Predictive Multiplicity in Classification

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ABSTRACT
In the context of machine learning, a prediction problem exhibits multiplicity if there exist several “good” models that attain identical or near-identical performance (i.e., accuracy, AUC, etc.). In this paper, we study the effects of multiplicity in human-facing applications, such as credit scoring and recidivism prediction. We introduce a specific notion of multiplicity — predictive multiplicity — to describe the existence of good models with conflicting predictions. Unlike existing notions of multiplicity (e.g., the Rashomon effect), predictive multiplicity reflects irreconcilable differences in the predictions of models with comparable performance, and presents new challenges for common practices such as model selection and local explanation. We propose measures to evaluate the predictive multiplicity in classification problems. We present integer programming methods to compute these measures for a given dataset by solving empirical risk minimization problems with discrete constraints. We demonstrate how these tools can inform stakeholders on a large collection of recidivism prediction problems. Our results show that real-world prediction problems often admit many good models that output wildly conflicting predictions, and support the need to report predictive multiplicity in model development.

KEYWORDS
multiplicity, classification, integer programming, recidivism prediction, measurement, contestability

1 INTRODUCTION
Many methods in machine learning are designed to fit the best predictive model. In modern empirical risk minimization, for example, we aim to choose a model that optimizes an objective function (e.g., expected error) from a set of models that satisfy a given set of constraints (e.g., linear classifiers with equal FPR between groups). Assuming that stakeholders agree on the formulation of this prediction problem [??], and that we have the tools to solve it, there is still key issue with this approach: there may be more than one “best” model.

In machine learning, this notion — that a prediction problem may not have one “best” model but many “good” models that attain near-identical performance — is called multiplicity. Several works mention that prediction problems can exhibit multiplicity [see 34, 36], but only few discuss its practical implications, or provide concrete recommendations. The work of Breiman [8] is a major exception. In a seminal position paper, Breiman describes how multiplicity challenges the inherent validity of models: if there exists several equally good models for a given dataset, each of which provides a different explanation of the data-generating process, then how can we tell which one is correct?

Drawing parallels between the discordant explanations of good models and the discordant testimonies of witnesses in the motion picture “Rashomon,” Breiman calls this dilemma the Rashomon effect. In the context of his paper, the Rashomon effect is — in fact — an argument against the misuse of predictive models in scientific applications. Seeing how prediction problems can exhibit multiplicity, a cautious scientist should not draw scientific conclusions by “explaining” a predictive model, at least until there is evidence against the existence of multiplicity.

Machine learning has changed fundamentally since Breiman introduced the Rashomon effect. Many models are now built merely to make accurate predictions [24, 45]. In human-facing applications, such as credit scoring and recidivism prediction, these predictions affect people [7]. In turn, multiplicity challenges key aspects of how we build, interact, and trust models. Consider the following examples:

Recidivism Prediction: Say we are given a recidivism prediction model that performs well, but there exists a “competing model” that performs just as well. If these models output different predictions, then some individuals who are predicted to recidivate by the model we deploy could be predicted not to recidivate by a model that is equally valid. In this case, competing models with conflicting predictions present irreconcilable differences in the predictions of individuals [similar to the impossibility results in e.g., 11, 12, 25, 29]. Ignoring the existence of competing models would mean that we would arbitrate conflicting predictions by brute luck. In the worst case, a malicious practitioner could exploit this degree of freedom to choose a model that optimizes a secondary objective (e.g., a competing model that is least accurate on a certain group).

Credit Scoring: Say we must explain the prediction of a credit scoring model to a person [by producing e.g., a counterfactual explanation 31, 50]. If there exists several models that performed equally well, with conflicting predictions would yield contradictory explanations for certain individuals. In turn, it would be misguided to trust the explanations of a model for a person who is assigned a conflicting prediction by a competing model. In this case, awareness of competing models with conflicting predictions would mitigate unwarranted rationalization of the model (e.g., via fairwashing [2] or explanation bias [23, 27]).

Stakeholders in machine learning — practitioners, policy-makers, decision-subjects — are broadly unaware that there may exist alternative models that output wildly different predictions from those in deployment. One possible reason for this is the hypothesis that “good” models are “good” because they output similar predictions [see e.g., 33, for a critique]. We believe that it is important not only to raise awareness that competing models can produce conflicting predictions, but also to develop the tools to test this claim [see e.g., 26]. The latter goal is crucial since the incidence and severity of
conflicting predictions inherently depends on elements of model development such as the training data and model class. In such cases, presenting stakeholders with salient information on the existence and severity of conflicting predictions allows them to challenge key aspects of modern machine learning [as per the principles of contestability 20, 26] – from model selection (e.g., how should we choose between competing models, if we should choose one at all, and who should have a say in this decision) to downstream tasks that depend on model selection (e.g., model validation, model regulation, explanation).

In this paper, we introduce a general framework to evaluate the multiplicity of predictions in classification problems. Our objective is to provide stakeholders with information on the incidence and severity of multiplicity. We introduce three measures to capture how predictions vary over the set of all good models:

1. **Individual Ambiguity**: Does there exist a good model that produces a conflicting prediction for a given person?

2. **Ambiguity**: How many individuals can be assigned a different prediction by at least one good model?

3. **Discrepancy**: What is the maximum number of conflicting predictions between a baseline model and any good model?

These are model-agnostic measures that capture meaningful aspects of how multiplicity affects individuals in general classification problems (binary or multiclass).

To compute these measures, one must find specific models within a set of “good” models (e.g., a model that maximizes discrepancy while achieving comparable accuracy with respect to a baseline model we would deploy). We present tools to compute these quantities exactly for linear classification problems, then apply our tools to recidivism prediction problems where predictive multiplicity has important ethical implications.

The main contributions of our paper are:

1. We present formal measures of how multiplicity affects individual predictions in a classification task: discrepancy and ambiguity.

2. We develop integer programming tools to compute these measures for linear classification problems in a way that is exact and efficient. This is non-trivial since computing these measures requires solving hard optimization problems over a user-defined set of good models. We present integer programming formulations to solve these problems, and pair them with path algorithms to efficiently compute these measures over all possible sets of good models.

3. We present an empirical study of predictive multiplicity in recidivism prediction. Our results show that many real-world datasets can admit good models with wildly conflicting predictions. For example, in the ProPublica COMPAS dataset [4], we find that a competing model that is only 1% less accurate than the most accurate model we can deploy, can disagree on over 17% of predictions, and that 44% of predictions are vulnerable to model selection (see Section 4).

4. We discuss how predictive multiplicity challenges key aspects of modern machine learning. We show how our tools can calibrate trust in explanations, or address performance disparities between protected groups.

