A COMBINATORIAL APPROACH TO FAIRNESS TESTING OF
MACHINE LEARNING MODELS

by

ANKITA RAMJIBHAI PATEL

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To my parents and Jagan
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ABSTRACT

A COMBINATORIAL APPROACH TO FAIRNESS TESTING OF MACHINE LEARNING MODELS

Ankita Ramjibhai Patel, MS

The University of Texas at Arlington, 2022

Supervising Professor: Jeff (Yu) Lei

Machine Learning (ML) models could exhibit biased behavior, or algorithmic discrimination, resulting in unfair or discriminatory outcomes. The bias in the ML model could emanate from various factors such as the training dataset, the choice of the ML algorithm, or the hyperparameters used to train the ML model. In addition to evaluating the model’s correctness, it is essential to test ML models for fair and unbiased behavior. In this thesis, we present a combinatorial testing-based approach to perform fairness testing of ML models. Our approach is model agnostic and evaluates fairness violations of a pre-trained ML model in a two-step process. In the first step, we create an input parameter model from the training data set and then use the model to generate a t-way test set. In the second step, for each test, we modify the value of one or more protected attributes to see if we could find fairness violations. We performed an experimental evaluation of the proposed approach using ML models trained with tabular datasets. The results suggest that the proposed approach can successfully identify fairness violations in pre-trained ML models.

This thesis is presented in an article-based format and includes a research paper. This paper reports our work on applying combinatorial testing to identify fairness violations in Machine Learning (ML) models. This paper has been accepted at a peer-reviewed venue (In press).
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CHAPTER 1. INTRODUCTION

Machine Learning (ML) model is a key component of Artificial Intelligence (AI)-based software systems and has demonstrated exemplary performance in accomplishing human intelligence tasks such as classification, prediction, language translation, and object detection. ML models are increasingly used in critical decision-making activities across different domains. For example, an AI-based application is used in banking to assess the credit risk of potential customers [1], to assess and predict the risk of defendants committing crimes in the future [2], to control and drive a car [3], and in medical diagnosis [4,5]. Despite their potential to perform intelligence tasks with higher precision, AI systems struggle when deployed in real-world conditions. Consider the case of an AI system used in a hospital to identify patients for extra care, which preferred patients belonging to a particular race over other patients [6]. In another scenario, a recruiting tool preferred male candidates over female candidates [7]; face-recognition software falsely classifies subjects [8, 9]. Incidents like these suggest that ML models, when deployed in a real-world environment, are vulnerable to the problem of generalizability – the ability of an ML model to adapt and perform well on new, unseen data and exhibit a discriminative behavior.

1.1. RESEARCH OVERVIEW

As ML models learn from a training dataset by discovering the underlying patterns, a trained ML model inadvertently reflects the inherent, underlying bias it infers either from the training dataset, the training algorithm, or its hyperparameters. A biased ML model on deployment poses the risk of exhibiting a discriminative behavior and adversely affecting the users and thus, posing a risk of diminishing trust among the users. Given the ever-increasing use of ML-based systems across domains, it is necessary to ensure that ML models exhibit a fair behavior. Hence,
in addition to functional testing, it is essential to test ML systems for discriminatory behavior (also referred to as fairness violations) and ensure the models exhibit fair behavior.

This thesis presents a combinatorial testing-based approach to perform fairness testing of ML models. First, we generate t-way test instances based on the training dataset. Next, we identify fairness violations by generating perturbations of test instances using a counterfactual approach. We evaluated our approach using twelve pre-trained ML models; the results suggest that the proposed approach can identify many fairness violations across ML models. Furthermore, results suggest that the proposed approach can detect discriminatory behavior introduced by both the dataset and the training algorithm.

1.2. SUMMARY OF PUBLICATIONS

This thesis is presented in an article-based format and includes a research paper. In Chapter 2, we present the paper titled, A Combinatorial Approach to Fairness Testing of ML Models. This paper is accepted at the IEEE 15th International Conference on Software Testing, Verification and Validation Workshops (ICSTW) in 2022. This paper is co-authored and includes the following authors: Jaganmohan Chandrasekaran, Yu Lei, Raghu Kacker, and D. Richard Kuhn. I am the primary author of this paper, and I was responsible for developing the approach, designing input parameter models, deriving constraints, conducting the experiments, and analyzing the results. Dr. Chandrasekaran and Dr. Lei advised in the design of experiments and helped significantly in improving the manuscripts. Additionally, Dr. Lei supervised the overall project. Dr. Kacker and Dr. Kuhn contributed to improving the final draft of the paper.

