Data-centric Reliability Evaluation of Individual Predictions

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ABSTRACT
At the same time that AI and machine learning are becoming central to human life, their potential harms become more vivid. In the presence of such drawbacks, a critical question one needs to address before using these data-driven technologies to make a decision is whether to trust their outcomes.

Aligned with recent efforts on data-centric AI, this paper proposes a novel approach to address the reliability question through the lens of data by associating data sets with distrust quantification that specifies their scope of use for predicting future query points. The distrust values raise warning signals when a prediction based on a dataset is questionable and are valuable alongside other techniques for trustworthy AI. We propose novel algorithms for efficiently and effectively computing distrust values. Learning the necessary components of the measures from the data itself, our sub-linear algorithms scale to very large and multi-dimensional settings. Furthermore, we design estimators to enable no-data access during the query time. Besides demonstrating the efficiency of our algorithms, our extensive experiments reflect a consistent correlation between distrust values and model performance. This highlights the necessity of dismissing prediction outcomes for cases with high distrust values, at least for critical decisions.

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The source code, data, and/or other artifacts have been made available at https://github.com/neemashahbazi/distrust2.

1 INTRODUCTION
AI and Machine Learning (ML) are becoming central to human life and societies. Increasingly, data is being used for building predictive models to help different entities and businesses make crucial decisions, not only efficiently and at scale but also wisely, accurately, and just. However, AI depends on data, and any data-driven algorithm is “only as good as the data it works with” [12]. As a result, “despite their huge promise, AI systems can be brittle and unfair” [78]. Unfortunately, examples of such failures are abundant. Bias in recidivism prediction scores used in the US jurisdictions [24, 29], in police decisions [32], in granting loans [28], in job screening [22], and in online advertising [74] are only a few examples underscoring the scope of the issue.

In the presence of such machine learning failures, any decision-maker using a data-driven predictive model faces a critical question: should they trust the outcome of the model for decision-making? To further motivate this, let us use the following example:

Example 1: Consider a judge who needs to decide whether to accept or deny a bail request. Using data-driven predictive models is prevalent in such cases for predicting recidivism [24]. Indeed, such models can be beneficial to help the judge make wise decisions. Suppose the model predicts the queried individual as high risk (or low risk). The judge is aware and concerned about the critics surrounding such models. A major question the judge faces is whether or not they should rely on the prediction outcome to take action for this case. Furthermore, if, for instance, they decide to ignore the outcome and hence they need to provide a statement supporting their action, what evidence can they provide? □

In line with the recent trend on data-centric AI [55], in this paper we propose a novel approach, complimentary to the existing work on trustworthy AI [41, 50, 69, 78], to address the aforementioned trust question through the lens of data. In particular, unlike existing works that generate proper trust information for a given model, we associate data sets with trust measures that specify their scope of use for predicting future cases. We note that a predictive model provides only probabilistic guarantees on the average loss over the distribution represented by the data set used for training it. As a result, these predictions may not be distribution generalizable [46]. Consequently, if the query point is not represented by the data, the guarantees may not hold, hence one cannot rely on the prediction outcome. Besides, we note that the bulk of work on trustworthy AI provides information that supports the outcome of an ML model. For example, existing work on explainable AI, including [33, 35, 62], aims to find simple explanations and rules that justify the outcome of a model. Conversely, motivated by Example 1, we aim to raise warning signals when the outcome of a model is not trustworthy. That is, to provide reasons that cast doubt on the reliability of the model outcome for a given query point.

To this end, given a data set, we introduce two probabilistic measures Strong Distrust Measure (SDT) and Weak Distrust Measure (WDT) that specify the reliability of the data set for predicting the outcome of a specific query point. The distrust measures are defined based on two components: (a) if the data set misses to represent the query point properly and (b) if the query point belongs to an uncertain neighborhood where data set tuples have different target values. The distrust measures can be embedded as widgets in data set profiles [2], nutritional labels [70, 73], and data sheets [31].

Example 1 (part 2): Distrust measures raise warning when the fitness of the data set used for drawing a prediction is questionable, helping the judge to be cautious when taking action. Besides, these
measures provide quantitative justification to support the judge’s action when they decide to ignore a prediction outcome that is not trustworthy. Suppose the WDT for the query point is low. Besides the score, our system specifies that, for example, lack of representation is the issue, reflected by the low representation score. The judge can then argue to ignore a model outcome for this case, justifying that the model has been built using a data set that misses to represent the given case.

While being agnostic to the choice of the uncertainty and lack of representation components, we propose an implementation based on the $k$-vicinity of a query point. In particular, given the radius of the $k$-vicinity and its uncertainty, we develop functions that return probabilities indicating the lack of representation and uncertainty. We propose methods to learn the probabilities from the data set itself. We devise proper indexing and algorithms that enable sublinear (near logarithmic) query processing that scales to large data sets.

Our work differs from existing literature in model-centric uncertainty quantification, local interpretation techniques, and data coverage in several radical ways:

- We offer a data-centric distrust measure, a quantitative warning signal that measures whether a query point is in the scope of use of a data set and if not, users should not rely on the outcome of any model constructed on top of this data for that query point. Despite model-centric uncertainty quantification techniques, our techniques reveal a property of the data set regardless of the constructed model this property stands still.

- While model-centric techniques such as [20, 42, 59] guarantee a user-specified assurance level of error, this error is still computed over the entire data and consequently may fail to focus the error on local regions in data, representing, for example, minority populations in social applications. However, the local fidelity of our techniques satisfies equal treatment for every query point.

- While some model-centric uncertainty quantification techniques [42, 59] claim considering lack of representation as a source of uncertainty, as we observed in our experiments, they fail to capture the associate uncertainty for such query points in sparse regions. This failure originates from the perfect sampling assumption in development and production data which may not hold in practice. Our measures however properly capture such cases and directly target the lack of representation of a query point.

- While techniques in data coverage [10, 11, 48] body of work only focus on enough representation of the query point in the data set, they fail to capture uncertainty. Additionally, they only return a binary signal of whether to trust the outcome of the model for a query point or not which practically is not very informative. Whereas our proposed measures target both sources of uncertainty and representation and return a quantitative probabilistic value that is easily interpretable.

- While techniques in interpretable machine learning [52] try to justify why a model performs in a certain manner regarding a particular query point and advocate the model’s behavior, our techniques instead try to question that by investigating whether it is reliable to trust the model for the query point or not.

