# Information-Theoretic Testing and Debugging of Fairness Defects in Deep Neural Networks

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Abstract—The deep feedforward neural networks (DNNs) are increasingly deployed in socioeconomic critical decision support software systems. DNNs are exceptionally good at finding minimal, sufficient statistical patterns within their training data. Consequently, DNNs may learn to encode decisions—amplifying existing biases or introducing new ones-that may disadvantage protected individuals/groups and may stand to violate legal protections. While the existing search based software testing approaches have been effective in discovering fairness defects, they do not supplement these defects with debugging aids-such as severity and causal explanations—crucial to help developers triage and decide on the next course of action. Can we measure the severity of fairness defects in DNNs? Are these defects symptomatic of improper training or they merely reflect biases present in the training data? To answer such questions, we present DAIKE: an information-theoretic testing and debugging framework to discover and localize fairness defects in DNNs.

The key goal of DAIKE is to assist software developers in triaging fairness defects by ordering them by their severity. Towards this goal, we quantify fairness in terms of protected information (in bits) used in decision making. A quantitative view of fairness defects not only helps in ordering these defects, our empirical evaluation shows that it improves the search efficiency due to resulting smoothness of the search space. Guided by the quantitative fairness, we present a causal debugging framework to localize inadequately trained layers and neurons responsible for fairness defects. Our experiments over ten DNNs, developed for socially critical tasks, show that DAIKE efficiently characterizes the amounts of discrimination, effectively generates discriminatory instances (vis-a-vis the state-of-the-art techniques), and localizes layers/neurons with significant biases.

### I. INTRODUCTION

AI-assisted software solutions—increasingly implemented as deep neural networks [1] (DNNs)-have made substantial inroads into critical software infrastructure where they routinely assist in socio-economic and legal-critical decision making [2]. Instances of such AI-assisted software include software deciding on recidivism, software predicting benefit eligibility, and software deciding whether to audit a given taxpayer. The DNN-based software development, driven by the principle of information bottleneck [3], involves a delicate balancing act between over-fitting and detecting useful, parsimonious patterns. It is, therefore, not a surprise that such solutions often encode and amplify pre-exisiting biases in the training data. What's worse, improper training may even introduce biases not present in the training data or irrelevant to the decision making. The resulting fairness defects may not only disadvantage protected groups [4], [5], [6], [7], [8], but may stand to violate statutory requirements [9], [10].

This paper presents DAIKE (pronounced as  $\Delta(\kappa\eta)$ ), an information-theoretic testing and debugging framework for fairness defects in deep neural networks.

Quantifying Fairness. Concentrated efforts from the software engineering and the machine learning communities have produced a number of successful fairness testing frameworks [11], [12], [13], [14]. These frameworks characterize various notions of fairness—such as group fairness [15] (decision outcome for various protected groups must be similar) and individual fairness [16] (individuals differing only on protected attributes must receive similar outcome)—and employ search-based testing to discover fairness defects. While a binary classification of fairness is helpful in discovering defects, developers may require further insights into the nature of these defects to decide on the potential "bug fix". Are some defects more severe than others? Whether these defects stem from biases present in the training data, or they are artifacts of an inadequate training? Is it possible to find an alternative explanation of the training data that does not use protected information?

Individual discrimination is a well-studied [17], [12], [18], [19] causal notion of fairness that defines a function being discriminant towards an individual (input) if there exists another individual (potentially counterfactual), differing only in the protected features, receives a more favorable outcome. We present a quantitative generalization of this notion as the quantitative individual discrimination (QID). We define QID as the amount of protected information—characterized by entropy metrics such as Shannon entropy and min entropy—used in deriving an outcome. Observe that a zero value for the QID measure implies the absence of the individual discrimination. The QID measure allows us to order various discriminating inputs in terms of their severity, as in an application that is not supposed to base its decisions on protected information, inputs with higher dependence indicate a more severe violation. Our first research question (**RQ1**) concerns the usefulness of QID measure in finding inputs with different severity.

**Search-Based Testing.** Search-based software testing provide scalable optimization algorithms to automate discovery of software bugs. In the context of fairness defects, the search of such bugs involves finding twin inputs exhibiting discriminatory instances. The state-of-the-art algorithms for fairness testing [20], [18], [19] explore the input space governed by a binarized feedback, resulting in a discontinuous search domain. On the other hand, QID-based search algorithms can benefit a smooth (quantitative) feedback during the optimiza-

tion, resulting in a more guided search. Our next research question (**RQ2**) is to investigate whether this theoretical promise materializes in practice in terms of discovering richer discriminating instances than using classic notions of discrimination.

Causal Explanations. While the discriminating instances (ordered by their severity) provide a clear evidence of fairness defects in the DNN, it is unclear whether these defects are inherent in the training data, or whether they are artifacts of the training process. Inspired by the AUDEE framework [21] for bug localization in deep learning models, we develop a layer and neuron localization framework for fairness defects. If the cause of the defects is found to be at the input layer, it is indicative of discrimination existing in the training data. On the other hand, if we localize the cause of the defect to some internal layer, we wish to further prod the DNN to extract quantitative information about neurons and their counterfactual parameters that can mitigate the defect while maintaining the accuracy. This debugging activity informed our next research question (RQ3): is it possible to identify a subset of neurons and their causal effects on QID to guide a mitigation without affecting accuracy?

Experiments. DAIKE implements a search algorithm (Algorithm 1) to discover inputs that maximize QID and a causal debugging algorithm (Algorithm 2) to localize layers and neurons that causally affect the amounts of QID. Using 10 socio-critical DNNs from the literature of algorithmic fairness, we show that DAIKE finds inputs that can use up to 76% of protected information in the decision making; outperforms three state-of-the-art techniques [20], [18], [19] in generating discriminatory instances; and localizes neurons that guides a simple mitigation strategy to reduce QID up to 88.8% with at most 5% loss of accuracy. The key contributions of this paper are listed next.

- 1) **Quantitative Individual Discrimination.** We introduce an information-theoretic characterization of discrimination, dubbed quantitative individual discrimination (QID), based on Shannon entropy and min Entropy.
- Search-based Testing. We present a search-based algorithm to discover circumstances under which the DNNs exhibit severe discrimination.
- 3) **Causal Debugging.** We develop a causal fairness debugging based on the language of interventions to localize the root cause of the fairness defects.
- 4) Experimental Evaluation. Extensive experiments over different datasets and DNN models that show feasibility, usefulness, and scalability (viz-a-viz state-of-the-art). Our framework can handle multiple protected attributes and can easily be adapted for regression tasks.

### II. PRELIMINARIES

**Fairness Terminology.** We consider decision support systems as *binary classifiers* where a prediction label is *favorable* if it gives a desirable outcome to an input (individual). These favorable predictions may include higher income estimations for loan, low risk of re-offending in parole assessments, and

high risk of failing a class. Each dataset consists of a number of *attributes* (such as income, experiences, prior arrests, sex, and race) and a set of *instances* that describe the value of attributes for each individual. According to ethical and legal requirements, data-driven software should not *discriminate* on the basis of an individual's *protected attributes* such as sex, race, age, disability, colour, creed, national origin, religion, genetic information, marital status, and sexual orientation.

