Integer Programming-based Error-Correcting Output Code Design for Robust Classification

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Abstract

Error-Correcting Output Codes (ECOCs) offer a principled approach for combining simple binary classifiers into multiclass classifiers. In this paper, we investigate the problem of designing optimal ECOCs to achieve both nominal and adversarial accuracy using Support Vector Machines (SVMs) and binary deep learning models. In contrast to previous literature, we present an Integer Programming (IP) formulation to design minimal codebooks with desirable error correcting properties. Our work leverages the advances in IP solvers to generate codebooks with optimality guarantees. To achieve tractability, we exploit the underlying graph-theoretic structure of the constraint set in our IP formulation. This enables us to use edge clique covers to substantially reduce the constraint set. Our codebooks achieve a high nominal accuracy relative to standard codebooks (e.g., one-vs-all, one-vs-one, and dense/sparse codes). We also estimate the adversarial accuracy of our ECOC-based classifiers in a white-box setting. Our IP-generated codebooks provide non-trivial robustness to adversarial perturbations even without any adversarial training.

1 Introduction

Error Correcting Output Codes (ECOCs) offer an effective and flexible tool to combine individually trained binary classifiers for multiclass classification. Prior research [Dietterich and Bakiri, 1995, Allwein et al., 2000] has shown that ECOCs can provide high multiclass classification accuracy using simple but powerful binary classifiers (e.g., Support Vector Machines and Adaboost). On the other hand, extensive body of work has emerged in recent years showing that, when large amount of training data is available, deep learning models [LeCun et al., 2015] outperform most multiclass classifiers. Still, further progress is needed for classification tasks when training data is limited or constrained, and model interpretability is preferred. In this paper, we consider the problem of ECOC-based multiclass classification, when individual binary classifiers are SVMs or deep learning models. We focus on the question of design of codebooks along with optimality guarantees.

Importantly, our approach to codebook design is distinct from the prior literature, which approaches the problem using a continuous relaxation of the inherently discrete optimization problem, and solving the relaxed problem using nonlinear optimization tools [Crammer and Singer, 2002, Zhao and Xing, 2013, Xiao Zhang et al., 2009, Martin et al., 2018]. In principle, this approach can be scaled to a large number of classes, but it does not provide any optimality guarantees. Another approach in the literature [Dietterich and Bakiri, 1995] casts the design problem as a propositional satisfiability problem that can be solved for using off-the-shelf SAT solvers. However, only a feasible solution may be readily computable using this approach. In contrast, we formulate the optimal codebook design problem as a large-scale Integer Program (IP), and exploit the structure of the problem to obtain a compact formulation that can be solved with modern IP solvers. Our resulting codebook has optimality guarantees. This also enables a systematic comparison with respect to several well-known fixed-size codebooks.

Our IP formulation is flexible in that it models various codebook (or coding matrix) generation criteria: (i) Sufficiently large Hamming distance between any pair of codewords (row separation); (ii) Uncorrelated columns (column separation); (iii) Relatively even distribution of data points across two classes (balanced columns); and (iv) Larger Hamming distance between pair of codewords whose corresponding classes are hard to separate from one another. These criteria are important
not only for the nominal error correction performance, but also promote adversarial robustness. However, this initial formulation can quickly become intractable for a classification problem of more than 10 classes.

To address the abovementioned computational bottleneck, we exploit the inherent graph-theoretic feature of the constraints that pertain to selecting an appropriate subset of columns. In particular, we prove that the constraints modeling the pair of columns that do not satisfy column separation criterion can be replaced by a much smaller set formed by an edge clique cover of the underlying graph. This result allows us to reformulate our original problem into another IP with a substantially smaller set of constraints.

A distinct advantage of our design approach is that it generates relatively small codebooks, which achieve a high nominal accuracy as well as robustness to adversarial perturbations [Szegedy et al., 2013, Goodfellow et al., 2015, Su et al., 2017]. In particular, we demonstrate that our IP-generated codebooks outperform the well-known codebooks such as one-vs-all and one-vs-one, and other dense or sparse designs. To evaluate the robustness of optimal codebooks to adversarial perturbations, we conduct experiments based on white-box attacks [Madry et al., 2018, Tramer et al., 2020]. Importantly, our codebooks achieve non-trivial robustness even without any adversarial training of the individual binary classifiers. Thus, our results suggest a strong potential of ECOCs for training robust classifiers.

The paper is organized as follows: Sec. 2 introduces the ECOC framework; Sec. 3 presents the design criteria for codebooks; Sec. 4 details our IP formulation; Sec. 5 provides computational experiments on numerous datasets; Sec. 6 outlines future work.

2 ECOCs for Classification

In the ECOC-based framework for $k$-class classification [Dietterich and Bakiri, 1995], each class is encoded with a unique codeword of length $l$, resulting in a codebook (coding matrix) $\mathcal{M} = (m_{ij})$ of size $k \times l$. For binary (resp. ternary) codes, the entries $m_{ij}$ of the coding matrix $\mathcal{M}$ belong to the set $\{+1, -1\}$ (resp. $\{+1, 0, -1\}$). The rows (resp. columns) of $\mathcal{M}$ correspond to distinct classes (resp. binary classifiers or hypotheses). Figure 1 shows examples of two standard codebooks.

In the learning problem corresponding to every column in $\mathcal{M}$, the set of training examples belonging to different classes $C_1, \ldots, C_k$ is partitioned into two groups: all examples from classes with entry $+1$ represent the positive class, and all examples from classes with entry $-1$ represent the other class. In the case of ternary codes, training examples with entry $0$ are not included in the training set and are considered irrelevant.

Let $f_1(\cdot), \ldots, f_l(\cdot)$ represent the learned binary hypotheses for the corresponding columns of $\mathcal{M}$. For a learned hypothesis $s \in \{1, \ldots, l\}$ and a test example $x$, let $f_{s,+}(x)$ (resp. $f_{s,-}(x)$) denote the output/score of the class $+1$ (resp. class $-1$). Then,

$$
\hat{f}_s(x) := \begin{cases} 
+1 & \text{if } f_{s,+}(x) > f_{s,-}(x) \\
-1 & \text{otherwise}
\end{cases} \quad \forall s \in \{1, \ldots, l\}.
$$