Our extensive proof-of-concept experiments verify a consistent correlation between distrust values and ML performance metrics on a variety of tasks, data sets, and ML algorithms. For tuples that have higher distrust values (meaning they are less reliable w.r.t. to our measures), an ML model is more likely to fail to capture the truth and make a correct decision.

**How to use?** The final message is when distrust values for a query point with regard to a data set are high, one should discard or at least not rely on the prediction outcome based on the data set for critical decisions.

In the end, we would like to reiterate that our proposal in this paper is complementary to the existing literature and should be used alongside other techniques and potential approaches for trustworthy AI.

**Summary of contributions:** In summary, our contributions in this paper include the following:

- We propose data set distrust measures to raise a warning when the fitness of a data set for drawing prediction for a given case is questionable. To the best of our knowledge, we are the first to propose data-centric distrust measures, a property associated with data sets.

- Our proposal is a probabilistic measure based on two components: the query’s lack of representation and uncertainty in the data set. The proposed measures can be extended to different data types and are independent from the model and prediction task (classification and regression). The measures are also agnostic to the choice of metric or approach for computing the two components. Proposing quantitative probabilistic outcomes, our measures are interpretable for the users since beyond the scores, the uncertainty and lack of representation components provide an explanation to justify them.

- We propose novel algorithms that consider the $k$-vicinity of a query point to compute the query’s lack of representation and uncertainty. In particular, we “learn” the measurements from the data set itself. We also propose proper preprocessing and algorithms that enable sub-linear query answering that scales to very large and multi-dimensional data sets. Furthermore, to enable no-data access during the query time, we build regression models to accurately estimate parameters needed to compute distrust measures. We design an exponential search strategy for constructing large-enough samples for training the estimators.

- We conduct comprehensive experiments on multiple synthetic and real-world data sets with various scales and dimensions, on different prediction tasks, using several models (such as Logistic Regression, DNN, Random Forest, etc), and distance measures to (i) validate the effectiveness and consistency of the distrust measures, (ii) evaluate the efficiency and scalability of our algorithms and (iii) evaluate the efficacy of the existing works.

## 2 RELATED WORK

Responsive data science has become a timely topic, to which the data management community has extensively contributions [8, 9, 45, 54, 63, 64, 66, 71, 77, 84, 85]. In particular [27] introduces a data profiling primitive conformance constraint to characterize whether inference over a tuple is untrustworthy. By the assumption that the conformance constraints always hold, they claim that they can use a tuple’s deviation from the constraint as proxy to whether trust model’s outcome for that tuple. Besides, extensive studies on
differing dimensions of trust in ML and AI have been presented in [41, 50]. It is also worth mentioning the body of work on the notion of trustworthiness of data sources that focuses on correctness and legitimacy of data sources [23, 37], however despite the similar terminology, it is a different concept from our problem.

Related work also includes [1, 13, 57, 86] that aim to estimate and quantify uncertainty in AI models, however, they have a different perspective on the issue as they extract the uncertainty from models, while our measures are data-centric. Probabilistic classifiers predict a probability distribution over the set of classes for a given query point instead of simply returning the most likely class [56, 60, 82, 83]. A given probability metric such as log loss or Brier score is calculated for each example to evaluate the predicted probabilities. Not all of the common classifiers are intrinsically probabilistic and some return distorted probabilities that need to be calibrated. Prediction probabilities are computed using the model trained for global performance and may not be accurate for the unrepresented regions. Prediction Intervals (PIs) are a common practice for quantifying the uncertainty associated with a model’s prediction of a query point in regression tasks [20, 42, 59]. PIs consist of a lower and upper bound that contain a future observation with a specified level of confidence. Although PIs can be constructed in multiple ways, there is a negative correlation between the quality of the PI and the computational load associated with it [43]. Conformal Prediction (CP) is another standard way of quantifying uncertainty in both classification and regression problems returning confidence intervals and confidence sets respectively, guaranteeing a user specified confidence level. Benefiting from a heuristic notion of uncertainty in the model of choice, a scoring function \( s(x, y) \) is defined that assigns uncertainty values to query point \( x \) given target variable \( y \) with larger values to the cases that \( x \) and \( y \) disagree more. Next, the \( 1 - \alpha \) quantile (\( \alpha \) being the user specified confidence level) of the calibration set scores is calculated and is used to form the prediction set for the new examples.

It is important to note that all aforementioned model-centric approaches, including PI and CP, estimate intervals, probabilities, and scores using model(s) built by maximizing the expected performance on random sample from the underlying distribution. As a result, while they may provide accurate estimations for the dense regions of data (e.g. majority groups), their estimation accuracy is questionable for the poorly represented regions (e.g. minority groups). In particular, [7] recognizes the lack of guarantees in the performance of CP for such regions. On the contrary, prediction outcomes are specifically unreliable for regions that are unlikely to be sampled. As a result, as we further discuss in § 4.1, such approaches fail for cases that are not represented by the training data. This is consistent with our experimental evaluations. PI and CP methods usually rely on techniques such as bootstrapping and constructing ensembles to elicit uncertainty, which regardless of the number of subsamples or ensembles created, fails to account for the regions that are not represented. Contrarily, our proposed measures are computed locally around the query point (in form of lack of certainty and lack of representation) and therefore are equally accurate for different regions of data. Finally, while PI and CP return an interval or set for each query point, the results may be too generic (e.g. including a large set) or lack a proper explanation for the user to make an informed decision.

The notion of data coverage is a related topic that has been studied across different settings [3, 4, 10, 11, 38, 48, 53, 75]. For categorical data, uncovered regions are identified in form of value combinations (e.g. Hispanic Females) called patterns. A pattern is uncovered if there are not enough samples matching it [10, 38, 48]. Coverage on continuous space is studied in [11]. Accordingly, lack of coverage is identified as any point in the data space that doesn’t have enough points in a fixed-radius neighborhood around it. Although coverage does not provide a score for an arbitrary query point, following the idea of whether the point is covered or not, users can decide whether to trust the outcome of the model for that query point.