There are several well-established fairness definitions. Fairness through unawareness (FTU) [16] requires removing protected attributes during training. However, FTU may provide inadequate support since protected attributes can influence the prediction via a non-protected collider attribute (e.g., race and ZIP code). Fairness through awareness (FTA) [16] is an individual fairness notion that requires that two individuals with similar non-protected attributes are treated equally. In contrast, group fairness requires that the statistics of ML outcomes for different protected groups to be similar [15] using metrics such as equal opportunity difference (EOD), which is the difference between the true positive rates (TPR) of two protected groups.

**Individual Discrimination.** Causal discrimination, first studied in THEMIS [22], measures the difference between two subgroups via *counterfactual* queries. It samples individuals with the protected attributes set to A and compares the outcome to a counterfactual scenario where the protected attributes is set to B. Individual discrimination (ID) is a prevalent notion that adapts counterfactual queries to find an individual such that their counterfactual with a different protected attributes receives more favorable outcome. This fairness notion is used by the state-of-the-art fairness testing to generate fairness defects [23], [20], [18], [19].

Information-Theoretic Concepts. The notion of Rényi entropy [24],  $H_{\alpha}(X)$  quantifies the uncertainty (randomness) of a system responding to inputs X. In particular, Shannon entropy  $(\alpha=1)$  and min-entropy  $(\alpha=\infty)$  are two important subclasses of Rényi entropy. Shannon entropy  $(H_1)$  measures the expected amounts of uncertainty over finitely many events whereas min entropy  $(H_{\infty})$  measures the uncertainty over single maximum likelihood event.

Consider a deterministic system (like pre-trained DNN) with a finite set of responses and assume that the input X is distributed uniformly. Thus, the system induces an equivalence relation over the input set X such that two inputs are equivalent if their system outputs are approximately close, i.e.  $x{\sim}x'$  iff  $DNN(x) \approx_{\epsilon} DNN(x')$ . Let  $X_o$  denote the equivalence class of X with output o. Then, the remaining uncertainty after observing the output of DNN over X can be written as:

$$H_1(X|O) = \sum_{O=o} \frac{|X_o|}{|X|} \cdot \log_2(|X_o|)$$
 (Shannon entropy)

where |X| is the cardinality of X and  $|X_o|$  is the size of equivalence class of output o. Similarly, the min-entropy is

given as

$$H_{\infty}(X|O) = \log_2(\frac{|X|}{|O|})$$
 (min-entropy)

where |O| is the number of equivalence classes over X [25], [26]. Given that the initial entropy is equal to  $\log_2(|X|)$  for both entropies, the amount of information from X used by the system to make decisions are

$$I_1(X;O) = \log_2(|X|) - H_1(X|O)$$
, and  $I_{\infty}(X;O) = \log_2(|O|)$ ,

under Shannon- and min- entropies with  $I_1 \leq I_{\infty}$ .

**Quantitative Notion and Fairness.** Our approach differs from these state-of-the-art techniques [27], [23], [20], [18], [28], [19] in that it extends the individual discrimination notion with quantitative information flow that enables us to measure the amount of discrimination in the ML-based software systems. Given non-protected attributes and ML outcomes, the *Shannon entropy* measures the expected amount of individual discrimination over all possible responses varying protected classes, whereas, *min entropy* measures the amount over a single response from the maximum likelihood class.

**Example 1.** Consider a dataset with 16 different protected values—sex(2), race(2), and age(4)—distributed uniformly, and suppose that we have 4 individuals in the system. We perturb the protected attributes of these individuals to generate 16 counterfactuals and run them through the DNN to get their prediction scores. Suppose that the outputs have all 16 outputs in the same class for the first individual (absolutely fair) and have 16 classes of size one for the second individual ( absolutely discriminatory). For the third individual, let the outputs be in 4 classes with  $\{4, 4, 4, 4\}$  elements in each class (e.g., there is one output class per each age group). For the fourth individual, let us consider outputs to be in 5 classes with  $\{8,4,2,1,1\}$  elements in each class (e.g., if race=1 then the output is class 1; else, if sex=1 then the output is 2; else if  $age=\{1,2\}$  then the output is 3; else there is one output class for each age= $\{3,4\}$ ).

We work with the following notions of discrimination.

- *Individual Notion*. The individual discrimination used by the state-of-the-art techniques can only distinguish between the first individual and the rest, but they cannot distinguish among individuals two to four. In fact, these techniques generate tens of thousands of individual discriminatory instances in a short amount of time [20], [18], [19]. However, they fail to prioritize test cases for mitigation and cannot characterize the amounts of discrimination (i.e., their severity).
- Shannon Entropy. Using the Shannon entropy, we have the initial fairness to be 4.0 bits, a maximum possible discrimination. The remaining fairness of DNN are 4.0, 0.0, 2.0 and 2.125, for the first to fourth individuals, respectively. The discrimination is the difference between the initial and remaining fairness, which are 0.0, 4.0, 2.0

- and 1.875 for the first to fourth individuals, respectively. It is important to note that beyond the two extreme cases, Shannon entropy deems perturbations to the third individual (rather than the fourth) create a higher amount of discrimination.
- Min Entropy. The initial fairness via min entropy is also 4 bits. The conditional min entropy is  $\log \frac{16}{1} = 4.0$ ,  $\log \frac{16}{16} = 0.0$ ,  $\log \frac{16}{4} = 2.0$ , and  $\log \frac{16}{5} = 1.7$ , for the four individuals, respectively. The amounts of discrimination thus are 0.0, 4.0,  $\log 4 = 2.0$  and  $\log 5 = 2.3$ , respectively. Beyond the two extreme cases where both entropies agree, the min entropy deems perturbations to the fourth individual create a higher amount of discrimination. This is intuitive since the discrimination on the fourth case is more subtle, complex, and significant. Therefore, the ML software developers might prioritize those cases characterized by the min entropy.

### III. OVERVIEW

**DAIKE in Nutshell.** Figure 1 shows an overview of our framework DAIKE. It consists of two components: (1) an automatic test-generation mechanism based on search algorithms and (2) a debugging approach that localizes the neurons with significant impacts on fairness using a causal algorithm. First, DAIKE searches through the space of input dataset to find circumstances on the non-protected attributes under which the DNN-under-test shows a significant dependency on the protected attributes in making decisions. In doing so, it works in global and local phases. In the global phase, the search explores the input space to increase the amount of discrimination in each step of search. On the other hand, in the local phase it exploits the promising seeds from the global phase to generate as many discriminatory instances as possible.

The key elements of search is a threshold-based clustering algorithm used for computing both gradients and objective functions that provide a smooth feedback. The search characterizes the amounts of discrimination and returns a set of interesting inputs. Second, DAIKE uses those inputs to localize neurons with the largest causal effects on the amounts of discrimination. In doing so, it intervenes [29] over a set of suspicious neurons. For every neuron, our debugging approach forces the neurons to be active (n>0) and non-active (n=0) over the test cases as far as the functional accuracy of DNN remains in a valid range. Then, it computes the difference between the amounts of discrimination in these two cases to characterize the causal effects of the neuron on fairness.

DAIKE reports top k neurons that both have positive impacts (i.e., their activation reduces the amounts of discrimination) and negative impacts (i.e, their activation increases the amounts of discrimination). A potential mitigation strategy is to intervene to keep a small set of neurons activated (for the positive neurons) or deactivated (for the negative neurons).

