An Algorithm for Learning Smaller Representations of Models With Scarce Data

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Abstract. We present a greedy algorithm for solving binary classification problems in situations where the dataset is either too small or not fully representative of the problem being solved, and obtaining more data is not possible. This algorithm is of particular interest when training small models that have trouble generalizing. It relies on a trained model with loose accuracy constraints, an iterative hyperparameter pruning procedure, and a function used to generate new data. Analysis on correctness and runtime complexity under ideal conditions and an extension to deep neural networks is provided. In the former case we obtain an asymptotic bound of $O(|\Theta|^2 (\log|\Theta| + |\theta|^2 + T_f(|D|)) + S|\Theta||E|)$, where $|\Theta|$ is the cardinality of the set of hyperparameters $\theta$ to be searched; $|E|$ and $|D|$ are the sizes of the evaluation and training datasets, respectively; $S$ and $f$ are the inference times for the trained model and the candidate model; and $T_f(|D|)$ is a polynomial on $|D|$ and $f$. Under these conditions, this algorithm returns a solution that is $1 \leq r \leq 2(1 - 2^{-|\Theta|})$ times better than simply enumerating and training with any $\theta \in \Theta$. As part of our analysis of the generating function we also prove that, under certain assumptions, if an open cover of $D$ has the same homology as the manifold where the support of the underlying probability distribution lies, then $D$ is learnable, and vice-versa.

Keywords: data augmentation · semi-supervised learning

1 Introduction

The goal of most machine learning systems is to, given a sample of an unknown probability distribution, fit a model that generalizes well to other samples of the same distribution. It is often assumed that said sample is fully representative of the unknown, or underlying, probability distribution being modeled, as well as being independent and identically distributed (Shalev-Shwartz and Ben-David, 2014). It occurs in many natural problems that at least one part of said assumption does not hold. This could be by either noisy or insufficient sampling of the underlying function, or an ill-posed problem, where the features of the data do not represent the relevant characteristics of the phenomenon being described (Hampel, 1998; Dundar et al., 2007). Some systems, such as deep neural networks, appear to be remarkably resilient to this situation. Often, this is due to the fact that overparametrized models are easier to train (Livni et al., 2014). This issue becomes more self-evident in situations where the presence of outliers may harm the overall experience, such as commercial voice assistants; as well as when training small, shallow models, where exposure to large amounts of data is critical for proper generalizability (Livni et al., 2014; Hanneke, 2016; Kawaguchi et al., 2017).

1.1 Contributions

We present an algorithm, which we dub Agora, for solving binary classification problems in situations when the data does not fully characterize the underlying probability distribution, chiefly

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1 This paper has not been fully peer-reviewed.

2 One of Plato’s Dialogues—Timaeus—involves a conversation between the eponymous character and Socrates, about the nature of the world and how it came into being. It fits well with the nature of our algorithm, and with the goal of machine learning.
having in mind the creation of smaller, non-linear models for these tasks whenever we are unable to further sample the underlying probability distribution.

Our algorithm works by training a model (Timaeus), through the output of a trained, but relatively low-performing, model (Socrates), along with a function to generate new samples (the $\tau$-function). The only condition imposed to Agora, outside of the characterization of the $\tau$-function, is that the evaluation set must be representative of the underlying distribution being learned. Similar constraints are not required for the training set.

We provide statements around the correctness and time bounds of this approach under ideal conditions by leveraging ideas from the field of topological data analysis. In particular, when the underlying probability distribution $P$ is describable as a Riemannian manifold and the size of the data is large enough to be representative of $P$; if Timaeus is unable to “forget” a correctly labeled point, then Agora’s solution is

$$1 \leq r \leq 2 \left( 1 - \frac{1}{2|\Theta|} \right)$$

times better, when compared to an enumeration of trained models with hyperparameters from $\Theta$.

Assuming a polynomial-time training algorithm, Agora converges in at most

$$O \left( |\Theta|^2 \left( \log |\Theta| + |\theta|^2 + T_f \left( |D| + \frac{|E|}{2|\Theta|-1} \right) \right) + \tilde{S} \left( |\Theta| \left[ \left( 1 - \frac{1}{2|\Theta|} \right) \right] \right) \right), \quad (1)$$

steps, where $|\Theta|$ is the cardinality of the set of hyperparameters $\theta$ to be searched; $|E|$ and $|D|$ are the sizes of the evaluation and training datasets, respectively; $\tilde{S}$ is the steps required to perform inference on Socrates; and $T_f(|D|)$ is the runtime of the training algorithm–assumed to be a polynomial on $|D|$ and on the inference time for Timaeus, $f$.

We further relax the–admittedly strong–assumption that there exists such a polynomial-time training algorithm, and consider the case where it is a neural network with a loss function that is $L$-Lipschitz, bounded from below and with stochastic gradients bounded by some $G$. We prove that whenever the learning rate $\eta$, batch size $|B|$, and random state $s$ is considered as part of the hyperparameter search, then the runtime of Agora is given by

$$O \left( |\Theta|^2 \left( \log |\Theta| + |\theta|^2 + f \left( |E| + \frac{|B|}{(LG\zeta)^{2/3}} \right) \right) + \tilde{S} |\Theta| \left[ \left( 1 - \frac{1}{2|\Theta|} \right) \right] \right) \quad (2)$$

steps, where $B \subset D$, with $|B| = \max_{\theta \in \Theta} \{|B| \in \theta\}$ and $\zeta = \min_{\theta \in \Theta} \{\eta^2 \in \theta\}$ is the square learning rate.

Additionally, we provide a proof that, under certain assumptions, if an open cover of $D$ has the same homology as the manifold where the support of $P$ lies, then $D$ is learnable, and viceversa. While we only leverage this result as a mechanism for our correctness proofs, we believe that this result is of interest to the community at large.

### 1.2 Outline

The remaining of this paper is structured as follows: we begin by providing a brief survey of related approaches to this and similar problems in Section 2. After establishing notational conventions, basic definitions, and assumptions in Section 3, we introduce Agora in Section 4. We provide an analysis of its correctness and asymptotic bounds in Section 5, before concluding in Section 6 with a discussion of our work, as well as potential applications–and pitfalls–when using this algorithm.

### 2 Related Work

The Socrates model in the Agora algorithm serves two purposes: it must act as a guide to the training of a candidate model, and it must judge membership of an unlabeled point with respect
to a given concept class. Both requirements are studied in multiple fields in the machine learning literature, in theory and in practice.

Socrates acting as a guide is more commonly known as knowledge distillation, and has multiple variants. It was originally repurposed by [Bucilu et al. (2006)] as a model compression technique, and subsequently applied to deep learning by [Hinton et al. (2015)]. The judgment of Socrates amounts to ensuring generated points belong to the domain being considered. For this reason, Agora and some of these techniques can be considered, from an algorithmic point of view, a type of active learning. See [Balasubramanian et al. (2009)] and [Sener and Savarese (2018)] in the context of deep learning; and [Settles (2012)] for a survey of earlier and foundational work on this area, in addition to the work by [Hanneke (2009)]. However, this discipline focuses on selecting a subset of the data to be labeled to guarantee efficient generalizability, and tends to concentrate on specific tasks and models. Our algorithm overlaps more with the subfield of membership query synthesis [Angluin, 2001]. That being said, Agora makes the makes no assumptions about the task or the model being input, and our setting disallows us from sampling more data. Moreover, Socrates is not constrained to have a good performance on the dataset, and our proofs impose a lower-bound accuracy of \( \frac{2}{3} \).

The third component of Agora—the \( \tau \)-function—can be seen as a general-purpose injector of noisy data. The idea of inducing perturbations in the data, or data augmentation, is comparatively new when applied to deep learning [Lin et al. (2013)]. This is a wide field of research, mainly due to the fact that it is known that perturbations improve a model’s generalizability, up to a point [Graham, 2014]. When facing a task with a small corpus, another technique commonly employed is the use of generative models to create synthetic data [Ratner et al. 2017; Zhang et al. 2019; Ho et al. 2019]. On the other hand, generating synthetic data is not always a reliable stratagem—otherwise, the generating model would have perfect accuracy on the task and there would be no need to train a second model. Theoretical research around the effectiveness of this work was done by [Dao et al. (2018)] by framing it as a kernel method, and [Wu et al. (2020)] studied its generalizability with respect to linear transforms. See [Oliver et al. (2018)] for an overview of both data augmentation and knowledge distillation, and how they fit on the wider field of semi-supervised learning. As mentioned earlier, these techniques often focus on the training set without consideration as to whether they properly belong to the support of the underlying probability distribution. In general, this implies that algorithms for synthetic data generation are task-dependent, unlike Agora. We circumvent the issue of reliability and potential overfitting with respect to the underlying probability distribution by providing tight bounds for which the correctness of Agora holds, with implications towards generalizability.