Chapter 3 presents the concluding remarks and directions for our future work.
1.3. REFERENCES

1. AI-powered decision making for the bank of the future -


4. AI In Medicine: Rise Of The Machines

5. AI just as good at diagnosing illness as humans

6. Racial Bias Found in Algorithms That Determine HealthCare for Millions of Patients -

7. Amazon scraps secret AI recruiting tool that showed bias against women


The chapter contains a paper accepted at the IEEE 11th International Workshop on Combinatorial Testing (IWCT), in 2022.
A Combinatorial Approach to Fairness Testing of Machine Learning Models

Ankita Ramjibhai Patel¹, Jaganmohan Chandrasekaran², Yu Lei¹, Raghu N. Kacker³, D. Richard Kuhn³

¹Dept. of Computer Science and Engineering, The University of Texas at Arlington, Arlington, Texas 76019, USA
²Commonwealth Cyber Initiative (CCI), Virginia Tech, Arlington, Virginia 22203, USA
³Information Technology Laboratory, National Institute of Standards and Technology, Gaithersburg, Maryland 20899, USA

Abstract — Machine Learning (ML) models could exhibit biased behavior, or algorithmic discrimination, resulting in unfair or discriminatory outcomes. The bias in the ML model could emanate from various factors such as the training dataset, the choice of the ML algorithm, or the hyperparameters used to train the ML model. In addition to evaluating the model’s correctness, it is essential to test ML models for fair and unbiased behavior. In this paper, we present a combinatorial testing-based approach to perform fairness testing of ML models. Our approach is model agnostic and evaluates fairness violations of a pre-trained ML model in a two-step process. In the first step, we create an input parameter model from the training data set and then use the model to generate a t-way test set. In the second step, for each test, we modify the value of one or more protected attributes to see if we could find fairness violations. We performed an experimental evaluation of the proposed approach using ML models trained with tabular datasets. The results suggest that the proposed approach can successfully identify fairness violations in pre-trained ML models.
Keywords — Fairness Testing, Algorithmic Discrimination, Bias Detection, Testing Model Bias, Testing ML model, Combinatorial Testing

2.1. INTRODUCTION

Machine Learning (ML) models are widely used across domains in automated decision-making processes. For example, ML-based recommender systems are used by banks to approve or deny loans for their applicants [29]. Companies use ML-based software applications to filter/select candidates in the hiring process [20][34]. Despite its impressive predictive capabilities, ML models inadvertently exhibit bias and result in discriminatory behavior, also referred to as algorithmic discrimination [3][7][18][34].

A bias in an ML model could be introduced via various factors such as the training dataset, the choice of the ML algorithm, or the hyperparameters used to train the ML model. Recent reports in [16][18] illustrate the biased behavior of ML models and their adverse effects on society. Thus, in addition to an ML model’s correctness, there is a need to test and ensure that the ML model behaves in an unbiased and non-discriminatory manner. In recent years, a significant amount of research has been reported on fairness testing [37]. From a testing perspective, the objective of fairness testing is to evaluate whether a model under test exhibits a consistent, non-discriminatory behavior for all its use cases.

ML models used in the automated decision-making process must avoid discriminating against sensitive characteristic features of individuals such as age, race, sex, and ethnicity [1]. The sensitive characteristics vary depending on the domain, and they are referred to as protected attributes. Assume a pre-trained model M, on receiving an input I, predicts a class label C. A discriminatory behavior (also referred to as fairness violation) of M can be broadly classified into two types: (1) individual discrimination and (2) group discrimination [1][12]. Model M exhibits
individual discrimination if M predicts a different outcome for two similar instances. Model M exhibits group discrimination if M favors or discriminates instances belonging to a specific group over the other groups.

Some recent work has been reported on fairness testing [1][2][6][10][21][33][36][38]. Galhotra et al. proposed THEMIS, a causality-based random test generation technique to identify discriminatory behavior of ML models [10]. Aggarwal et al. proposed a symbolic execution-based approach to generate test instances and then use a local explanation tool called LIME to identify individual discriminations in an ML model [1]. Udeshi et al. proposed Aeqitas, a testing technique to discover discriminatory inputs by randomly sampling the input space [33]. The results from existing studies suggest that traditional testing techniques can effectively be adapted to identify the discriminatory behavior of ML models.

In this paper, we present a combinatorial approach to test ML models for individual discriminations. We believe that the key insight that has allowed combinatorial testing to be effective for general software testing could also apply to fairness testing. That is, while the behavior of an entire model could be affected by many factors, individual fairness violations may be caused by only a few factors. Our approach consists of two phases: Generating T-Way Tests and Identifying Fairness Violation. In Phase 1, we generate t-way tests based on a training dataset. We begin this phase with the design of an Input Parameter Model (IPM). All attributes excluding the class label attribute from the training dataset are mapped as parameters. Then, we identify representative values for each parameter based on the corresponding attribute’s data type. In the case of categorical (string) attribute(s), we identify and map its unique values as representative values. For numerical attribute(s), we identify its representative values via discretization, a process of converting numerical (continuous) values into a set of discrete values [15].
Next, we identify constraints using an unsupervised learning algorithm that infers the underlying relationships among different attributes (excluding the class label) from the training dataset. The relationships identified by the learning algorithm are mapped as constraints in our IPM. Finally, we generate abstract t-way tests that are later converted into concrete t-way tests.