Out-of-distribution generalizability is another related topic from the ML community that quantifies the degree to which a query point is an outlier in the underlying distribution. Specifically, [18] proposes five metrics for identifying well-represented examples. These metrics are shown to be highly correlated, stable, and model-agnostic. The metrics rank examples based on different measures within ensembles, distance to the decision boundary, or prediction difference of two models for the same query point (holdout retraining). It is important to note that these techniques are model-agnostic in the sense that they have consistent results for different models and parameters, however, unlike our techniques that merely assess representation from the data, they still measure representation within model properties.

**Table 1: Descriptive comparison of distrust measures and related work**

| line of work                     | target     | fidelity | output           | task           | components           | model advocacy | data profiler |
|----------------------------------|------------|----------|------------------|----------------|----------------------|----------------|---------------|
| distrust measures (this work)     | data       | local    | probabilistic score | classification regression | lack of certainty lack of representation | challenge | yes           |
| prediction probabilities [56, 60, 82, 83] | model     | global   | probabilistic score | classification | lack of certainty | challenge | no            |
| prediction intervals [20, 42, 59]  | model      | global   | interval          | regression     | lack of certainty | challenge | no            |
| conformal prediction [7, 65]      | model      | global   | interval          | classification regression | lack of certainty | challenge | no            |
| data coverage [10, 11, 48]        | data       | local    | binary signal     | classification regression | lack of representation | challenge | yes           |
| local interpretation [51, 62]     | model      | local    | prediction probability | feature effect | classification regression | n/a | support | no |
| out-of-distribution generalizability [18] | model     | global   | continuous score  | classification regression | lack of representation | challenge | yes           |

**Figure 1: Descriptive comparison of distrust measures and related work**
Another related topic is the body of work on local interpretation methods for explaining individual predictions [52]. LIME provides local explanations for a model's prediction behavior on query points by substituting the original complex model with a locally interpretable surrogate model. Being a model-agnostic technique, to realize what parts of the input are involved in the prediction, LIME perturbs the query point by creating samples around its neighborhood and observes how the model performs for the perturbed samples. Next, the samples are weighted with regard to their proximity to the original query point, and an interpretable model is constructed on the new samples. The learned model should be locally a good approximation and is used to interpret the original model. We note that interpretation methods justify a model's reasoning for a particular behavior. Conversely, our measures raise warnings to cast doubt when the prediction outcome is not reliable for a specific case.

Figure 1, presents an extensive comparison between the related body of work and our proposed measures and demonstrates how our measures stand out in the skyline. The techniques are examined based on the following properties:

- **target** specifies whether the technique targets data or model.
- **fidelity** specifies whether the technique evaluates trust locally or only provides global assurance (may fail for sparse regions in the data).
- **output** specifies the outcome of the technique.
- **task** specifies the learning problem.
- **component** specifies the considered complications causing the trust problems.
- **model advocacy** specifies whether the technique questions the outcome of the model or tries to justify it.
- **data profiler** specifies whether or not the outcome of the technique is considered as a property of the data.

To the best of our knowledge, our paper is the first to provide data-centric distrust measures to identify the scope of use of data sets or only provides global assurance (may fail for sparse regions in the data). Hence, our proposal does not make the iid assumption, which we shall further explain in § 3.2. Prediction models assume that \( D \) is a set of iid (independent and identically distributed random) samples\(^2\), drawn from an (unknown) underlying distribution \( \xi \). Attribute values may be discrete ordinal, continuous-valued, or non-ordinal categorical. Throughout the paper, we assume ordinal attributes are normalized in the range [0, 1], with values drawn from the set of rational or real numbers. For non-ordinal attributes, we assume one-hot encoding is considered. We use \( t^j \) to refer to the \( j \)-th tuple in the data set \( D \) and its values of the observation attributes in particular. Similarly, we use \( y^j \) to refer to the value of the target attribute of \( t^j \). For every tuple \( t \in D \), we use the notation \( t_j \) to show the value of \( t \) on attribute \( x_j \in x \).

### 3.2 Query and Prediction Model

The goal of prediction is to guess the target value \( y \) of a query point based on the observations on \( x \). In other words, given a point \( q = (q_1, q_2, \ldots, q_d) \), the goal is to predict the value of the target attribute of \( q \). We consider the prediction model \( h : \mathbb{R}^d \rightarrow \mathbb{R} \) as a function that predicts the target value of \( q \) as \( h(q) \). When \( y \) is categorical, the task is classification, while regression is considered when \( y \) is continuous.

The underlying assumption is that \( q \) is drawn from the same distribution \( \xi \) from which \( D \) has been generated. Now, consider the Cartesian product of the input and output space \( x \times y \), and fix the hypothesis universe \( \mathcal{H} \) of prediction functions. A learning algorithm \( A \) takes as input the set of samples in the data set \( D \) and finds a specific function \( h = A(D) \) by minimizing the empirical risk (maximizing the empirical accuracy or minimizing empirical loss) over \( D \). Empirical accuracy for classification is computed as the sum of samples in \( D \) for which the true label is the same as the predicted label. That is,

\[
\max \sum_{j=1}^{n} \mathbb{1}\{y_j = h(t_j)\} \tag{1}
\]

The equivalent objective for regression is to minimize the empirical error between the target variable and predicted values. Sum of Squares Error (SSE) is the de-facto error measure for regression:

\[
\min \sum_{j=1}^{n} (y_j - h(t_j))^2 \tag{2}
\]

Having a prediction model \( h \) trained by maximizing its empirical accuracy over the sample points in \( D \), the model is then used to predict the value of unseen target attribute of each query point \( q \), observed after model deployment, as \( h(q) \). A central question at this point is whether a decision-maker should rely on the model prediction (at least for critical decisions). In the next section, we propose data-centric measures generated to answer this concern.

### 4 DISTRUST MEASURES

Not every data set is fit for all data science tasks [10, 73]. An essential requirement for a learning algorithm is that its training data \( D \) should represent the underlying distribution \( \xi \). Even if so, the trained model guarantees to perform well only on average over the query points drawn from \( \xi \), not necessarily on a specific query point. To further explain this, let us remind some background from the machine learning theory.