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### Figure 1: Toy example showing how multiple classifiers can perform equally well while assigning conflicting predictions. We train linear classifiers on perfectly sampled dataset with 400 points. Here, $n^+$ and $n^-$ denote the number of examples with $y = +1$ and $y = -1$ for each $(x_1, x_2) \in \{0, 1\}^2$, $\hat{h}_0, \hat{h}_a, \hat{h}_b, \hat{h}_c$ represent linear classifiers that minimize training and test error (25%). The predictions of any 2 classifiers differ on 200 points (50% of the training sample). Thus, the discrepancy is 50% among the set of optimal classifiers. Moreover, there exists a classifier that can predict +1 or −1 for each point. Thus, the ambiguity is 100% among optimal classifiers.

| $(x_1, x_2)$ | $n^+$ | $n^-$ | $\hat{h}_0$ | $\hat{h}_a$ | $\hat{h}_b$ | $\hat{h}_c$ |
|---------------|-------|-------|-------------|-------------|-------------|-------------|
| (0, 0)        | 0     | 100   | −           | −           | +           | +           |
| (0, 1)        | 100   | 0     | +           | +           | −           | +           |
| (1, 0)        | 100   | 0     | +           | −           | +           | +           |
| (1, 1)        | 0     | 100   | +           | −           | +           | +           |

| Training Error of Optimal Classifier | 25% |
| Test Error of Optimal Classifier    | 25% |
| Discrepancy among Optimal Classifiers | 50% |
| Ambiguity among Optimal Classifiers  | 100% |

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5. We provide a software implementation of our tools in Python at https://github.com/charliemarx/pmtools

### 1.1 Related Work

**Multiplicity.** The potential for predictive models to exhibit multiplicity has been known since at least the 1980s [see e.g., 36]. McCullagh and Nelder [34], for example, write “data will often point with almost equal emphasis on several possible models, and it is important... to recognize and accept this.”

Breiman [8] presents an early discussion of the practical implications of multiplicity. He argues that the existence of alternative models undermines the validity of using a single model to support broader claims about the data-generating mechanism (e.g., conflating the important variables of a recidivism prediction instrument with the root causes of criminal behavior). Breiman does not advocate a prescription to resolve multiplicity. Instead, he cautions against “automatic methods of model selection” and warns that “the multiplicity problem and its effect on conclusions drawn from models needs serious attention.”

Recent work in machine learning tackles multiplicity from the “Rashomon” perspective. Fisher et al. [15] and Dong and Rudin [14] present methods to evaluate variable importance over the set of good models. Semenova and Rudin [44] propose a measure for the relative size of the set of good models, and use it to characterize prediction problems where simple models perform well. Our work differs from this stream of research in that we focus on problems where good models output conflicting predictions (see e.g., Figure 2). This type of multiplicity leads to irreconcilable differences between subsets of predictions, which is similar to the impossibility results in the fair machine learning literature [e.g., 11, 12, 25, 29].
We consider a standard binary classification problem. We are given a baseline classifier  and denote an optimal classifier as:

\[ h_0 = \text{argmin}_{h \in \mathcal{H}} R(h) \]

Formally, a prediction problem consists of an empirical risk minimization (ERM) problem, a dataset, and a hypothesis class. We then use the posterior distribution to construct a single model for deployment [e.g., via a majority vote or a randomization procedure as in PAC Bayesian approaches, 18, 32].

These approaches, which are typically designed to improve out-of-sample performance, may not be appropriate to handle all incidences of multiplicity. In some prediction problems, for instance, tie-breaking between models would be ill-motivated since it would not achieve its intended goal of improving out-of-sample performance (e.g. in Figure 1 if we assume that the training data is drawn according to the true underlying distribution).

Other approaches include choose a single model to “break ties” between equally good models on the basis of secondary criteria, such as simplicity [44] or operational cost [46].

2 FRAMEWORK

In this section, we introduce measures to describe the multiplicity of predictions in classification. We will restrict our attention to binary classification problems where we want to maximize accuracy. Note, however, that our measures can be generalized to settings where we care about different performance metrics (e.g., AUC, TPR), where models must obey constraints [e.g., fairness constraints 10, 13, 53], or where we work with three or more outcomes.

2.1 Preliminaries

We consider a standard binary classification problem. We are given a training dataset of \( n \) examples \( \{(x_i, y_i)\}_{i=1}^n \) where each example consists of a vector of \( d+1 \) features \( x_i = (1, x_{i1}, \ldots, x_{id}) \in \mathbb{R}^{d+1} \) and a label \( y_i \in \{-1, +1\} \).

Our goal is to train a classifier \( h : \mathbb{R}^{d+1} \to \{-1, +1\} \) from a fixed hypothesis class \( \mathcal{H} \) that optimizes the true risk (i.e., test error). To this end, we minimize the empirical risk (i.e., the training error):

\[ \hat{R}(h) := \sum_{i=1}^n I \left[ h(x_i) \neq y_i \right] . \]

Formally, a prediction problem consists of an empirical risk minimization (ERM) problem, a dataset, and a hypothesis class. We denote an optimal classifier as:

\[ h_0 = \text{argmin}_{h \in \mathcal{H}} \hat{R}(h) . \]

Unless otherwise specified, we will assume that we deploy a baseline classifier \( h_0 = \hat{h} \) that optimizes performance on training data.\(^1\) This practice implicitly assumes that we expect the performance of \( \hat{h} \) on the training data to generalize to test data, which is a reasonable assumption for the applications that we consider as we often fit classifiers from a simple hypothesis class using datasets where \( n > d \) (see also our empirical results in Table 1 in Section 4).

Our framework and tools also apply for baseline models \( \hat{h}_0 \) that do not optimize training performance.

The Set of Good Models. We measure the multiplicity of predictions among the set of “good” models – i.e., a subset of classifiers in \( \mathcal{H} \) whose performance differs from the performance of a baseline classifier by a fixed amount. Given a baseline classifier \( \hat{h} \), we refer to the set of classifiers whose performance differs by at most \( \epsilon \) as the \( \epsilon \)-level set.

Definition 2 (\( \epsilon \)-Level Set). Given any classifier \( h \) and a hypothesis class \( \mathcal{H} \), the \( \epsilon \)-level set around \( h \) is the set of all models \( h' \in \mathcal{H} \) that make at most \( \hat{R}(h) + \epsilon \) mistakes over the training data:

\[ S_\epsilon(h) := \{ h' \in \mathcal{H} : |\hat{R}(h') - \hat{R}(h)| \leq \epsilon \} . \]

Since we measure performance in terms of the error rate, we refer to \( \epsilon \) as the error tolerance. We refer to models in the \( \epsilon \)-level set as competing models.

Definition 2 (Multiplicity). Given a baseline classifier \( \hat{h}_0 \) and an error tolerance \( \epsilon \), a prediction problem exhibits multiplicity if the \( \epsilon \)-level set around \( \hat{h}_0 \) is non-trivial. Formally, a problem exhibits multiplicity if \( |S_\epsilon(\hat{h}_0)| > 1 \).

It is possible for prediction problems to admit several models that optimize performance while producing conflicting predictions (see e.g., Figure 1). This corresponds to multiplicity over the level set where \( \epsilon = 0 \). In spite of this, there is good reason to measure multiplicity over an \( \epsilon \)-level set where \( \epsilon > 0 \). Specifically, while it is reasonable to expect that a model that optimizes performance on the training data to exhibit a similar level of performance in deployment, it not reasonable to expect that this model will actually optimize performance in deployment. Competing models – i.e., models that attain near-optimal performance on the training set – can perform better than the optimal model in deployment (see e.g., Section 4 for empirical evidence). In such settings, it would not be defensible to rule out near-optimal models on the basis of small differences in training error.

In practice, one should therefore evaluate multiplicity among a set of models that plausibly contains a model that performs the best in deployment. That is, we should set \( \epsilon \) so that the \( \epsilon \)-level set will, with high probability, contain the model that optimizes performance in deployment.\(^2\)

\(^1\) Deploying a model that optimizes performance on training data also reflects best practice in settings where a model that optimizes performance on the training data can overfit, and we control overfitting using techniques that estimate the performance of the model in deployment. In empirical risk minimization problems where we control overfitting by tuning hyperparameters, for example, we would first determine a value of the hyperparameters that optimizes an estimate of error in deployment (e.g., mean 5-CV test error). Given these hyperparameters, however, we still deploy the model that optimizes performance on the training data for these hyperparameters [9].