Using the concrete t-way tests, in phase 2, we identify individual fairness violations using a counterfactual approach. Given a t-way test instance, we generate perturbations that are similar to the t-way instance by modifying the value of one or more protected attributes while retaining the values of non-protected attributes and respecting all the constraints. On receiving the perturbated instance(s) as input, if the ML model results in an outcome that differs from the outcome produced for the original t-way instance, then the ML model is considered to exhibit an individual fairness violation.

We report an experimental evaluation of the proposed approach. Three widely used datasets, namely Adult Income [31], German Credit [32], and COMPAS [25], are used as our subject datasets. We build ML classifiers (models) for each dataset using four popular Machine Learning algorithms, namely Logistic Regression, Random Forest, Support Vector Machines, and Deep Neural Network. We generate t-way test sets based on the datasets and test the ML models for fairness violations. Our results suggest that the combinatorial approach can successfully identify fairness violations in ML models. In some cases, more than 40% of t-way test cases resulted in a fairness violation. Furthermore, the results indicate that t-way test cases generated using our approach can identify a substantial number of fairness violations across different types of ML classifiers. This suggests that the proposed approach is model-agnostic and can be adopted to test fairness violations for different ML models.
The remainder of this paper is organized as follows. Section II provides an introduction of fairness testing. Section III presents our approach, illustrated with an example. In Section IV, we present our experimental design and discuss the results. Section V discusses the existing work on fairness testing. Section VI provides the concluding remarks and plans for future work.

2.2. BACKGROUND

In this section, we introduce several concepts that are important in fairness testing.

**ML Model:** To build an ML model, first, a practitioner selects an ML algorithm; provides a training dataset and a set of hyperparameters as input to the ML algorithm. Then, the ML algorithm infers a decision logic based on the underlying patterns discovered from the training dataset. The derived decision logic is referred to as the ML model. An ML model exhibits fair behavior if it does not favor or discriminate against a specific individual or a particular group.

**Protected Attributes:** The attributes from the training dataset that are sensitive and need to be protected against discrimination are referred to as protected attributes [37]. Example of protected attributes includes Race, Color, Religion, Sex, and Familial Status [14]. Fairness testing aims to evaluate and assure that the ML model exhibits a non-discriminatory behavior.

**Individual Discrimination:** Given two valid inputs (instances) that differ only by the protected attribute(s), an ML model is expected to predict the same outcome for both the inputs. Otherwise, the ML model is considered to exhibit individual discrimination [1]. For example, consider two applicants with an identical credit history but differ only by their Race. If an ML model approves the loan for one applicant while rejecting the other, the model exhibits individual discrimination. In the rest of the paper, we refer to individual discrimination simply as a fairness violation unless otherwise specified.
**Group Discrimination:** If an ML model favors or discriminates instances belonging to a specific group over the other groups, it is considered group discrimination. For example, the Amazon AI recruiting tool preferred male candidates over female candidates in the candidate hiring process [3]. As another example, Buolamwini et al. demonstrated that a commercially available facial recognition software misclassifies more female faces than male faces [7].

**Counterfactual Explanation:** Explainable Artificial Intelligence (XAI) tools generate explanations for decisions made by ML models [4]. A counterfactual approach is one of the two commonly used approaches to explain a model’s decision. Assume a pre-trained model M, on receiving an input I, predicts a class label C. A counterfactual approach identifies a minimum set of features that, if removed, shall result in a different prediction [11]. That is, a counterfactual is generated by making minor change(s) to the original instance, resulting in a different outcome than the original prediction.

### 2.3. APPROACH

This section presents a combinatorial approach to identify fairness violations of pre-trained ML models. Figure 2-1 presents an overview of our approach. It consists of two major phases: (1) Generating T-Way Tests, where a t-way test set is generated; and (2) Identifying fairness violations, where the t-way tests are executed to detect fairness violations.
2.3.1. Phase 1: Generating T-Way Tests

In Phase 1, we generate t-way test cases (instances) based on the training dataset. A training dataset consists of numerical attributes, categorical attributes, or a combination of both. We first create an Input Parameter Model (IPM) for the training dataset. All attributes except the class label attribute from the training dataset are mapped as a parameter in the IPM. Next, we identify representative values for each identified parameter (attribute) based on its data type (numeric or categorical).

For a categorical attribute, we identify and map all its unique values as the parameter values. For a numerical attribute, we identify the parameter values using an entropy-based discretization approach. Discretization is a process of converting numerical (continuous) values into a set of discrete values. A numerical attribute is divided into a small number of intervals, where each interval is mapped to a bin [15]. In entropy-based discretization, the entropy of a bin
is calculated based on the frequencies of the class labels to which the values in the bin belong. The entropy-based approach tries to find the best splits (bins) where the majority of values in a bin belong to the same class label [28]. The bins identified using the discretization approach are mapped as the parameter values. That is, if a numeric attribute is divided into n bins using the discretization approach, then the attribute has n values one for each bin.