**Test Cases.** Consider the *adult census income* [30] dataset with a pre-trained model with 6 layers [18] to overview DAIKE in practice. We ran DAIKE for 1 hours and obtain 230, 593

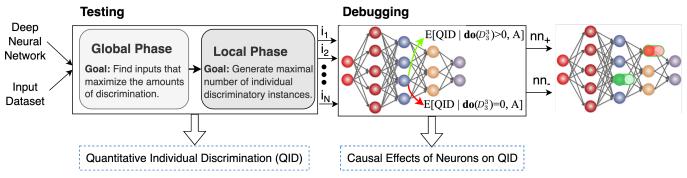


Fig. 1: Workflow of DAIKE.

test cases. It discovered 35.61 clusters from the initial of 13.54 clusters, and the amounts of discrimination are 4.05 and 2.64 bits for min entropy and Shannon entropy, respectively, out of maximum 5.3 bits of information. These numbers show averages over 10 runs. In average, we observe 85,311 instances of individual discriminatory; have 1 test case with maximum discrimination of 5.3 bits; and 17, 77, and 296 cases with 5.2, 5.17, and 5.13 bits of discrimination.

Localization and Mitigation. DAIKE uses the generated test cases to localize layers and neurons with a significant causal contribution to the discrimination. For the census dataset, it identifies the second layer as the layer with largest sensitivity to protected attributes. Among the neurons in this layer, DAIKE found that 24th neuron has the largest negative influence on fairness (the discrimination increased by 17.8% when it is activated vs. deactivated) and 13the neuron has the largest positive influence on fairness (the discrimination decreased by 13.8% when it is activated vs. deactivated). Following this localization, a simple mitigation strategy of activating or deactivating these neuron reduces the number of clusters by 12.5% with 1% accuracy loss.

Comparison to the State-of-the-art. We compare DAIKE to the state-of-the-art techniques in terms of generating individual discrimination (ID) (rather than the quantitative notion) per each protected attribute. Our goal is to evaluate whether the clustering-based search is effective in generating discriminatory instances. We run DAIKE and baseline for 15 minutes, and report average of results over 10 runs. The baseline includes AEQUITAS [20], ADF [18], and NEURONFAIR [19]. Considering sex as the protected attribute in the census dataset, DAIKE generated 61,246 instances whereas AE-QUITAS, ADF, and NEURONFAIR generated 9, 243, 16, 299, and 17,172 discriminatory instances, respectively. Overall, DAIKE generate  $9 \times$  more ID instances with  $3 \times$  more success rates. However, DAIKE is slower in finding the first ID instance in order of 2 seconds (in average), possibly due to extra clustering computations. Since the fairness notion is the same for all tools, we conjecture that the improvements are due to smooth search space via quantitative feedback.

### IV. PROBLEM STATEMENT

We consider DNN-based classifiers with the set of input variables A partitioned into protected set of variables Z (such as race, sex, and age) and non-protected variables X (such as profession, income, and education). We further assume the output to consist of t prediction classes.

**Definition IV.1** (DNN: Semantics). A deep neural network (DNN) encodes a function  $\mathcal{D}: X \times Z \to [0,1]^t$  where  $X = X_1 \times X_2 \cdots \times X_n$  is the set of non-protected input variables,  $Z = Z_1 \times Z_2 \cdots \times Z_r$  is the set of protected input variables, and the output is t-dimensional probabilistic vector corresponding to t prediction classes. The predicted label  $\mathcal{D}_{\ell}(x,z)$  of an input pair (x,z) is the index of the maximum score, i.e.  $\mathcal{D}_{\ell}(x,z) = \max_i \mathcal{D}_{\ell}(x,z)(i)$ . We assume that the set of protect input variables are finite domain, and we let m be the cardinality of the set of protected variables Z.

**Definition IV.2** (DNN: Syntax). A DNN  $\mathcal{D}$  is parameterized by the input dimension n+r, the output dimension t, the depth of hidden layers N, and the weights of its hidden layers  $W_1, W_2, \ldots, W_N$ . Our goal is to test and debug a pre-trained neural network with known parameters and weights. Let  $D_i$  be the output of layer i that implements an affine mapping from the output of previous layer  $D_{i-1}$  and its weights  $W_{i-1}$  for  $1 \le i \le N$  followed by

- 1) a fixed non-linear activation unit (e.g., ReLU defined as  $D_{i-1} \mapsto \max\{W_{i-1}.D_{i-1},0\}$ ) for  $1 \le i < N$ , or
- 2) a SoftMax function that maps scores to probabilities of each class for i = N.

Let  $D_i^j$  be the output of neuron j at layer i.

**Individual Discrimination.** We say a DNN  $\mathcal{D}$  is biased based on causal discrimination notion [17], [12], [18], [19] if

$$\exists z_1, z_2 \in Z, x \in X \text{ s.t. } \mathcal{D}_{\ell}(x, z_1) \neq \mathcal{D}_{\ell}(x, z_2),$$

for  $z_1 \neq z_2$  of protected inputs. Intuitively, the idea is to find an individual such that their counterfactual with different protected attributes such as race receives a different outcome.

**Quantitative Individual Discrimination.** In the setting of fairness testing, it is often desirable to quantify the *amounts* 

of bias for individuals. We define the notion quantitative individual discrimination (QID) based on the equivalence classes induced from the output of DNN over protected attributes. Formally,  $QID(Z, X = x) = \langle Z_1, \ldots, Z_k \rangle$  that is the quotient space of Z characterized by the DNN outputs under an individual with non-protected value x. Using this notion, we say a pair of protected values z, z' are in the same equivalence class i (i.e.,  $z, z' \in Z_i$ ) if and only if  $\mathcal{D}(z, x) \approx \mathcal{D}(z', x)$ .

Given that Z is uniformly distributed and  $\mathcal{D}$  is a deterministic function, we can quantify the QID notion for an individual (z,x) according to the Shannon and min entropy, respectively:

$$Q_1(Z, x) = \log_2(m) - \sum_{i=1}^k \frac{|QID_i(Z, x)|}{m} \cdot \log_2(|QID_i(Z, x)|)$$

$$Q_{\infty}(Z, x) = \log_2(m) - \log_2(\frac{m}{k}) = \log_2(k).$$

where m is the cardinality of Z,  $|QID_i(Z, x)|$  is the size of equivalence class i, and k is the number of equivalence classes.

**Debugging/Mitigating DNN for QID.** After characterizing the amounts of discrimination via QID, our next step is to localize a set of layers and neurons that causally effect the output of DNN to have k equivalence classes.

Causal logic [29] provides a firm foundation to reason about the causal relationships between variables. We consider a structural causal model (SCM) with exogenous variables U over the unobserved input factors, endogenous variables V over  $(X, Z, D_i^j)$ ; the set of functions  $\mathcal F$  assign variables in V using the DNN function  $\mathcal D$  and exogenous variables U. Using the SCM, we aim to estimate the average causal effect (ACE) [29] of neuron  $D_i^j$  on the QID.