Let \( L \) be the loss function used by the learning algorithm. Considering the underlying distribution \( \xi \), the optimal model \( h^* \in \mathcal{H} \)
as opposed to the average performance of the model over a set

As the running example in this section, let us consider the following

Example 2: Consider a binary classification task where the input
space is $x = \langle x_1, x_2 \rangle$ and the output space is the binary label $y$

with values $\{-1, +1\}$. Suppose the underlying data distribution $\xi$ follows a 2D Gaussian, where $x_1$ and $x_2$ are positively correlated as shown in Figure 2a. The figure shows the data set $\mathcal{D}$ drawn independently from the distribution $\xi$, along with their labels as their colors. Using $\mathcal{D}$, the prediction model $h$ is constructed as shown in Figure 2b. The decision boundary is specified in the picture; while any point above the line is predicted as +1, a query point below it is labeled as -1. The classifier has been evaluated using a test set that is an iid sample set drawn from the underlying data set $\xi$. The accuracy on the test set is high (above 90%), and hence, the model gets deployed for predicting the outcome of unseen query points. We cherry-picked four query points, $q_1$ to $q_4$, that are also included in Figure 2b. Using $h$ for prediction, $h(q_1) = -1$, $h(q_2) = +1$, $h(q_3) = +1$, and $h(q_4) = -1$. Figure 2c adds the ground-truth boundary to the search space, revealing the true label of the query points: every point inside the red circle has the true label +1 while any point outside of it is labeled as -1. Looking at the figure, $y_1 = +1$ while the model predicted it as $h(q_1) = -1$.

Let us take a closer look at the four query points in this example and their placement with regard to the tuples in $\mathcal{D}$ used for training $h$. $q_3$ belongs to a dense region with many training tuples in $\mathcal{D}$ surrounding it. Besides, all of the tuples in its vicinity have the same label $y = +1$. As a result, one can expect that the model’s outcome $h(q_3) = +1$ should be a reliable prediction. Similar to $q_2$, $q_4$ also belongs to a dense region in $\mathcal{D}$; however, $q_4$ belongs to an uncertain region, where some of the tuples in its vicinity have a label $y = +1$, and some others have the label $y = -1$. Considering the uncertainty in the vicinity of $q_4$, one cannot confidently rely on the outcome of the model $h$. On the other hand, the neighbors of $q_1$ (resp. $q_3$) are not uncertain, all having the label $y = -1$ (resp. $y = +1$). However, the query points $q_1$ and $q_4$ are not well represented by $\mathcal{D}$, as those would be outliers with respect to $\mathcal{D}$. In other words, $q_1$ and $q_4$ are unlikely to be generated according to the underlying distribution $\xi$, represented by $\mathcal{D}$. As a result, following the no-free-lunch theorem,
one cannot expect the outcome of model \( h \) to be reliable for these points. Note that, as we observed in our experiments, model-centric techniques such as prediction intervals and conformal prediction fail to detect \( q^1 \) and \( q^3 \) as not trustworthy.

Looking at the ground-truth boundaries in Figure 2c, \( h \) luckily predicted the outcome for \( q^3 \) correctly, but it was not fortunate to predict the \( y^3 \) correctly. Nevertheless, since the model has not reliably been trained for these outlier points, its outcome may or may not be accurate for these query points, hence is not trustworthy.

4.2 Strong and Weak Distrust Measures

From Example 2, we observe that the outcome of a model \( h \), trained using a data set \( \mathcal{D} \) is not reliable for a query point \( q \), if:

- **Lack of representation**: \( q \) is not well-presented by \( \mathcal{D} \). In other words, \( q \) is an outlier with respect to the tuples in \( \mathcal{D} \). In such cases, the model has not seen “enough” samples similar to \( q \) to reliably learn and predict the outcome of \( q \).
- **Lack of certainty**: \( q \) belongs to an uncertain region, where different tuples of \( \mathcal{D} \) in the vicinity of \( q \) have different target values. In a classification context, that means the tuples have different labels (similar to \( q^3 \) in Example 2). Similarly, in a regression setting, \( q \) belongs to a high-fluctuating area, where tuples in the vicinity of \( q \) have a wide range of values on the target variable.

We design the data-centric distrust measures based on these two observations. In particular, given a query point \( q \), let \( P_o \) be the probability indicating if \( q \) is an outlier and let \( P_u \) be the probability indicating if \( q \) belongs to an uncertain region. Before formally defining the distrust measures, we would like to emphasize that our definitions are agnostic and independent from how \( P_o \) and \( P_u \) are computed. We still shall provide the details of how to compute these probabilities in § 5.

**Definition 1 (Strong distrust measure (SDT)).** The strong distrust measure is a probabilistic measure that considers the outcome of a model for a query point \( q \) untrustworthy if \( q \) is not represented by \( \mathcal{D} \) and it belongs to an uncertain region. Formally, the strong distrust measure is:

\[
SDT(q) = P((q \text{ is outlier}) \land (q \text{ belongs to uncertain region}))
\]

Since \( P_o \) and \( P_u \) are independent:

\[
SDT(q) = P_o(q) \times P_u(q)
\]  

\[\tag{5}\]

SDT raises the distrust warning signal only when the query point fails on both conditions of being represented by \( \mathcal{D} \) and not belonging to an uncertain region. For instance, in Example 2 none of the query points fail both on representation and on uncertainty; hence neither has a high SDT score. On the other hand, a high SDT score for a query point \( q \) provides a strong warning signal that one should perhaps reject the model outcome and not consider it for decision-making.

SDT is a strong signal that raises warning only for the fearfully-concerning cases that fail both on representation and uncertainty. However, as observed in Example 2 a query points failing at least one of these conditions may also not be reliable, at least for critical decision making. We define the weak distrust measure to raise a warning for such cases.

**Definition 2 (Weak distrust measure (WDT)).** The weak distrust measure is a probabilistic measure that considers the outcome of a model for a query point \( q \) untrustworthy if \( q \) is not represented by \( \mathcal{D} \) or it belongs to an uncertain region. Formally, the weak distrust measure is computed as follows:

\[
WDT(q) = P((q \text{ is outlier}) \lor (q \text{ belongs to uncertain region}))
= P_o(q) + P_u(q) - P_o(q) \times P_u(q)
\]  

\[\tag{6}\]

5 IMPLEMENTATION OF THE MEASURES

5.1 Lack of Representation Oracle

The first component of the distrust measures identifies if the data set \( \mathcal{D} \) misses to represent the query point \( q \). The oracle returns the probabilistic measure \( P_o \), indicating if \( q \) is an outlier in \( \mathcal{D} \). Different techniques have been proposed to identify the outliers and the anomalies [16, 19, 26, 49, 61] of a data set. The distrust measures proposed in this paper are agnostic to the choice of the outlier detection technique, and alternative approaches that can compute \( P_o \) are equally applicable. Still, we note that existing approaches are designed to identify the entire set of outliers of a given data set. Conversely, our goal is to determine if a given query point \( q \) is an outlier in \( \mathcal{D} \). As a result, those approaches are inefficient for our goal. Besides, existing approaches such as [11] often require extensive parameter tuning, and those are usually not probabilistic. Therefore, this section provides a new approach for computing the probability \( P_o \), indicating if \( q \) is an outlier. In particular, we follow the existing work [11, 16, 26, 61] by considering the \( k \) nearest neighbors of \( q \) in \( \mathcal{D} \) for studying if it is an outlier.