Next, to derive constraints, we first modify the dataset by mapping all the numeric attributes to their respective bins identified via discretization. Our goal is to identify the relationships among all attributes, excluding the class label attribute. Hence, we remove the class label attribute from the dataset. Then, the modified dataset is provided as an input to Apriori, an association rule mining algorithm [2]. The Apriori algorithm discovers association rules in a two-step process. First, they identify the relationship among attributes that appear together more frequently in the training dataset. Next, the algorithm calculates association rules between frequently appearing attributes (identified in the previous step) using a statistical score. These association rules are mapped as constraints in our IPM. Using constraints enables us to generate valid test cases.

After we create the IPM, we generate an abstract t-way test set using ACTS [9][35], and derive a concrete test set from the abstract test set. Recall that our approach discretizes the numeric attributes. Therefore, in this step, for numeric attributes, we replace the abstract value with a value (selected randomly) from the corresponding bin. The t-way concrete test set, where each test case is a test instance, is used to identify the fairness violations of the pre-trained ML model.

2.3.2. PHASE 2: IDENTIFYING FAIRNESS VIOLATION

In Phase 2, we identify fairness violations by perturbing the test instances using a counterfactual approach. First, each test instance (i.e., a concrete test generated from Phase 1) is
provided as an input to the pre-trained ML model, and its predicted class label is recorded. Then, we generate a set of perturbated instances (from the test instance) by changing the value of one or more protected attribute(s) while retaining the value of non-protected attributes. We modify the value of the protected attribute(s) such that the perturbated instances satisfy the constraints (identified in Phase 1). Then, we execute the model with the perturbated instances and record its predicted class label. If the predicted class label for any of the perturbated instances differs from the predicted class label of the original test instance, then it is considered a fairness violation. Otherwise, the model is considered to exhibit fair behavior.

2.3.3. Example

We illustrate our approach using an example. Assume that an ML classifier is used to predict the admission decisions for prospective candidates. The ML classifier is trained using a dataset that consists of 5 attributes, namely Gender, Race, State, Final Score, and Decision. Gender, Race, and State are categorical attributes with 3, 4, and 10 unique values, respectively. Final Score is a numerical attribute. Decision is a class label with two values – Accept, Reject. Based on domain knowledge, we identify Gender and Race as protected attributes among the four attributes.

We begin the first phase by generating an IPM. We identify the four attributes (excluding the class label attribute) Gender, Race, State, Final Score as parameters. For the three categorical attributes (Gender, Race, State), their unique values are identified as parameter values. We discretize Final Score into eight bins, and they (bins) are identified as its parameter values. Next, to identify constraints, we use the Apriori algorithm. The algorithm identifies two association rules by analyzing the training dataset \{State = CA \Rightarrow Final Score \geq 40, State = GA \Rightarrow Final Score <
We map these association rules as constraints in our IPM. Next, we generate 80 abstract t-way test cases \((t=2)\) followed by deriving the concrete test cases.

Using constraints allows us to generate t-way tests that correspond to more realistic test instances. That is, in the generated t-way tests, if the state is CA, then the final score will always be greater than or equal to 40. Similarly, if the state is GA, then the final score will always be less than 95.

In the second phase, we use a counterfactual XAI tool to identify if there exists a counterfactual for any test instance from the t-way test set. We provide the ML classifier, dataset, test instance, constraints and a list of protected attributes \((\text{Gender, Race})\) as an input to the counterfactual tool. Recall that our goal is to identify if changing the protected attributes results in a different outcome. The tool successfully identifies a counterfactual for one of the test instances from the concrete test set: \((\text{male, white, CA, 92})\). The ML classifier predicts Admit for the test instance \((\text{original prediction})\). For one of the perturbated instances: \((\text{female, black, CA, 92})\), we observe that the model predicts Reject. As the counterfactual indicates, modifying the protected attribute(s) results in a different outcome, suggesting a fairness violation of the ML classifier.

2.4. EXPERIMENTS

In this section, we first present the design of our experiments, including the research question, the datasets, the subject models, discretization techniques, the counterfactual generation tool, and the metrics used to identify fairness violations. Next, we present and discuss the results of our experiments. Finally, the threats to validity are discussed.
2.4.1. Research Questions

Our experiments are designed to answer the following research question:

- How effective is our combinatorial testing-based approach in fairness testing of ML models?

2.4.2. Datasets

In our experiments, we use three datasets, namely the Adult Income [31], German-Credit [32], and COMPAS [25] datasets, that are among the most widely used in the fairness testing domain [1][8][10][13]. Bellamy et al. presented IBM AI Fairness 360, a software library to detect and mitigate bias in AI models [5]. They made their data wrangling scripts publicly accessible. We refer to their scripts and preprocess the subject datasets [30].

- The German credit dataset is used to classify individuals as either good or bad credit risk based on their personal and financial information. The dataset consists of 1000 instances and 21 attributes (8 numerical + 13 categorical). Similar to AI Fairness 360, we replace the Status attribute with a new attribute Sex. The Sex attribute has two possible values – Male and Female [5][30]. Among the 20 attributes (excluding the class label), Sex and Age are treated as protected attributes.