A primary tool for performing such computation is called do logic [31]. We write  $\mathrm{do}(i,j,y)$  to indicate that the output of neuron j at layer i is intervened to stay y. In doing so, we remove the incoming edges to the neuron and force the output of neuron to take a pre-defined value y, but we are not required to control back-door variables due to the feedforward structure of DNN. Then, the ACE of neuron  $D_i^j$  on the quantitative individual discrimination with min entropy can be written as  $E[Q_{\infty}|\mathrm{do}(i,j,y),k,l]$ , which is the expected QID after intervening on the neuron given that the non-intervened DNN characterized k classes with an accuracy of k. Our goal is to find neurons with the largest causal effects on the QIDs, requiring that such interventions are faithful to the functionality of DNN.

**Definition IV.3** (Quantitative Fairness Testing and Debugging). Given a deep neural network model  $\mathcal{D}$  trained over a dataset A with protected  $(Z \subset A)$  and non-protected  $(X \subset A)$  attributes; the search problem is to find a single non-protected value  $x \in X$  such that the quantitative individual discrimination (QID), for a chosen measure  $Q_1$  or  $Q_{\infty}$ , is maximized over the m protected values  $\Sigma = \{z_1, \ldots, z_m\}$ . Given the inputs  $(\Sigma, x)$  characterizing the maximum QID, our debugging problem is to find a minimal subset of layers  $l \subset \{1, \ldots, N\}$  and neurons  $D_l^{(J)}$  for  $J \subseteq |W_l|$  such that the average causal effects of  $D_l^J$  on the QID are maximum.

# **Algorithm 1:** DAIKE (SEARCH)

Input: Dataset A, deep learning model  $\mathcal{D}$ , the loss function for the DNN J, protected attributes P, non-protected attributes NP, the number of partitions over the dataset p, the step size in global perturbation  $s_g$ , the step size in local perturbation  $s_l$ , the maximum number of global iterations  $N_g$ , the maximum number of local iterations  $N_l$ , the tolerance  $\epsilon$ , and time-out T.

Output: Num. Clusters and (local+Global) Test Cases.

```
1 A', cur \leftarrow \text{KMeans}(A, p), time()
2 while time() - cur < T do
         x, i, k, \delta \leftarrow \operatorname{pick}(A'), 0, 1, 0.0
         while i < N_q do
 4
               I_m, S_m \leftarrow \text{Generate\_Predict}(a, P)
 5
               X_k, \, \delta' \leftarrow \operatorname{Clust}(S_m, \, \epsilon)
 6
 7
               a, a' \leftarrow \text{Choose Pair Max}(X_k)
 8
               Gs \leftarrow (\nabla J(a), \nabla J(a'))
               d \leftarrow \text{choose common direct}(Gs, NP)
 9
               x' \leftarrow \text{perturb}(x, d, s_q)
10
              if (|X_k| > k) or (|X_k| = k \text{ and } \delta' > \delta) then
11
                    eval_f(x) {
12
                      \begin{array}{l} I_m', S_m' \leftarrow \texttt{Generate\_Predict}(x, \, P) \\ X_{k'} \leftarrow \texttt{Clust}(S_m', \, \epsilon) \end{array}
13
14
                      \Delta \leftarrow arg. \max(X_{k'}) - arg. \min(X_{k'})
15
                      local\_inps.add(x)
16
                      Return -\Delta
17
                    \texttt{step\_f} \leftarrow \lambda_x \; \texttt{perturb\_local}(x, s_l)
18
                    LBFGS(x, eval_f, step_f, N_l)
19
               global\_inps.add(a)
20
               k, x \leftarrow \max(k, |X_k|), x'
```

# V. APPROACH

22 return k,  $I = global\_inps \cup local\_inps$ 

Characterizing Quantitative Individual Discrimination. Given a DNN  $\mathcal D$  over a dataset A, our goal is to characterize the worst-case QID over all possible individuals. Since min entropy characterizes the amounts of discrimination from one prediction with  $Q_\infty(Z,x) \geq Q_1(Z,x)$ , it is a useful notion to prioritize the test cases. Therefore, we focus on  $Q_\infty$  and propose the following objective function:

$$\max_{x \in X} 2^{Q_{\infty}(Z,x)} + (1 - exp(-0.1 * \delta))$$

where  $2^{Q_{\infty}(Z,x)}=k$  and  $\delta$  is the maximum distance between equivalence classes, normalized with the exponential function to remain between 0 and 1. The term is used to break ties when two instances characterize the same number of classes, by preferring one with the highest distance. Overall, the goal is to find a single value of non-protected attribute x such that the neural network model  $\mathcal D$  predicts many distinguishable classes of outcomes when x is paired with m protected values. However, finding those inputs requires an exhaustive search in the exponential set of subsets of input space, and hence

is clearly intractable. We propose a gradient-guided search algorithm that aims to search the space of input variables (attributes) to maximize the number of equivalence classes and generate as many discrimination instances as possible.

**Search Approach.** Our search strategy consists of global and local phases as in some of the prior work [18], [28], [19]. The goal of the global phase is to find the maximum quantitative individual discrimination via gradient-guided clustering. The local phase uses the promising instances to generate a maximum number of discriminatory instances (ID).

Global Phase. Given a current instance x, the global stage first uses m different values from the space of protected attributes, while keeping the values of non-protected attributes the same. Then, it receives m prediction scores from the DNN and partitions them into k classes. We adapt a constrained-based clustering with  $\epsilon$  where two elements cannot be in the same cluster if their scores differ more than  $\epsilon$ . Now, the critical step is to perturb the current instance over a subset of non-protected attributes with a direction that will likely increase the number of clusters induced from the perturbed instance in the next step of global search.

In doing so, we first compute the gradients of DNN loss function for a pair of instances (say a,a') in the cluster with the maximum elements. The intuition is that we are more likely to split the largest cluster into 2 or more sub-clusters and increase the number of partitions in the next step. For the pair of samples, we use the non-protected attributes that have the same direction of gradients d since it shows the high sensitivity of loss function with respect to small changes on those common features of the pair. If we were to use gradients of opposite directions, we will neutralize the effects of gradients since we only perturb one instance over the non-protected attributes. Finally, we perturb the current sample x to generate x' using the direction d and step size  $s_q$ .

Local Phase. Once we detect an instance with more than 2 clusters, we enter a local phase where the goal is to generate as many discriminatory instances (ID) as possible. In our quantitative approach, we say that an unfavorable decision for an individual x is discriminatory if there is a counterfactual individual x' that received a favorable outcome. Similar to the state-of-the-art [20], [18], [19], we use non-linear optimizer that takes an initial instance x, a step function to generate the next instance around the neighborhood of the current instance, and an objective function that quantifies the discrimination of the current instance. Since our approach uses a continuous objective based on the characteristics of clusters, it enables us to guide the local search to generate discriminatory instances.

**Search Procedure.** Algorithm 1 sketches our search algorithm to quantify the amounts of bias. We first use the clustering (KMeans algorithm) to partition the data points into p groups (line 1). Next, we run the algorithm until the time-out T reaches where in each iteration we seed a sample randomly from one of the partitions p (line 2). Then, we proceed into global and local phases of search.