Considering scenarios where some parts of the i.i.d. assumption do not hold has become a more active field of research, as the emerging field of decentralized learning gains momentum. See, for example the applied works by [Dundar et al. (2007)], and [Hsieh et al. (2020)] from a deep learning point of view. Yet, there is a trove of work done in learning theory with respect to under which conditions a hypothesis class is able to learn and generalize to an input task [Valiant, 1984; Kearns and Valiant, 1994; Balcan et al. 2010; Hanneke, 2016], and more specialized to deep neural networks [Kawaguchi et al. 2017], as well as online learning [Littlestone, 1988; Shalev-Shwartz, 2012]. Furthermore, it is known [Kearns, 1998] that most learning algorithms allow some form of error-tolerant statistical query akin to the relationship between Timaeus and Socrates. We leverage these results for our proofs, in addition to several elements of the field of topological data analysis, and more specifically, the techniques used in persistent homology. The interested reader is highly encouraged to review the survey by [Wasserman (2018)], and the brief but thorough note by [Weinberger (2011)], for introductions to this very active field. Finally, we must highlight that our proof of the correspondence between homology and learnability is, to the best of our knowledge, new. A similar argument using the packing number is given by [Mohri et al. (2012)], along with a
number of related works (Haussler, 1995; Alon et al., 1997); however, it is used to bound various complexity measures, rather than the data itself. More importantly, they do not leverage the homology of the manifold on which the support of the probability distribution lies, which, as we will point out, it is easier to work with than other similarity measures.

3 Background

3.1 Motivation

Consider the problem of learning a probability distribution \( P \) via a dataset \( D = \{\langle x_i, y_i \rangle \}_{i \in [1,n]} \), where \( D \) is sampled from \( P \) with a function \( \sigma: P \to X \times Y \) for some measurable sets \( X \) and \( Y \). Here we implicitly assume \( \sigma \) assigns a label \( y \in Y \) to every \( x \sim P \), where \( x \in X \). The goal of statistical learning is then, following the model by Valiant (1984), to output a function ("hypothesis") \( f: X \to Y \) via a polynomial-time algorithm such that the true error,

\[
\Pr_{\langle x,y \rangle \sim P}[f(x) \neq y] \leq \epsilon, \tag{3}
\]

is minimized with probability at least \( 1 - \delta \) for some \( 0 < \epsilon, \delta \leq 1/2 \), and for any element of the codomain of \( \sigma \) as described by any \( P \).

It is common to approximate Equation 3 by considering the empirical error rate

\[
\text{err}(f(\cdot), E) = \sum_{\langle x_i, y_i \rangle \in E} \mathbb{1}[f(x_i) \neq y_i] \tag{4}
\]
on a separate evaluation dataset \( E \sim P \), \( E \cap D = \emptyset \), as the main predictor of generalizability of the model. Solving this problem directly, however, is known to be hard for multiple problems.\(^3\)

In this paper we concern ourselves with the setting where \( D \) is not representative of a specific \( P \): that is, that in a given hypothesis class \( W \), there does not exist a guarantee under which a function \( f(\cdot) \in W \) trained with \( D \) will be able to properly generalize to other subsets \( E \sim P \). Formally, we assume \( \delta \) in Equation 3 is fixed and hence

**Definition 1 (\( \epsilon \)-representativeness of \( P \)).** A dataset \( D \sim P \) is \( \epsilon \)-representative (or \( \epsilon \)-learnable) of \( P \) with \( f(\cdot) \) if and only if the relation

\[
\Pr_{\langle x,y \rangle \sim P}[f(x) \neq y] \leq \frac{1}{|D|} \left( \sum_{\langle x_i, y_i \rangle \in D} \mathbb{1}[f(x_i) \neq y_i] \right) + \epsilon \tag{5}
\]

holds for a given \( \epsilon \in [0,1/2] \) and polynomial-time algorithm.

This definition is not new, and it is merely a notational convenience. Some equivalent measures are the \( \epsilon \)-representativeness of \( P \) in the sense of Shalev-Shwartz and Ben-David (2014), which is defined as the difference between the empirical error and the true error; and, following a result by Hanneke (2016), the minimum sample size for binary function classes of finite VC dimension can also be considered equivalent in the converse.\(^3\)

\(^3\) For example, agnostically learning intersections of half-spaces (Klivans and Sherstov, 2006; Daniely, 2016).

\(^4\) The result by Hanneke (2016) concerns the minimum size of \( D \) such that Equation [4] holds. It follows that if the sample size doesn’t meet that bound, the probability distribution is not \( \epsilon \)-learnable. We will revisit this result in Section 5.
3.2 Assumptions

We will assume a binary classification task, \( y_i \in \{0, 1\} \), over \( x_i \in X \subset \{0, 1\}^m \) \( \forall (x_i, y_i) \in D \); and adopt a narrower view of this problem by considering our hypothesis space to be a finite set of valid weight assignments \( w \in W \) to a fixed architecture or model \( f(\cdot; w) \), and our goal to be learning a specific \( \mathcal{P} \) defined over \( X \).

We will make the assumption that, at all times, we have a validation set \( E \) which is \( \epsilon \)-representative of \( \mathcal{P} \), and concern ourselves with the case when the training set \( D \) is not. The scenario where neither \( D \) nor \( E \) are \( \epsilon \)-representative of \( \mathcal{P} \) is readily seen to be impossible to solve\(^5\) and thus we will not consider it further. It could be argued that this problem could easily be worked around by switching \( E \) and \( D \). We will assume that this can’t be done, due to—for example—an evaluation dataset that varies over time and whose only invariant is that it remains \( \epsilon \)-representative of \( \mathcal{P} \). More importantly, we assume we are unable to sample more data; i.e., we no longer have access to \( \sigma \).

Remark 1. Balcan et al. (2010) showed that the sample complexity bound for an active learning algorithm dominates that of a passive algorithm. However, the conditions required to maintain this remarkable result do not hold in our setup, as we no longer have access to the sampling function needed in active learning. Nonetheless, we provide similar bounds for this scenario in Lemma 3.

Likewise, we will only consider, for simplicity, that \( \sigma \) is noise-free, and for some proofs we will assume that both \( X \) and the support of \( \mathcal{P} \) lie on some compact Riemannian submanifold of a Euclidean space, and that all sets involved are measurable\(^6\). Positive results around the reconstructability of a manifold under noisy conditions can be found in Niyogi et al. (2011); Genovese et al. (2014) and Chazal et al. (2017b). Still, in Section 6 we discuss further improvements to Agora that do not rely on these constraints. We also provide in Corollary 2 an analysis of the runtime of Agora under more relaxed assumptions, for the case where the input is a neural network and, as discussed, the existence of a polynomial-time algorithm that satisfies Equations 4 and 5 is not guaranteed.

With these constraints we are able to restate the problem as the one of finding the best weight assignment \( w^* \) from a set \( W = \{w_1, \ldots, w_k\} \) such that the accuracy

\[
\text{acc}(f(\cdot; w^*), E) = 1 - \text{err}(f(\cdot; w^*), E)
\]

is maximized. This last convention is for practical purposes only, and does not affect the mathematics governing the problem.

We will use \( \tilde{f} \) to denote the number of steps required to obtain an output from a function \( f(\cdot; \cdot) \) given a fixed-size input \( x \) regardless of other parameters, that is, \( \tilde{f} = \Theta(f(x; w)), \forall w \in W \). Likewise, we will refer to the training algorithm used to assign a set of weights to \( f(\cdot; w) \) as \textsc{train-model}(\( f, D, \theta \)), and remark that it runs, by definition, in a number of steps polynomial in \( |D| \), \( \tilde{f} \), and \( \theta \). In this context, \( \theta \) is a set of \textit{hyperparameters} that control the algorithm’s behavior and are not learned by the architecture itself. The choice of \( \theta \) influences directly the accuracy that can be attained by \( f(\cdot; w) \) on \( E \), especially in cases where Equations 4 and 5 are non-convex. We will revisit this assumption in Section 5. Finally, we will write use \( B_\rho(x) \) to refer to a \( m \)-ball of radius \( \rho \) and centered at some \( x \in \mathbb{R}^m \).

\(^5\) There is insufficient data to provide a meaningful answer in polynomial time.
\(^6\) Real data tends to be high-dimensional, sparse, and not necessarily lying on a manifold. See Niyogi et al. (2011) and Section 6 for a discussion on this assumption.
3.3 The $\tau$-function

The $\tau$-function is Agora’s central mechanism to improve the performance of Timaeus. It exploits the structure of $X$ to generate points, which in turn are used by the algorithm to obtain a dataset that is $\epsilon$-representative of $\mathcal{P}$. We will discuss this function in detail in Section 5.

**Definition 2 (The $\tau$-function).** Let $D = \{(x_i, y_i)\}_{i=1}^n$ be a dataset sampled from a distribution $\mathcal{P}$. Let $X = \{x_i \in D\}$ be the set of all the points contained in $D$, and let $Q_{x, \rho}$ be a uniform probability distribution with support $\text{supp}(Q_{x, \rho}) = \{x : x' \in B_{\rho/4}(x) \land x' \in Z \land x' \neq x\}$, for some $\rho > 0$ and $X \subset Z \subset \{0, 1\}^n$. The $\tau$-function, parametrized by $\rho$, is then defined as:

\[
\tau_\rho : \hat{X} \to Z, \\
\tau_\rho(x) : \hat{X} \mapsto \hat{x} \sim Q_{x, \rho}.
\]

4 The Agora Algorithm

The Agora algorithm takes as an input a tuple $(f, S, D, E, \Theta, \tau_\rho)$, where $f(\cdot; \cdot)$ is an untrained, fixed architecture (Timaeus) $f : X \times W \to Y$; $S(\cdot; \cdot)$ is a trained model (Socrates) $S : X \times \{w^S\} \to Y$; and $D$ and $E$ are datasets with $D, E \sim \mathcal{P}$, $D \cap E = \emptyset$, and $E$ is $\epsilon$-representative of $\mathcal{P}$ for some, perhaps unknown, $\epsilon$. Agora also has access to a training subroutine $\text{TRAIN-MODEL}(\cdot, \cdot, \cdot)$, as described in Section 3.2, with a corresponding set of possible hyperparameter configurations $\Theta = \{\theta_1, \ldots, \theta_t\}$, and a $\tau$-function $\tau_\rho(\cdot)$ parametrized by some $\rho$.