- The Adult dataset contains census information of individuals that is used to determine if an individual can earn more than $50,000 per year. The dataset has 13 attributes with five numerical and eight categorical attributes. The Adult dataset has two protected attributes: Sex and Race. Similar to AI Fairness 360 [5][30], we preprocessed the dataset and dropped the fnl_weight attribute from the dataset.

- The Correctional Offender Management Profiling for Alternative Sanctions (COMPAS) dataset consists of information of defendants such as criminal history, prison time, demographics, and it is used to predict the likelihood of a defendant to re-offend (recidivism). The dataset contains
74 records with four categorical and five numerical attributes. Sex and Race are treated as protected attributes. Note that the original COMPAS dataset had 52 attributes. We preprocessed the dataset as per AI Fairness 360 [5][30] and retain ten attributes.

2.4.3. Subject Models

We evaluate our approach using four ML classifiers. Three (out of four) ML classifiers are implemented using classical ML algorithms, namely Logistic Regression (LR), Random Forest (RF), and Support Vector Machines (SVM) that are commonly used in fairness testing studies [1][10][13][21]. In addition to this, we also use a fourth ML classifier, a simple Deep Neural Network (DNN) model with two hidden layers, in our experiments. Thus, for each dataset, we train and build four ML classifiers. Overall, we use twelve 12 ML classifiers (subject models) in our experiments. Similar to earlier studies [13], we train the ML classifiers using their default configuration, provided by the sci-kit learn library [24].

2.4.4. Discretization

We use a decision-tree (entropy-based) algorithm to discretize numeric attributes [24][27]. The user can specify the depth of the decision tree. A decision tree of depth n will generate a maximum of 2n bins. Note that the depth of a decision tree could affect the size of the t-way test cases generated using our approach. A higher value (tree depth) can result in a significantly large number of t-way test cases, thus making it computationally expensive to identify fairness violations in ML models. As a trade-off, similar to LIME, a state-of-the-art XAI tool [17][26], in our experiments, we limit the depth of the decision tree to a value of 3. Thus, a numeric attribute can be discretized into a maximum of 23 bins (8 bins). That is, a discretized numeric attribute will have at most eight bins.
In our experiments, we identify representative values for numerical attributes as follows: First, we calculate the total number of unique values for each numerical attribute. If the number of unique values is less than or equal to 8, we map the unique values as the representative values for the attribute. Otherwise, we use a decision tree algorithm with its default configuration value (not explicitly specifying the depth of the tree) and identify the representative values until either of the two conditions is satisfied. (1) the number of bins identified by the algorithm is less than or equal to 8; or (2) the number of bins is greater than 8. In the first case, we map the identified bins as the representative values for the attribute. In the second case, we re-execute the decision tree algorithm by setting the depth (of the tree) to 3 and discretizing the numerical attribute into eight bins. These bins are identified as representative values.

2.4.5. CONSTRAINTS

In our experiments, we use Waikato Environment for Knowledge Analysis (WEKA), an open-source ML workbench tool, to identify the association rules from the training dataset. We preprocess the training dataset by converting all attributes to nominal datatype as required by WEKA.

Next, we provide the modified dataset (input) to WEKA and execute the Apriori algorithm with its default configuration values. The Apriori algorithm identifies a list of the top 10 association rules from the dataset. These association rules are used as constraints in the t-way test generation.

Recall that if any constraints involve protected attributes, then they will be used in counterfactual generation. However, the constraints derived for all three datasets do not contain any protected attributes. Thus, no constraints are used in counterfactual generation.
2.4.6. Test Generation

Using ACTS, a combinatorial test generation tool [9][35], we generate t-way (t=2) abstract tests, which are then converted into concrete t-way tests.

2.4.7. Counterfactual Generation

We use DiCE, a state-of-the-art XAI tool, to identify a counterfactual by modifying the values of protected attributes while retaining the values of the non-protected attributes [22]. The DiCE tool allows a user to generate a counterfactual based on specific attribute(s) [22]. Therefore, we provide a pre-trained model, the concrete t-way test instance, and protected attribute(s) as input to the DiCE tool. If successful, DiCE generates a test instance that is almost identical to the original instance but differs by the value of its protected attribute. In other words, DiCE identifies a scenario where the model predicts a different outcome on changing the protected attribute while retaining the value of all other attributes. This is considered as a fairness violation exhibited by the model.

2.4.8. Metrics

We assess our approach's effectiveness in terms of the number of fairness violations revealed by a t-way test set. The more fairness violations identified by a t-way test set, the more effective the t-way test set is considered.

2.4.9. Results and Discussion

We present and discuss our experimental results. The source code, data, and/or artifacts have been made available at [23].
Table 2-1 presents the results of fairness violations of ML models identified using t-way test sets. The column headers in Table 2-1 are self-explanatory.