In the global phase, we first use the seed instance x and perturb the protected attributes P to generate m possible instances  $X_m$  with different protected values and the same non-protected ones. Then, we run  $X_m$  through the DNN model to get the probability scores  $S_m$  (line 5). Then, we cluster the scores  $S_m$  into k groups using the tolerance  $\epsilon$  (line 6). Afterward, we compute the gradients over two random instances (from the cluster with the largest size) and use a subset of non-protected features that have the largest number of agreements on the gradient directions. Then, we use those features and their directions to perturb the inputs x and generate the next instance x' (line 7-10). Then, we enter the local phase if the number of clusters or distance between are increased (line 11).

In the local phase, we use the general-purpose optimizer, known as LBFGS [32], which takes an initial seed x, an objective function, a step function, and the maximum number of local iterations  $N_l$ ; it returns the generated instances during the optimization (Line 12-19). In the objective function shown with eval\_f (Line 12-17), we generate m instances with the same non-protected values but different protected ones (Line 13). We generate prediction scores for those instances and cluster them with tolerance parameter  $\epsilon$  (line 14). Then, we compute the difference between the indices of two clusters with the smallest and largest scores (line 15). Finally, we record the generated sample and return the difference as the evaluation of optimizer at the current sample (line 16-17). The step function is shown with perturb local (Line 18) where it guides the optimizer to take one step in the input space. Our step function uses a random sample from a different cluster compared to the current sample. Then, it computes the normalized sum of gradients and perturbs it using the smallest gradients to remain in the neighborhood of the current sample.

**Debugging Approach.** Since it is computationally difficult to intervene over all possible neurons in a DNN, we first adapt a layer-localization technique from the literature of DL framework debugging [33], [21] where we detect a layer with the largest sensitivity to the protected attributes. Let  $D_i(z,x)$  be the output of layer i over protected value z and non-protected value x. Let  $\Delta_i(x): \mathbb{R}^{|D_i|} \times \mathbb{R}^{|D_i|} \to \mathbb{R}$  be the distance between the outputs of DNN at layer i as triggered by m different protected values and the same non-protected value x, and let  $\delta_i$  be the  $\max_x \Delta_i(x)$ . The rate of changes in the sensitivity of layer i (w.r.t protected attributes) is

$$\rho_i = \frac{\delta_i - \max_j \delta_j}{\max_i \delta_i + \epsilon}, \text{ with } 0 \le j < i$$

where  $\delta_0=0.0$  and  $\epsilon=10^{-7}$  (to avoid division-by-zero [33], [21]). Let  $l=\arg\max_i\rho_i$  be the layer index with the maximum rate of changes. Our next step is to localize neurons in the layer l that have significant positive or negative effects on fairness. Let  $V_l^j$  be the set of possible values for neuron j at later l (recorded during the layer localization). We are interested in computing the average causal effects when the neuron  $D_l^j$  is activated vs. deactivated, noting that

# Algorithm 2: DAIKE (DEBUGGING).

**Input:** Dataset  $A = (A_X, A_Z)$ ,  $\mathcal{D}$  with accuracy  $\mathcal{A}_{\mathcal{D}}$ , Test cases I, the distance function  $\Delta$ , the tolerance of layer localization  $\epsilon_1$ , the tolerance of accuracy loss  $\epsilon_2$ , and k top items.

of accuracy loss  $\epsilon_2$ , and k top items. **Output:** Layer Index, Negative, and Positive Neurons. /\* Layer Localization \*/

1  $\delta \leftarrow \lambda_l \max \sum_{x \in I} \Delta \left( D_l(z, x), D_l(z', x) \right)$ 2  $\delta[0], \delta_{max} \leftarrow 0.0, \lambda_i \max_{j < i} \delta[j]$ 3  $\rho \leftarrow \lambda_l \frac{\delta[i] - \delta_{max}[i]}{\delta_{max}[i] + \epsilon_1}$ 4  $l \leftarrow \arg \max_i \rho[i]$ /\* Neuron Localization \*/
5  $V_l \leftarrow \lambda_i$  stats( $D_l^i$ )
6  $v_l \leftarrow \lambda_i \lambda_j |\mathcal{A}_{\mathcal{D}} - \mathcal{A}_{\mathcal{D}} \leftarrow do(l,i,V_l[j])| \leq \epsilon_2$ 7  $ACD_l \leftarrow \lambda_i \mathbb{E} \left( k' | \operatorname{do}(l,j,v_l^j > 0) - \mathbb{E}(k'|\operatorname{do}(l,j,v_l^j = 0)) \right)$ 8 **return** l,  $top_k(\max ACD_l)$ ,  $top_k(\min ACD_l)$ .

such interventions might affect the functionality of DNN. Therefore, among a set of intervention values, we choose one activated value  $v_1 \in V_l^j > 0$  and one deactivated value  $v_2 \in V_l^j \approx 0$ , considering the functional accuracy of DNN within  $\epsilon$  of original accuracy A. Therefore, we define average causal difference (ACD) for a neuron  $D_l^j$  as:

$$\mathbb{E}[Q_{\infty} \mid \operatorname{do}(l, j, v_1 > 0), k, A] - \mathbb{E}[Q_{\infty} \mid \operatorname{do}(l, j, v_2 \approx 0), k, A],$$

where do notation is used to force the output of neuron j at layer l to a fix value v. We then return the neuron indices with the largest positive (aggravating discrimination) and smallest negative (mitigating discrimination). Let  $\hat{i}$  and  $\hat{j}$  be the layer and neuron with the largest positive ACD. One simple mitigation strategy is thus to deactivate the neuron  $D_l^{\hat{j}}$ , expecting to reduce QID by ACD/k percentage. Similarly, activating the neuron with the smallest negative ACD is expected to reduce QID by ACD/k percentage.

**Debugging Procedure.** Algorithm 2 shows the debugging aspect of DAIKE. Given a set of test cases from the search algorithm, we first use a notion of distance (e.g,  $\Delta = L_1$ ) to compute the difference between any pair of protected values z,z' w.r.t the outputs of layer  $l \in \{1,\ldots,N\}$  (line 1). Then, we compute the rate of changes (line 2-3) and return a layer l with the largest change (line 4). We compute various statistics on the output of every neuron i at layer l such as the minimum, maximum, average, average $\pm$ std. dev, average $\pm$ 2\*std. dev, etc (line 5). Among those values, we take the smallest and largest values such that the intervention on the neuron i at layer l has the minimal impacts on the accuracy of DNN (line 6). Finally, we compute the average causal difference (line 7) and return the indices of layer, neurons with large negative influence, and neurons with large positive influence.

# VI. EXPERIMENTS

**Datasets and DNN models.** We consider 10 socially critical datasets from the literature of algorithmic fairness. These

datasets and their properties are described in Table I. For the DNN model, we used the same architecture as the literature [18], [19], [28] and trained all datasets on a six-layers fully-connected neural network with  $\langle 64, 32, 16, 8, 4, 2 \rangle$  neurons. We used the same hyperparameters for the all training with num\_epochs, batch\_size, and learning\_rate are set to 1000, 128, and 0.01, respectively. The accuracy of trained models are reported in Table V.