The full procedure is displayed in Algorithm 1. It alternates between selecting the highest-performing Timaeus over multiple sets of hyperparameters, and augmenting the training set with elements generated by $\hat{x} = \tau_\rho(x)$ and scored with Socrates, $S(\hat{x}; w^S)$. Specifically, at the $k$th iteration, the algorithm will execute the following steps:

- Train $|\Theta^{(k)}|$ Timaeus models $f(\cdot; w_{i}^{*,(k)})$ on $D^{(k)}$ corresponding to every $\theta_i \in \Theta^{(k)}$, and select the highest-accuracy model. Tabulate all the scores for the current iteration.
- Create a set $M^{(k)} = \{\tau_\rho(x) : (x, y) \in E \land f(x; w_i^{*,(k)}) \neq y \land \tau_\rho(x) \notin E\}$, label it with Socrates, and append it to the training set, $D^{(k+1)} = D^{(k)} \cup \{\langle \hat{x}, S(\hat{x}, w^S) \rangle : \hat{x} \in M\}$.
- Sort the tabulated performances along with their hyperparameters in non-decreasing order. Select the hyperparameter $\theta_{0,j}^{(k)}$ belonging to the longest sequence of contiguous hyperparameters rooted at the first element, $\theta_{0,j}^{(k)} \in \Theta^{(k)}$; finally, remove all the hyperparameter sets from $\Theta^{(k)}$ that contain $\theta_{0,j}^{(k)}$, $\Theta^{(k+1)} = \{\theta_t : \theta_{0,j}^{(k)} \notin \theta_t, \forall \theta_t \in \Theta^{(k)}\}$.

5 Analysis

We begin this section by proving properties of the $\tau$-function. This is done by leveraging some assumptions and techniques from the field of topological data analysis, and then use these results to provide bounds regarding Agora’s correctness and runtime.

5.1 Properties of the $\tau$-Function

We provide proofs around two basic facts needed for the correctness of Agora: first, that the $\tau$-function is able to generate a dataset that, when labeled correctly, is $\epsilon$-representative of $\mathcal{P}$ (shown in Lemma 3); and second, that in the (ideal) case where the $\tau$-function is equivalent to $\sigma$ and Socrates
Theorem 1 (Theorem 3.1 of [Niyogi et al. 2008]). Let $\mathcal{M}$ be a compact submanifold of $\mathbb{R}^n$ with condition number $\mu = \inf_{x \in \mathcal{M}} \|x - m\|_{\mathbb{R}^N}$, where $m$ is its medial axis. Let $X = \{x_1, \ldots, x_n\}$ be a set of $n$ points drawn i.i.d. according to the uniform probability measure with support on $\mathcal{M}$. Let $0 < \rho < \mu/2$. Let $U = \cup_{x_j \in X} B^m_\rho(x_j)$ be a correspondingly random open subset of $\mathbb{R}^N$.

Let 
\[
\beta(\rho) = \frac{\cos^m (\arcsin (\frac{\rho}{2m}))}{\text{vol}(B^m_\rho)},
\]
for $m = \text{dim}(\mathcal{M})$, and $\text{vol}(B^m_\rho)$ the volume of a $m$-ball of radius $\rho$.

Then, for all
\[
 n > \beta(\rho/4) \left( \ln \beta(\rho/8) + \ln \left( 1/\delta \right) \right),
\]
the homology of $U$ equals the homology of $\mathcal{M}$ with probability greater than $1 - \delta$.

Intuitively, the proof for Theorem 1 relies on the fact that the homologies are equal whenever $X$ is dense (in a precise sense) in $\mathcal{M}$, and hence the number of samples required to ensure such a condition is lower-bounded by Equation 9. To analyze the correctness of the $\tau$-function, however, it suffices to enforce the sample size as in Equation 9 and note that our ambient space and our noisy sampled space are roughly the same; specifically, they both have the same dimension, and the former is contained in the latter. We formalize these observations in Lemma 1.

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The constraint around the condition number (often known referred to as reach, as introduced by Federer (1959)) being strictly positive can be weakened to a certain degree (Chazal et al., 2006). It is known (Chazal et al., 2017a) that a smooth compact submanifold of $\mathbb{R}^n$ always has positive reach.
Lemma 1. Let $D$ be a dataset sampled from a probability distribution $\mathcal{P}$ with support $X$. Assume $X$ lies on a compact Riemannian submanifold of $\mathbb{R}^m$, $\mathcal{X}$, with condition number $\mu$ in the sense of Niyogi et al. (2008). Let $\{f(\cdot; w): w \in W\}$ be a set of classifiers with VC dimension $d$.

Let $\rho$ correspond to a choice of $\rho/4$-covering number for $\mathcal{X}$ such that $0 < \rho < \mu/2$, and let

$$
A_\rho = \left( \frac{\rho \sqrt{\pi}}{4} \right) \left( 1 - \frac{\rho^2}{64 \mu^2} \right)^{1/2}.
$$

Also let $0 < \delta \leq 1/2$. Then the homology of an open subset $\bigcup_{x_i \in D} B_\rho(x_i)$ equals the homology of $\mathcal{X}$ with probability at least $\delta$, if and only if $D$ is $\epsilon$-representative of $\mathcal{P}$ with $f(\cdot; \cdot)$, when

$$
\epsilon \in \Omega \left( \left( \frac{A_\rho^m}{(2^m)! \text{vol}(\mathcal{X})} \right)^{1/2} \right),
$$

$$
d \in \Omega \left( \log \left( 2^m \left( \frac{64 - \rho^2 / \mu^2}{256 - \rho^2 / \mu^2} \right)^{m/2} \frac{(2^m)! \text{vol}(\mathcal{X})}{A_\rho^m} \right) \right).
$$

Proof. In Appendix A.

Remark 2. The results from Lemma 1 are applicable to a range of models wider than fixed-architecture classifiers, which are the main focus of this paper.

Lemma 2. Let $D \sim \mathcal{P}$ be a dataset that is $\epsilon$-representative of $\mathcal{P}$ for a set of classifiers $\{f(\cdot; w): w \in W\}$ with VC dimension $d$, and assume the support of $\mathcal{P}$ lies on a manifold $\mathcal{X}$ as described in Lemma 1. Then, if for any other dataset $E \sim \mathcal{P}$, the homology of some open cover of $\mathcal{X}$, $U_D = \bigcup_{x_i \in D} B_\rho(x_i)$, equals the homology of another open cover $U_E = \bigcup_{x_i \in E} B_\rho(x_i)$, then $E$ is also $\epsilon$-representative of $\mathcal{P}$ for the same set of classifiers, and appropriate choices of $\rho$, $d$, $|E|$, and $\epsilon$.

Proof. It follows immediately from Lemma 1.

With both results we are now able to prove a key result: the dataset generated by the $\tau$-function will also be $\epsilon$-learnable. Our proof follows closely the techniques from Niyogi et al. (2008), as this problem has a natural solution in terms of their homology-based framework.

Lemma 3. Let $E \sim \mathcal{P}$ be a dataset that is $\epsilon$-representative of a probability distribution $\mathcal{P}$ with support $X$, for a set of classifiers $\{f(\cdot; w): w \in W\}$ with VC dimension $d$, for $\epsilon$, $|E|$ and $d$ as stated in Lemma 1. Let $\tau_\rho(\cdot)$ be a $\tau$-function parametrized by $0 < \rho < \mu/2$.

Assume that the domain $Z$ of $\tau_\rho(\cdot)$ is describable as a compact Riemannian submanifold of $\mathbb{R}^m$ with the same condition number as $\mathcal{X}$. Consider the set

$$
\tilde{E}^{(k)} = \bigcup_{j=1}^{\kappa} \{\tau_\rho(x): \forall x \in E \land \tau_\rho(x) \notin E \}
$$

formed by $\kappa$ calls to $\tau_\rho(\cdot)$ on elements of $E$.

Then, for $0 < \delta \leq 1/2$ and $\Delta = Z \setminus E$; with $|E \cup \Delta| \leq c|X|$ for $0 < c < 1$; if

$$
\kappa \geq \left( \frac{|X| + |\Delta|}{X(1-c) + 2|\Delta|} \right) \ln \left( \frac{|E|}{\delta} \right)
$$

then $\tilde{E}^{(k)}$ is $\epsilon$-representative of $\mathcal{P}$ with probability at least $1 - \delta$. 

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Proof. In Appendix B.