\(^2\) The value of \( \epsilon \) can be determined systematically by generalization bounds, or by computing confidence intervals of out-of-sample performance (e.g., via bootstrapping or cross-validation).
2.2 Predictive Multiplicity
A prediction problem exhibits predictive multiplicity if there exist several models that attain similar performance but that produce conflicting predictions on the training data.

Definition 3 (Predictive Multiplicity). Given a baseline classifier \( \hat{h}_0 \) and an error tolerance \( \epsilon \), a prediction problem exhibits predictive multiplicity over the \( \epsilon \)-level set \( S_\epsilon (\hat{h}_0) \) if there exists a model \( h \in S_\epsilon (\hat{h}_0) \) such that \( h(x_i) \neq \hat{h}_0(x_i) \) for some \( x_i \) in the training dataset.

Predictive multiplicity ignores instances of multiplicity where “good models are good because they produce the same predictions” (see e.g., Figure 2). Any incidence of predictive multiplicity implies that there is concrete evidence of irreconcilable differences between the predictions of good models.

2.3 Measures of Predictive Multiplicity

Discrepancy. Given a baseline classifier \( \hat{h}_0 \), we measure the severity of predictive multiplicity by counting the number of conflicting predictions between \( \hat{h}_0 \) and a model in the \( \epsilon \)-level set.

Definition 4 (Discrepancy). The discrepancy of a baseline classifier \( \hat{h}_0 \) over the \( \epsilon \)-level set \( S_\epsilon (\hat{h}_0) \) is the maximum number of conflicts over points in a training set \( x_i \in X \) between \( \hat{h}_0 \) and any competing classifier \( g_\epsilon \in S_\epsilon (\hat{h}_0) \):

\[
\delta_\epsilon (h) := \max_{\hat{h}_0 \in S_\epsilon (\hat{h}_0)} \# (x_i \in X : h(x_i) \neq \hat{h}_0(x_i)).
\]

If the discrepancy is small, it means that near-optimal models must output similar predictions. This reflects the common intuition that models which perform similarly output similar predictions. If the discrepancy is large, this means there exists a near-optimal solution which makes very different predictions than the baseline classifier. Such a result signals inherent trade-offs between predictions, possibly resulting from noisy data or structure in the data the model class cannot fit. Large discrepancies also means practitioners should consider choosing between models on the basis of secondary objectives, and rule out the possibility of adversarial model selection.

Ambiguity. We define the ambiguity of a model as the number of instances that exhibit individual ambiguity. While discrepancy reflects the maximum number of predictions that can change between the baseline model and a single model in the \( \epsilon \)-level set, ambiguity measures how many individual predictions are determined by the choice of one model between a set of good models.

Definition 5 (Ambiguity). The ambiguity of a baseline classifier \( \hat{h}_0 \) over the \( \epsilon \)-level set \( S_\epsilon (\hat{h}_0) \) is the number of points in a training dataset \( x_i \in X \) that can be assigned a conflicting prediction by a competing classifier \( g_\epsilon \in S_\epsilon (\hat{h}_0) \):

\[
\alpha_\epsilon (\hat{h}_0) := \# (x_i \in X : \exists h' \in S_\epsilon (\hat{h}_0) \text{ s.t. } h'(x_i) \neq \hat{h}_0(x_i)).
\]

Canonical Measures. Ambiguity and discrepancy capture salient aspects of predictive multiplicity for a given prediction problem. Considering the fact that these measures depend our choice of baseline model, we view the ambiguity and discrepancy of an optimal model as the canonical measures of predictive multiplicity for a given prediction problem, and denote these quantities as \( \alpha_\epsilon^* \) and \( \delta_\epsilon^* \), respectively. We observe that \( \delta_\epsilon^* \leq \alpha_\epsilon^* \), since the predictions flipped by a single model are a subset of those flipped by any model.

Since different subsets of predictions can be flipped by different models within a level set, there may be prediction problems where ambiguity far exceeds the discrepancy. This would reflect an unintuitive case where all good models make similar decisions, but many points are given conflicting predictions by good models. In other cases, ambiguity and discrepancy are similar to one another. This reflects that a single model is capable of expressing most of the predictive multiplicity.

2.4 Formal Guarantees
We conclude this section with simple bounds that illustrate the relationship between accuracy and predictive multiplicity.

In Proposition 2.1, we bound the number of distinct prediction profiles produced by models in the \( \epsilon \)-level. In Proposition 2.2, we bound the number of conflicts between the optimal model and any single model in the \( \epsilon \)-level set. We include proofs for all results in Appendix A.
Proposition 2.1 (Bound on the Number of Good Models). Given any value of \(\varepsilon \in \{0, \ldots, n\}\), the number of distinct classifiers in an \(\varepsilon\)-level set of a baseline classifier \(\hat{h}_0\) is bounded by

\[
|S_\varepsilon(\hat{h}_0)| \leq \sum_{i=\varepsilon}^{n} \binom{n}{\varepsilon, i, n-i} \hat{R}(\hat{h}_0) + i
\]

Here, \(\hat{e}^l = \max(-\varepsilon, -\hat{R}(\hat{h}))\) and \(\hat{e}^{ub} = \min(\varepsilon, n - \hat{R}(\hat{h}))\) represent lower and upper bounds for error tolerance given a baseline classifier that makes \(\hat{R}(\hat{h}_0) \in [0, n]\) mistakes.

Proposition 2.2 (Bound on the Discrepancy). The discrepancy between \(h_0\) and any competing classifier in the \(\varepsilon\)-level set \(h \in S_\varepsilon(\hat{h}_0)\) obeys:

\[
\delta_\varepsilon \leq 2\hat{R}(\hat{h}_0) + \varepsilon.
\]

Propositions 2.1 and 2.2 demonstrate how the severity of predictive multiplicity depends on the accuracy of a baseline model. These bounds illustrate the "pinching" effect of accuracy on multiplicity. As the number of mistakes decreases, the maximum number of possible trade-offs between conflicting points also decreases. In other words, there is more "room" for predictive multiplicity in settings where models perform poorly.

3 Methodology

In this section, we present integer programming tools to compute our measures of multiplicity for linear classification problems.

3.1 Preliminaries

Overview. Our methods compute the values of discrepancy and ambiguity in Section 2 by training linear classifiers of the form \(h(x) = \text{sign}(\langle w, x \rangle)\). We describe methods to train three kinds of linear classifiers:

1. \(\hat{h}\): a baseline classifier that minimizes the training error. While we can compute ambiguity and discrepancy with respect to any baseline classifier, computing them with respect to \(\hat{h}\) yields meaningful measures of multiplicity since it reflects the best possible model that can be produced for a given prediction problem.

2. \(\ell_i\): a classifier in the \(\varepsilon\)-level set that maximizes the number of conflicting predictions. This classifier will be used to compute discrepancy.

3. \(g_i\): a pathological classifier that minimizes training error subject to the constraint that it must flip the prediction of \(\hat{h}\) on \(x_i\). We will use \(g_i\) to determine the individual ambiguity of \(i\). By training \(g_i\) for all \(i \in \{1, \ldots, n\}\), we will be able to compute ambiguity.