**Technical Details.** We implemented DAIKE with TensorFlow v2.7.0 and scikit-learn v0.22.2. We run all the experiments on an Ubuntu 20.04.4 LTS OS sever with AMD Ryzen Threadripper PRO 3955WX 3.9GHz 16-cores X 32 CPU and two NVIDIA GeForce RTX 3090 GPUs. We choose the values 10, 1000, 0.025, 1, and 1 for max\_global, max\_local,  $\epsilon$ ,  $s_g$ , and  $s_l$  in Algorithm 1, respectively, and take the average of 10 multiple runs for all experiments. In Algorithm 2, we used  $L_1$ -norm,  $10^{-7}$ , 0.05, and 3 for  $\Delta$ ,  $\epsilon_1$ ,  $\epsilon_2$ , and k, respectively.

**Research Questions.** We seek to answer the following three questions using our experimental setup.

- **RQ1** Can DAIKE characterize the amounts of information from protected attributes used for the inferences?
- **RQ2** Is the the proposed search algorithm effective and efficient (vis-a-vis the state-of-the-art techniques) in generating individual discrimination instances?
- **RQ3** Can the proposed causal debugging guide us to localize and mitigate the amounts of discrimination?

### A. Characterizing QID via Search (RQ1)

An important goal is to characterize the amount of information from protected attributes used during the inference of DNN models. Table II shows the result of experiments to answer this research question. The left side of table shows the initial characteristics such as the number of protected values (m), the maximum possible amounts of discrimination  $(Q_I)$ based on  $\min(\epsilon^{-1}, m)$ , and the initial number of clusters found using samples from the dataset  $(K_I)$ . The right side of table shows the results after running our search for 1 hour. The column #I is the number of instances generated, and  $K_F$ is the maximum number of clusters discovered by DAIKE. The columns  $T_{K>1}$  and  $T_{K_F}$  are the time to find the first instance with more than one cluster and the time taken to find the maximum number of clusters from an input with initial clusters  $K_I$  (in seconds). The columns  $Q_{\infty}$  and  $Q_1$  are the quantitative individual discrimination based on min entropy and Shanon entropy, respectively. The columns  $\#I_{K_n^1}$ ,  $\#I_{K_n^2}$ , and  $\#I_{K_n^3}$  show the number of test cases with the highest, second-highest, and third-highest QIDs, respectively. Overall, the results show that DAIKE can find  $2.8\times$  more clusters (in average) from the initial characteristics within 1 minute of search. The DNN for Students dataset showed the largest increase in the number of clusters going from 1.9 to 10.9 in 14 seconds. DAIKE found that Census dataset has the largest amounts of OID where 4.05 out of 5.3 bits (76.4%)from protected variables are used to make decisions. The German dataset with 1.61 out of 4.0 bits (40.0%) showed the

TABLE I: Datasets used in our experiments.

Dataset	#Instances	#Features	Protected Groups	Num. Protected	Outcome Label			
Dataset	#Ilistances	#reatures	Name Size	Values (m)	Label 1	Label 0		
Adult			Sex 2					
Census	32, 561	13	Race 5	90	High Income	Low Income		
Income [30]			Age 9					
			Sex 2					
Compas [34]	7,214	12	Race 2	12	Did not Reoffend	Reoffend		
			Age 3					
German	600	20	Sex 2	16	Good Credit	Bad Credit		
Credit [35]			Age 8					
Default	13,636	23	Sex 2	12	Default	Not Default		
Credit [36]	,		Age 6					
Heart	297	13	Sex 2	14	Disease	Not Disease		
Health [37]			Age 7					
Bank Marketing [38]	45,211	16	Age 9	9	Subscriber			
Diabetes [39]	768	8	Age 9	9	Positive	Negative		
Students	1044	32	Sex 2	16	Pass	Not Pass		
Performance [40]	1011	02	Age 8	10	1 433	1101 1 455		
			Age 9					
MEPS15 [41]	15,830	137	Race 2	36	Utilized Benefits	Label 0  Low Income  Reoffend  Bad Credit  Not Default		
			Sex 2					
			Age 9					
MEPS16 [41]	15,675	137	Race 2	36	Utilized Benefits	Not Utilized Benefits		
			Sex 2					

least amounts of discrimination. For test-case prioritizing, the column  $\#I_{K_F^1}$  shows our approach to be useful in finding a small percentage of generated test cases with the worst-case discrimination. In 7/10 experiments, DAIKE found less than 50 test cases with severe discrimination (out of hundreds of thousands inputs).

Answer RQ1: The search algorithm is effective in characterizing the amounts of discrimination via QID. Within 1 hour, it increased the number of clusters by  $2.8 \times$  in average, and found instances that used up to 76% of protected information (4.05 out of 5.3 bits) to infer DNN decisions. DAIKE is found to be helpful in prioritizing the test cases.

### B. Individual Discriminatory Instances (RQ2)

In this section, we compare the efficiency and effectiveness of our search algorithm to the state-of-the-art techniques in searching individual discrimination (ID) instances (as defined in Section IV). Our baselines are AEQUITAS [20], ADF [18], and NEURONFAIR [19]. We obtained the implementations of these tools from their GitHub repositories and configured them according to the prescribed setting to have the best performance. Following these techniques, we report the results for each protected attribute separately. Table III shows the results of baselines and DAIKE in runs of 15 minutes. The results are averaged over 10 repeated runs. The column #IDis the total number of generated individual discriminatory instances. The column  $l\_succ$  is the success rate of local stage of searches. We exclude the global success rate since the goal of global phase in our search is to maximize QID whereas the local phase focuses to generate many ID instances. We calculate success rate as the number of ID found over the total number of generated samples. The column T.1st is the time taken to find the first ID instance. The result shows that DAIKE outperforms the-state-of-the-art in generating many ID instances. In particular, DAIKE finds  $16.7 \times$ ,  $12.2 \times$ , and  $15.0 \times$  more IDs in the best case and  $4.6 \times$ ,  $2.9 \times$ , and  $2.8 \times$ 

more IDs in the worst case compare to AEQUITAS, ADF, and NEURONFAIR, respectively. The success rate of local search are 19.3%, 30.5%, 26.8%, and 79.0% in average for AEQUITAS, ADF, NEURONFAIR, and DAIKE, respectively. For the time taken to find the first ID, NEURONFAIR achieves the best result in most of the cases with an average of 0.014 (s) whereas it took DAIKE 2.4 (s) in average to find the first ID. Overall, our experiments indicate that DAIKE is effective in generating ID instances compared to three state-of-the-art techniques, largely due to the smoothness of the feedback during the local search.

Answer RQ2: Our experiments demonstrate that DAIKE outperforms the state-of-the-art fairness testing techniques [20], [18], [19]. In average, our approach found  $9 \times$  more individual discrimination (ID) instances than these techniques with  $3 \times$  more success rates. However, we found that DAIKE is slower than those techniques in finding the first ID instance in the order of a few seconds.

# C. Causal Debugging of DNNs for Fairness (RQ3)

We perform experiments over the DNN models to study whether the proposed causal debugging approach is useful in identifying layers and neurons that significantly effect the amounts of discrimination as characterized by QID. Table IV shows the results of experiments (averaged over 10 independent runs). The first two columns show the localized layer and its influence (i.e., l and  $\rho$  in Algorithm 2). The next six columns show top 3 neurons with the positive influence on fairness (i.e., activating those neurons reduce the amounts of discrimination based  $Q_{\infty}$ ). The last six columns show top 3 neurons with the negative influence on fairness (i.e., activating those neurons increase the amounts of discrimination based  $Q_{\infty}$ ). Except for the DNN of Heart dataset where DAIKE points to the layer 4 with the largest rate of changes, the layer 2 has the largest rate of changes in all the DNN models. Overall, the average causal difference (ACD) range

TABLE II: DAIKE characterizes QID for 10 datasets and DNNs in 1 hour run (results are average of 10 runs).