It is important to highlight that equivalence up to homology is a weak relation, in comparison to, say, equivalence up to homeomorphism. Unfortunately, this is an undecidable problem for dimensions larger than 4 (Markov, 1958). One implication of Lemma 3 is that, if \( Z = X \), the number of calls to \( \tau_\rho(\cdot) \) is minimal for any input problem. We leverage these ideas to obtain the notion of a faithful \( \tau \)-function:

**Definition 3 (The Faithful \( \tau \)-Function).** Let \( \tau_\rho: X \rightarrow Z \) be a \( \tau \)-function parametrized with some \( \rho \). We say that \( \tau_\rho(\cdot) \) is faithful whenever \( Z = X \) and \( \rho \) corresponds to the minimum \( \rho/4 \)-covering number of \( X \).

We prove in Lemma 4 that it is possible to be able to increase the performance of the model through a faithful \( \tau \)-function.

**Lemma 4.** Let \( D, E \sim P \) be datasets such that \( D \cap E = \emptyset \), and let \( F = \{ f(\cdot;w) : w \in W \} \) be a set of classifiers with VC dimension \( d \), trained on \( D \), and with \( \sup\{ \text{acc}(f, E) : f(\cdot) \in F \} = \alpha \) for some \( f(\cdot;\cdot) \). Assume we have an oracle \( O(\cdot;w^o) \) for \( P \) such that \( \text{acc}(O, F) = 1 \), \( \forall F \sim P \), and a faithful \( \tau \)-function \( \tau_\rho(\cdot) \). Assume that the conditions from Lemmas 2 and 3 hold.

Then training \( f(\cdot;\cdot) \) on a dataset

\[
D' = D \cup \{ (\tilde{x}, O(\tilde{x};w^o)) : \tilde{x} = \tau_\rho(x) \land x \in E \land \tilde{x} \notin E \}
\]

and evaluating it on \( E \) will have accuracy \( \text{acc}(f, E) \geq \alpha \).

**Proof.** From Lemma 3 it can be seen that, if \( F \) has the appropriate size, \( D' \) will be at least \((1 - \alpha)\)-learnable by some \( f(\cdot;w \in W) \). Given that \( O(\cdot;w^o) \) has zero error across \( X \), it follows that we can guarantee that the labeling produced by \( O(\tau_\rho(x);w^o) \) will be correct for any \( x \in X \). The VC dimension of \( F \) remains unchanged, but adding a new point to \( D \) lowers the Rademacher complexity of this problem,

\[
\sqrt{\frac{2d \ln (|D| + |F|)}{|D| + |F|}} < \sqrt{\frac{2d \ln (|D|)}{|D|}},
\]

and hence \( E \) remains at least \((1 - \alpha)\)-learnable.

In practice we might not have access to the conditions from Lemma 4 around a faithful \( \tau \)-function and an oracle—indeed, one of the constraints for our problem is the lack of access to \( \sigma \). Nonetheless, these assumptions allow us to simplify the analysis of Agora. In the case where the \( \tau \)-function is not faithful, the bounds still hold as long as the conditions of Lemma 4 are met, as it is a probabilistic argument. Indeed, we are still able to work around such limitations to an extent, which is be the topic of Sections 4 and 5.

### 5.2 Correctness

We state bounds for the accuracy of Socrates, such that it allows us to maintain the invariants from Lemma 4 and then prove correctness of Algorithm 1. To begin, we introduce the notions of a random classifier and perfect memory which, like Definition 3, are meant to simplify our analysis. Then we show that for a random classifier, Agora is able to return a trained model with arbitrarily low error rate (Lemma 5) and then we extend the results to obtain correctness conditions for our algorithm (Theorem 2).
Definition 4 (The Random Classifier). Let $D \sim \mathcal{P}$ be a dataset with $p$ positive labels and $1 - |D|/p$ negative labels. A random classifier $f$ outputs, when called, 1 with probability $1/p$, and 0 otherwise, regardless of its input.

It is clear that a (specific) model that actually learns the input dataset will almost always have a better performance than a random classifier. Moving forward, we will consider the results involving a random classifier a lower bound on the performance of any other model, so long as the data remains balanced.

Definition 5 (Perfect Memory of a Classifier). Let \( \langle f, D, \theta \rangle \) be an input to \textsc{train-model}(\cdot, \cdot, \cdot), such that \( \text{acc}(f(\cdot; w^D), D) = a \) for some trained model \( f(\cdot; w^D) \). We say that an architecture \( f(\cdot; \cdot) \) has perfect memory with a given training algorithm, if its performance does not change when augmenting the dataset and retraining it.

That is, for some \( \langle x, y \rangle \notin D \), if for any input \( \langle f, D' = D \cup \{\langle x, y \rangle\}, \theta' \rangle \), \( \text{acc}(f(\cdot; w^{D'}), D') = a' \), then the following relation holds:

\[
a - \frac{1}{|D| + 1} \leq a' \leq a + \frac{1}{|D| + 1}.
\] (17)

Lemma 5. Let \( I = \langle f, S, D, E, \Theta, \tau_\rho \rangle \) be an input to Agora, such that \( f(\cdot; \cdot) \) is a random classifier with perfect memory, and \( \tau_\rho(\cdot) \) is faithful. Assume Socrates has accuracy \( \text{acc}(S, D') \geq 2/3, \forall D' \sim \mathcal{P} \), and, for simplicity, that the problem has equal proportion of negative and positive labels. Then the accuracy of \( f(\cdot; \cdot) \) on \( E \) at the end of the \( k \)-th iteration of Agora is given by:

\[
\text{acc}^{(k)}(f, E) \geq 1 - \frac{1}{2^k}.
\] (18)

Proof. Assume, for simplicity, \( \Theta = \{\theta_1, \ldots, \theta_k : \theta_i \cap \theta_j = \emptyset \forall \theta_i, \theta_j\} \) and \( f(\cdot; w \in \{w\}) \). The other cases follow immediately from Lines 10 and 20 and the proof for this base case.

Let \( D^{(1)} \) be the dataset at the beginning of the first iteration of Agora. Since \( f(\cdot; \cdot) \) is a random classifier, its performance on \( E \) is at least \( a_f^{(1)} \geq 1/2 \), and hence its error rate is \( e_f^{(1)} \leq 1/2 \).

Let the dataset constructed by Lines 15 and 16 be \( M^{(1)} \). Clearly, \(|M^{(1)}| \leq |E|/2 \), and hence

\[
|D^{(2)}| \leq |D| + \frac{|E|}{2}.
\] (19)

On the next iteration, the labels of every element in \( |M^{(2)}| \) have a chance \( \text{acc}(S, M^{(2)}) \geq 2/3 \) of being correct, and hence the number of points that are misclassified is at most \(|E \cap M^{(1)}|/2 \), or

\[
|M^{(2)}| \leq \frac{|E|}{4},
\] (20)

since \( \tau_\rho(\cdot) \) is faithful. Hence each \( \langle x_i, y_i \rangle \in E \) is classified correctly with probability \( \text{Pr}[f(x_i) = y_i] \geq 1/3 \) in the case where Socrates correctly predicted the label for its corresponding point \( \langle \tilde{x}_i, S(\tilde{x}_i) \rangle \in D^{(2)} \).

If, for some \( \langle x_i, y_i \rangle \in E \), \( f(x_i) = y_i \), but its corresponding point was incorrectly labeled by Socrates, it will not appear again in any \( M^{(k)} \) due to the perfect memory of \( f(\cdot; \cdot) \).

Generalizing the above, it can be seen that at any iteration \( k \) the size of \( M^{(k)} \) will be given by

\[
|M^{(k)}| \leq \frac{|E|}{2^k}.
\] (21)

Induction on Equation 21 concludes the proof.

---

\* This statement does not hold in all cases. If the data were imbalanced across all \( \mathcal{P} \), “dumber” models could actually perform better, e.g., guessing all zeros in a problem with \( |X| - 1 \) negative labels.
Remark that the assumption that the dataset is balanced can be removed and Lemma 5 would still hold, but now as a function of the proportion of labels.

Regardless, if the convergent hyperparameter set—that is, the final hyperparameter in the algorithm’s run—is optimal with respect to $\Theta$, the output of Agora is correct.

**Theorem 2.** Let $I = \langle f, S, D, E, \Theta, \tau_\rho \rangle$ be an input to Agora, such that Timaeus is a random classifier with perfect memory, and $\tau_\rho(\cdot)$ is faithful. Let $\theta^*$ be the convergent hyperparameter set for the entire run of Agora, with a corresponding trained model $f(\cdot; w^* \in W)$. Then, for any $\theta_1 \in \Theta$, if Socrates has accuracy $\text{acc}(S, D') \geq 2/3$, $\forall D' \sim \mathcal{P}$, and the problem has equal proportion of positive and negative labels, the following holds:

\[
\text{acc}(f(\cdot; w^*), E) \geq \text{acc}(f(\cdot; w_i), E),
\]

where $f(\cdot; w_i \in W)$ is the output of $\text{train-model}(f, D, \theta_i)$.

