Unsupervised Estimation of Ensemble Accuracy

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Abstract

Ensemble learning combines several individual models to obtain a better generalization performance. In this work we present a practical method for estimating the joint power of several classifiers. It differs from existing approaches which focus on "diversity" measures by *not relying on labels*. This makes it both accurate and practical in the modern setting of unsupervised learning with huge datasets.

The heart of the method is a combinatorial bound on the number of mistakes the ensemble is likely to make. The bound can be efficiently approximated in time linear in the number of samples. We relate the bound to actual misclassifications, hence its usefulness as a predictor of performance.

We demonstrate the method on popular large-scale face recognition datasets which provide a useful playground for fine-grain classification tasks using noisy data over many classes.

1 Introduction

Classifier ensembles allow combining several classifiers into a possibly more accurate one. Traditionally features and "weak learners" were used in boosting [4, 18, 16]. Nowadays it is common to combine several deep learning networks or random forests into an ensemble classifier [14, 15, 5]. Each component in the ensemble is chosen according to some specific principle or is randomly selected. In Ensemble Learning there is empirical evidence that ensembles tend to yield better results when there is significant diversity among the models, with several definitions of the term [17, 10, 3] that are useful when labeled data exists.

In this paper we devise a computationally efficient bound for the number of errors an ensemble will make — even without using labeled data or joint optimization. It therefore extends existing approaches to unsupervised learning regime over massive datasets. This is also true for many modern datasets which are labeled automatically and contain mistakes such as wrong or duplicate identities [19]. To the best of our knowledge this is the first time that the idea of "diversity" is extended to unsupervised setting.

Intuitively, weak-learners are useful together when they split the input space differently. Specifically, they need to disagree on their mistakes. The suggested bound is computed over the observed mapping of the inputs by the classifiers, essentially ignoring their labels. We show that this information suffices to surface errors the ensemble will produce by posing it as an optimal assignment problem which can be efficiently approximated in $O(N)$ where N is the number of samples. The bound relies on reasonable assumptions and is verified to work well experimentally.

To give a numeric example, we can check an ensemble of three classifiers over a face recognition dataset with ten million samples of one million identities by picking about a hundred random samples and testing the joint classification on them.

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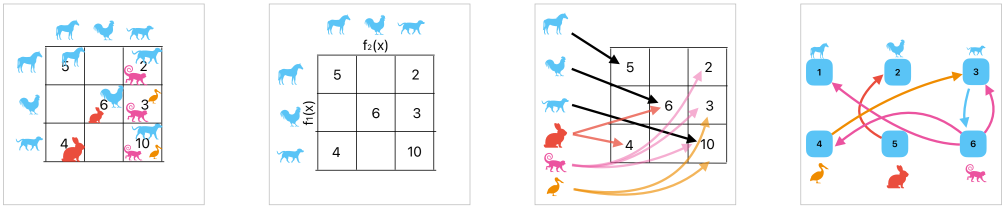


(a) Ground truth (unknown)

(b) Cell Occupancy **C** (visible)

(c) Bipartite graph representation

(d) Mistakes multigraph

Figure 1: A schematic example of the approach where we wish to estimate the potential ensemble performance of $Q = 2$ classifiers over $K = 6$ classes projected onto $L = 3$ classes. Panel **(a)** shows the (unknown) true mapping. Note that monkey class is split among several cells thus limiting the potential accuracy. Panel **(b)** shows the count of the number of elements in the mapping $x_i \mapsto (f_1(x_i), f_2(x_i))$ which is our only observable. Panel **(c)** illustrates the bipartite graph of the same mapping where multiplicity of edges is counted. Panel **(d)** shows the multigraph used in the proof of Claim 5.

Figure **1** illustrates the method for an ensemble of two classifiers $f_1, f_2 : \mathcal{X} \mapsto [L]$. We count duplicity of tuples $(f_1(x_i), f_2(x_i))_{i=1}^{N}$ creating the matrix C (Panel **1b**, where rows are the output of f_1 and columns of f_2). The count enables efficient approximation of a lower bound for the number of mistakes over all possible mappings from a class into (one or more) matrix cell (Panel **1c**) such that all samples are accounted for. This without knowing the ground truth (Panel **1a**).

The paper is organized as follows: In Section 2, we show how two or more metric-learner based classifiers can be used to construct a joint space partitioning scheme. In Section 3 we formally define and analyze the proposed bound. In Section 4 we verify the method on real data and conclude.

2 Problem Formulation

Let $\{x_i \in \mathcal{X}\}_{i=1}^{N}$ be samples from K classes. Let $\{f_q\}_{q=1}^{Q}$ be multi-class classifiers. We aim to estimate their potential accuracy over the samples without using labels.