After evaluating $x$ on all the $l$ hypotheses, we obtain an encoding $\hat{f}(x) = [f_1(x), \ldots, f_l(x)]$. To associate $\hat{f}(x)$ with a class (i.e., a row of coding matrix $\mathcal{M}$), we can use a decoding scheme based on a similarity measure such as Hamming distance. Particularly, one can compute the Hamming distance $d_H(\cdot, \cdot)$ between $\hat{f}(x)$ and each codeword $\mathcal{M}(r, \cdot)$ and select the class, denoted $\hat{y}$, that corresponds to the minimum distance:

$$
d_H(\mathcal{M}(r, \cdot), \hat{f}(x)) = \sum_{s=1}^{l} \left(1 - \frac{\mathcal{M}(r,s) \times f_s(x)}{2}\right) \tag{1}
$$

$$
\hat{y} = \arg\min_r d_H(\mathcal{M}(r, \cdot), \hat{f}(x)). \tag{2}
$$

3 Codebook Generation Criteria

The final prediction accuracy of ECOC scheme introduced in Sec. 2 crucially depends on the error correction ability of the coding matrix $\mathcal{M}$. To ensure low test error, the coding matrix must be chosen carefully. Below we introduce the key properties that serve as guidelines for our design of binary codes.\footnote{Similar codebook design approach can be developed for ternary codes (not presented here due to space constraints).}

Row Separation: It is well-known that more separation between pairs of codewords (i.e., rows in the coding matrix $\mathcal{M}$) improves the error correction capability. Particularly, if every pair of distinct codewords has a hamming distance of at-least $d$, then such a code can correct at-least $\left\lfloor \frac{d-1}{2} \right\rfloor$ errors. Thus, we seek coding matrix with a high row separation between any pair of codewords.
**Column Separation:** Additionally, every pair of distinct columns in $\mathcal{M}$ should be uncorrelated. The benefit of large column separation can be understood by drawing analogy with error correction in communication over a noisy channel. Encoding a signal and transmitting the codeword over a noisy channel is highly effective when the errors introduced during transmission are random. By maintaining a sufficiently large encoding, one can recover the original signal at the receiving end with high accuracy. Analogously, in our setup, if any two columns (classifiers) make errors in their predictions on the same inputs (i.e., their outputs are highly correlated), then the effectiveness of encoding in correcting errors will be reduced.

**Balanced Columns:** On the other hand, to prevent over-fitting of individual hypotheses, it is important to prioritize selection of columns for which the $k$ class data points are evenly distributed across the two classes. This criterion is particularly relevant when the test examples are adversarially perturbed [Tsipras et al., 2018].

**Data Distribution:** Finally, in multi-class problems, some class pairs are more difficult to separate than others. This makes the prediction of these classes more vulnerable to adversarial attacks. Therefore, it is desirable to have larger Hamming distances among pairs of codewords corresponding to hard-to-separate class pairs. This hardness of separation can be estimated from the training data for different class pairs, either using the semantics of classes [Zhao and Xing, 2013], or by calculating similarity measures between classes for small datasets [Xiao Zhang et al., 2009, Martin et al., 2018, Pujol et al., 2006, Gao and Koller, 2011, Griffin and Perona, 2008].

**4 Integer Programming Formulation**

In this section, we embed the abovementioned guidelines into a discrete optimization formulation for generating an optimal codebook.

To begin with, note that for a $k$-class problem a coding matrix can have at most $(2^k-2)/2 = 2^{k-1} - 1$ columns. However, such an exhaustive coding might be feasible only for a small $k$ (2 to 5). As $k$ increases, the number of binary classifiers that need to be trained for exhaustive coding increase exponentially. Practically, it is desirable to select a small subset (say of $L$ columns) from $2^{k-1} - 1$ possible columns. This subset should be selected in accordance with the codebook generation criteria described in Sec. 3.

One way to formulate the column subset selection problem is to cast it as a propositional satisfiability problem, and solve it using an off-the-shelf SAT solver. For example, the authors in [Dietterich and Bakiri, 1995] considered the following problem for $8 \leq k \leq 11$: For a predefined number of columns $L$ and some value $\rho$, is there a solution such that the Hamming distance between any two columns is between $\rho$ and $L - \rho$? However, this approach only leads to a feasible (not necessarily optimal) solution. In contrast, we present an Integer Programming (IP) problem that captures the design criteria in a more flexible manner and can be used to find an optimal codebook.

For sake of simplicity, we first consider the row and column separation criteria; the remaining criteria on balanced columns and data distribution can be addressed in our IP formulation, as discussed subsequently at end of this section. In its basic form our problem is the following: We want to find a solution which maximizes the minimum Hamming distance between any two rows (or the error-correcting property).

Let $x_i$ denote the binary variable associated with each column $i$ of the exhaustive code for $i \in \{1, \ldots, 2^{k-1} - 1\}$, i.e. the decision variable whether or not column $i$ is selected in the final solution. Also, let $x_{ij}$ be the binary variable which represents the outcome of AND operation between variables $x_i$ and $x_j$ for all distinct $i,j$ pairs, i.e. $(i,j) \in \{1, \ldots, 2^{k-1} - 1\}^2 | i < j$. Essentially, when $x_{ij} = 1$ means that columns $i$ and $j$ satisfy the column separation criterion. We can now write the IP formulation to generate an optimal codebook as follows:

$$\mathcal{IP}_1: \max_{x_i, x_{ij}} \min \{d_h^2(x_i), \ldots, d_h^{k-1,k}(x_i) \}$$

s.t.

$$\sum_{i=1}^{2^{k-1}-1} x_i \leq L$$

$$\rho x_{ij} \leq d_h(\mathcal{M}(\cdot, i),\mathcal{M}(\cdot, j)) x_{ij} \leq (L - \rho) x_{ij} \quad \forall (i,j) \in \{1, \ldots, 2^{k-1} - 1\}^2 | i < j$$

$$x_{ij} \leq x_i$$

$$x_{ij} \leq x_j$$

$$x_i + x_j - 1 \leq x_{ij}$$

$$d_h^{s,t}(x_i) = \sum_{i=1}^{2^{k-1}-1} \left( \frac{1 - \mathcal{M}(s, \cdot) \times \mathcal{M}(t, \cdot)}{2} \right) x_i$$

$$\forall (s, t) \in \{1, \ldots, k\}^2 | s < t$$

$$x_i \in \{0, 1\} \quad \forall i \in \{1, \ldots, 2^{k-1} - 1\}$$

$$x_{ij} \in \{0, 1\} \quad \forall (i, j) \in \{1, \ldots, 2^{k-1} - 1\}^2 | i < j$$
In IP1, max-min objective can be simplified by introducing an auxiliary variable \( t \), where \( t = \min \{ d^{1,2}_H(x_1), d^{1,3}_H(x_1), \ldots, d^{k-1,k}_H(x_1) \} \), and adding the corresponding constraints \( t \leq d^{1,2}_H(x_1) \), \( t \leq d^{1,3}_H(x_1) \), \ldots, \( t \leq d^{k-1,k}_H(x_1) \). Eq. (5) ensures large column separation for \( x_{ij} = 1 \). Constraints (6) and (7) ensure that if \( x_{ij} = 1 \) then both columns \( i \) and \( j \) are included in the solution, i.e. \( x_i = 1 \) and \( x_j = 1 \). Conversely, Equation (8) ensures that if columns \( i \) and \( j \) are selected then \( x_{ij} = 1 \).