**Proof.** By a straightforward application of Agora and Lemma 5. To begin, assume for simplicity that we run the algorithm on $I' = \langle f, S, D, E, \{\theta_1, \theta_2\}, \tau_\rho \rangle$, such that $|\theta_1 \cap \theta_2| \leq \min(|\theta_1|, |\theta_2|) - 1$. Agora only runs for $k = 2$ iterations, evaluating three models. On the first iteration, it obtains two models corresponding to $\theta_1$ and $\theta_2$, $f(\cdot; w_1^{(k=1)})$ and $f(\cdot; w_2^{(k=1)})$, and prunes out the lowest performing hyperparameter set—say, $\theta_1$. Let $f(\cdot; w_2^{*(1)})$ be the trained model at $k = 1$.

On the second iteration, it evaluates only one model, $f(\cdot; w_2^{(2)})$. Call the trained version $f(\cdot; w_2^{*(2)})$. Since $f(\cdot; \cdot)$ has perfect memory, by Lemma 5 and Lines 10 and 20 we know that

\[
\text{acc}(f(\cdot; w_1^{*(1)}), E) \leq \text{acc}(f(\cdot; w_2^{*(1)}), E) \leq \text{acc}(f(\cdot; w_2^{*(2)}), E),
\]

and hence $\theta^{(2)} = \theta_2$ is the convergent hyperparameter set for Agora for $I'$.

Since the performance of $f(\cdot; \cdot)$ does not decrease when calling Socrates, in general we can see that, across the entire run of the algorithm, the convergent hyperparameter set will not be removed. In other words, if $\theta_j$ is the aforementioned set, and $k$ the total number of iterations, for any $i < k$,

\[
\text{acc}(f(\cdot; w_i^{*(k-i)}), E) \leq \text{acc}(f(\cdot; w_j^{*(k)}), E),
\]

for any $\theta_i \in \Theta, \theta_i \neq \theta_j$.

It follows that the performance of $f(\cdot; \cdot)$ on the convergent hyperparameter set, for any instance of Agora, will upper bound the other members of $\Theta$.

**Corollary 1.** Let $I = \langle f, S, D, E, \Theta, \tau_\rho \rangle$ be an input to Agora, where $\tau_\rho(\cdot)$ is a faithful $\tau$-function and Timaeus has perfect memory, but is not necessarily a random classifier. Let $f(\cdot; w^*)$ be the model obtained returned by Agora. Let $f(\cdot; w^\circ)$ be the model obtained from an enumeration over all $\Theta$. Then

\[
\text{acc}(f(\cdot; w^*), E) = r \cdot \text{acc}(f(\cdot; w^\circ), E),
\]

for $1 \leq r \leq 2 \left(1 - \frac{1}{2^{\rho \tau}}\right)$.

**Proof.** By Lemma 5 if $\tau_\rho(\cdot)$ is faithful and $f(\cdot; \cdot)$ has perfect memory, Agora converges in $1 \leq k \leq |\Theta|$ iterations to a specified accuracy which is lower-bounded by $1 - 2^{-k}$.

An enumeration over $\Theta$ is equivalent to the first iteration of Agora. It follows immediately from Lemma 5 that an upper bound is given when $k = |\Theta|$, or:
\[
\text{acc}(f(\cdot; w^\theta), E) \geq 1 - \frac{1}{2^{\theta}}, \quad (26)
\]
\[
\text{acc}(f(\cdot; w^e), E) \geq 1 - \frac{1}{2^{|\Theta|}}. \quad (27)
\]

Hence:
\[
r = \frac{\text{acc}(f(\cdot; w^\theta), E)}{\text{acc}(f(\cdot; w^e), E)} \leq 2 \left( 1 - \frac{1}{2^{|\Theta|}} \right), \quad (28)
\]

as desired. The lower bound follows from the fact that the case where \( \Theta = \{\theta\} \) means that Agora is equivalent to an enumeration, and \( k = 1 \).

Note that the bounds obtained in Corollary 1 are fairly loose, and can be tightened on a model-by-model basis.

5.3 Time Bounds
In this section we provide runtime bounds for Agora. Unlike our earlier results, we are no longer able to assume that a random classifier will bound the performance of most models of interest. The runtime of this algorithm is highly dependent on how long it takes for an arbitrary input to converge. We show in Theorem 3 that the runtime for Agora is polynomial on \( \text{train-model}(\cdot, \cdot, \cdot) \), the cardinalities of \( |\Theta| \) and \( |E| \), and the inference times for Timaeus and Socrates. We conclude this section by narrowing down these results in Corollary 2 for a large class of inputs.

**Theorem 3.** Let \( I = (f, S, D, E, \Theta, \tau_\rho) \) be an input to Agora, where Timaeus has perfect memory and Socrates has accuracy \( \text{acc}(S, D') \geq 2/3, \forall D' \sim \mathcal{P} \).

Assume \( \tau_\rho(\cdot) \) is faithful, and the assumptions from Lemma 3 hold. Assume \( \text{train-model}(f, D, \theta) \in O(|\Theta| + |E|) \). If the problem has balanced positive and negative labels, then Agora terminates in
\[
O\left( |\Theta|^2 \left( \log |\Theta| + |\theta|^2 + T_f \left( |D| + \frac{|E|}{2^{|\theta|-1}} \right) \right) + S|\Theta||E| \left( 1 - \frac{1}{2^{|\Theta|}} \right) \right) \quad (29)
\]
steps, where \( T_f(|D|) \in O(\text{poly}(f, |D|, \theta)), \forall \theta \in \Theta \) and any \( f(\cdot; w \in W) \).

**Proof.** Let \( k \) be an iteration of Agora, and let \( T_f(|D|) \) be the upper bound number of steps required to train each of the \( \Theta(\cdot) \) Timaeus models \( f(\cdot; \cdot) \) on \( D^{(k)} \). Then the cost, per iteration, of Line 6 to Line 14 is
\[
O\left( |\Theta|^2 \left( |\Theta| + |\theta|^2 + T_f \left( |D| + \frac{|E|}{2^{|\theta|-1}} \right) \right) + S|\Theta||E| \left( 1 - \frac{1}{2^{|\Theta|}} \right) \right). \quad (30)
\]

Lines 15 and 16 involve \( |M^{(k)}| \) calls to \( \tau_\rho(\cdot) \), and \( |M^{(k)}| \) calls to Socrates. Both operations can be executed at the same time, and, since Timaeus has perfect memory, we know that the bound corresponding to this step is tight. Moreover, Line 17 is a simple sorting statement, which we assume to be comparison-based, while Lines 19 and 20 can be executed with a naïve implementation that compares every element and employs a counting argument, in time \( O(|Q^{(k)}| |\theta|^2) \), for \( \theta \in \Theta^{(k)} \).

This yields:
\[
O\left( |M^{(k)}| S + |Q^{(k)}| |\theta|^2 + |Q^{(k)}| \log |Q^{(k)}| \right). \quad (31)
\]
Adding both equations together, and using the fact that $|Q^{(k)}| = |\Theta^{(k)}|$, gives a total time per iteration of

$$\text{Cost}(k) = O\left(|\Theta^{(k)}| \left( T_f(|D^{(k)}|) + \bar{f}|E| + |\theta|^2 + \log |\Theta^{(k)}| \right) + |M^{(k)}| S \right). \quad (32)$$

Since in the worst case Agora will prune exactly one member of $\Theta$ on every iteration, Equation (32) can be expressed in terms of $|\Theta|$. By using Lemma 5 we obtain:

$$\sum_{k=1}^{|\Theta|} \text{Cost}(k) = \sum_{k=1}^{|\Theta|} |\Theta^{(k)}| \left( \bar{f}|E| + T_f(|D^{(k)}|) \right) + \sum_{k=1}^{|\Theta|} |\Theta^{(k)}| \left( \log |\Theta^{(k)}| + |\theta|^2 + \log |\Theta^{(k)}| \right) + |M^{(k)}| S \text{log (}|\Theta^{(k)}|) \right). \quad (33)$$

Note that, for $k \geq 2$,

$$\sum_{k=1}^{|\Theta|} |\Theta^{(k)}| T_f(|D^{(k)}|) = |\Theta| T_f(|D|) + \sum_{k=2}^{|\Theta|} (|\Theta| - (k - 1)) T_f \left( |D| + \frac{|E|}{2^{k-1}} \right), \quad (34)$$

and so

$$\sum_{k=1}^{|\Theta|} \left( \bar{f}|E| + T_f(|D^{(k)}|) \right) \in O\left( |\Theta|^2 \left( \log |\Theta| + |\theta|^2 + T_f \left( |D| + \frac{|E|}{2^{k-1}} \right) \right) + S|\Theta||E| \left( 1 - \frac{1}{2^{|\Theta|}} \right) \right). \quad (35)$$

It then follows that Equation (35) simplifies to

$$\sum_{k=1}^{|\Theta|} \text{Cost}(k) \in O\left( |\Theta|^2 \left( \log |\Theta| + |\theta|^2 + T_f \left( |D| + \frac{|E|}{2^{|\Theta| - 1}} \right) \right) + S|\Theta||E| \left( 1 - \frac{1}{2^{|\Theta|}} \right) \right), \quad (36)$$

as desired.

The key assumption behind Theorem 5 and Agora, for that matter—is that the hypothesis class is able to learn, with high probability, $\mathcal{P}$ in a polynomial number of steps. As mentioned in Section 5.1, this is an unrealistic assumption for most systems of interest given that there is no guarantee that an algorithm fulfilling the conditions for $\text{train-model}(\cdot, \cdot, \cdot)$ exists.