Mixed Integer Programming. We train each classifier by solving an empirical risk minimization (ERM) problem with discrete constraints. We express each problem as a mixed integer program (MIP) and solve with a MIP solver such as CPLEX [22], Gurobi [1], or CBC [16]. MIP solvers return the global optimum of non-convex optimization problems using a principled exhaustive search process such as branch-and-bound [see 32]. In our setting, solving a MIP would produce: (i) an upper bound on the objective value; (ii) a lower bound on the objective value; and (iii) the coefficients of a linear classifier that achieve the upper bound. When the upper bound (i) and the lower bound (ii) match, the solution is said to be certifiably optimal.

Path Algorithms. We will present path algorithms to efficiently compute our measures for all possible sets of good models - i.e., \(\varepsilon\)-level sets for all possible values of the error tolerance \(\varepsilon\). [see e.g., algorithms to train machine learning models over the full regularization path such as glmnet 17].

3.2 Training the Baseline Classifier

We train a classifier that directly minimizes the training error (i.e., the 0-1 loss function) by solving an optimization problem of the form:

\[
\min_{h \in \mathcal{H}} \sum_{i=1}^{n} I[h(x_i) \neq y_i] \tag{1}
\]

We train a linear classifier \(h(x) = \text{sign}(\langle w, x \rangle)\) that optimizes the 0-1 loss by solving the MIP formulation:

\[
\begin{align*}
\min & \sum_{i=0}^{n} l_i \\
\text{s.t.} & M_i l_i \geq y_i (\| - \sum_{j \in K} w_j x_j \|) & i = 1, \ldots, n \tag{2a} \\
& 1 = l_i + l_{i'} & (i, i') \in K \tag{2b} \\
& w_j = w_j' + w_j'' & j = 0, \ldots, d \tag{2c} \\
& 1 = \sum_{j \in K} w_j' - w_j'' & \tag{2d}
\end{align*}
\]

Here, constraints (2a) set the mistake indicators \(l_i \leftarrow I[h(x_i) \neq y_i]\). These constraints depend on: (i) a margin parameter \(\gamma > 0\), which should be set to a small positive number (e.g., \(\gamma = 10^{-4}\)); (ii) the "Big-M" parameters \(M_i\), which can be set as \(M_i = \gamma + \max_{x \in X} \|x\|_{\infty}\) since we have fixed \(\|w\|_{\infty} = 1\) in constraint (2d). Constraint (2b) produces an improved lower bound by encoding the necessary condition that any classifier must make exactly one mistake between any two points \((i, i') \in K\) with identical features \(x_i = x_{i'}\) and conflicting labels. Here, \(K = \{(i, i') : x_i = x_{i'}, y_i = +1, y_{i'} = -1\}\) is the set of points with conflicting labels.

3.3 Computing Discrepancy

Given a training dataset, a baseline classifier \(\hat{h}_0\), and a specific error tolerance \(\varepsilon\), we compute the maximum discrepancy among all models within the \(\varepsilon\)-level set of \(\hat{h}_0\) by solving the following optimization problem:

\[
\begin{align*}
\min & \sum_{i=1}^{n} I[h(x_i) = \hat{h}_0(x_i)] \\
\text{s.t.} & |\hat{R}(\hat{h}) - \hat{R}(\hat{h}_0)| \leq \varepsilon
\end{align*}
\]

The optimization problem in (3) minimizes the agreement between \(g_\varepsilon\) and \(\hat{h}_0\) (which is equivalent to maximizing discrepancy). This
problem can be viewed as a standard ERM problem where we train a model using the dataset \( \{(x_i, -\hat{h}_0(x_i))\}_{i=1}^{n} \) (i.e., where we train a model to predict \(-\hat{h}_0(x_i)\) rather than \(y_i\)). The solution to this optimization problem is a classifier in the \(\epsilon\)-level set that maximizes discrepancy with respect to the baseline classifier, which we denote as \(\hat{q}_\epsilon\).

We train a linear classifier \(\hat{q}_\epsilon\) that maximizes discrepancy with the baseline classifier \(\hat{h}_0\) by solving the MIP formulation:

\[
\max \sum_{i=1}^{n} \delta_i \quad \text{s.t.} \quad M_i \delta_i \geq y_i (y - \sum_{j=0}^{d} w_j x_{ij}) \quad i = 1, \ldots, n \tag{4a}
\]

\[
M_i (1 - \delta_i) \geq y_i (y - \sum_{j=0}^{d} w_j x_{ij}) \quad i = 1, \ldots, n \tag{4b}
\]

\[
\epsilon \geq \sum_{i=1}^{n} \delta_i (1 - 2l_i) \tag{4c}
\]

\[
1 = l_i + l_i' \quad (i, i') \in K \tag{4d}
\]

\[
w_j = w_j^+ + w_j^- \quad j = 0, \ldots, d \tag{4e}
\]

\[
1 = \sum_{j=0}^{d} (w_j^+ - w_j^-) \tag{4f}
\]

Here, the objective maximizes the expression \(\sum_{i=1}^{n} \delta_i\), where \(\delta_i\) is an indicator variable that is set as \(1\) if \(h(x_i) \neq \hat{h}_0(x_i)\). These variables are set via the "Big-M" constraints (4a) and (4b), which have the same form as constraints (2a). The \(\hat{y}_i\) represent the prediction of the baseline classifier on point \(x_i\). Constraint (4c) enforces that any classifier must belong to the \(\epsilon\)-level set, i.e. that \(|\hat{R}_p(h) - \hat{R}_p(\hat{h}_0)| \leq \epsilon\). All other constraints and variables are identical to those in MIP (2).

Given a baseline classifier \(\hat{h}\) that is provably optimal, we reduce computation by adding the constraint \(\sum_{i=1}^{n} \delta_i (1 - 2l_i) \geq 0\). This constraint reflects the fact that we cannot increase the error rate by using an optimal baseline.

For the discrepancy MIP, the objective value is the maximum discrepancy found by the solver in the \(\epsilon\)-level set. The upper bound is the maximum possible discrepancy. When the objective value equals the upper bound, the solution provably maximizes the number of conflicts with the baseline classifier.

**Computing Discrepancy for all Values of \(\epsilon\)**

In Algorithm 1, we present an simple algorithm to computing discrepancy for all possible values of \(\epsilon\) for this task. While there are systematic ways to set the error tolerance, this algorithm avoids the need to set \(\epsilon\) a priori. The procedure solves the MIP (4) for all values of the error tolerance from \(\epsilon_{lb}\) to \(\epsilon_{ub}\). At each iteration, it uses solutions obtained from earlier iterations to initialize the current MIP. This resulting process is many times faster than solving the MIP separately for various error tolerances.