Given a distance metric \( \Delta \), let \( \rho_q = \Delta_k(q, \mathcal{D}) \) be the distance of the \( k \)-th nearest tuple in \( \mathcal{D} \) to \( q \). Considering euclidean\(^3\) distance measure for \( \Delta \), \( \rho_q \) is the radius of the \( k \)-vicinity of \( q \), the tight hypersphere (circle in 2D) centered at \( q \) that includes exactly \( k \) tuples from \( \mathcal{D} \). For example, Figure 3 shows the \( k \)-vicinity of the query points \( q^1 \) to \( q^4 \) in Example 2. It is easy to see that smaller values of \( \rho_q \) correspond to denser \( k \)-vicinities around \( q \), meaning that the data set \( \mathcal{D} \) is more representative of the query point. We use this observation to develop the lack of representation component \( P_o \). That is, we consider the \( k \)-vicinity of \( q \) and the value of \( \rho_q \) to identify whether or not \( q \) is represented by \( \mathcal{D} \).

In particular, we would like to develop the function \( O : \mathbb{R} \rightarrow [0, 1] \) that given the value of \( \rho_q \) returns the probability \( P_o(q) \). That is, \( P_o(q) = O(\Delta_k(q, \mathcal{D})) \). The function \( O \) takes a distance value as the input and returns a probability indicating if the query point with that \( k \)-vicinity radius is not represented by \( \mathcal{D} \). It is clear that as the distance values increase, the probability \( P_o \) should monotonically increase as well. However, translating the distances to the probabilities is unclear and may vary from one data set to another.

Our idea is to learn the function \( O \) using the tuples in the data set \( \mathcal{D} \). Specifically, we note that the probability of sampling an outlier tuple according to the underlying distribution \( \xi \) is low, and hence most of the tuples in \( \mathcal{D} \) are not outliers. Therefore, the comparison
between $\rho_0$ and the k-vicinity radii of the tuples in $\mathcal{D}$ can reveal if $q$ is an outlier. As a result, instead of directly translating the distance values to probabilities, we can first identify the rank of $\rho_q$ in comparison with other tuples in $\mathcal{D}$ and use this information to specify if $q$ is an outlier. For example, if $\rho_q$ is smaller than more than half of k-vicinity radii of the tuples in $\mathcal{D}$, one can conclude that $q$ is not an outlier. On the other hand, if $\rho_q$ is larger than the k-vicinity radii of all tuples in $\mathcal{D}$, it should be an outlier. Besides, it is often the case in practice that data sets are associated with information such as outlier ratio, showing approximately what percentage of its samples are outliers. We use such information to develop the function $O$.

In particular, since the ratio of the outliers in $\mathcal{D}$ is often an estimation by the experts, we consider a Normal distribution $\mathcal{N}(\mu, \sigma)$, where the user-specified outlier ratio is $(1 - \mu)$ and $\sigma$ is the standard deviation specifying the outlier ratio estimation variance. Figure 4 demonstrates such a distribution as a bell curve centered at one minus expected outlier ratio. Note that we define the probability distribution on the ratio of outliers in $\mathcal{D}$ instead of directly defining it on the distance values.

Let $\Gamma_D$ be the multi-set (including duplicate values) of k-vicinity radii of the tuples in $\mathcal{D}$. Let $r_q$ be the percentage of values in $\Gamma_D$ that are not larger than $\Delta_k(q, \mathcal{D})$. That is

$$r_q = \frac{|\{r \in \Gamma_D | r \leq \Delta_k(q, \mathcal{D})\}|}{n} \quad (7)$$

The query point $q$ is an outlier if its k-vicinity radius falls within the range of outlier radii. That is, if the boundary of outlier values in $\Gamma_D$ is smaller than $r_q$, $q$ is considered an outlier. Now to compute the probability $P_o(q)$, the function $O$ can use the probability distribution $\mathcal{N}(\mu, \sigma)$. As shown in Figure 4, $P_o(q)$ is the probability that the outlier boundary $r$ is less than or equal to $r_q$, i.e., $P_o(q) = \mathbb{P}(r \leq r_q)$.

Converting the values to the standard-Normal distribution and using the $Z$-table:

$$P_o(q) = \mathbb{P}(r \leq r_q) = Z\left(\frac{r_q - \mu}{\sigma}\right) \quad (8)$$

To further elaborate on how $P_o(q)$ is computed, let us consider the following example:

**Example 3:** Consider the 2D data set $\mathcal{D}$ with $n = 10$ tuples shown in the table of Figure 5. In addition to the tuple values on $x_1$ and $x_2$, the table also includes the k-NN ($k = 2$) of the tuples and the radius $\rho$ of their k-vicinity. Let the outlier ratio of the data set be 20% ($\mu = 1 - 0.2 = 0.8$) with a standard deviation of $\sigma = 0.1$. Now consider the query point $q = (0.81, 0.76)$. The 2-NN of $q$ are $\{t_1, t_6\}$, and $\rho_q = 0.286$. Looking at the last column of Figure 5, only $t_6$ has a larger k-vicinity radius than $\rho_q$, i.e., for 90% of tuples the k-vicinity radius is smaller than $\rho_q$. Therefore, using Equation 8, $P_o(q) = Z((0.9 - 0.8)/0.1) = 0.84$.

Computing Equation 8 requires (i) computing $\Delta_k(q, \mathcal{D})$, which requires finding the k-NN of $q$, and (ii) computing the value of $r_q$. The baseline approach for computing these values makes a linear pass over $\mathcal{D}$ to identify the k-NN of $q$. Besides, it requires $O(n^2)$ to compute the multi-set of k-vicinity radii $\Gamma_D$ for the tuples in $\mathcal{D}$ and then it needs $O(n)$ to make a pass over $\Gamma_D$ to compute $r_q$.