We can, however, prove similar results to Theorem 5 for a specific subset of inputs to Agora where the problem is non-convex, but the training algorithm does run in polynomial time with respect to $\bar{f}$, $D$, $\theta$, and an extra set of parameters $\pi$. To see this, let us now shift our analysis to the case where Timaeus and Socrates are piecewise-continuous, real-valued functions with their output mapped consistently to $\{0, 1\}$. Due to the nonconvexity and discontinuities present in Equations 11 and 12, a carefully-chosen surrogate loss is commonly employed in tandem with a polynomial-time (or better) optimization algorithm, such as stochastic gradient descent (SGD).

If we choose the optimizer for $\text{train-model}(\cdot, \cdot, \cdot)$ to be SGD, and the surrogate loss is $L$-Lipschitz smooth, bounded from below and with bounded stochastic gradients for some $G$, then $\text{train-model}(\cdot, \cdot, \cdot)$ will return an $\epsilon$-accurate solution in $O(|B| \bar{f}/\epsilon^c)$ steps, for some constant $c \leq 2$, $B \subseteq D$, and an appropriate choice of learning rate $\eta$. Most SGD-based training procedures present...
such a runtime, even in the non-convex setting (Reddi et al., 2018; Nguyen et al., 2020), as long as the surrogate loss function fulfills the conditions mentioned above. Indeed, Nguyen et al. (2020) showed that, for a specific variant of SGD referred to as shuffling-type SGD, this algorithm converges to a choice of $E||\nabla F(\cdot; w)||^2 \leq \gamma$ with $c = 2/3$ whenever $\eta = \sqrt{\gamma}/(LG)$, for some (not necessarily convex) function $F$. Note that $\gamma$ may be a stationary point, and that, for an appropriate choice of loss function, $\gamma \propto \epsilon$.

**Corollary 2.** Assume Timaeus and Socrates are both piecewise-continuous, real-valued functions with their output mapped consistently to $\{0, 1\}$, and that the rest of the assumptions for Theorem 3 hold. Also assume that TRAIN-MODEL($\cdot$, $\cdot$, $\cdot$) uses shuffling-type SGD as its optimizer.

If for every $\theta \in \Theta$ there exists a subset $\pi \subset \theta$ which encodes the learning rate, batch size, and random seed for TRAIN-MODEL($\cdot$, $\cdot$, $\cdot$), and if the surrogate loss is is $L$-Lipschitz smooth, bounded from below and where all gradients are stochastic and bounded by some $G$, then Agora converges in

$$O\left(\left|\Theta\right|^2 \left(\log \left|\Theta\right| + \left|\Theta\right|^2 + \bar{f} \left(\left|E\right| + \frac{|B|}{(LG\zeta)^{2/3}}\right)\right) + \bar{S}(\Theta || E) \left(1 - \frac{1}{2|\Theta|}\right)\right) \quad (37)$$

steps, where $B \subset D$, with $|B| = \max_{\theta \in \Theta} \{ |B| \in \theta \}$ and $\zeta = \min_{\theta \in \Theta} \{ \eta^2 \in \theta \}$.

**Proof.** The extra set of parameters in this case is the choice of learning rate $\eta$, as well as the characterization of the batch $B \sim D$ with respect to the state $s$ of some random number generator. Since our setting assumes that $D$ is not $\epsilon$-representative of $\mathcal{P}$—at least not in the first iteration—batch-based optimization methods will be sensitive to the algorithm’s stochasticity. Let $\pi_i = \{ \eta_i, s_i, |B_i| \}$, and note that every combination of elements of $\pi_i$ guarantees an $\epsilon_i$-accurate solution (w.p.1) in polynomial time under the assumptions given. The unknown $\epsilon_i$ is fully characterized by $\pi_i$ and, by definition, the rest of the hyperparameters from $\theta_i$.

It follows that constructing a hyperparameter set $\theta'_i = \theta_i \cup \pi_i$ will allow Agora to search over $\pi_i$, and select the appropriate values based on $\epsilon_i$, hence maintaining the invariants from Lines 10 and 20 which, by Lemma 5 and Theorem 3 ensure correctness.

The bound for Equation 37 is obtained by a simple substitution in Equation 29 of $T_f(D)$, coupled with the facts that TRAIN-MODEL($f, B_i, \theta'_i$) with shuffling-type SGD runs in $O(|B| / \bar{f} / \epsilon_i^{2/3})$ steps, and that, $\forall \pi_i, \theta_i, \epsilon_j$, TRAIN-MODEL($f, B_i, \theta_i$) defines a surjection $\pi_i \cup \theta_i \mapsto \epsilon_j$.

Note that this result is not necessarily applicable to all machine learning models, or all neural networks for that matter, as their convergence conditions differ. Moreover, this makes the ratio from Corollary 1 more dependent on the choice of $\Theta$, as neural networks, without accounting for finite-precision computing, belong to hypothesis classes of infinite size.

**Remark 3.** Training Timaeus—especially when it is a neural network—may become computationally costly, and dominate the other terms in the equation. Still, the “wall clock” runtime of Agora can be improved by a factor of $|\Theta|$, by parallelizing Line 7 across multiple nodes.

6 Concluding Remarks

We presented an algorithm to obtain models under low-resource and ill-posed settings. Our analysis of Agora shows that this procedure is able to generate a dataset that is provably a part of the underlying distribution, and thus return an optimal solution by making the problem easier to learn—all while maintaining generalizability.

The runtime of this algorithm can be improved algebraically by employing a generalized suffix tree in the longest common substring search part of the procedure. Most practical problems have
a near-negligible runtime dependency with respect to this step, since, as mentioned, the training procedure signifies the largest drain in terms of computational steps and tends to dominate the other quantities. On the other hand, although Agora’s intended use is to simplify the training of smaller models, it can be seen from Lemma 3 that this algorithm can be used to improve the performance of any model. Indeed, Theorem 3 shows a linear dependency of the runtime of Agora with respect to the steps needed to perform inference on both Timaeus and Socrates, and hence it performs better when the time needed to train the former is minimized.

By design, our setup focused on binary classifiers, but the results from this work can easily be extended to multi-class classification problems by reducing membership of each class to a binary classification problem, and breaking ties arbitrarily and consistently. The correctness analysis would vary slightly, as the VC dimension, which is an integral part of our proofs, is defined only over binary classification problems.

Another central part of our correctness results is the assumption that the support lies on or around a manifold. This is a fairly strong constraint—perhaps even unrealistic. Yet, the work by Genovese et al. (2014) focused on the existence of density ridges, as opposed to a fully-fledged manifold, and showed that a well-defined ridge can be topologically similar, in a certain sense, to such a manifold. Similar to Niyogi et al. (2008), this result is also resilient to noise from the sampling procedure, and indeed appears to be a stronger basis from which to analyze the behavior of the $\tau$-function. Nonetheless, unless the support fulfills the density requirements from this paper, this algorithm—like all manifold learning methods—are not guaranteed to yield good results within a practical timeframe. On the other hand, density can be achieved by a dimensionality reduction step. This has the benefit of re-establishing the performance bounds under smaller constants, at the cost of some preprocessing overhead.

Finally, we would like to point out that Agora is not optimal for all possible hypothesis classes, and its convergence and runtime properties rely on assumptions that may or may not hold in realistic scenarios. Nevertheless certain models are remarkably robust to ill-posed problems (e.g., deep neural networks). A derivative of this algorithm that maintains the invariances from the $\tau$-function in tandem with better rules for hyperparameter pruning would, without a doubt, present even better convergence and generalizability guarantees.

Acknowledgments

To my grandfather.
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Appendices

A Proof of Lemma 1

“If” direction: We show that an open set \( U = \bigcup_{x_i \in D} B_\rho(x_i) \) that has the same homology as \( X \) is \( \epsilon \)-representative of \( P \), and that Equation 3 holds when the conditions for the lemma are met.

Fix an arbitrary confidence \( 0 < \delta \leq \frac{1}{2} \). Then, from Theorem 1 the minimum sample size \( |D| \) needed to construct such a set \( U \) with probability greater than \( 1 - \delta \) has to be at least

\[
|D| > \beta(\rho/4) (\ln \beta(\rho/8) + \ln (1/\delta)),
\]

for \( \beta(\rho) = \frac{\text{vol}(X)}{\cos^m(\arcsin(\rho/\mu)) \text{ vol}(B^m_{\rho/4})} \), and where \( \mu \) is the condition number, \( \dim(X) = m \), and \( \rho \) the radius \( 0 < \rho < \mu/2 \) of the \( m \)-balls covering \( X \).

On the other hand, Hanneke (2016) showed that the minimum sample size needed for Equation 3 to hold with probability at least \( 1 - \delta \) is given by

\[
|D| \geq c \left( \frac{d + \log (1/\delta)}{\epsilon^2} \right),
\]

for some constant \( c \) and \( 0 < \epsilon, \delta \leq \frac{1}{2} \). This bound is tight, but we are only concerned with the lower bound.