Recall that we identify fairness violations by perturbing each test instance using a counterfactual approach. Given a test case, if we successfully identify a counterfactual (a perturbation of the test case whose output differs from the original prediction), we consider that the test case resulted in a fairness violation.

**Adult Income:** For the Adult Income dataset, our approach generates 676 t-way tests ($t=2$). The results indicate that a substantial number of t-way test cases result in a fairness violation. For the LR-based model, out of 58 tests, we observe that 27 tests result in a fairness violation on modifying either one of the two protected attributes: 16 tests cases result in a fairness violation on modifying attribute Race whereas 11 test cases result in a fairness violation on modifying attribute Sex. The remaining 31 test cases (out of 58) result in a fairness violation on modifying both of the protected attributes. In the case of the RF-based model, ten tests result in a fairness violation on modifying the Race attribute, and one test results in a fairness violation on changing the Sex attribute. Fourteen tests result in a fairness violation on modifying the value of both the protected

<table>
<thead>
<tr>
<th>Datasets</th>
<th>Number of t-Way tests</th>
<th>Protected Attributes</th>
<th>Number of fairness violations</th>
</tr>
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<tbody>
<tr>
<td>Adult Income</td>
<td>676</td>
<td>Sex, Race</td>
<td>58</td>
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<td>German Credit</td>
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<td>Sex, Age</td>
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<tr>
<td>COMPAS</td>
<td>64</td>
<td>Sex, Race</td>
<td>27</td>
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Datasets | Number of t-Way tests | Protected Attributes | Logistic Regression (LR) | Random Forest (RF) | Support Vector Machines (SVM) | Deep Neural Network (DNN) |
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<tbody>
<tr>
<td>Adult Income</td>
<td>676</td>
<td>Sex, Race</td>
<td>58</td>
<td>25</td>
<td>23</td>
<td>11</td>
</tr>
<tr>
<td>German Credit</td>
<td>81</td>
<td>Sex, Age</td>
<td>5</td>
<td>10</td>
<td>9</td>
<td>26</td>
</tr>
<tr>
<td>COMPAS</td>
<td>64</td>
<td>Sex, Race</td>
<td>27</td>
<td>37</td>
<td>24</td>
<td>4</td>
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attributes. For the SVM-based model, out of 23 tests, we observe that eight tests result in a fairness violation on modifying either one of the two protected attributes (Race = 5, Sex = 3), and 16 tests result in a fairness violation modifying both protected attributes.

**German Credit:** Based on the IPM derived from the German Credit Dataset, we generate 81 t-way test cases. The results indicate that t-way tests can detect fairness violations among models trained using different ML algorithms. We observe that across three ML models, t-way tests result in a fairness violation on modifying both the protected attributes (Sex and Age).

**COMPAS dataset:** Out of the 64 t-way test cases generated using our approach, for the RF-based ML model, more than 50% of tests (37 tests) result in a fairness violation. Among these 37 tests, 19 tests result in a fairness violation on modifying the Race attribute; three tests result in a fairness violation on modifying the Sex attribute. The remaining 15 (out of 37) tests result in a fairness violation on modifying both the protected attributes. For the LR-based ML model, 11 tests result in a fairness violation on modifying the Race attribute, one test results in a fairness violation on modifying the Sex attribute, and 15 tests result in a fairness violation on modifying both the protected attributes. In the case of the SVM-based ML model, 18 tests result in a fairness violation on modifying both protected attributes, while the remaining six tests result in a fairness violation on modifying either one of the two protected attributes (Race = 5, Sex = 1).

For DNN based classifiers, we noticed DiCE takes longer to identify a counterfactual. For example, to identify a counterfactual for a pre-trained DNN model (trained with the Adult Income dataset), on average, DiCE takes 2 minutes per test case. So, it will take \((676*2)/60= 22.5\) hours to complete the execution. Therefore, for DNN models, we follow a brute-force approach as a workaround. That is, for each test case, using a script, we generate and execute all possible
perturbations and identify if there exists a counterfactual by comparing the output with the original prediction.

Our results indicate that for the Adult Income dataset (DNN model), nine tests result in a fairness violation on modifying either of the protected attributes (Race = 4, Sex = 5), while the remaining two tests result in a fairness violation on modifying both the protected attributes. For the German Credit dataset (DNN model), twelve tests result in a fairness violation on modifying both the protected attributes. Additionally, fourteen tests resulted in a fairness violation on modifying either Age (4 instances) or Sex (10 instances) attributes. For the COMPAS dataset (DNN model), we observed two tests result in a fairness violation on modifying both of the protected attributes, while the other two tests result in a fairness violation on modifying either of the two protected attributes. Due to space limitations, we only discuss the number of t-way tests that result in a fairness violation. A comprehensive result analysis with additional information such as the original value vs. modified value of a protected attribute original vs. modified prediction of a classifier is made available at [23].

Overall, the results suggest the following major points:

(1) The t-way test sets generated based on the three subject datasets can identify fairness violations in pre-trained ML models.