However, given the interactive nature of query answering for ML systems and potentially large size of $\mathcal{D}$, we are interested in designing an algorithm that runs in a sublinear time to $n$. Theoretically speaking, finding the $k$ nearest neighbors of a point can be done in $O(\log n)$ using k-voronoi diagrams\footnote{A k-voronoi diagram is a partitioning of the query space into convex cells where the k-NN of all points in each cell is the same set of tuples.} [5, 14, 21, 47], while constructing the k-voronoi cells takes polynomial time for a constant number of dimensions [5, 25] ($O(k^2 n \log n)$ for 2D [47]). Besides, practically efficient algorithms have been proposed [36, 72, 79], construct data structures in preprocessing time that enables identifying k-NN is near-logarithmic time. We rely on the off-the-shelf techniques for finding the k-NN of a query point.

During the preprocessing time, we first construct the k-NN data structure. Next, for every tuple in $\mathcal{D}$, we identify its k-vicinity radius and add it to the list $\Gamma_D$. Finally, to quickly identify the value of $r_q$ in query time, we sort the list $\Gamma_D$.

The preprocessing algorithm and the function for identifying $P_o(q)$ are provided in Algorithm 1. To compute $r_q$ for a query point $q$, the algorithm first finds the k-vicinity of $q$ and identifies the tuple in $\mathcal{K}$-vicinity with maximum distance from $q$. Next, it applies a binary search on the sorted list $\Gamma$ to identify the number of cells
Algorithm 1

Input: data set $D$; $k$; expected outlier ratio $r$; standard deviation $\sigma$; query point $q$

1: function $\text{preprocess}(D, k)$
2: $M \leftarrow$ build the $k$-NN index of $D$; $\Gamma \leftarrow [ ]$
3: for $t \in D$ do
4: $V \leftarrow k$-NN$(t)$
5: add $\max_{t' \in V} \Delta(t, t')$ to $\Gamma$
6: return $M$, sort($\Gamma$)

7: function $\mathcal{P}_u(q)$
8: $\rho_q \leftarrow \max \{ \Delta(q, t'), \forall t' \in k$-NN$(q, M) \}$
9: $r_q \leftarrow \frac{1}{n} \text{binary search}(\rho_q, \Gamma)$
10: return $\mathcal{Z}^T\Delta(y - \mu)$

in $\Gamma$ that have a value not larger than $\rho_q$, and use it to compute $r_q$. At last, it uses Equation 8 and returns the value of $\mathcal{P}_u(q)$.

Let $T_n$ be the time to construct the $k$-NN index. Also, let $T_{kn} = O(\log n)$ be the time to identify the $k$-NN of a query point, using the constructed index. The preprocessing function constructs the $k$-NN index, identifies the $k$-NN of each tuple in $D$, and finally spends $O(n \log n)$ to sort the list $\Gamma$. Therefore, the total preprocessing time is $O(T_n + n^2)$. Computing $\mathcal{P}_u(q)$ requires $T_{kn}$ to identify the $k$-NN of $q$ and $O(\log n)$ for the binary search. As a result, the time to compute $\mathcal{P}_u(q)$ is $O(T_{kn} + \log n) \approx O(\log n)$.

5.2 Lack of Certainty Oracle

After the lack of uncertainty oracle, we now turn our attention to the uncertainty oracle that, given the query point, the data set $D$, and the target variable $y$, returns $\mathcal{P}_u$, the probabilistic measure that indicates if $q$ belongs to an uncertain region. There has been extensive research, and there exist different metrics for computing uncertainty, namely, entropy, Gini impurity, Brier score, and probability calibration [15, 17, 30, 57, 68]. Indeed, we are agnostic to the choice of the technique for developing the uncertainty oracle, and any method that can compute the probabilistic measure $\mathbb{P}_u$ is equally applicable. Even so, in the rest of this section, we provide a development of the uncertainty oracle, following the technique proposed in § 5.1. Similar to § 5.1, we use the $k$-vicinity of a query point $q$ as the region for studying uncertainty.

Binary classification is among the most popular ML tasks. A straightforward approach for developing the uncertainty oracle for such cases is to use the Shannon entropy ($\mathcal{H}$) [68]. Let $y_1, \ldots, y_t$ be the set of possible values for a target variable $y$. Known as a measure of uncertainty, the entropy of the random variable $y$ is

$$\mathcal{H}(y) = -\sum_{i=1}^{t} \mathbb{P}(y_i) \log \mathbb{P}(y_i)$$

(9)

Higher entropy values refer to higher uncertainty, while values close to zero indicate a high certainty in the value of $y$. For a binary variable $y$, the maximum value of entropy is one, and it refers to the cases where the probability of each value is 0.5. Using entropy to measure uncertainty for binary classification, we consider the set of tuples $V_k(q) \subseteq D$ in the $k$-vicinity of the query point $q$ and compute $\mathcal{P}_u(q)$ as the entropy among them. Let $p_1$ be the ratio of tuples in $V_k(q)$ with label 1. Then,

$$\mathcal{P}_u(q) = -p_1 \log p_1 - (1 - p_1) \log (1 - p_1)$$

(10)

Entropy can also be used for non-binary classification. However, when the cardinality of $y$ is larger than 2, entropy is not bounded by 1 anymore. While different approaches can be applied for transforming the entropy values to probabilistic measures, we choose a method similar to our proposal in § 5.1. That is, we use the uncertainty values in $k$-vicinities of the tuples in $D$ as an indicator showing if $q$ belongs to an uncertain region. Assuming that a model trained using $D$ has high accuracy (or it will not get deployed in practice), one can conclude if the model should perform well for a query point that its uncertainty is comparable with the uncertainty of the tuples in $D$. In other words, one can identify the tuples in $D$ that their uncertainty is considered outlier compared to other tuples in the data set. Let $r_u$ be the expected percentage of the tuples in $D$ that have an uncertain $k$-vicinity. We consider a Normal distribution $\mathcal{N}(\mu_u, \sigma_u)$ where $\mu_u = (1 - r_u)$ and $\sigma_u$ is the standard deviation of uncertain ratio estimation. During the preprocessing, we construct $\Gamma_{ud}$, the sorted list of uncertainty values for the tuples in $D$. Then, given a query point $q$, we first compute $\mathcal{H}(q)$, the uncertainty in the $k$-vicinity of the tuples in $D$. Then, applying a binary search on $\Gamma_{ud}$, we compute $r_u$, the ratio of uncertainty values in $\Gamma_{ud}$ that are not larger than $r_u$. Finally, converting the values to standard-Normal distribution, $\mathcal{P}_u(q)$ is computed as following:

$$\mathcal{P}_u(q) = \mathbb{P}(r \leq r_u) = \mathcal{Z} \left( \frac{r_u - \mu}{\sigma_u} \right)$$