We note that in IP1 there are \( 2^{k-1} - 1 \approx O(2^{k-1}) \) binary variables for each column, and for each pair of columns there are \( (2^{k-2} - 1) \approx O(2^{2k-3}) \) binary variables. Thus, the total number of binary variables is \( O(2^{2k-3}) \). Similarly, the total number of constraints is \( O(2^{2k-1}) \). For \( k = 10 \), this would entail solving an IP of approximately 130,000 variables and 650,000 constraints. Modern IP solvers like Gurobi and CPLEX can handle such problem instances.

However, for \( k > 10 \), the above optimization problem quickly becomes intractable. The main reason is that we have a binary variable \( x_{ij} \) for each pair of columns to capture the large column separation criterion; see (5). We now propose a second formulation which does not involve a new variable for every pair of columns.

Let \( S_p \) denote the set of all distinct pairs of columns in the exhaustive code \( M \), i.e. \( S_p = \{(i,j) \in \{1, \ldots, 2^{k-1} - 1\} | i < j \} \) and \( |S_p| = \binom{2^{k-1}-1}{2} \). We now consider two mutually disjoint subsets \( S_p^{\text{feas}} \) and \( S_p^{\text{inf}} \), such that \( S_p = S_p^{\text{feas}} \cup S_p^{\text{inf}} \); the set \( S_p^{\text{feas}} \) (resp. \( S_p^{\text{inf}} \)) contains only those \( i,j \) pairs that satisfy (resp. do not satisfy) the column separation criterion (5).

Mathematically, we can write:

\[
S_p \quad = \quad \{(i,j) \in \{1, \ldots, 2^{k-1} - 1\} | i < j \}, \\
S_p^{\text{feas}} \quad = \quad \{(i,j) \in \{1, \ldots, 2^{k-1} - 1\} | i < j \} \text{ and } \\
\rho \leq d_H(M(:,i), M(:,j)) \leq (L - \rho), \\
S_p^{\text{inf}} \quad = \quad S_p \setminus S_p^{\text{feas}}. 
\]

In this new representation, the constraint (5) is captured by the construction of \( S_p^{\text{feas}} \), which eliminates the need of variables \( x_{ij} \) for column pairs. Similarly, we no longer need the constraints (6), (7) and (8). Now, for any \( (i,j) \) pair of columns in the set \( S_p^{\text{inf}} \), at-most one of the columns can be included in the final solution. This can be achieved by setting \( x_{ij} = 0 \) in (8). Equivalently, for every \( (i,j) \) pair in \( S_p^{\text{inf}} \), it is sufficient to impose the constraint \( x_i + x_j - 1 \leq 0 \).

We can now write IP1 as the following equivalent form:

\[
\text{IP2: max min } \{ d^{1,2}_H(x_1), \ldots, d^{k-1,k}_H(x_1) \} \\
\text{s.t. } \sum_{i=1}^{2^{k-1}-1} x_i \leq L, \\
x_i + x_j \leq 1 \forall (i,j) \in S_p^{\text{inf}} \\
d^{\rho}_H(x_1) = \sum_{i=1}^{2^{k-1}-1} \left( \frac{1}{\rho} \cdot M(s,.) \times M(t,.) \right), \forall (s,t) \in \{1, \ldots, k\}^2 \ s < t, \\
x_i \in \{0,1\} \forall i \in \{1, \ldots, 2^{k-1} - 1\}
\]

Since IP2 does not contain any \( x_{ij} \) variables, this formulation has significantly less number of variables and constraints in comparison to (IP1). The computational complexity of IP2 is mainly governed by the size of \( S_p^{\text{inf}} \), which determines the number of constraints in (15). However, even in this new representation, the size of the set \( S_p^{\text{inf}} \) increases prohibitively large as \( k \) increases. Table 1, column 4 shows how quickly \( |S_p^{\text{inf}}| \) increases with \( k \) for an appropriately chosen \( \rho \).

Fortunately, the constraints (15) for the set \( S_p^{\text{inf}} \) can be represented on a graph \( G_p^{\text{inf}} \), in which each node corresponds to a column \( x_i \) and each constraint \( x_i + x_j \leq 1 \) corresponds to an edge between the node \( i \) and node \( j \); see Figure 2 for an illustration.

![Figure 2: An example of \( S_p^{\text{inf}} \) and corresponding \( G_p^{\text{inf}} \).](image)

In fact, the above graphical interpretation leads to a reduction in the number of constraints involving \( (i,j) \) column pairs in the set \( S_p^{\text{inf}} \). Before presenting this result, we recall that a clique is a set of nodes in a graph such that there is an edge between any two distinct nodes of this set. Proofs of all results are provided in the supplementary material.

**Theorem 1.** The feasible space enclosed by the constraints constituting the edges of any clique \( C \) in \( G_p^{\text{inf}} \) is same as that enclosed by the single constraint:

\[
\sum_{i \in C} x_i \leq 1.
\]

From theorem 1, we obtain that for a clique of size \( n \), \( n(n-1)/2 \) constraints of form \( x_i + x_j \leq 1 \) between all \( (i,j) \) node pairs in the clique can be substituted.
with a single constraint (16). This constraint captures the requirement that out of all the columns in $\mathcal{M}$ forming a clique, at most one can be present in a feasible solution. Before introducing our next result, we recall the following useful definition.

**Definition 1** (Edge Clique Cover [Conte et al., 2016, Gramm et al., 2009, Kou et al., 1978]). An edge clique cover for a graph $\mathcal{G}$, denoted as $\text{ECC}(\mathcal{G})$, is a set of cliques $\mathcal{ECC}(\mathcal{G}) = \{C_1, C_2, \ldots, C_k\}$ such that:

1. No clique $C_i$ is contained in another clique $C_j$, i.e $C_i \not\subseteq C_j$ for all $i \neq j$, and
2. Every edge in the graph $\mathcal{G}$ is included in at least one clique.

**Corollary 1.1.** The feasible space enclosed by the constraint set $\mathcal{S}_p^{inf}$ (or its graphical equivalent $\mathcal{G}_p^{inf}$) in $\mathcal{IP}_2$ is same as that enclosed by a much smaller constraint set formed by $\text{ECC}(\mathcal{G}_p^{inf})$.

A given graph can have many possible edge clique covers; see for example Fig. 3. To reduce the size of the constraint set $\mathcal{S}_p^{inf}$ as much as possible, we would need to find an edge clique cover of the smallest size. However, the minimum edge cover problem is known to be NP-hard [Garey and Johnson, 1990]. Fortunately, several heuristics have been proposed to [Kellerman, 1973, Gramm et al., 2009, Kou et al., 1978, Conte et al., 2016] find edge clique cover of a graph, and they have been very effective in many practical applications. The heuristic [Conte et al., 2016] is particularly well-suited for large graphs – in practice, it shows a linear runtime in the number of edges. We therefore use this heuristic for our analysis.