### Algorithm 1 Compute discrepancy for all possible values of \(\epsilon\)

**Input**

- \(\hat{h}_0\) baseline classifier
- \(\epsilon_{lb}, \epsilon_{ub}\) bounds on the error tolerance \(\epsilon\) (see Section 2)

**Initialize**

- \(S \leftarrow \emptyset\) pool of classifiers for initialization
- \(\mathcal{P} \leftarrow \emptyset\) value of discrepancy for each \(\epsilon\)

**for** \(\epsilon \in \{\epsilon_{lb}, \epsilon_{lb} + 1, \ldots, \epsilon_{ub}\}\) **do**

- MIP \(\leftarrow\) Instance of MIP (4) for error tolerance of \(\epsilon\)
- Set lower bound of MIP to discrepancy in \(\mathcal{P}\)
- \(\delta_\epsilon\) \(\leftarrow\) number of conflicts between \(\hat{q}_\epsilon\) and \(\hat{h}_0\)
- \(S \leftarrow S \cup (\hat{q}_\epsilon)\)
- \(\mathcal{P} \leftarrow \mathcal{P} \cup (\epsilon, \delta_\epsilon)\)

**end for**

**Output:** \(\mathcal{P}\) the discrepancy for each \(\epsilon\) considered

### 3.4 Computing Ambiguity

Given a training dataset and a baseline classifier \(\hat{h}_0\), we compute the value of ambiguity for all possible values of \(\epsilon\) by training a pathological classifier \(\hat{q}_\epsilon\) for each point \(i \in \{1, \ldots, n\}\).

Given the baseline classifier \(\hat{h}_0\) and the instance \(x_i \in X\), the pathological classifier for point \(i\) \(\hat{q}_\epsilon\) is the most accurate linear classifier that outputs a conflicting prediction on point \(i\). We can train \(\hat{q}_\epsilon\) by solving an optimization problem of the form:

\[
\min_{h \in \mathcal{H}} \sum_{k=1}^{n} \mathbb{I}[h(x_k) \neq y_i]
\]

s.t. \(h(x_i) \neq \hat{h}_0(x_i)\) \hspace{1cm} (5)

Here, \(h(x_i) \neq \hat{h}_0(x_i)\) is a constraint that forces any feasible classifier \(h\) to assign \(x_i\) a prediction that is in conflict with \(\hat{h}_0(x_i)\). Seeing how this optimization problem is identical to the optimization problem in (1), we train this model using a variant of MIP in (2) which contains the same variables and constraints and includes one additional constraint of the form:

\[
y_i \leq -\hat{h}_0(x_i) \sum_{j=0}^{d} w_j x_{ij} \hspace{1cm} (6)
\]

Constraint (6) ensures that \(h(x_i) \neq \hat{h}_0(x_i)\). The solution to this MIP returns the coefficients and training error of \(\hat{q}_\epsilon\).

With these quantities in hand, we can determine if point \(i\) exhibits individual ambiguity over the set of \(\epsilon\)-good models by checking if the following inequality holds:

\[
\hat{R}(g_i) \leq \hat{R}(\hat{h}_0) + \epsilon
\]

Given a set of pathological classifiers \(\hat{q}_\epsilon\) for each point \(i \in \{1, \ldots, n\}\), we can recover the ambiguity over the \(\epsilon\)-level set as:

\[
\alpha_{\epsilon} = \#(x_i \in X : \hat{R}(g_i) \leq \hat{R}(\hat{h}_0) + \epsilon)
\]

The expression in Eq. (7) states that the ambiguity over the \(\epsilon\)-level set is equivalent to the number of pathological classifiers whose performance is within \(\epsilon\) of the baseline model.

Our approach to evaluate ambiguity has the benefit that it computes this value for all possible values of \(\epsilon\). In practice, however, it may involve substantial computation since it requires training a
Algorithm 2 Compute ambiguity for all possible values of $\epsilon$

**Input**
- $h_0$, $\epsilon^{lb}$, $\epsilon^{ub}$
  - $h_0$: baseline classifier
  - $\epsilon^{lb}$, $\epsilon^{ub}$: bounds on the error tolerance $\epsilon$ (see Section 2)

**Initialize**
- $S \leftarrow \emptyset$
  - pool of classifiers for initialization
- $\Delta \leftarrow 0$
  - training error increase to change each prediction
- $\mathcal{P} \leftarrow \emptyset$
  - value of ambiguity for each $\epsilon$

**for** $i \in \{1, 2, \ldots, n\}$
- MIP $\leftarrow$ Instance of MIP (6) for point $x_i$
  - MIP: Mixed-Integer Programming
- Initialize MIP to best solution in $S$ satisfying Equation (6)
- $g_i \leftarrow$ solution to MIP
- $\Delta_i \leftarrow$ increase in train error of $g_i$ versus $h_0$
- $S \leftarrow S \cup \{g_i\}$
- $\Delta \leftarrow \Delta \cup \{\Delta_i\}$

**end for**

**for** $\epsilon \in \{\epsilon^{lb}, \epsilon^{ub} + 1, \ldots, \epsilon^{ub}\}$
- $\alpha_{\epsilon} \leftarrow$ number of $\Delta_i$ less than $\epsilon$
- $\mathcal{P} \leftarrow \mathcal{P} \cup \alpha_{\epsilon}$

**end for**

**Output:** $\mathcal{P}$, the ambiguity for each $\epsilon$ considered

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pathological classifier for each $x_i$. In our implementation, we aim to reduce the computation in several ways:

- We initialize the lower bound of the MIP that we use to train $g_i$ to the lower bound of the baseline MIP (since the baseline solution space is a subset of the solution space of the baseline MIP).
- Since $h_0$ and $g_i$ must output conflicting predictions, it follows that exactly one of these classifiers must make a mistake on $x_i$. Thus, we can also add the constraint to MIP (6) that $l_i = I[h_0(x_i) = g_i]$.
- When solving a MIP to train $g_i$, we can reduce computation by collecting the solutions from previous MIPs and initializing each MIP problem with the best solution that obeys $h_0(x_i) \neq h_0(x_i)$.

### 3.5 Discussion

**Design Considerations.** Our use of integer programming is motivated by the fact that it can directly optimize and constrain the exact quantities that we care about. In effect, integer programming trains models in a way that is guaranteed to consider all possible models in an $\epsilon$-level set. In this setting, popular approaches to reduce computation (e.g., solving a convexified ERM problem with a surrogate loss function such as the hinge loss) would return unreliable estimates since they may neglect salient models within the full $\epsilon$-level set (i.e., the optimal model, or the models that define the discrepancy).

Although integer programming is computationally intractable, modern solvers can solve empirical risk minimization for many real-world problems [see e.g., 6, 37, 47–49]. When integer programs do not produce a certifiably optimal solution, they will return a feasible solution along with meaningful bounds on the objective value. For example, in cases where the discrepancy MIP does not solve to optimality, the MIP returns the best solution found along with a lower bound on the minimum agreement (i.e., an upper bound on the discrepancy).

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**Extensions.** Our MIP formulations can be modified to optimize other objectives (e.g., class-based accuracy measures) or to incorporate constraints on model form or predictions (e.g., parity constraints). In addition, we can train a large class of “linearizable” rule-based models. Our measures can be evaluated without these tools, and provide useful information (albeit in a heuristic manner that can underestimate or overestimate these measures).

### 4 EXPERIMENTS

In this section, we present experiments where we apply our tools to evaluate predictive multiplicity in recidivism prediction problems. We have four goals: (i) to test the incidence and severity of multiplicity in real-world classification problems; (ii) to show how our tools can inform stakeholders in such settings; (iii) to discuss the implications of multiplicity with respect to transparency and accountability; (iv) to show that we can repurpose existing tools to capture some, but not all of the predictive multiplicity. For the sake of reproducibility, we include the software, scripts, and datasets to generate these results at https://github.com/charliemarx/pmtools.

#### 4.1 Setup

**Datasets.** We define a set of recidivism prediction problems from 3 studies of recidivism in the United States:
- *pretrial*: Felony Defendants in Large Urban Counties [40];
- *recidivism*: Recidivism of Prisoners Released in 1994 [39];
- *compar*: ProPublica COMPAS repository [4].