Assume \( |D| \) satisfies Equation 38. Then there is an assignment of \( \beta(\rho) \) that allows Equation 39 to hold. Solving Equation 39 for \( \beta(\rho) \) with the ansatz:

\[
\epsilon = \sqrt{c/\beta(\rho/4)},
\]

\[
d = c' \log \beta(\rho/8),
\]

where \( c' = \ln(2) \), yields:

\[
\epsilon = \sqrt{c} \left( \frac{\cos^m(\arcsin(\rho/\mu)) \text{ vol}(B^m_{\rho/4})}{\text{ vol}(X)} \right)^{1/2},
\]

\[
d = c' \log \left( \frac{\text{ vol}(X)}{\cos^m(\arcsin(\rho/\mu)) \text{ vol}(B^m_{\rho/8})} \right).
\]

We can refine this result, and obtain the same as Equations 11 and 12 by noting that the volume \( \text{ vol}(B^m_\rho) \) is given in the \( m \)-dimensional ambient space, which is Euclidean and equipped with the canonical Euclidean metric, and that \( \Gamma(\frac{x}{2} + 1) = (x/2)! \):

\[
\epsilon = \sqrt{c} \left( \frac{\cos^m(\arcsin(\rho/\mu))\pi^{m/2} (\frac{\mu}{\rho})^m}{(\frac{\mu}{2})! \text{ vol}(X)} \right)^{1/2},
\]

\[
d = c' \log \left( \frac{\text{ vol}(X)(\frac{\mu}{2})!}{\cos^m(\arcsin(\rho/\mu))\pi^{m/2} (\frac{\mu}{8})^m} \right).
\]

Letting \( \Lambda_\rho = \left( \frac{\sqrt{\pi}}{4} \right) \left( 1 - \frac{\rho^2}{64\mu^2} \right)^{1/2} \), we obtain
\( \varepsilon \in \Omega \left( \left( \frac{A^m_{\rho}}{(\frac{\mu}{2})! \vol(\mathcal{X})} \right)^{1/2} \right) \) \hspace{1cm} (46)

\( d \in \Omega \left( \log \left( 2^m \left( \frac{64 - \rho^2}{256 - \rho^2/\mu^2} \right)^{m/2} \frac{(\frac{\mu}{2})! \vol(\mathcal{X})}{A^m_{\rho}} \right) \right) \) \hspace{1cm} (47)

as desired. It follows that, when the homology of \( \cup_{x_i \in D} B_\rho(x_i) \) equals the homology of \( \mathcal{X} \), \( D \) is \( \varepsilon \)-learnable, if \( \varepsilon \) and \( d \) satisfy Equations 11 and 12.

"Only if" direction: We show that a dataset that is \( \varepsilon \)-representative of \( \mathcal{P} \) with its size determined by Equations 11 and 12 and Equation 39 has the same homology as \( \mathcal{X} \).

Fix an arbitrary confidence \( 0 < \delta \leq 1/2 \). Assume there exists an assignment of \( \varepsilon \) and \( d \) that satisfies Equation 39, such that \( D \) is \( \varepsilon \)-representative of \( \mathcal{P} \) under these conditions. Then

\[
|D| > c \left( \frac{c' \log \left( 2^m \left( \frac{64 - \rho^2}{256 - \rho^2/\mu^2} \right)^{m/2} \frac{(\frac{\mu}{2})! \vol(\mathcal{X})}{A^m_{\rho}} \right) + \log \frac{1}{\delta} }{c_\varepsilon \left( \frac{A^m_{\rho}}{(\frac{\mu}{2})! \vol(\mathcal{X})} \right)} \right)
\]  

for some positive, nonzero constants \( c \geq \ln(2) \), \( \log c' = c_d \geq 1/8 \), and \( c_\varepsilon \geq 1 \) encoding the respective constants for Equations 11 and 12.

From the derivation of Equation 38 by Niyogi et al. (2008) we know that the confidence \( \delta \) is lower-bounded by the \( \rho/4 \)-packing number \( z \), times the minimum probability \( 1 - \alpha \) that the intersection of the cover with a nontrivial subset \( F \subset D \), \( |F| < |D| \) is empty, that is:

\[
z(1 - \alpha)^{|F|} \leq z e^{-|F|\alpha} \leq \delta
\]  

(49)

for \( \alpha = \min_{x_i \in F} \vol(B_{\rho/4}(x_i) \cap \mathcal{X})/\vol(\mathcal{X}) \). Crucially, if \( |F| \) is larger than a carefully-chosen lower bound, it follows that the homology of a cover of \( F \) equals the homology of \( \mathcal{X} \). From the same work we know that \( \alpha \) and \( z \) are invariants of the manifold, and are unrelated to the dataset itself. In particular,

\[
\frac{1}{\alpha} \leq \frac{\vol(\mathcal{X})}{\cos^m \left( \arcsin \left( \frac{\rho}{8\mu} \right) \right) \vol(B_{\rho/4})},
\]

(50)

\[
z \leq \frac{\vol(\mathcal{X})}{\cos^m \left( \arcsin \left( \frac{\rho}{16\mu} \right) \right) \vol(B_{\rho/8})}.
\]

(51)

Solving for \( |F| \) in Equation 49, we obtain:

\[
|F| \geq \frac{1}{\alpha} \ln \frac{z}{\delta},
\]

(52)

which is precisely the statement from Equation 38. Plugging in Equation 48 in Equation 49 along with the fact that \( |D| \geq |F| \), it follows that:

\[
\frac{1}{\alpha} \ln \frac{z}{\delta} \leq c \left( \frac{c_d \log \left( 2^m \left( \frac{64 - \rho^2}{256 - \rho^2/\mu^2} \right)^{m/2} \frac{(\frac{\mu}{2})! \vol(\mathcal{X})}{A^m_{\rho}} \right) + \log \frac{1}{\delta} }{c_\varepsilon \left( \frac{A^m_{\rho}}{(\frac{\mu}{2})! \vol(\mathcal{X})} \right)} \right)\]

(53)
\[ \leq \left( \frac{c}{\ln (2)} \right) \left( c_e \frac{(m^2)! \text{vol} (\mathcal{X})}{\Lambda^m_p} \right) \ln \left( c_d 2^m \left( \frac{64 - \rho^2 / \mu^2}{256 - \rho^2 / \mu^2} \right)^{m/2} \frac{(m^2)! \text{vol} (\mathcal{X})}{\delta \Lambda^m_p} \right). \]  

(54)

Our work is limited to show variable-per-variable bounds. Note, however, that from Equations 50 and 51 we do not obtain any information with respect to the relationship of these bounds and the ones from Equations 11 and 12. Thus the best we can do expect that the bounds from Equations 50 and 51 are at least a lower bound for Equations 11 and 12:

\[ z \leq c_d 2^m \left( \frac{64 - \rho^2 / \mu^2}{256 - \rho^2 / \mu^2} \right)^{m/2} \frac{(m^2)! \text{vol} (\mathcal{X})}{\Lambda^m_p}. \]  

(55)

We can drop the dependence on the volume of the manifold, and recall that \( \text{vol} (\mathcal{B}_{\rho/8}) \) is defined over the tangent space, which is Euclidean. Using this, along with the fact that \( \cos (\text{arcsin} (x)) = \sqrt{1 - x^2} \), we obtain:

\[ \frac{1}{\cos (\text{arcsin} \left( \frac{\rho}{16\mu} \right))} \leq c_d \left( \frac{64 - \rho^2 / \mu^2}{256 - \rho^2 / \mu^2} \right)^{1/2} \left( 1 - \frac{\rho^2}{64\mu^2} \right)^{-1/2}, \]  

(58)

\[ 1 \leq 8(c_d), \]  

(59)

which is true by the definition of \( c_d \).

Similarly, for \( \alpha \), we obtain another inequality:

\[ \frac{1}{\alpha} \leq c_e \left( \frac{(m^2)! \text{vol} (\mathcal{X})}{\Lambda^m_p} \right). \]  

(61)

\[ \frac{\text{vol} (\mathcal{X})}{\cos^m \left( \text{arcsin} \left( \frac{\rho}{8\mu} \right) \right)} \frac{\text{vol} (\mathcal{B}_{\rho/4})}{\text{vol} (\mathcal{B}_{\rho/8})} \leq c_e \left( \frac{(m^2)! \text{vol} (\mathcal{X})}{\left( \frac{\sqrt{\pi}}{4} \right)^m \left( 1 - \frac{\rho^2}{64\mu^2} \right)^{m/2}} \right). \]  

(62)

\[ \frac{1}{\cos^m \left( \text{arcsin} \left( \frac{\rho}{8\mu} \right) \right)} \leq c_e \left( 1 - \frac{\rho^2}{64\mu^2} \right)^{-m/2}. \]  

(63)

\[ 1 \leq c_e, \]  

(64)

which is true by the definition of \( c_e \).

It follows that if \( D \) satisfies Equation 39 with Equations 11 and 12 and \( c \geq \ln (2) \), the homology of \( \cup_{x_i \in D} B_{\rho}(x_i) \) equals the homology of \( \mathcal{X} \).

This last assumption is not necessary, given that the definition of the lower bound of \( d \) in Equation 12 implies a constant \( c_d \) which can be made arbitrarily large with respect to the volume form of \( B_{\rho/8} \) on a chosen (oriented) manifold.