Finally, using corollary 1.1 (or its extension lemma 1) we can reduce $\mathcal{IP}_2$ to the following integer program:

$$\mathcal{IP}_3 : \max_{x_i} \min \{d_H^{k,2}(x_i), \ldots, d_H^{k-1,k}(x_i)\}$$

s.t.

$$\sum_{i=1}^{2^k-1} x_i \leq L$$

$$\sum_{i : \forall \mathcal{C}_i \in \text{ECC} \mathcal{G}_p^{inf}} x_i \leq 1 \quad \forall \mathcal{C}_i \in \text{ECC} \mathcal{G}_p^{inf}$$

$$d_H^{k,i}(x_i) = \sum_{i=1}^{2^k-1} \left(1 - \frac{M(s, \cdot) \times M(t, \cdot)}{2}\right) x_i$$

$$\forall (s, t) \in \{1, \ldots, k\}^2, s < t, \quad \forall i \in \{0, 1\}$$

Finally, the last two criteria mentioned in Sec. 3 can be easily incorporated in $\mathcal{IP}_3$. Specifically, the requirement for balanced columns can be incorporated by setting the $x_i$’s violating this criterion to 0 in $\mathcal{IP}_3$. Equivalently, since each $x_i \in \{0, 1\}$ corresponds to whether a column is selected from the exhaustive code.
Table 1: Reducing the size of the constraint set $|S_p^{inf}|$ in $\mathcal{IP}_2$ by finding the Edge Clique Cover of $G_p^{inf}$.

| No. of classes $k$ | No. of Columns $2^{k-1} - 1$ | $\rho$ | No. of constraints $|S_p^{inf}|$ | No. of constraints (Reduced) | Reduction Factor | Time Taken (in sec.) |
|------------------|-----------------|------|-----------------|-----------------|-----------------|------------------|
| 10               | 511             | 3    | 11,475          | 695             | 16              | 0.146            |
| 11               | 1,023           | 3    | 28,105          | 1,404           | 20              | 0.208            |
| 12               | 2,047           | 4    | 236,313         | 8,165           | 28              | 0.991            |
| 13               | 4,095           | 4    | 610,006         | 18,472          | 33              | 2.573            |
| 14               | 8,191           | 4    | 1,543,815       | 41,088          | 37              | 7.350            |
| 15               | 16,383          | 5    | 12,040,770      | 44,916          | 268             | 58.957           |
| 16               | 32,767          | 5    | 31,783,020      | 91,304          | 348             | 240.53           |
| 17               | 65,535          | 5    | 62,241,772      | 185,661         | 444             | 935.26           |
| 18               | 131,071         | 6    | 616,094,535     | 1,073,248       | 574             | 1,007.58         |

We run all our experiments on a system with a single 1080Ti Nvidia GPU, Intel Core i7-6800K CPU and 128 GB RAM. We use Gurobi as our IP solver.

Table 2: $\mathcal{IP}_3$: Optimality Gap (max. time 2000s).

| $k$ | $L$ | $f_{best}$ | Best Bound | Gap | Optimality Gap $|f_{best} - f^*|$ |
|-----|-----|------------|------------|-----|-----------------|
| 10  | 20  | 10         | 10         | 0%  | 0%              |
| 11  | 22  | 12         | 12         | 0%  | 0%              |
| 12  | 24  | 12         | 12         | 0%  | 0%              |
| 13  | 26  | 14         | 14         | 7.60%| 7.7%            |
| 14  | 28  | 14         | 14         | 7.14%| 0%              |
| 15  | 30  | 16         | 16         | 6.67%| 0%              |
| 16  | 32  | 16         | 17         | 6.25%| 0%              |
| 17  | 34  | 16         | 18         | 12.2%| 6.25%           |
| 18  | 36  | 17         | 19         | 11.8%| 5.5%            |

Our computational experiments focus on solving $\mathcal{IP}_3$ which uses the edge-clique-cover approach to reduce

$\mathcal{M}$, we can simply reduce $\mathcal{M}$ by removing the unbalanced columns and then form $\mathcal{IP}_3$. In contrast to [Xiao Zhang et al., 2009], in our formulation, the requirement for balanced columns further reduces the final problem size and complexity.

The remaining criterion of data distribution can be also incorporated by modifying the objective function. Previous works such as [Martin et al., 2018, Zhao and Xing, 2013, Xiao Zhang et al., 2009], pre-compute a similarity measure between every pair of classes (from training data) and use this computation to estimate the desirable class-pairwise hamming distances $d_{p,q}$. Finally, they optimize to obtain codebooks which attain these distance values. This can be easily incorporated in our formulation by changing the objective function (17) in $\mathcal{IP}_3$ to the following:

$$\min_{x_i} \sum_{(p,q)\in\{1,\ldots,k\}^2\mid p \neq q} |d_H^p(x_i) - \hat{d}_{p,q}|. \quad (19)$$

5 Experiments

We run all our experiments on a system with a single 1080Ti Nvidia GPU, Intel Core i7-6800K CPU and 128 GB RAM. We use Gurobi as our IP solver.

Table 2: $\mathcal{IP}_3$: Optimality Gap (max. time 2000s).

5.1 Natural Classification Performance

Toy Dataset (2d): We generate a synthetic dataset of 10 classes where points in each class are sampled from a 2d Gaussian distribution. Here we use SVMs with Rbf kernels as our binary classifier for individual hypotheses in all our codebooks. Figure 5 shows the decision boundaries of all hypotheses for three codebooks along with the training set. The prediction accuracy on the test set is reported in Table 3. Our $\mathcal{IP}_3$ generated codebook easily outperforms other codebooks, and almost matches the accuracy of 1-vs-1. Note that this codebook only used $L = 20$ columns while 1-vs-1

$^2$Please see the supplementary section for more details.
used $L = 45$ columns. This highlights the benefit of ECOC theory: high accuracy can be achieved with a carefully chosen compact codebook.

Table 3: Performance on 2d Toy dataset ($k = 10$).

| Codebook | Dense | Sparse | 1-vs-All | 1-vs-1 |
|----------|-------|--------|----------|--------|
| IP3      | $L = 10$ | $L = 20$ | $L = 10$ | $L = 10$ | $L = 45$ |
|          | 89.8%   | 90.8%   | 88.1%    | 66.8%   | 80.6%    | 91.2%    |

Real-world Datasets (Small/Medium): We evaluate the performance of different codebooks on small to medium sized, real-world datasets. We consider Glass, Ecoli and Yeast datasets taken from UCI repository [Dua and Graff, 2017]. Details such as the number of samples, features and classes for each dataset are provided in the supplementary material. For Dense, Sparse, and IP generated codebook we set $L = 2k$. We again use SVMs with Rbf kernel as the binary classifier for training different hypotheses in our IP-generated and other codebooks. We set aside 30% of the samples as our test set and used them to evaluate the performance of different codebooks. The final test set accuracies are reported in Table 4. Our codebook provides best accuracy on Ecoli and second-best accuracy on Glass and Yeast, thus providing best performance on an average.