Every multi-class classifier partitions $\mathcal{X}$ into (not necessarily connected) parts, one for each class. Two classifiers splitting the space differently have the potential to jointly refine the partition of $\mathcal{X}$, thus possibly enabling higher accuracy. At high dimension the number of parts in the joint partition is likely to grow exponentially while the likelihood of a sample to appear in a part diminishes. We therefore pick a small random set of $L \ll K$ samples from distinct classes and observe the joint behavior of f_q on them. A good choice is $L > \sqrt[Q]{K}$ yielding more cells than classes. This forces some cells to be empty in a perfect classification which increases the probability of visible errors.

We start with the following claim:

Claim 1. *Every multi-class classifier can be converted to a metric-learner and vice-versa.*

Proof. By construction for each direction separately:

$\Leftarrow$ Given a multi-class classifier $f(x) \mapsto [K]$ define a metric learner $g(x) := e_{f(x)}$ which maps the class k into the unit vector $e_k \in R^K$ in the standard basis.

$\Rightarrow$ Given a metric learner $f(x) \mapsto R^d$ satisfying $||f(x) - f(y)|| \leq ||f(x) - f(z)||$ for x, y in one class and z in another, and given a one or more (sample, class) pair from each class (x_i, y_i). Define $g(x) := y_j$ where $j := \text{argmin}_i ||f(x) - f(x_i)||$.

It is immediate to verify that this mapping preserves mistakes and hence also accuracy. □

By claim 1 we can assume w.l.o.g. that f_q are metric-learners. Therefore any choice of a random set of L samples induces a mapping of samples $x_i \mapsto \vec{i} \in [L]^Q$ where $\vec{i} := (\, f_1(x_i), \cdots, f_Q(x_i)\,)$. The structure $\mathbf{C} = [c_{\vec{i}}]$ counts how many samples are mapped into each tuple (also called Cell). When

$Q = 2$ the structure $\mathbf{C}$ is a matrix. This count is our only observable. We next show it is indicative of ensemble accuracy.

3 Approach and analysis

The core idea for our error analysis is that any cell $c_{\vec{i}}$ which is not of a class size must contain an error. We seek a mapping matching classes to cells such that all samples are accounted for. Given such mapping we count the number of samples that are mapped incorrectly. This approach may miss cells that unknowingly mix several classes, a point which we address in 5.

We define the bound by considering bipartite multi-graphs (see Panel **1c**) with two types of nodes $N = [K] \cup \{\vec{i}\}$. On the left the nodes represent the K classes and on the right the nodes represent the L^Q cells. Denote by $H^k_{\vec{i}}$ the (unknown) number of elements from class k that are mapped into cell $\vec{i}$. Out of all possible bipartite multigraphs on this vertex set with left degrees S and right degrees $c_{\vec{i}}$, we seek H^* maximizing $\sum_{\vec{i}} \sum_k (H^k_{\vec{i}})^2$. The objective function counts pairs of samples of the same class that end up in the same cell and penalizes the rest.

This leads to the following definition:

Definition 2. *Given a list of cell sizes* $\mathbf{C}$ *and class size* S *we define*

$$\mathrm{CB}(\mathbf{C}) = \max_H \sum_{\vec{i}} \sum_k (H^k_{\vec{i}})^2, \quad \textit{s.t.} \quad \sum_{\vec{i}} H^k_{\vec{i}} = S \,, \sum_k H^k_{\vec{i}} = c_{\vec{i}}.$$

Computing $\mathrm{CB}(\mathbf{C})$ is NP-hard, being a generalization of the Multiway Number Partitioning problem [6]. Yet it is sometimes called "The easiest NP-hard problem" [13] as it can be approximated efficiently. In some cases we can find $\mathrm{CB}(\mathbf{C})$ exactly:

Claim 3. *There is a pseudopolynomial algorithm for exact computation of* $\mathrm{CB}(\mathbf{C})$ *requiring* $O(L^2(K_r - 1)C_m^{K_r - 1})$ *memory where* C_m *is the size of the largest cell and* K_r *is the number of classes after removal of classes and cells of equal size.*

The proof follows [9] with two adaptations. First, as long as there is a cell of size S, we remove it from $\mathbf{C}$. The second modification is that we allow cells to be split between classes and vice-versa. As K tends to be large the above does not provide a practical solution in most cases.

Claim 4. *There is a polynomial time approximation scheme (PTAS) for finding* $\mathrm{CB}(\mathbf{C})$ *with runtime* $O(K_r)$ *with exponential dependence in the reciprocal of the precision.*

Here we apply a PTAS of Alon et al. [1], again after removal of cells and classes of equal size.