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[10] This last assumption is not necessary, given that the definition of the lower bound of \( d \) in Equation 12 implies a constant \( c_d \) which can be made arbitrarily large with respect to the volume form of \( B_{\rho/8} \) on a chosen (oriented) manifold.
Conclusion: From both parts it follows that $D$ is $\epsilon$-learnable if and only if the homology of a cover for $\mathcal{X}$ with elements of $D$, $\cup_{x_i \in D} \mathcal{B}_\rho(x_i)$, equals the homology of $\mathcal{X}$, as long as $\epsilon$ and $d$ satisfy Equations 11 and 12. This concludes the proof.

Remark 4. A consequence of the second part of the proof of Lemma 1 is that the Big Omega notation can be substituted with an inequality.

B Proof of Lemma 3

By Lemma 2 we know that a dataset is $\epsilon$-representative if (and only if) an open cover of the dataset has the same homology as the support from which it was drawn. We can then prove Lemma 3 by showing that an open cover $\cup_{x_i \in \mathcal{E}(\kappa)} \mathcal{B}_\rho(x_i)$ of $\mathcal{E}(\kappa)$ has the same homology as a respective cover $\cup_{x_i \in \mathcal{E}} \mathcal{B}_\rho(x_i)$ of $\mathcal{E}$ via Theorem 1 and then leverage Lemma 2 to state that such a dataset is $\epsilon$-representative of $\mathcal{P}$. We begin by arguing that building said cover is possible, and then proceed to establish bounds on $\kappa$.

Fix an arbitrary probability $0 < \delta < 1/2$.

It is possible to build a $\rho/4$-cover of $\mathcal{X}$ by sampling $\tau_\rho(\cdot)$, even though the codomain of the $\tau$-function excludes the center of the sphere: since $\mathcal{E}$ is $\epsilon$-representative of $\mathcal{P}$, from Lemma 2 we know that the open cover $\cup_{x_i \in \mathcal{E}} \mathcal{B}_\rho(x_i)$ has the same homology as $\mathcal{X}$, and so $\mathcal{E}$ is $\rho/2$-dense on $\mathcal{X}$.

Then there exists at least one $\tilde{x}_i \in X$ on every $\mathcal{B}_{\rho/4}(x_i) \setminus \{x_i\}$, such that it is possible to construct a $\rho/4$-cover $V = \cup_{i=1}^{|E|} \mathcal{B}_{\rho/4}(\tilde{x}_i^k)$ of a manifold on which $X \setminus E$ lies. Hence such a cover is also a $\rho/4$-cover for $\mathcal{X}$. The second condition for $\mathcal{E}(\kappa)$, that the elements are not repeated from $E$, holds because of the constraint $|E \cup \Delta| \leq c|X|$. Given that $E$ was sampled i.i.d. from $\mathcal{P}$, it is hence possible to sample $\kappa$ times from every $m$-ball a point that, with probability at most $1/c$, is not in $E$.

We now establish the bounds around $\kappa$ for which this holds by a use of the union bound on a nonempty $\Delta$, and remark that the case for $\Delta = \emptyset$ follows from this result.

When $\Delta \neq \emptyset$, a sampled $\tilde{x}_i$ might not belong to $X$, but, by Lemma 2, the cover realized by some subset $F \subset \mathcal{E}(\kappa)$, $\cup_{x_i \in F} \mathcal{B}_{\rho/4}(\tilde{x}_i)$, will have the same homology as the homology of $\mathcal{X}$ as long as $|F| \geq |E|$ and $F \subset X$. To see this, note that if all the points corresponding to $Z = X \cup \Delta$ lie on some manifold $\mathcal{M}$, then there exists a map that can construct a submanifold $\mathcal{X}$ of $\mathcal{M}$ containing only elements of $X$ (resp. $\Delta$); hence a cover for $\mathcal{M}$ will be a cover for $\mathcal{X}$, but a cover for $\mathcal{X}$ will not necessarily be a cover for $\Delta$. It follows that, since we only sample elements within a radius $\rho/4$ of a valid element from $X$, any cover constructed in such a way will be a cover for $\mathcal{X}$, and thus the homology of a cover realized by $F \subset \mathcal{E}(\kappa)$ equals the homology of $\mathcal{X}$.

It then suffices to establish the number of tries $\kappa$ needed to obtain the centers for said cover. For this we rely on the fact that there are two natural partitions of $\mathcal{E}(\kappa)$: one corresponding to the results of every sampling round, as displayed in Equation 13 and another mapping the index of every $i$th element of $E$ to a set tabulating the result of the $j$th sampling with $\tau_\rho(\cdot)$. Partition $\mathcal{E}(\kappa)$ based on the latter strategy, that is, $\tilde{E}(i) = \{\tau_\rho(x_i)(j) : x_i \in E \wedge j \in [1, \ldots, \kappa]\}$, for $E(\kappa) \subset \mathcal{E}(\kappa)$. Let $A_i$ be the event that the $i$th subset of $\mathcal{E}(\kappa)$ under this partition contains solely elements of $E$; that is, $A_i = \Pr[E(\kappa) \cap E \neq \emptyset]$.

Via the union bound, we get:
\[
\Pr \left[ \bigcup_{i=1}^{[E]} [A_i = 1] \right] \leq \sum_{i=1}^{[E]} \Pr [A_i = 1], \tag{65}
\]

\[
\leq \sum_{i=1}^{[E]} \prod_{j=1}^{\kappa} \left( 1 - \frac{\text{vol}((Z \setminus E) \cap (B_{\rho/4}(x_i) \setminus \{x_i\}))}{\text{vol} (Z \cap (B_{\rho/4}(x_i) \setminus \{x_i\}))} \right) \tag{66}
\]

\[
\leq \sum_{i=1}^{[E]} \left( 1 - \frac{\text{vol}((Z \setminus E) \cap (B_{\rho/4}(x_i) \setminus \{x_i\}))}{\text{vol} (Z \cap (B_{\rho/4}(x_i) \setminus \{x_i\}))} \right)^\kappa , \tag{67}
\]

since all elements in \( Q_{x_i, \rho} \) are equally probable. Let

\[
\alpha = \min_{i \in \{1, \ldots, [E]\}} \frac{\text{vol}((Z \setminus E) \cap (B_{\rho/4}(x_i) \setminus \{x_i\}))}{\text{vol} (Z \cap (B_{\rho/4}(x_i) \setminus \{x_i\}))}. \tag{68}
\]

By again relying on the \( \rho/2 \)-density of \( E \) on \( X \), we can see that \( \alpha > 0 \); more importantly, we can observe that the relevant (that is, inside the cover realized by \( E \)) subspace of \( M \) has the same condition number as \( X \), and relax the geometry of this problem. We then lower bound Equation 68 with a counting argument: since \( \tilde{x}_i \) is obtained i.i.d. from \( Z \) with a uniform probability distribution, we can assume that every draw for every \( B_{\rho/4}(x_i) \) is identical, at least with respect to \( Z \). Indeed, remark that all \( x_i \in E \) were also sampled in an i.i.d. fashion. Furthermore, we can drop the dependence on the volume of \( B_{\rho/4}(x_i) \) by noting that we do not need to sample elements strictly from \( X \). From the constraint \( |E \cup \Delta| \leq c|X| \), then \( |Z| = |X| + |\Delta| \), and \( |E| \leq c|X| - |\Delta| \).

Putting it all together, we obtain:

\[
\alpha \geq \frac{|\{ \tilde{x}_i : \tilde{x}_i \in (Z \setminus E) \cap (B_{\rho/4}(x_i) \setminus \{x_i\})\}|}{|\{ \tilde{x}_i : \tilde{x}_i \in Z \cap (B_{\rho/4}(x_i) \setminus \{x_i\})\}|} \tag{69}
\]

\[
\alpha \geq \frac{|Z \setminus E|}{|Z|} \tag{70}
\]

\[
\alpha \geq \frac{|X| (1 - c) + 2|\Delta|}{|X| + |\Delta|} \tag{71}
\]

Following Niyogi et al. (2008) we can simplify Equation 71 to

\[
\Pr \left[ \bigcup_{i=1}^{[E]} [A_i = 1] \right] \leq |E| (1 - \alpha)^\kappa \leq |E| e^{-\kappa \alpha} \leq \delta, \tag{72}
\]

where we used the fact that \( (1 - \beta) \leq e^\beta \) for \( \beta \geq 0 \). Choose \( \kappa \) to be

\[
\kappa \geq \frac{1}{\alpha} (\ln |E| + \ln (1/\delta)) \tag{73}
\]

\[
\kappa \geq \left( \frac{|X| + |\Delta|}{|X|(1 - c) + 2|\Delta|} \right) \ln \left( \frac{|E|}{\delta} \right). \tag{74}
\]

From the above, whenever \( \kappa \) is as specified in Equation 74, \( \bar{E}^{(\kappa)} \) has a subset \( F \subset \bar{E}^{(\kappa)} \) that realizes a cover of \( X \), and such that \( |F| \geq |E| \). It follows from this and from Theorem 1 that a cover of \( F \) has the same homology as \( E \); by Lemma 2 we conclude that \( \bar{E}^{(\kappa)} \) is \( \epsilon \)-learnable.
Remark 5. It is possible to obtain a tighter bound on Equation 68 (and thus on Equation 74) by employing a geometric argument. We leave this question open for further research.