Dataset	m	$Q_I$	$K_I$	#I	$K_F$	$T_{K>1}$	$T_{K_F}$	$Q_{\infty}$	$Q_1$	$\#I_{K_{F}^{1}}$	$\#I_{K_F^2}$	$\#I_{K_{F}^{3}}$
Census	90	5.3	13.54	230,593	35.61	0.0012	21.04	4.05	2.64	6.0	28.6	111.6
Compas	12	3.6	3.12	157,968	10.24	0.0305	6.50	1.81	1.40	35.2	338.7	1,016.9
German	16	4.0	2.34	245,915	9.56	0.0300	13.14	1.61	1.10	6.6	16.2	54.8
Default	12	3.6	5.58	258,105	11.26	0.0285	10.94	2.10	1.78	3,528.8	9,847.2	9,771.0
Heart	14	3.8	4.54	270,029	10.01	0.0307	11.88	2.31	1.80	21.7	135.2	579.7
Bank	9	3.2	1.45	172,686	8.93	0.0297	3.68	2.25	1.98	5, 118.5	13,513.3	20,438
Diabetes	10	3.3	2.39	504, 414	7.90	0.0281	0.016	1.40	1.11	89.7	609.6	2,310.1
Students	16	4	1.90	133, 221	10.90	0.0896	14	1.93	1.35	16.0	130.7	128.7
MEPS15	36	5.2	7.03	19,673	18.52	0.0318	31.62	2.61	1.62	2.6	3.5	6.0
MEPS16	36	5.2	9.06	14, 266	19.25	0.0309	49.16	2.21	1.52	2.0	3.5	6.0

TABLE III: Comparison of generating discriminatory instances to the state-of-the-art in 900 seconds. SENs is the the protected attributes; #ID is the number of individual discriminatory instances;  $l\_succ$  is the success rate of the local search; and T.1st is the time takes to find the first discriminatory instance. The results are averaged over 10 runs of each tool.

Dataset	Sens	AEQUITA	s [20]		ADF [18]			NEURON	FAIR [19]		DAIKE		
Dataset	Selis	#ID	l_succ	T.1st	#ID	$l\_succ$	T.1st	#ID	$l\_succ$	T.1st	#ID	l_succ	T.1st
	sex	9,243	10.14	0.028	16,299	18.74	0.785	17,172	18.11	0.014	61,246	74.0	0.085
Censes	age	7,565	29.10	0.051	17, 363	54.41	0.566	19, 130	56.39	0.014	77,961	85.38	0.029
	race	12,157	27.15	0.025	18,566	40.27	0.586	21,708	42.03	0.014	72,048	81.13	0.043
	sex	10,419	12.92	0.024	14,725	17.46	0.046	15,022	14.26	0.015	54,454	65.47	0.495
Compas	age	6,117	10.70	0.026	11,159	17.13	0.014	12,158	13.35	0.016	51,792	71.54	0.371
	race	5,602	7.24	0.026	9,038	9.76	0.017	9,899	9.12	0.014	32,097	58.40	0.967
German	sex	7,273	12.84	0.016	12,400	22.56	0.034	12,137	17.59	0.016	48,529	80.03	0.015
German	age	7,482	40.47	0.016	12,029	59.56	0.015	10,505	44.43	0.014	61,622	93.67	0.015
Default	sex	3,816	5.59	1.125	10,162	14.06	0.508	1.02	13.84	0.014	44,942	73.61	0.657
Default	age	4,705	11.31	1.784	9,698	32.4	0.498	9, 191	31.00	0.014	54,047	83.11	0.540
Heart	sex	7,950	11.73	0.019	10,375	13.44	0.012	10,032	9.69	0.018	68,418	85.24	0.016
Heart	age	14,589	46.40	0.013	24,994	69.00	0.012	25,777	65.99	0.013	71,546	95.16	0.017
Bank	age	9,166	37.9	0.052	6,822	35.84	0.030	6,966	30.80	0.014	41,943	88.94	0.968
Diabetes	age	14,633	82.99	0.011	46,917	76.7	0.013	45,305	75.02	0.014	138,025	94.30	0.017
Student	sex	2,442	6.13	0.041	4,504	11.84	0.013	4,012	9.38	0.014	24,052	72.06	0.552
Student	age	1,493	13.43	0.045	2,736	23.6	0.085	2,227	17.68	0.013	33,298	89.38	0.489
	sex	591	8.31	0.019	1,028	16.24	0.013	806	11.10	0.014	4,931	68.07	14.47
MEPS15	age	300	15.06	0.038	856	38.48	0.013	1,030	44.57	0.014	5,011	79.05	27.20
	race	693	9.43	0.018	1,376	21.88	0.023	750	10.72	0.014	4,821	71.54	0.069
	sex	615	8.53	0.016	972	14.62	0.012	920	11.94	0.014	4,260	72.98	0.782
MEPS16	age	316	16.01	0.022	790	35.1	1.475	469	23.82	0.013	4,707	78.16	0.014
	race	979	13.91	0.013	1,675	26.96	0.275	1,320	18.39	0.013	4,882	78.48	4.571

from 0.04 to 0.675 for neurons with positive fairness effects and from 0.002 to 0.178 for neurons with negative fairness effects. Guided by localization, DAIKE intervenes to activate neurons with positive fairness influence or de-activate those with negative influence. Table V shows the results of this mitigation strategy. The results indicate that the activation interventions can improve the fairness by at least 6.3% with 3% loss of accuracy (up to 88.8% with 2% loss of accuracy) whereas the de-activation can improve the fairness by at least 4.5% with 3% loss of accuracy (up to 49.5% with 5% loss).

Answer RQ3: The debugging approach implemented in DAIKE identified neurons that have at least 4% and up to 67.5% positive causal effects on the fairness and those which have at least 0.2% and up to 17.8% negative causal effects. A mitigation strategy followed by the localization can reduce the amounts of discrimination by at least 6.3% and up to 88.8% with a tolerable loss of accuracy.

### VII. DISCUSSION

*Limitation*. In this work, we consider all set of protected values and perturb them to generate counterfactual. This might introduce false positive since such person might not possibly

exist in the real world w.r.t their non-protected characters. One idea to overcome this limitation is to use causal diagrams over the input variables to filter out inputs.

Threat to Validity. To address the internal validity and ensure our finding does not lead to invalid conclusion, we follow established guideline and take average of repeated experiments. To ensure that our results are generalizable and address external validity, we perform our experiments on 10 DNN models taken from the literature of fairness testing. However, it is an open problem whether these datasets and DNN models are sufficiently representative for fairness testing.