We use the raw data from each study to define training datasets by following standard practice in the development of recidivism prediction instruments [see e.g., guidelines for the development of an instrument by the Pennsylvania Sentencing Commission 41]. Each dataset consists of a binary outcome (e.g., a proxy variable such as arrest, arrest for violent crime) and a set of features for prisoners released in a specific state (e.g., NY, CA). We process each dataset by dropping instances with missing entries, binarizing features, and oversampling the minority class to equalize the number of instances with positive and negative labels. We present an overview of the number of instances and features in each dataset in Table 1.

**Measurement with Our Tools.** We evaluate the incidence and severity of predictive multiplicity for each of the datasets as follows. We first split each training dataset into a training set composed of 80% of points, and a test set composed of 20% of the points. For each dataset, we use the training data to fit a baseline classifier – i.e., an optimal classifier that we would deploy – by solving the MIP in Section 3.2. Given the baseline classifier, we measure the discrepancy and ambiguity among the set of good models by solving the IPs in Sections 3.4 and 3.3 for all possible values of the error tolerance $\epsilon$. To measure discrepancy, we solve MIP (4) for all possible values of

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1These are rule-based models that can be expressed as special kinds of linear classifiers, such as decision sets [28], decision lists [3], or and-or rules [51].
2We consider recidivism prediction net not in an effort to build new recidivism prediction instruments, but because it is a domain where the existence of predictive multiplicity has serious ethical implications and may present an additional critique [see e.g., 5, 19, 30, for a critique.]
3Oversampling ensures that we can directly minimize the training error without producing trivial classifiers. This also allows us to report meaningful measures of the error rate as opposed to class-specific error rates. We find that oversampling has a trivial effect on our measures of multiplicity (< 1%).
We present the values of discrepancy and ambiguity across all datasets. We train all discrepancy models, and 6 hours to train the baseline model, 6 hours to train all ambiguity models. We allocate at most 6 hours to train the individual ambiguity models.

**Measurement using Standard Methods.** We also consider an alternative analysis where we compute our proposed measures over a large pool of linear classifiers. We include this analysis to show that a systematic evaluation of predictive multiplicity can still reveal salient information even without using specialized techniques.

We construct a pool of linear classifiers via penalized logistic regression using the glmnet package of [17]. Each model is trained using logistic regression along with a weighted combination of the $\ell_1$ and $\ell_2$ penalties. Thus, the coefficients of each model are the solution to the optimization problem:

$$\min_{w \in \mathbb{R}^{d+1}} \frac{1}{2n} \sum_{i=1}^{n} \log(1 + \exp(-(w, y_i x_i))) + \lambda \cdot (\alpha \|w\|_1 + (1 - \alpha)\|w\|_2^2)$$

Here $\alpha \in [0, 1]$ is the elastic-net mixing parameter and $\lambda \geq 0$ is a regularization penalty. We train 1,100 models by choosing 1,100 combinations of $(\alpha, \lambda)$: 11 values of $\alpha \in \{0.0, 0.1, \ldots, 0.9, 1.0\} \times 10$ values of $\lambda$ (chosen automatically by glmnet for each $\alpha$). This produces 1,100 models that include models obtained by: (i) Lasso ($\ell_1$-penalty), which corresponds to when $\alpha = 1.0$; (ii) Ridge ($\ell_2$-penalty), which corresponds to when $\alpha = 0.0$; (iii) standard logistic regression, which corresponds to when $\alpha = 0.0$ and $\lambda$ is small.

In this setting, we choose our baseline model as the model that minimizes the 5-fold cross-validation error. We then compute discrepancy and ambiguity by comparing the baseline model to models in the pool that attain at most $\epsilon$ additional training error.

## Table 1: Performance of baseline classifiers for all datasets.

| Dataset         | $n$  | $d$  | Baseline Error (Train) | Baseline Error (Test) |
|-----------------|------|------|------------------------|-----------------------|
| compas_arrest   | 5,380| 18   | 32.7%                  | 33.4%                 |
| compas_violent  | 8,768| 18   | 37.7%                  | 37.9%                 |
| prettrial_CA_arrest | 9,926| 22   | 34.1%                  | 34.4%                 |
| prettrial_CA_fta | 8,738| 22   | 36.3%                  | 36.3%                 |
| prettrial_NY_fta | 730  | 22   | 25.9%                  | 29.9%                 |
| recidivism_CA_arrest | 114,522| 20  | 34.4%                  | 34.4%                 |
| recidivism_CA_drug | 96,664| 20  | 36.3%                  | 36.2%                 |
| recidivism_NY_arrest | 31,624| 20  | 31.0%                  | 31.8%                 |
| recidivism_NY_drug | 27,526| 20  | 32.5%                  | 33.6%                 |

*Table 1: Performance of baseline classifiers for all datasets. Here, $n$ is the number of instances in the dataset and $d$ is the number of features. We train each model by minimizing the 0-1 loss function on the training data. All 9 models generalize as shown training error is close to test error. This is expected given that we fit models from a simple hypothesis class on datasets where $n >> d$."

4.2 Results

We present the values of discrepancy and ambiguity across all possible values of the error tolerance $\epsilon$ in Figure 3. Due to space restrictions, we show plots of the measures computed using our tools for 3 datasets, and plots of the measures computed by standard tools on 1 dataset. We include for plots for all other datasets in Appendix B. In Table 2, a comparison of the competing classifiers trained on compas_arrest in Table 2. In what follows, we discuss these results.

**On the Incidence and Severity of Predictive Multiplicity.** Our results in Figure 3 shows how predictive multiplicity arises often in recidivism prediction tasks. Our results across all 9 datasets show that between 4% and 53% of individuals are assigned ambiguous predictions by models in the 1%-level set. In compas_arrest, for example, we observe an ambiguity of 44% – this means that 2,355 individuals (44%) are assigned different predictions by a competing model with an error tolerance of $\epsilon = 1\%$. For compas_violent, ambiguity over the 1%-level set is 53%, which means the the majority of predictions are affected by the decision to choose a model within the 1% training error. Considering discrepancy, we see that compas_arrest and compas_violent we can find a single competing model in the 1% level set that assigns 17% of individuals a different prediction. As shown in Figure 3, these measures of multiplicity also generalize to the test set.

Our results also illustrate why it not be defensible to rule out in model selection competing models due to minute differences in training performance. Even in setting where we train the best possible model that optimizes our performance objectives on the training data, this model – which is most likely to generalize does not actually represent the model that performs the best in deployment. In compas_arrest, for example, we find that the model that optimizes test error is only in the set of good models when $\epsilon \geq 1\%$.

As shown in Table 1, we can train baseline classifiers that perform well and do not overfit for all 9 datasets.8

**On the Implications of Predictive Multiplicity.** These results illustrate why it is important to report ambiguity and discrepancy as one would report estimates of test error. Ambiguity and discrepancy capture salient aspects of how the decision to choose a model affects individual predictions. Large values of these measures draw attention to model selection, and motivate the need for greater scrutiny. In compas_arrest, for example, one could justify the choice of a particular model since it optimizes training error, and appears to generalize. However, there exists a model with similar train and test performance that makes 17% of predictions differently. In turn, these measures signal the need for greater scrutiny and support the need for stakeholder involvement in model selection decisions (as per the principles of contestability).