(11)

The residual sum of squares (RSS) is a popular measure for regression. In regression trees [15], for example, the objective is to split the search space into regions with high certainty, where the RSS values in each region are minimized, i.e., the certainty in each region is maximized. We also use RSS for measuring $\mathcal{P}_u(q)$ for the regression tasks. Let $V_k(q) \subseteq D$ be the set of tuples in the $k$-vicinity of $q$. Also, let $m_{qy}$ be the average of $y$ values in $V_k(q)$.

That is, $m_{qy} = (\sum_{t' \in V_k(q)} y_t)/k$. Then the uncertainty around $q$ is computed as

$$\text{RSS}_q(y) = \sum_{t' \in V_k(q)} (y_t - m_{qy})^2$$

(12)

The process for computing $\mathcal{P}_u(q)$ is the same as the one for classification, with the only difference being that RSS should be used for computing uncertainty (instead of entropy).

The pseudo-code of the function $\mathcal{P}_u(q)$, along with preprocessing steps, are provided in Algorithm 2. Following a similar procedure as of Algorithm 1, the time to compute $\mathcal{P}_u(q)$ is $O(T_{kn} + \log n) \approx O(\log n)$. Using the functions $\mathcal{P}_o$ and $\mathcal{P}_u$, it takes a (near) logarithmic time to compute the uncertainty measures STD and WDT.

5.3 No Data Access During the Query Time

During the query answering phase, Algorithms 2 and 1 require to compute the $k$-vicinity radius and the entropy with the $k$-NN of a query point $q$. Although off-the-shelf $k$-NN indices are used to find this information, one could view it as requiring to access the training data after preprocessing. Our practical approach to address this is to learning these values. That is, to create two models that take as the input a query point as the input, returning the $k$-vicinity radii
and the entropy values. Creating these models requires sampling from the query space, i.e., to generate a large-enough training set with observations being i.i.d samples from the query space, while the target variables are the $k$-vicinity radius and entropy. On the positive side, one can generate an arbitrarily large training set by generating i.i.d sample queries and then computing the target values using their $k$-NN. On the flip side, however, as proven in [11], the theoretical upper bound on the number of samples needed is exponential. In other words, theoretically speaking, the size training set may need to be exponential in $d$ for adversarial cases, in order to guarantee a given error $\epsilon$. Fortunately, as we observe in our experiments, the theoretical upper bound is not tight, and in practice, the training set size is much smaller.

We still need to specify the proper training set size for our learning tasks. To do so, we design an exponential search algorithm as follows: the algorithm starts by setting the sample set size $N_0$ to an initial value ($O(n)$). It then collects $N_0$ i.i.d samples $S$ from the query space and finds the $k$-vicinity of each sample $s_i$ and identifies the $k$-vicinity radius$^5$ of $s_i$ as $r_i \leftarrow \max \Delta(s_i, t')$, $\forall t' \in k$-NN($s_i$). Next, the algorithm builds a regression model $M$ using $S$ as the training set. After building the model, the algorithm checks if $M$ has the error of at most $\epsilon$, for a user-specified error $\epsilon$. To check this, the model uses the test set $T$. If $error > \epsilon$, the algorithm doubles the sample size and repeats the process until it reaches the right sample size for $N_r$.

Let $Reg_0$ and $Reg_1$ be the trained regression models that return the $k$-vicinity radius and the $k$-NN entropy of a query point $q$, respectively. Then, the only changes in the proposed algorithms are (i) replace Line 8 of Algorithm 1 with $p_q \leftarrow Reg_0(q)$ and (ii) replace Line 8 of Algorithm 2 with $u_q \leftarrow Reg_1(q)$.

$^5$The process to learn the entropy values is the same as learning the $k$-vicinity radius.

6 EXPERIMENTS

We conduct comprehensive experiments on multiple synthetic and real-world data sets of diverse sizes and dimensions using a variety of models (Logistic Regression, K-Nearest-Neighbor, Artificial Neural Networks, Deep Neural Networks, ElasticNet, Random Forest, and SVM), and distance measures (Braycurtis, Canberra, Chebyshev, Cityblock, Manhattan and Euclidean) to validate the effectiveness and consistency of our proposal and evaluate the efficiency and scalability of our algorithms. In summary, our supplementary experiment (i) demonstrate the failure of existing work such as Conformal Prediction, Prediction Probabilities, and data coverage for cases that are not represented by the data, (ii) provide extended proof of concept experiments with large data sets and deep neural network models, and (iii) study the impact of similarity measures on the distrust values.

6.1 Experiments Setup

The experiments were conducted using a 2.5 GHz Quad-Core Intel Core i7 processor, 16 GB memory, running macOS. The algorithms were implemented in Python.

6.1.1 Data Sets. For evaluation purposes, we used (i) a collection of synthetic data sets and (ii) five real-world data sets for classification and regression.

Challenge: In the evaluation of our distrust measures, we needed to generate samples with different distrust values. However, since the tuples with high distrust values are unlikely to be drawn from the underlying distribution $\xi$, it is challenging to collect enough samples (as a test set) to evaluate the effectiveness of our measures. A comprehensive evaluation requires query points drawn uniformly from the query space to cover different parts of it. To achieve this, we need to have access to a ground truth oracle that for any given sample taken from the query space returns the value of target variable. However, finding a real-world data set in a context where the ground truth oracle exists (publicly) is challenging. To overcome this challenge, we take three directions: first, to have full control of the shape and complexity of the ground truth labels over different data sets, we generate synthetic data; second, we find a real-world data set and a third party (public) service that provides access to ground truth labels; and third, we find a very large data set that contains samples from different parts of the query space and apply sub-sampling on it. Next, we remove the outliers from each sample and split each cleaned sample into train and test sets, and add the outliers to the test set to cover larger parts of the query space.
Real Data Sets: We use multiple real data set, as briefly explained in the following:

- 3D Road Network (RN) [40]: Containing 434,874 records, this data set is used to predict the elevation of a location based on the coordinates.
- House Sales in King County (HS) [34]: A regression data set to predict the selling price of a house, containing 21,614 records over 21 attributes.
- Diamond (DI) [6]: A regression data set to predict the price of a diamond given its properties. It contains 53,941 records and 14 attributes.
- Default of Credit Card Clients (DCC) [81]: A binary classification data set with 30,000 records and 23 attributes to predict whether an individual pays their default payment.
- Adult (AD) [44]: A binary classification data set (containing 32,561 records with 14 attributes) to predict whether an individual makes more than $50K annually.