Table 4: Performance of various codebooks on different real-world (small) datasets.

| Codebook | Dense | Sparse | 1-vs-all | 1-vs-1 |
|----------|-------|--------|----------|--------|
| IP3      |        |        |          |        |
|          | 67.69% | 75.38% | 67.69%   | 59.99% | 66.15%  |
| Glass    | 90.09% |        |          |        |
| Ecoli    | 51.79% | 50.67% | 43.04%   | 48.20% | 52.91%  |
| Yeast    |        |        |          |        |

We now evaluate the performance of different codebooks on real-world image datasets: MNIST and CIFAR10.

MNIST: We run two set of experiments: In the first set, we use SVMs (with both Linear and Rbf kernel) on PCA-transformed MNIST dataset (using 25 principal components). In the second set, we use binary Convolutional Neural Networks CNNs to train different hypotheses in our codebooks. Tables 5 and 6 provide the test set accuracy of different codebooks from both sets of experiments. We observe that in the case of

Table 5: Performance of different codebooks using SVM on PCA transformed MNIST dataset.

| Codebook | Dense | Sparse | 1-vs-all | 1-vs-1 |
|----------|-------|--------|----------|--------|
| IP3      |        |        |          |        |
|          | 80.37% | 75.74% | 68.87%   | 76.82% | 92.01%  |
| Linear   |        |        |          |        |
| Rbf      | 97.59% | 97.5%  | 79.18%   | 96.95% | 98.01%  |

Table 6: Performance of Different Codebooks with binary CNN on MNIST dataset.

| Codebook | Dense | Sparse | 1-vs-all | 1-vs-1 |
|----------|-------|--------|----------|--------|
| IP3      |        |        |          |        |
|          | 98.84% | 98.8%  | 95.05%   | 84.17% | 98.65%  |
| Normalized |      |        |          |        |
| Linear   |        |        |          |        |
| Rbf      | 100.0% | 95.0%  | 84.17%   | 98.65% | 94.51%  |

CIFAR10: Since running SVMs on this dataset is expensive computationally, we resort to CNNs here. In particular, we use ResNet18 [He et al., 2015] as our binary classifier to train the individual hypotheses in different codebooks. As shown in Table 7, IP3 achieves the best performance. Note that our experiments on CIFAR10 should be viewed only in terms of evaluating the relative performance of different codebooks. We are
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aware that modern multi-output CNNs have achieved an accuracy of around 95% (or higher) on CIFAR10 dataset. However, recall that in this work our goal is to highlight the benefit of using ECOCs when working with binary classifiers.

Table 7: Performance of Different Codebooks with binary CNN (ResNet18) on CIFAR10 dataset.

| Codebook | Dense | Sparse |
|----------|-------|--------|
|          | Normalized | Raw    |
| IP3      | 76.25%  | 75.47% |
|          | 68.15%  | 61.53% |
| 1-vs-all | 71.25%  | 68.76% |
| 1-vs-1   | 72.63%  | 68.76% |

5.2 Adversarial Robustness

We now evaluate the robustness of different codebooks against white-box attacks. For further comparison, we also evaluate the robustness of a naturally trained multiclass CNN with our IP-generated codebook in the final layer – this is somewhat similar to the recent approach in [Verma and Swami, 2019].

However, note that all our binary hypotheses are naturally trained, i.e. without any adversarial training. We first discuss how to obtain the class probability estimates that are necessary to evaluate the adversarial robustness.

Recall from Sec. 2 the procedure of assigning a class to an input $x$ using Hamming decoding. However, this decoding scheme in itself does not provide us with class probability estimates, which are essential for evaluating the robustness of an ECOC-based classifier with respect to white-box attacks [Madry et al., 2018, Goodfellow et al., 2015]. Particularly, we need probability estimates to compute the adversarial loss function. Furthermore, we need to be able to compute the gradients of the loss-function with respect to input $x$.

We adopt the procedure of calculating the class probability estimates for general codebooks, as proposed in [Zadrozny, 2002, Hastie and Tibshirani, 1998]. After evaluating an input $x$ on each binary classifier, we obtain a probability estimate (or score$^5$), denoted $r_l(x)$, for each column $l$ (i.e., binary classifier) in $M$. Let $I$ denote the set of classes for which $M(i,l) = 1$ and $J$ denote the set of classes for which $M(i,l) = -1$. Then the class probability estimate for $i \in \{1, \ldots, k\}$ on an input $x$ is given as follows:

$$
\hat{p}_i(x) = \frac{1}{|J|} \sum_{l: M(i,l) = 1} r_l(x) + \frac{1}{|I|} \sum_{l: M(i,l) = -1} (1 - r_l(x)), \quad (20)
$$

where differentiability with respect to $x$ is maintained. Using these estimates, we can compute a loss function (e.g., cross-entropy Loss) and then generate white-box PGD-attacks [Madry et al., 2018] to evaluate the robustness of the overall classifier. Note that we use the same differentiable class scores (or decoding scheme) for both prediction and to generate a white-box attack in order to prevent gradient-obfuscation [Athalye et al., 2018, Tramer et al., 2020]. For all our experiments, we work with perturbations based on $l_{\infty}$-norm. In particular, for a given input $x'$, the allowed set of perturbations are given by set:

$$
Q(x') = \{x \in R^d | \|x - x'\|_{\infty} \leq \epsilon : l \leq x \leq u\}.
$$

MNIST: We run an $l_{\infty}$-norm based 100-step PGD attack with multiple values of $\epsilon$ on different codebooks; Table 8 summarizes these results. In terms of the overall performance, our IP3-generated codebook significantly outperforms all other codebooks except the Dense codebook. In this codebook, different pairs of codewords have different hamming distances, ranging from 8-14. On the other hand, in IP3, all codeword pairs have identical hamming distance of 10 as result of the max-min objective function (17). This disparity in performance can therefore be mitigated by incorporating the underlying data distribution (via class pair similarity measures) using the objective function (19). However, note that efficiently computing similarity measures for large image datasets is in itself a research problem. Finally, as we discuss in the next set of experiments, the performance of Dense codebook deteriorates as the data-distribution changes.