# VIII. RELATED WORK

**Fairness Testing of ML systems.** THEMIS [22] presents a causal discrimination notion where they measure the difference between the fairness metric of two subgroups by *counterfactual* queries; i.e., they sample individuals with the protected attributes set to A and compare the outcome to a counterfactual scenario where the protected attributes are set to B. Symbolic generation (SC) [27], [23] presents a black-box testing that approximates the ML models with decision trees and leverage symbolic execution over the tree structure to find individual discrimination (ID). AEQUITAS [20] uses a two-step approach that first uniformly at random samples instances

TABLE IV: Localization of layers and neurons that causally influence fairness. Neuron $_i^+$  shows the index of i-th top neuron that has positive influence on fairness once activated; Neuron $_i^-$  shows the index of i-th top neuron that has negative influence on fairness once activated; ACD $_i^+$  shows the (normalized) average causal difference of i-th top neuron with positive fairness influence; ACD $_i^-$  shows the (normalized) average causal difference of i-th top neuron with negative fairness influence.

Dataset	Layer Index	Layer Influence	Neuron <sub>1</sub> <sup>+</sup>	$ACD_1^+$	Neuron <sub>2</sub> <sup>+</sup>	$ACD_2^+$	Neuron <sub>3</sub> <sup>+</sup>	$ACD_3^+$	Neuron <sub>1</sub>	$ACD_1^-$	Neuron <sub>2</sub>	$ACD_2^-$	Neuron <sub>3</sub>	$ACD_3^-$
Census	2	9.15	$N_{13}$	0.138	$N_{18}$	0.115	$N_4$	0.109	$N_{24}$	0.178	$N_{15}$	0.177	$N_{14}$	0.096
Compas	2	37.42	$N_{25}$	0.378	$N_{28}$	0.320	$N_7$	0.298	N/A	N/A	N/A	N/A	N/A	N/A
German	2	1.78	$N_{29}$	0.176	$N_{15}$	0.146	$N_5$	0.145	$N_9$	0.059	$N_{19}$	0.046	$N_0$	0.042
Default	2	4.51	$N_{12}$	0.675	$N_9$	0.623	$N_{14}$	0.488	$N_{16}$	0.004	N/A	N/A	N/A	N/A
Heart	4	1.58	$N_4$	0.078	$N_5$	0.046	$N_3$	0.041	N/A	N/A	N/A	N/A	N/A	N/A
Bank	2	6.19	$N_0$	0.500	$N_7$	0.322	$N_1$	0.321	$N_6$	0.077	$N_{11}$	0.038	$N_{12}$	0.019
Diabetes	2	17.27	$N_{19}$	0.041	$N_{22}$	0.032	$N_{31}$	0.016	$N_0$	0.012	$N_{29}$	0.015	N/A	N/A
Students	2	3.99	$N_{22}$	0.401	$N_{24}$	0.373	$N_{30}$	0.252	N/A	N/A	N/A	N/A	N/A	N/A
MEPS15	2	37.41	$N_6$	0.162	$N_{29}$	0.129	$N_{16}$	0.121	$N_{24}$	0.017	N/A	N/A	N/A	N/A
MEPS16	2	58.70	$N_8$	0.110	$N_1$	0.103	$N_{20}$	0.096	$N_{13}$	0.002	N/A	N/A	N/A	N/A

TABLE V: A is accuracy, K is the average number of clusters from test cases;  $A^{=0}$  is the accuracy after deactivating the neuron with the highest negative fairness impacts;  $K^{=0}$  is the average number of clusters after the deactivation;  $A^{>0}$  is the accuracy after activation the neuron with the highest positive fairness impacts; and  $K^{>0}$  is the average number of clusters after the activation.

Dataset	A	K	$A^{=0}$	K=0	$A^{>0}$	$K^{>0}$
Census	0.88	20.56	0.87	18.48	0.86	18.27
Compas	0.97	4.57	N/A	N/A	0.971	2.94
German	1.0	4.20	0.954	2.81	0.97	2.92
Default	0.83	5.82	0.824	4.67	0.825	4.33
Heart	0.96	6.12	N/A	N/A	0.933	5.66
Bank	0.92	5.50	0.901	4.862	0.897	3.73
Diabetes	0.99	3.37	0.961	2.78	0.962	3.17
Students	1.0	5.25	N/A	N/A	0.98	2.78
MEPS15	0.94	8.33	0.914	7.97	0.913	7.64
MEPS16	0.95	6.46	0.944	5.68	0.925	5.54

from the input dataset to find a discriminatory instance and then locally perturb those instances to further generate biased test cases. EXPGA [17] proposed a genetic algorithm (GA) to generate ID instances in natural language processes. The proposed technique used a prior knowledge graph to guide the perturbation of protected attributes in the NLP tasks. While these techniques are black-box, they potentially suffer from the lack of local guidance during the search. ADF [18] utilized the gradient of the loss function as guidance in generating ID instances. The global phase explores the input space to find diverse set of individual discrimination whereas the local phase exploits each instance to generate many individual discriminatory (ID) instances in their neighborhoods. EIDIG [28] follows similar ideas to ADF, but uses different computations of gradients. First, it uses the gradients of output (rather than loss function) to reduce the computation cost at each iteration. Second, it uses momentum of gradients in global phase to avoid local optima. NEURONFAIR [19] extends ADF and EIDIG to support unstructured data (e.g., image, text, speech, etc.) where the protected attributes might not be well-defined. In addition, NEURONFAIR is guided by the DNN's internal neuron states (e.g., the pattern of activation and deactivation) and their activation difference. Beyond the capability of these techniques, DAIKE quantifies the amounts

of discrimination, enables software developers to prioritize test cases, and searches multiple protected attributes at one time.

Beyond the scope of this paper, a body of prior work [42], [43], [44], [45], [46] considered testing for group fairness. FAIRWAY [43] mitigates biases after finding suitable ML algorithm configurations. In doing so, they used a multi-objective optimization (FLASH) [47]. PARFAIT-ML [46] searches the hyperparameter space of classic ML algorithms via a gray-box evolutionary algorithm to characterize the magnitude of biases from the hyperparameter configuration.

Debugging of Deep Neural Network. CRADLE [33] traced the execution graph of a DNN model over two different deep-learning frameworks and used the differences in the outcomes to localize what backend functions might cause a bug. However, since CRADLE did not use causal analysis, it showed a high rate of false positive. AUDEE [48] used a similar approach, but it leveraged causal-testing methods. In particular, it designed strategies to intervene in the DNN models and tracked how the intervention affected the observed inconsistencies. We adapted the layer localization of CRADLE and AUDEE; but our causal localization is developed using do logic for a meta-property (fairness). AUDEE used a simple perturbation of neuron values for functional correctness (i.e., any inconsistency shows a bug) without considering the accuracy or the severity of neuron contributions to a bug.

**In-process mitigation.** A set of work considers in-process algorithms to mitigate biases in ML predictions [49], [50], [51]. Adversarial debiasing [49] and Prejudice remover [50] improve fairness by adding constraints to model parameters or the loss function. Exponentiated gradient [51] uses a meta-learning algorithm to infer a family of classifiers that maximizes accuracy and fairness. We left further investigation on using DAIKE for in-process mitigation to the future work.

# IX. CONCLUSION

DNN-based software solutions are increasingly being used in socio-critical applications where a bug in their design may lead to discriminatory behavior. In this paper, we presented DAIKE: an information-theoretic model to characterize the amounts of protected information used in DNN-based decision making. Our experiments showed that the search and debugging algorithms, based on the quantitative landscape, are effective in discovering and localizing fairness defects.

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