(2) The results also indicate that the proposed approach can successfully detect fairness violations across different ML model architectures. Furthermore, on executing a t-way set across ML models (LR, RF, SVM, and DNN), we observe in the case of the Adult Income dataset and German Credit dataset, there is no overlap among the t-way test cases that result in a fairness violation across all four ML models. In the case of the COMPAS dataset, out of t-way tests that result in fairness violations, there are only four tests that are common among all ML models. This
suggests a minimal overlap among the t-way test cases (from the test set) that resulted in a fairness violation across different ML models. That is, not the same set of t-way test cases triggers a fairness violation across ML models. We believe this indicates that t-way tests are effective in identifying biases introduced by both the training dataset and the learning algorithm.

(3) The results also indicate that the proposed approach can identify fairness violations with a relatively small number of test cases compared to the existing work [1]. We plan to perform a detailed comparison as part of future work.

2.4.10. Threats to Validity

Threats to external validity occur when the results from our experiments could not be generalized to other subjects. The datasets and ML models used in our study have been used in other studies in the fairness testing domain [1][10][13][21]. We use four different algorithms (model architectures) to train ML models. This reduces the risk of a lack of representatives in the model architecture used in our study.

Threats to internal validity are factors that may be responsible for the experimental results without our knowledge. To mitigate the risk of human errors, we tried to automate the experimental procedure as much as possible. In particular, all the steps are automated except the identification and mapping of constraints. Further, we have performed manual verification whenever we observe any surprising results. For example, on executing the t-way test cases (676 tests) generated for the Adult Income dataset, 23 tests and 25 tests resulted in a fairness violation for SVM and RF models, respectively. However, for the LR model, we observed 58 tests (times 2, compared to SVM and RF) that resulted in a fairness violation. In such a scenario, we manually verified the counterfactuals identified by DiCE.
2.5. RELATED WORK

This section discusses existing work on fairness testing that is closely related to our work. First, we discuss existing work that focuses on testing individual discriminations of ML models. Udeshi et al. proposed Aqueitas, a testing technique to discover discriminatory inputs that result in an individual fairness violation [33]. In phase 1, they identify a set of discriminatory inputs from a test set generated by randomly sampling the input space (global search). In phase 2, they identify additional discriminatory inputs by changing the values of the non-protected attributes for the discriminatory instance found in the global search. Furthermore, they demonstrate that retraining the model with portions of the discriminatory inputs improves its performance. Our work is similar to theirs in generating test instances to identify individual fairness violations. However, our work differs in the following two ways: 1) Aqueitas generates test instances using a random testing approach, whereas we use a combinatorial approach to generate test instances. 2) Their approach identifies discriminatory instances from the random test set, and they (discriminatory instances) are further perturbated by searching the neighborhood. In contrast, we identify discriminatory instances using a counterfactual approach by perturbing the protected attributes defined by the user.

Galhotra et al. proposed THEMIS, a causality-based technique to measure discrimination in software [10]. They use a random test generation technique to identify discriminatory test instances. In contrast, we use combinatorial testing, a systematic test generation technique to generate test cases and identify fairness violations.

Zhang et al. proposed an approach that generates discriminatory test instances for Deep Neural Network (DNNs)-based models [38]. Their work adopts a gradient descent and clustering-based approach to identify individual discriminatory instances. In contrast, we use a combinatorial
testing-based approach to generate test instances. Their approach focuses on testing individual fairness violations in DNN models, whereas our approach is model agnostic and can be used to test ML models trained using different architectures.

Aggarwal et al. proposed an approach to generate test inputs and identify individual discriminations in ML models [1]. Their approach uses a combination of symbolic execution and LIME, a local explainer tool to generate test instances and identify individual discriminations. Once they identify a test instance that identifies individual discrimination, they perturb the test instance further by modifying its non-protected attributes and generating additional test instances to test the ML model for fairness violations. Similar to their work, the goal of our approach is to generate test instances and identify individual discriminations in an ML model. However, our work differs in the following ways: 1) We generate test instances using a combinatorial testing approach. 2) Our approach identifies individual discrimination by perturbating a test instance using a counterfactual approach. 3) We do not perturb discriminatory inputs further.

Next, we discuss the existing literature on applying combinatorial testing for fairness testing. Morales et al. proposed Coverage-Guided Fairness Testing (CGFT) that aims to improve the performance of Aequitas, a testing technique that identifies individual discriminations in a two-step test generation process, namely global search and local search. CGFT aims to leverage combinatorial testing by replacing the random test generation process in the global search phase of Aequitas with a t-way test generation approach to reduce the execution cost [21]. Our work is similar to theirs in using combinatorial testing to generate t-way test cases that are later used to identify individual discrimination. However, our work differs in the following way. CGFT uses an algorithm to control the number of t-way test cases generated. Hence, the test set generated using their algorithm is of mixed strengths. In contrast, all test cases generated in our approach belong
to the same test strength (t=2). Furthermore, they do not use constraints in their test generation process. In contrast, we derive (from the training dataset) and use constraints in our test generation and perturbation process. We believe using constraints enables our approach to generate more realistic t-way test cases to detect discriminations compared to their approach.