Table 8: Adversarial Accuracy of Nominally Trained Codebooks on MNIST.

| Codebook   | $\epsilon = 0.05$ | $\epsilon = 0.1$ | $\epsilon = 0.15$ | $\epsilon = 0.2$ | $\epsilon = 0.25$ | $\epsilon = 0.3$ |
|------------|-------------------|-------------------|-------------------|-------------------|-------------------|-------------------|
| IP3        | 93.46%            | 84.64%            | 75.74%            | 69.89%            | 58.96%            | 45.81%            |
| 1-vs-1     | 84.48%            | 79.17%            | 69.57%            | 62.89%            | 54.96%            | 46.81%            |
| 1-vs-All   | 83.04%            | 77.74%            | 68.89%            | 64.89%            | 57.86%            | 49.80%            |
| Sparse     | 86.12%            | 85.62%            | 74.12%            | 68.12%            | 64.96%            | 57.60%            |
| Dense      | 95.17%            | 84.08%            | 62.95%            | 53.54%            | 38.64%            | 28.64%            |
| Multiclass | 94.35%            | 70.29%            | 21.72%            | 2.19%             | 0.04%             | 0.00%             |

CIFAR10: Finally, we evaluate the robustness of different codebooks on CIFAR10 by running 30-step PGD attack; see table 9. In this case, our IP3 codebook outperforms all other codebooks including Dense codebook. Note that since the data-distribution changed from MNIST to CIFAR10, Dense codebook now shows lower performance than IP3, particularly for larger perturbations of $\epsilon = 4/255$ and $\epsilon = 8/255$.

Importantly, the adversarial accuracy achieved by our IP3 is by no means trivial as under the exactly same setting other codebooks like 1-vs-1, 1-vs-All, Sparse do not show any robustness. In similar setting, a multi-
Table 9: Adversarial Accuracy of Nominally Trained Codebooks on CIFAR10.

| ϵ        | IP3  | 1-vs-1 | Sparse | Dense | Multiclass |
|----------|------|--------|--------|-------|------------|
| ϵ = 2/255 | 24.04% | 4.65%  | 5.05%  | 24.2% | 15.46%     |
| ϵ = 4/255 | 19.24% | 0.11%  | 0.08%  | 12.79%| 2.55%      |
| ϵ = 8/255 | 16.48% | 0.0%    | 0.0%    | 11.63%| 0.27%      |

class CNN of similar network capacity also does not provide any robustness to adversarial perturbations. This highlights the impressive capability of ECOCs to handle adversarial perturbations even though the individual binary hypotheses are all nominally trained. Our approach provides robustness-by-design, and does not make any specific assumptions about the adversary model in the design of codebook.

6 Conclusion and Future Work

Our computational results validate the merit of our optimal codebook design approach. Importantly, our IP-based formulation achieves small (or zero) optimality gaps while maintaining tractability for reasonable problem sizes. This is possible mainly due the graph-theoretic viewpoint we adopted in applying the edge-clique-cover, which substantially reduced the constraint set of original IP formulation. In the nominal setting, our compact IP generated codebooks outperform commonly used standard codebooks on most datasets.

In the adversarial setting, our IP-generated codebooks achieve non-trivial robustness. This is surprising due to three main reasons: (1) We do not employ any adversarial training; (2) Most other codebooks (except Dense) do not exhibit any robustness even when they use more than twice the number of columns; (3) The robustness that we obtain is not simply because of the large network capacity. To the best of our knowledge, we are the first ones to report that adversarial robustness can be achieved by a careful codebook design approach, while only using nominally trained binary classifiers.

Our results provide guidance for further research in the use of ECOCs for robust classification. We plan to study the effect of robustifying the individual hypotheses. Another variant would be to use a combination of nominally and adversarially trained hypotheses. We plan to pursue these aspects in our future work.

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1 Proofs

Theorem 1 The feasible space enclosed by the constraints constituting the edges of any clique $C$ in $G^m$ is same as that enclosed by the single constraint:

$$\sum_{i \in C} x_i \leq 1.$$  \hspace{1cm} (16)

Proof: We use mathematical induction to show that the result holds for any clique $C_n$, of size $n \geq 3$. Assume that the theorem holds for a clique of size $n - 1$. We know that a clique $C_n$ (size $n$) contains $n$ distinct cliques $C^1_{n-1}, \ldots, C^n_{n-1}$ of size $n - 1$ such that $C^1_{n-1} \cup C^2_{n-1} \cup \ldots \cup C^n_{n-1} = C_n$. Under induction hypothesis, we can write the following set of $n$ equations:

\[
\begin{align*}
    x_1 + x_2 + \cdots + x_{n-1} &\leq 1 \\
    x_1 + x_2 + \cdots + x_n &\leq 1 \\
    \vdots & \quad \vdots & \quad \vdots \\
    x_1 + x_{n-1} + x_n &\leq 1 \\
    x_2 + x_{n-1} + x_n &\leq 1 \\
\end{align*}
\]

Adding these equations, we obtain:

$$x_1 + x_2 + \cdots + x_{n-1} + x_n \leq \frac{n}{n-1}$$  \hspace{1cm} (21)

For $n \geq 3$, we know the following trivial bound:

$$\frac{n}{n-1} < 2$$  \hspace{1cm} (22)

Using (21) and (22):

$$x_1 + x_2 + \cdots + x_{n-1} + x_n < 2$$  \hspace{1cm} (23)

Since $x_i \in \{0, 1\}$ $\forall i \in \{1, \ldots, n\}$:

$$x_1 + x_2 + \cdots + x_{n-1} + x_n \in \mathbb{Z}^+ \cup \{0\}$$  \hspace{1cm} (24)

Using (23) and (24):

$$x_1 + x_2 + \cdots + x_{n-1} + x_n \leq 1$$  \hspace{1cm} (25)

Thus, (16) holds for a clique of size $n$. To complete the induction argument, we need to show that the result holds for $n = 3$. For $n = 3$, we have:

$$x_1 + x_2 \leq 1$$
$$x_1 + x_3 \leq 1$$
$$x_2 + x_3 \leq 1$$

Summing the above equations, we get:

$$x_1 + x_2 + x_3 \leq 1.5$$
Supplementary Material

Again, since \( x_i \in \{0, 1\} \forall i \in \{1, 2, 3\} \):

\[
x_1 + x_2 + x_3 \in \mathbb{Z}^+ \cup \{0\},
\]

and we conclude that:

\[
x_1 + x_2 + x_3 \leq 1.
\]

Therefore, the result also holds for \( n = 3 \).

\[ \blacksquare \]

**Corollary 1.1** The feasible space enclosed by the constraint set \( S_{p}^{inf} \) (or its graphical equivalent \( G_{p}^{inf} \)) in \( T\Pi^2 \) is same as that enclosed by a much smaller constraint set formed by \( \mathcal{ECC}(G_{p}^{inf}) \).