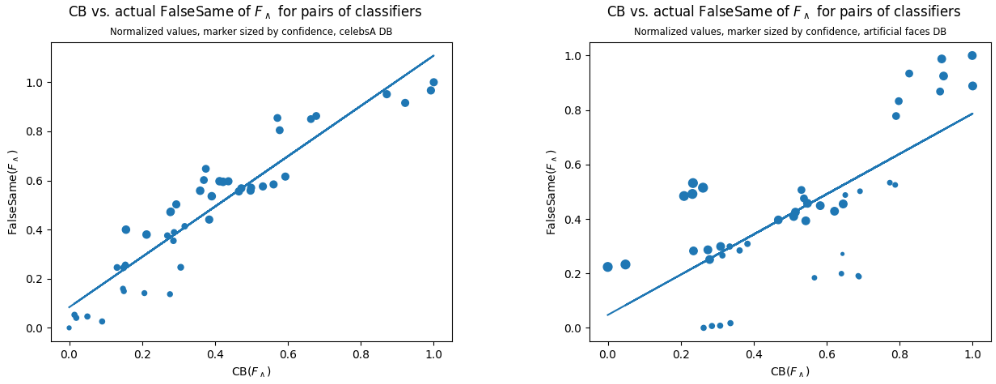
Finally, a greedy algorithm gives a $4/3$ approximation ratio [6]. Our experiments demonstrate this suffices in some cases.

We next prove that the number of "hidden" mistakes is likely to grow as $\mathrm{CB}(\mathbf{C})$ grows, something that is also shown empirically in Section 4. Intuitively, some misclassifications may change cell counts and be visible to us, while others are not. We do not expect classifiers to have a tendency towards detectable vs. invisible errors, so it is not surprising the two grow together. Hence we hypothesize that the number of visible errors increases monotonically with the total number of mistakes.

Let φ^* be an optimal mapping of classes to cells achieving $\mathrm{CB}(\mathbf{C})$. Whenever a sample from class c is mapped to a different cell than $\varphi^*(c)$ we consider it a mistake. We can show the following:

Claim 5. *Let* F *be a classifier and assume that when* F *misclassifies, the target class is chosen uniformly at random. Then the expectation of* $\mathrm{CB}(\mathbf{C})$ *is monotonically increasing with the total number of mistakes.*

For the proof we define the mistakes graph — a directed multigraph where each sample not mapped into the correct cell is represented by an arc between the correct cell and the mapped cell (see Fig. **1d**). Hidden mistakes are those appearing in a cycle or in a path besides the first and last edges. Hence counting such errors amounts to finding an edge maximum cover of the multi-graph by edge disjoint directed cycles and paths. We complete the proof by analyzing edge-maximal edge-disjoint collection of cycles in the appropriate random graph model



(a) CelebsA dataset

(b) artificial faces dataset - DigiFace1M

Figure 2: Real True-same counts vs. CB estimation

The approach of the last proof yields a polynomial relation: $\mathrm{CB}(\mathbf{C}) = O(f^c)$ where f is the number of errors and $c > 1/5$ is constant. We believe that a stronger result, $c \geq 1/2$, may be obtained by finding an analog to the main result of [12] for the mistakes graph — showing essential independence between degrees and analyzing cell size distribution widths. In silico, when using two similar classifiers, we get heavy counts on the diagonal of $\mathbf{C}$, in which case the number of visible errors grows linearly with the number of total mistakes.

4 Experiments

We created a collection of ten classifiers f_q and measured CB for all 45 pairs on two datasets. We have used the `Dlib` [8, 7] as a base. This metric learner maps a photo into $\mathcal{R}^{128}$. The authors recommend a distance threshold of 0.6 when deciding if two photos are of the same origin. Representatives from L random classes were randomly chosen, and proximity to them was used in classification. We have created our metric learners in a few different ways:

- d pairs of samples were randomly chosen. For each pair we took the line connecting the two samples and projected each sample on it, with an affine correction making the center of the segment the origin. This projection bisects the samples along probable interesting affine hyperplanes.
- Using only randomly chosen d coordinated from the original 128.
- Same as above, but using more representatives from each class.

Table **1** lists the datasets we used. Figure **2** presents the results, Panel **2a** for the CelebsA dataset [11] and Panel **2b** for DigiFace1M [2]. In both charts the x-axis is CB and y-axis is the real False-Same error measured using labels. Pairs of samples were considered Same when both classifiers agreed they are the same. Markers are sized according to the sum of real performances of each classifier. Regression lines were added for convenience.

Table 1: Datasets characteristics

Name	Identities	Samples	Reference	Remarks
CelebaA	10,000	200,000	[11]	
DigiFace1M	100,000	1,220,000	[2]	Artificially generated

5 Conclusion

We presented a combinatorial bound on the number of mistakes an ensemble is likely to make, without relying on labeled data. The bound can be approximated efficiently while still agreeing with real data. As such it is useful in modern settings of huge datasets in the unsupervised learning regime.

Due to space limitations we left out some proofs to be added in a longer version of this manuscript. We would like to thank the anonymous referee for keen reading and insightful suggestions that improved this manuscript.

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