We also note that there is a significant number of existing studies in the literature, and we refer the reader to [19][37] for a comprehensive report on existing work on fairness testing for machine learning systems.

### 2.6. Conclusion and Future Work

In this paper, we presented a combinatorial approach to identify individual fairness violations in pre-trained ML models. Our approach consists of two phases. In the first phase, based on the training dataset, we develop an IPM, derive constraints and generate t-way test instances. In the second phase, we identify fairness violations by perturbing the t-way instances using a counterfactual approach. The key idea is to generate counterfactuals by modifying the protected attribute(s) while retaining the value of non-protected attributes of the t-way test instance. Using constraints that are discovered from the training dataset helps us to generate valid t-way test sets (Phase 1) and valid counterfactuals (Phase 2), which in turn improve the validity of fairness violations identified by our approach. We performed an experimental evaluation of our approach using twelve ML classifiers (4 ML classifiers * 3 datasets). Our results suggest that our approach can successfully identify fairness violations in ML models. Furthermore, our approach identifies a substantial number of fairness violations for different ML model classifiers. This suggests t-way tests are effective in identifying biases introduced by both the training dataset and the learning algorithm.
There are a few directions to continue our work. First, in our current approach, for a categorical attribute, we identify and map all its unique values as representative values in IPM. A significantly large number of t-way tests cases will be generated if the training dataset consists of one or more categorical attributes with many unique values. We plan to investigate how to adapt the entropy-based discretization technique for categorical attributes. Second, after we detect fairness violations from a model, the next step is to identify the root cause and modify and/or retrain the model to remove those violations. We plan to explore how to leverage the t-way instances that identified fairness violations for model debugging and for model modification and retraining activities. Third, we plan to extend this approach to identify group discriminations in pre-trained ML models. Finally, we plan to conduct more empirical studies to further evaluate the effectiveness of our approach. In particular, we plan to compare the effectiveness of our approach to existing approaches such as the symbolic generation (SG) approach [1] and the CGFT approach [21].

2.7. ACKNOWLEDGEMENT

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Disclaimer: Certain software products are identified in this document. Such identification does not imply recommendation by the NIST, nor does it imply that the products identified are necessarily the best available for the purpose.
2.8. REFERENCES


CHAPTER 3. CONCLUSION

This thesis presented a combinatorial testing-based approach to test individual fairness violations of pre-trained ML models. On receiving the training dataset as input, in phase 1, we design the input parameter model, derive constraints, and generate t-way tests. Next, in phase 2, we identify fairness violations by generating perturbations of the t-way tests using a counterfactual approach. That is, on executing the ML model with the original test instance and the perturbated instance(s), if the pre-trained ML model generates different outcomes (predictions), then the model is considered to exhibit an individual fairness violation. The result from our experimental evaluation showcases that the approach is model-agnostic, and the approach can successfully identify fairness violations in pre-trained ML models. The result further indicates that the approach can identify discriminative behavior (bias) introduced by the training dataset and the learning algorithm. Furthermore, in our approach, we generate t-way tests and counterfactuals such that they satisfy the constraints identified from the training dataset. This improves the validity of the fairness violations identified using our approach. This thesis has demonstrated that combinatorial testing can be successfully adopted to perform fairness testing in ML models.

The approach presented in this thesis can be further extended in several directions. 1). Although the approach in this thesis has successfully demonstrated that the combinatorial testing-based approach can identify fairness violations, it has certain limitations in terms of identifying representative values for String attributes. In our current approach, during input parameter modeling, in the case of a string attribute, we map all the unique values as its representative values. This could impact the performance of our approach in the case of a string attribute having a significantly larger number of unique values (>10). Future studies should explore possible ways to identify truly representative values for the string attributes (like entropy-based
discretization for integer datatypes). 2). A natural progression of this work is to extend the approach to identify group fairness violations in pre-trained ML models. 3). Further work is needed to understand the effectiveness of our approach compared to the other existing work (fairness testing approaches) from the literature. 4). The ML models used in our evaluation are trained using the default hyperparameters. Future studies should explore the use of fine-tuned ML models (with higher accuracy), and more research is needed to understand the fairness-accuracy tradeoff in testing ML models. 5). Another possible area of future research would be to investigate leveraging the t-way test instances that detected the fairness violations in model retraining activities.
BIOGRAPHICAL STATEMENT

Ankita Ramjibhai Patel received her Bachelor of Technology in Information Technology in 2008 from Nirma University, Ahmedabad, India. She worked in the industry for 10 years in various roles including Software Developer, Project Lead, and Project Manager. She started her graduate studies in computer science at The University of Texas at Arlington in 2020 and joined Dr. Jeff Lei’s research group in Spring 2021. Her research interest is in the area of Software Engineering for Artificial Intelligence systems, focusing on the test and evaluation of AI-based software systems.