**Proof:** Since the graph \( G_{p}^{inf} \) does not contain any isolated nodes and loops, and every edge in \( G_{p}^{inf} \) is covered in atleast one clique, therefore we can write:

\[
\bigcup_{i=1}^{k} C_i = G_{p}^{inf}.
\]

Also, \( G_{p}^{inf} \equiv S_{p}^{inf} \), therefore \( \{C_1, \ldots, C_k\} \equiv S_{p}^{inf} \).

\[ \blacksquare \]

**Lemma 1** Suppose \( G_1, \ldots, G_m \) are edge-disjoint subgraphs of \( G_{p}^{inf} \), such that:

1. \( G_i \cap G_j = \emptyset \ \forall \ i, j \in \{1, \ldots, m\} | i < j \)
2. \( \bigcup_{i=1}^{m} G_i = G_{p}^{inf} \)

The union of the edge clique covers of individual subgraphs \( G_1, \ldots, G_m \) is a valid edge clique cover of \( G_{p}^{inf} \):

\[
\bigcup_{i=1}^{m} \mathcal{ECC}(G_i) = \mathcal{ECC}(G_{p}^{inf}).
\]

**Proof:** Recall from the definition of Edge Clique Cover, a set of cliques is a valid edge-clique-cover of a given graph, if the following two requirements are satisfied by the clique set:

I. Every edge of the graph is covered in atleast one clique.

II. No clique is completely contained in another clique.

Consider the following arguments:

1. For any \( i \in \{1, \ldots, m\} \), \( \mathcal{ECC}(G_i) \) is a valid edge-clique-cover for subgraph \( G_i \).
2. Every edge in \( G_{p}^{inf} \) is covered in atleast one subgraph as \( \bigcup_{i=1}^{m} G_i = G_{p}^{inf} \), therefore every edge in \( G_{p}^{inf} \) is contained in atleast one of the cliques in the set: \( \bigcup_{i=1}^{m} \mathcal{ECC}(G_i) \). Thus requirement I is satisfied.
3. For a clique to be completely contained in another clique, there should be atleast one common edge between any two distinct subgraphs \( G_i \) and \( G_j \). Since, the subgraphs are edge-disjoint, i.e. \( G_i \cap G_j = \emptyset \), therefore no clique can be completely contained in another clique. Thus requirement II is also satisfied.

\[ \blacksquare \]

2 A sample exhaustive code

Table 1: Exhaustive code (all possible valid columns) for \( k = 5 \)

| Classes | \#1 | \#2 | \#3 | \#4 | \#5 | \#6 | \#7 | \#8 | \#9 | \#10 | \#11 | \#12 | \#13 | \#14 | \#15 |
|---------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| 1       | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   |
| 2       | -1  | -1  | -1  | -1  | -1  | -1  | -1  | -1  | -1  | -1  | -1  | -1  | -1  | -1  | -1  |
| 3       | -1  | -1  | -1  | -1  | 1   | 1   | 1   | 1   | 1   | -1  | -1  | -1  | -1  | -1  | -1  |
| 4       | -1  | -1  | 1   | 1   | -1  | -1  | -1  | -1  | 1   | 1   | 1   | 1   | -1  | -1  | -1  |
| 5       | -1  | 1   | -1  | 1   | -1  | 1   | -1  | 1   | -1  | 1   | -1  | 1   | -1  | 1   | -1  |
3 Dense/Sparse Codes

Random codes is another way of generating codebooks as proposed in [Allwein et al., 2000]. Here, authors propose generating 10000 matrices, whose entries are randomly selected. If the elements are chosen uniformly at random from \{+1, -1\}, then the resulting codebooks are called dense codes and if the elements are taken from \{-1, 0, +1\} then the resulting codebooks are called sparse codes. In sparse codes, 0 is chosen with probability \(\frac{1}{2}\) and \(\pm 1\) are each chosen with probability \(\frac{1}{4}\). Out of the 10,000 random matrices generated, after discarding matrices which do not constitute a valid codebook, the one with the largest minimum Hamming distance among rows is selected. Note that since out of the 10,000 matrices the one with the largest minimum hamming distance is selected, therefore despite the matrices being generated randomly, the final codebook can have high row-separation.

4 Details about Real-world datasets(Small/Medium)

In table 2 we provide details about Glass, Ecoli and Yeast datasets taken from the UCI repository [Dua and Graff, 2017].

|      | # of samples | # of features | # of classes (k) |
|------|--------------|---------------|------------------|
| Glass| 214          | 9             | 6                |
| Ecoli| 336          | 7             | 8                |
| Yeast| 1484         | 8             | 10               |

5 Class Probability Estimates

In section 5.2 under Adversarial Robustness, we discussed how class probability estimates enable us to estimate the adversarial robustness of ECOC based classifiers using white-box attacks. For binary codebooks we obtain class probability estimates using the procedure from [Zadrozny, 2002, Hastie and Tibshirani, 1998]. After evaluating an input \(x\) on each binary classifier, we obtain a probability estimate, denoted \(r_l(x)\), for each column \(l\) (i.e., binary classifier) in \(\mathcal{M}\). Let \(I\) denote the set of classes for which \(\mathcal{M}(i,l) = 1\) and \(J\) denote the set of classes for which \(\mathcal{M}(i,l) = -1\). Then the class probability estimate for \(i \in \{1, \ldots, k\}\) on an input \(x\) is given as follows:

\[
\hat{p}_i(x) = \sum_{l: \mathcal{M}(i,l)=1} r_l(x) + \sum_{l: \mathcal{M}(i,l)=-1} (1 - r_l(x)),
\]  

(20)

where differentiability with respect to \(x\) is maintained.

The above estimates work well for binary codes, however we need to be careful for ternary (or sparse) codes. For ternary codes, hypotheses which have zero (for a particular class) do not contribute to the above sum in (20). Therefore due to zero entries, estimates for different classes can significantly vary in relative magnitude. This can be easily fixed by simple normalization. Raw estimates in (20) can be normalized as follows:

\[
\hat{p}_i^* = \frac{1}{\sum_{l=1}^L 1\{ \mathcal{M}(i,l)=1\vee\mathcal{M}(i,l)=-1 \}} \left( \sum_{l: \mathcal{M}(i,l)=1} r_l(x) + \sum_{l: \mathcal{M}(i,l)=-1} (1 - r_l(x)) \right),
\]

(26)

where \(1\{\pi\}\) is the indicator function which evaluates to 1 when the predicate \(\pi\) is true and 0 otherwise.

In figure 1, we show how these estimates can be computed for 1-vs-1 codebook, when working with binary deep neural networks. Since, each row in 1-vs-1 has the same number of zeros therefore normalization is not necessary.
6 Adversarial Accuracy and Different types of Attacks

For ECOC based classifiers, evaluation of natural or clean accuracy over an example (generally from test-set) is straightforward, and can be easily done either by using a decoding scheme such as Hamming decoding or by calculating class probability estimates and choosing the class with the highest probability.

We now mathematically define the problem of evaluating the adversarial accuracy using class probability estimates. Suppose $c$ be the true class associated with a given input $x'$ and let $i \in \{1, \ldots, k\} \backslash \{c\}$ be the target class for which the attacker is trying to generate an adversarial perturbation. Attacker aims to solve the following non-convex problem:

$$f^*(x') = \max_{\delta} \{ \hat{p}_i(x' + \delta) - \hat{p}_c(x' + \delta) \}$$  \hspace{1cm} (27)

In (27), set $Q(x')$ for $l_{\infty}$-norm based perturbations is given as follows:

$$Q(x') = \{ x \in \mathbb{R}^d \mid \|x - x'\|_{\infty} \leq \epsilon ; l \leq x \leq u \}.$$ 

For a valid\(^1\) adversarial perturbation $\delta$, the objective function value of (27) would be strictly positive for some target class $i$. Different attacks such as black-box and white-box attacks attempt to solve the above outlined problem (27) under different settings (or threat model).