Large values of ambiguity and discrepancy also lead us to calibrate trust in downstream processes. For example, awareness that 44% of predictions are determined by model selection in the 1% level set calibrates our trust in downstream processes that depend on predicted outcomes. Consider the process of explaining individual predictions.

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8We discuss these values at for an error tolerance of $\epsilon = 1\%$, which represents a conservative default.

This is expected given that we are fitting linear classifiers on large datasets via 0-1 loss minimization. Here, we expect the models generalize since we are fitting classifiers from a simple hypothesis class, using a large dataset, and with an algorithm that is robust to outliers [see e.g., 38].
predictions. In this case, an ambiguity of 44% of points means we could produce conflicting explanations for individual predictions (e.g., a counterfactual explanation for the deployed model could explain how to change \( h(x_p) = -1 \) to \(+1\) while a counterfactual explanation for a competing model could explain how to change \( h(x_p) = -1 \) to \(+1\)). While both explanations would reflect how the model itself operates, awareness of the fact that these explanation would change based on model selection would calibrate trust in explanations and potentially avoid rationalization of the model by a process of explanation – thus, reflecting a sort of localized Rashomon effect.

On the Burden of Multiplicity. We find that the incidence of multiplicity can differ significantly between subgroups. In \( \text{compas-violent} \), for example, the proportion of individuals whose predictions are ambiguous within the 1% level set is: 72.9% among African-American individuals \((n = 4,042)\), 37.2% among Caucasian individuals \((n = 3,923)\), 32.5% among Hispanic individuals \((n = 579)\), and 34.4% among Other individuals \((n = 224)\). In this case, we find that multiplicity disproportionately affects African-Americans compared to individuals of other ethnic groups. Groups with a larger burden of multiplicity are more vulnerable to model selection, and more likely to be affected by the ignorance of competing models.

On Choosing between Competing Models. When presented with a set of near equivalent models, a natural solution is to choose among them to optimize other goals. We support this practice in cases where secondary objectives are justified (see Section 5 for a discussion). Nevertheless, tie-breaking does not always yield a unique model. For the \( \text{compas-arrest} \) dataset we find 102 unique models (i.e. distinct predictions) that differ from the optimal model by less than 1% train error and 1% disparity between African-American individuals and individuals of other ethnicities. Thus, there are cases where secondary objectives fail to sufficiently distinguish between good models.

On Measurement via Ad Hoc Analysis. Our results show that multiplicity can arise even in settings where we train classifiers using an objective function that is guaranteed to produce a unique optimal solution.\(^7\) These findings illustrate how evaluating and reporting multiplicity can reveal useful information even without specialized tools. In \( \text{compas-arrest} \), for example, an ad hoc analysis of multiplicity among models that achieve an error within 1% of optimal reveals an ambiguity of 10% and a discrepancy of 7% (i.e., 10% of predictions can be flipped by any "good model", and 7% can be flipped by a single "good model"). These estimates are far less than those produced using our tools (44% and 17% respectively) since are using a suboptimal baseline model and evaluating the

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\(^7\)The objective is strongly convex since all instances, even Lasso, include a tiny \( \ell_2 \) penalty.

\begin{table}[h]
\centering
\begin{tabular}{llll}
\hline
 & Baseline Model & Individual Ambiguity Model & Max Discrepancy Model \\
\hline
\( h(x_p) \) & +1 & -1 & -1 \\
Error (Train) & 32.7\% & 32.7\% & 33.6\% \\
Error (Test) & 33.4\% & 33.4\% & 34.5\% \\
Discrepancy (Train) & 0.0\% & 0.0037\% & 16.8\% \\
Discrepancy (Test) & 0.0\% & 0.0\% & 15.1\% \\
\hline
\end{tabular}
\caption{Competing linear classifiers for \( \text{compas-arrest} \), and their predictions on a person with features \( x_p \). We show the baseline model that we would deploy (left) and the models trained to evaluate individual ambiguity (middle) and discrepancy (right). Here, the baseline model predicts \( h(x_p) = +1 \) while the other models predict \( h(x_p) = -1 \). As shown, there exists at least two models with only 1% additional training error that predict that \( x_p \) would not recidivate. Moreover, the coefficients and importance among the models changes. Models in the 1%-level set exhibit an ambiguity of 44%, meaning that 44% of individuals (2355 individuals) could have been assigned a different prediction by a model with comparable error.}
\end{table}
### Measurement with Our Tools

| Dataset | Discrepancy | Ambiguity |
|---------|-------------|-----------|
| compas arrest | ![Discrepancy Graph](image1) | ![Ambiguity Graph](image2) |
| recidivism NY arrest | ![Discrepancy Graph](image3) | ![Ambiguity Graph](image4) |
| pretrial CA arrest | ![Discrepancy Graph](image5) | ![Ambiguity Graph](image6) |

### Measurement with Standard Tools

| Dataset | Discrepancy | Ambiguity |
|---------|-------------|-----------|
| compas arrest | ![Discrepancy Graph](image7) | ![Ambiguity Graph](image8) |

Figure 3: Overview of predictive multiplicity measures obtained with our tools (top) and using standard tools (bottom). We plot the values of discrepancy (left) and ambiguity (right) computed over the $\epsilon$-level set (i.e., the set of models whose training error is within $\epsilon$ of the optimal training error) Our analysis for *compas_arrest* shows that the set of models for $\epsilon = 1\%$ exhibit a discrepancy of 17%, and an ambiguity of 44%. This means that one can change 17% of predictions by switching the baseline model with a model that is only 1% less accurate. Ambiguity reflects the fact that 44% of predictions are susceptible to model selection within this set. We observe that the values of discrepancy and ambiguity are similar on both the training and test set. We include results for other datasets in Appendix B.
measures over an incomplete set of "good" models. These results show that ad hoc approaches for generating alternative models can confirm the presence of predictive multiplicity, but should not be used to guarantee the absence of multiplicity.

5 CONCLUDING REMARKS

Predictive multiplicity can arise in many real-world problems, and has important implications for how we choose and interact with predictive models. In applications such as recidivism prediction and credit scoring, predictive multiplicity implies irreconcilable differences in individual predictions. Thus, when a prediction problem exhibits severe predictive multiplicity, we need to carefully justify our decision to choose one model over other models that perform equally well. If there exists different models that produce conflicting predictions on individuals, and no justification to support one model over another, then it may be a better choice to forgo deployment entirely, or to assign favorable predictions to individuals who receive ambiguous predictions.

Even as there exists several established techniques to choose between competing models (see Section 1.1), we do not advocate for a general prescription to “resolve” predictive multiplicity. Instead, we argue that one should measure and report multiplicity in the same way that we measure and report other kinds of model statistics [21, 35, 42, 43]. In this way, problems that exhibit predictive multiplicity can be handled on a case-by-case basis, and in a way that allows for input from stakeholders [as per the principles of contestable design; see e.g., 20, 26]. The measures and machinery in this work provide a first step towards this goal.

Our proposed approach, which mirrors Breiman’s recommendations against the use of “automatic methods for feature selection,” [8], presents a series of technical and procedural benefits. Real-world problems can exhibit predictive multiplicity due to a host of reasons (e.g., the use of feature selection, training data that has missing features or latent groups, or a poorly specified model class). The process of evaluating predictive multiplicity may guide us in choosing a suitable solution. In Figure 1, for example, all models perform equally well and tie-breaking between models on the basis of out-of-sample accuracy would not achieve the goal of improving out-of-sample accuracy. Likewise, evaluating predictive multiplicity requires a systematic way to search for and evaluate alternative models, which can lead to improvements in the model in deployment, or provide safeguards against a malicious practitioner.

