitively, this additional degree of freedom can increase the growth function at most by a factor of $n + 1$, which is due to the following argument: For any $S \in S_K$ and $n$ generally-positioned points in $\mathbb{R}^K$, consider the subset of $n$ points outside of $S$, which currently are labeled as $-1$. Then, by increasing $\varepsilon$ (starting from 0), they start to fall inside the simplex (at worst one-by-one), which means only $n + 1$ more different labelings can occur. This completes the proof.

**Lemma 6** (Restricted Isoperimetry). For $K \in \mathbb{N}$, assume $S_{reg} \in S_K$ to be a perfectly regular simplex with equal side lines. Then for all $K$, $S_{reg}$ is $(\lambda, \bar{\lambda})$-isoperimetric where $\lambda$ and $\bar{\lambda}$ can be chosen to be as small as 1 and $e$, respectively.

**Proof.** For a perfectly regular simplex $S_{reg}(\Theta)$ with all side lines equal to $d \geq 0$, i.e. $\|\theta_k - \theta_{k'}\|_2 = d$, $\forall k \neq k'$, the Lebesgue measure $\text{Vol}(S_{reg})$ is already shown to be

$$
\text{Vol}(S_{reg}) = \frac{\sqrt{K + 1}}{K! \sqrt{2^K}} d^K.
$$

Thus, we have

$$
\max_{k,k'} \|\theta_k - \theta_{k'}\|_2 = d = \left(\frac{K! \sqrt{2^K}}{\sqrt{K + 1}}\right)^{1/K} \text{Vol}^{\frac{1}{K}}(S_{reg}).
$$

On the other hand, the following lower and upper bounds for $K!$ hold for all $K \in \mathbb{N}$: $e \left(\frac{K}{e}\right)^K \leq K! \leq K e \left(\frac{K}{e}\right)^K$, which leads us to the following relations:

$$
\max_{k,k'} \|\theta_k - \theta_{k'}\|_2 \leq \left[\left(\frac{K e}{\sqrt{K + 1}}\right)^{1/K} \sqrt{\frac{2}{e}}\right] K \text{Vol}(S_{reg})^{1/K} \leq K \text{Vol}(S_{reg})^{1/K},
$$

and means $\bar{\lambda}$ can be chosen to be as small as 1.

For the other claim, we should note that the maximal facet of $S_{reg}$ (noting the fact that for a perfectly regular simplex all facets are equal), can be attained by computing the volume of a perfectly regular $(K - 1)$-simplex with all side lines equal to $d$. In other words:

$$
\max_k \text{Vol}(S_{reg-k}) = \frac{\sqrt{K} d^{K-1}}{(K-1)! \sqrt{2^{K-1}}} = \frac{K! 2^{1-K}}{(K-1)!} \left(\frac{K! \sqrt{2^K}}{\sqrt{K + 1}}\right)^{\frac{K-1}{K}} \text{Vol}(S_{reg})^{\frac{K-1}{K}}.
$$
which, again by using the previously-mentioned lower and upper-bounds on $K!$, can be bounded as

$$\max_k \text{Vol}(S_{\text{reg},k}) = \left[ \sqrt{\frac{K}{(K+1)^{\frac{K+1}{2}}} (K!)^{-1/K}} \right] K \text{Vol}(S_{\text{reg}})^{\frac{K-1}{K}}$$

$$\leq \left[ e^{\sqrt{(K/e^2)^{1/K}}} \right] \text{Vol}(S_{\text{reg}})^{\frac{K-1}{K}}$$

$$\leq e \text{Vol}(S_{\text{reg}})^{\frac{K-1}{K}},$$

Again, it means $\lambda$ can be chosen to be as small as $e$. This completes the proof. \qed