In black-box setting, only the output of the classifier i.e. the class probabilities or score of each class is known to the attacker. No model information is available to the attacker, i.e. the network architecture and the weights of the network. In this setting, since only class probability estimates are available, therefore analytical computation of gradients is not possible. The problem is generally solved using off-the-shelf black-box optimizers comprising of heuristics based algorithms such as Particle Swarm Optimization (PSO), Genetic Algorithms (GAs) etc. However, given the efficacy of gradient based attacks, one can also try to compute an estimate of the gradient and then use this estimate to run gradient-based attacks, for details see [Ilyas et al., 2018]. SPSA proposed in [Spall, 1992] is another black-box optimization method which is based on gradient estimation.

\(^1\)An adversarial perturbation $\delta$ does not necessarily need to be the arg max of (27)
In white-box setting, the class probability estimates along with the model architecture and weights are known to the attacker. White-box setting can also be referred to as complete information setting. In white-box setting, the projected gradient descent or the PGD-attack proposed in [Madry et al., 2018] has emerged as one of the strongest known attack. Another popular gradient based attack known as Fast-Gradient-Sign method (FGSM) was proposed in [Goodfellow et al., 2015]. FGSM can be viewed as simply a single step PGD attack and therefore is a much weaker attack in comparison to PGD-attack.

Given the non-concave nature of the problem (27), the above attacks do not provide any guarantee in terms of finding the optimal solution, and mainly aims at finding a feasible solution to (27) with positive objective function value. If these attacks fail in generating an adversarial perturbation (especially if the attack is weak), we conclude that the model is robust against that particular attack. Therefore, to estimate the adversarial robustness accurately it is important to evaluate against strongest possible attack.

7 Comparison with Multiclass CNN

In section 5.2 we compared the adversarial robustness of our IP generated codebook IP3 with other standard codebooks such as 1-vs-1, 1-vs-All, Sparse and Dense codes. We reported our results on MNIST and CIFAR10 datasets in table 8 and 9 respectively. We note that our IP generated codebook achieves non-trivial robustness without any adversarial training. On CIFAR10, our codebook outperforms all other standard codebooks, achieving an adversarial accuracy of $\sim 16\%$ with $\epsilon = 8/255$. However, given that we are combining the output of 20 binary classifiers, each of which is a ResNet-18, a natural question arises:

Is network capacity (of the overall classifier) the main reason for this robustness?

Recall that to evaluate the robustness we combine the outputs of each of the hypotheses (individually trained before) using our IP generated codebook and form a multi-class classifier. Figure 1 shows this for 1-vs-1 codebook for 3 classes. We then do a PGD based evaluation of the resulting multiclass classifier. To investigate the role of network capacity, we now in the same manner, combine 20 untrained hypotheses (ResNet-18) to form a multi-class classifier (say $F(x)$). We now nominally train this 10-class classifier $F(x)$ end-to-end using the entire training set. $F(x)$ has exactly the same network architecture and capacity as our multiclass ECOC based classifier resulting from our IP generated codebook.

We now evaluate the adversarial accuracy of $F(x)$ using the same PGD attack which we used for different codebooks including our IP generated codebook. We report our results in the last row of table 8 and 9 with type as Multiclass. The lack of robustness of $F(x)$ or Multiclass shows that network capacity alone in itself is not the reason for robustness of IP generated ECOC based classifier.

Finally, we note that since the individual untrained hypotheses are combined using a codebook in the final layer, therefore $F(x)$ is similar to the approach taken in [Verma and Swami, 2019].

8 Estimating Error-Correlation between individual hypotheses of a codebook

In our discussion in section 3, we highlighted that in communicating over a noisy channel, Error-Correcting Codes are powerful only when the errors made due to noise are random. For classification setup like ours, this implies that any two hypotheses (or classifiers) should not make errors on the same inputs. To avoid this, we ensured large column separation in our IP formulation. However, we may still end up with hypotheses whose final predictions (or errors) are correlated. Therefore, measurement of such pairwise correlations between hypotheses can provide us with insights to better understand the final performance of a particular codebook. Moreover, it also will provide us with corroborative evidence to the fact that correlation between hypotheses should be avoided.

Assuming that we have already trained each of our individual hypotheses for a given codebook. Also, let $N_{test}$ denote the number of images in our test-set. For every binary classifier (corresponding to a column) in the codebook, we can compute the 0-1 loss for all images in the test set so that we have a vector $h_l \in \{0, 1\}^{N_{test}} \forall l \in \{1, \ldots, L\}$. We can now compute the error-correlations between these binary vectors $h_i$ & $h_j$, $(i, j) \in \{1, \ldots, L\}^2$. This can be represented in a $L \times L$ matrix, which we will refer to as the correlation matrix (denoted as $P$) in our subsequent discussion. We propose the following measure:
\[
\mathcal{P}_{i,j} = \frac{\sum_{n=1}^{N_{\text{test}}} 1\{h_i[n] = 1 \land h_j[n] = 1\}}{\sum_{n=1}^{N_{\text{test}}} 1\{h_i[n] = 1 \land h_j[n] = 1\} + \sum_{n=1}^{N_{\text{test}}} 1\{h_i[n] = 0 \land h_j[n] = 0\}},
\]

(28)

where \(1\{\pi\}\) is the indicator function which evaluates to 1 when the predicate \(\pi\) is true and 0 otherwise.

The above measure (28) accounts for both the correct and incorrect predictions made by individual hypotheses. The magnitude of this error-correlation measure (or the values in the error-correlation matrix \(\mathcal{P}\)) will help us in understanding the accuracy of the overall classifier or codebook.

We estimate the error-correlation matrix using the natural images from CIFAR10 dataset for the nominally trained hypotheses of our IP generated codebook. For the same hypotheses, we also estimate the error-correlation matrix using the adversarial images obtained from the PGD-attack with \(\epsilon = 8/255\) on the overall classifier. We plot both the matrices in figure 2.

![Error-Correlation Matrices](image)

(a) Natural (Accuracy: 76.25 %)  (b) Adversarial (Accuracy: 16.48 %)

Figure 2: Error-Correlation matrices estimated using the hypotheses of the IP-generated codebook on natural and adversarial images of CIFAR10 dataset.

From figure 2, we note that the error-correlation values on the natural and adversarial dataset differ by almost an order of magnitude. On natural images, much higher accuracy is achieved as the error-correlation is low, while on adversarial images higher error-correlation values result in lower accuracy. Therefore for higher accuracy, error-correlation between hypotheses should be avoided.
9 Various IP Generated Codebooks

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