One potential approach to handle predictive multiplicity is to circumvent difficult choices between competing models by adapting the training process to provide a forcibly unique solution. For example, by incorporating unnecessary constraints to the problem, or by choosing an algorithm that is guaranteed to produce a single model. If such changes are only motivated by the need to produce a unique model, rather than to achieve other desirable objectives, then this would effectively relegate model selection to the training process – and thereby “automate” model selection in an unwarranted way.

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9We do not consider the full set of linear classifiers in the 1%-level set; only models that are produced by varying $\ell_1$ and $\ell_2$ penalties in Eq (??)
A OMITTED PROOFS

Proof of Proposition 2.1. We proceed by a simple counting argument. First, note that in the context of predictive multiplicity we consider unique models to be models which differ in at least one observed prediction. Now, there are \( \binom{n}{R(\hat{h}_0)} \) ways to choose \( R(\hat{h}_0) \) instances on which to make a mistake. Denote the effective lower and upper bounds of the \( \epsilon \)-level set by \( \epsilon^l = \max(-\epsilon, -R(\hat{h}_0)) \) and \( \epsilon^u = \min(\epsilon, n - R(\hat{h}_0)) \) respectively, since the number of mistakes of any model must be in the interval \([0, n]\). Since the \( \epsilon \)-level set is comprised only of models making a number of mistakes in the interval \([R(\hat{h}_0) + \epsilon^l, R(\hat{h}_0) + \epsilon^u]\), we see that there are at most \( \sum_{i=\epsilon^l}^{\epsilon^u} \binom{n}{R(\hat{h}_0)+i} \) unique prediction vectors a model in the \( \epsilon \)-level set could generate. Thus, this supplies an upper bound on the number of unique models in the \( \epsilon \)-level set. Note that the number of these prediction vectors that will be achievable will vary between model classes.

Proof of Proposition 2.2. We will use the Triangle Inequality to bound the distance between the vector of predictions of the baseline model, and let \( \hat{y} = (\hat{h}_0(x_i))_{i=1}^n \) be the vector of predictions of the baseline model, and let \( y' = (h'(x_i))_{i=1}^n \) be the predictions of a competing model \( h' \) in the \( \epsilon \)-level set. Note that \( y, y', \hat{y} \in \{+1, -1\}^n \). Now, we can express the risk of each model, \( \hat{h} \) and \( h' \), as well as the discrepancy between the two models, denoted \( \delta(\hat{h}, h') \), in terms of these three vectors by

\[
\delta(\hat{h}, h') = \frac{1}{4}||y - \hat{y}||
\]

Next, consider the triangle formed in \( \mathbb{R}^n \) by the points \( y, y' \) and \( \hat{y} \). This triangle has side lengths \( ||y - \hat{y}|| \), \( ||y' - \hat{y}|| \) and \( ||y - y'|| \). The Triangle Inequality then gives us that

\[
||y' - \hat{y}|| \leq ||y - y'|| + ||y - \hat{y}||.
\]

Substituting using the three equations above, we have

\[
\delta(\hat{h}, h') \leq \hat{R}(\hat{h}_0) + \hat{R}(h').
\]

Since \( h' \in S_\epsilon(\hat{h}_0) \), we have by the definition of the \( \epsilon \)-level set that \( \hat{R}(h') \leq \hat{R}(\hat{h}_0) + \epsilon \). We can then rewrite the above expression to yield

\[
\delta(\hat{h}_0, h') \leq 2\hat{R}(\hat{h}_0) + \epsilon
\]

Recall that \( \delta_\epsilon := \max_{h' \in S_\epsilon(\hat{h}_0)} \delta(\hat{h}_0, h') \). Since each \( h' \in S_\epsilon(\hat{h}_0) \) satisfies \( \delta(\hat{h}_0, h') \leq 2\hat{R}(\hat{h}_0) + \epsilon \), we have the result that \( \delta_\epsilon \leq 2\hat{R}(\hat{h}_0) + \epsilon \).

B SUPPORTING EXPERIMENTAL RESULTS

| Dataset             | \( n \) | \( d \) | Outcome Variable                  |
|---------------------|---------|-------|-----------------------------------|
| compas_arrest       | 5,380   | 18    | rearrest for any crime            |
| compas_violent      | 8,768   | 18    | rearrest for violent crime        |
| pretrial_CA_arrest  | 9,926   | 22    | rearrest for any crime            |
| pretrial_CA_fta     | 8,738   | 22    | failure to appear                 |
| pretrial_NY_fta     | 730     | 22    | failure to appear                 |
| recidivism_CA_arrest| 114,522 | 20    | rearrest for any crime            |
| recidivism_CA_drug  | 96,664  | 20    | rearrest on drug crime            |
| recidivism_NY_arrest| 31,624  | 20    | rearrest for any crime            |
| recidivism_NY_drug  | 27,526  | 20    | rearrest for drug crime           |

Table 3: Overview of recidivism prediction datasets considered in Section 4. All datasets are publically available. We include a copy of compas_violent and compas_arrest with our submission. The remaining datasets must be requested from ICPSR due to privacy restrictions.
Figure 4: Multiplicity profiles for the compas and pretrial datasets. The maximum percent of conflicts between the optimal model and any model within the error tolerance (discrepancy) is shown on the left. The percent of individuals who could have been given a different prediction by some model within the error tolerance (ambiguity) is shown on the right.
**Measurement with Our Tools**

| Dataset      | Discrepancy | Ambiguity |
|--------------|-------------|-----------|
| recidivism NY arrest | ![Graph](image) | ![Graph](image) |
| recidivism CA arrest     | ![Graph](image) | ![Graph](image) |
| recidivism NY drug       | ![Graph](image) | ![Graph](image) |
| recidivism CA drug       | ![Graph](image) | ![Graph](image) |

Figure 5: Multiplicity profiles for the recidivism datasets. The maximum percent of conflicts between the optimal model and any model within the error tolerance (discrepancy) is shown on the left. The percent of individuals who could have been given a different prediction by some model within the error tolerance (ambiguity) is shown on the right.
Figure 6: Multiplicity profiles for the \texttt{compas} and \texttt{pretrial} datasets, using standard methods ($\ell_1$ and $\ell_2$ penalty grid) to generate the level sets. The maximum percent of conflicts between the optimal model and any model within the error tolerance (discrepancy) is shown on the left. The percent of individuals who could have been given a different prediction by some model within the error tolerance (ambiguity) is shown on the right.
### Measurement with Standard Tools

| Dataset     | Discrepancy | Ambiguity |
|-------------|-------------|-----------|
| **recidivism NY arrest** | ![Graph](#) | ![Graph](#) |
| **recidivism CA arrest** | ![Graph](#) | ![Graph](#) |
| **recidivism NY drug** | ![Graph](#) | ![Graph](#) |
| **recidivism CA drug** | ![Graph](#) | ![Graph](#) |

Figure 7: Multiplicity profiles for the recidivism datasets, using standard methods ($\ell_1$ and $\ell_2$ penalty grid) to generate the level sets. The maximum percent of conflicts between the optimal model and any model within the error tolerance (discrepancy) is shown on the left. The percent of individuals who could have been given a different prediction by some model within the error tolerance (ambiguity) is shown on the right.