Synthetic (SYN) Data Sets: To fully investigate the relationship between the distrust measures and the model performance, we generated a collection of 60 data sets and repeated each experiment 60 times, using different data sets. Each data set is a random sample following a 2D Gaussian distribution with $\mu = [0, 0]$ and $\Sigma = \begin{bmatrix} 6 & 4 \\ 3 & 1 \end{bmatrix}$ over the input space $x = (x_1, x_2)$ where $x_1$ and $x_2$ are positively correlated and the output space is the binary label $y$ with values $\{-1, +1\}$. To create the binary classes for each data set, we randomly moved the samples over each shape in Figure 6 in a way that the sample and shape have an intersection. As a result, each shape is the ground truth for 15 data sets but with different placements. A data point belongs to $-1$ class, if it falls into the corresponding shape, otherwise, it belongs to the $+1$ class. To address what we discussed in the evaluation challenge, we create a uniform sample of size 6400 over $[0, 1]$ and will label the points with respect to each shape and its placement in the space, generating a total of 60 uniform samples corresponding to each data set. In particular, following Example 2, we consider a binary classification task over the observation variables $x_1$ and $x_2$. We chose a 2D setting for visualization purpose.

All continuous values used are normalized in the range $[0, 1]$, using $(x_i - \min)/(\max - \min)$ and the non-ordinal ones are one-hot encoded using scikit-learn OneHotEncoder.

Default values: To evaluate the performance of our algorithms under different settings, we vary the value of a parameter, while fixing the value of the other ones. The default value for neighborhood size $k$ is 10. The outlier ratio $c$ is set to 0.1 suggesting that a mean $\mu = 0.9$ is chosen for outlier distribution with a standard deviation $\sigma = 0.1$. We adopt a technique proposed in [80] to jointly tune $k$ and $c$ parameters for a given data set. The tuning procedure for these two parameters alongside uncertainty ratio parameter $\alpha$ is discussed in detail in the appendix. The default value for $d$ (number of attributes) is 2 for SYN and RN data sets, while it is 20, 18, 9, and 14 for DCC, HS, DI, and AD respectively. The default value of $n$ (size of data set) for the SYN, RN, HS, DCC, DI, and AD data sets are 1000, 10000, 10000, 5000, 43150, and 32560. The uncertainty ratio $\alpha$ is set to 0.1, therefore, a mean $\mu_u = 0.9$ is chosen for uncertainty distribution with a standard deviation $\sigma_u = 0.1$.

6.2 Proof of Concept

We start our experiments by evaluating the effectiveness of distrust measures across different data sets, ML models, and different parameters. Since the distrust measures are task-independent, we perform the effectiveness validation experiments for both classification and regression tasks. For the classification tasks, we use SYN and DCC data sets and for the regression tasks, we employ RN and HS data sets. To demonstrate the effectiveness of the distrust measures we first provide a visual validation, using one of the 2D SYN data sets. We then present a comprehensive validation over all our data sets by providing the correlation between the distrust values and the performance of an ML model’s prediction on the same data. To do so, we deliver the results as bar graphs in which the x-axis is a bucketization of the ranges of the distrust measures and the y-axis is the ML model’s evaluation score. Each bar represents the performance of the ML model for all the tuples that have a distrust value in the same range as the bar.

Visual validation: Consider the 2D data set $D$ shown in Figure 7a. $D$ is borrowed from SYN as one of the 60 data sets with the shape of the cat as the ground truth (we obtained similar results for other data sets, as reflected in the aggregate values we shall report next). We compute SDT and WDT values for each query point in the uniform sample over the space using the default settings. In Figures 7b and 7c, the query space is colored by assigning a tone based on the corresponding values of SDT and WDT respectively. As shown in Figure 7b, the untrustworthy regions are the set of query points in the space that are both outliers with respect to the tuples in $D$ and also uncertain since the entropy in their $k$-vicinity is high. On the other hand, in Figure 7c, the untrustworthy regions are the set of query points that are either outliers or uncertain. The closer the color to red, the more trustworthy the region will be and the opposite goes for green. Next, we train an arbitrary classifier (LR in this case) on data set $D$ and evaluate the model’s prediction. In this regard, we bucketize the uniform query space in a $10 \times 10$ grid and we evaluate the model for each cell to see where it fails short and then we create a heatmap on top of the grid based on the values for each cell. Results are provided in Figures 7d and 7e. In a side-by-side comparison between the heatmaps and the colored space based on SDT and WDT, it is easy to see that the model is failing in the regions where the distrust measures are producing large values. Finally, we generate the bar graphs with a similar procedure as later discussed in 6.2 and are shown in Figures 7f and 7g. As the distrust value increases, the F1 score of the model drops while the FPR rises meaning that, the model fails for the regions that are untrustworthy with regard to our distrust measures. In Figure 7f, as SDT increases, the performance measures for the model rapidly drop, and for the 0.5-0.6 bucket, F1 is near zero. This confirms that while WDT is a weaker warning, SDT should be viewed as a red flag.

Validation on Classification: Having provided the visual validation results, we next validate our distrust measures on classification tasks. In this regard, using SYN data set, we first computed the distrust measures for all the query points in the uniform sample and bucketized the points with respect to their distrust values in
ranges of length 0.1. We repeated this for both SDT and WDT measures. Next, using a classification model that we trained on the (training) data set, we predict the model’s outcome for the points in each range of distrust measure. The performance of the classifier over each bucket of distrust values is provided in Figure 7h and 7i for SDT and WDT respectively. As the distrust values increases, the accuracy of the model drops while the FNR and FPR rise, and therefore, the model fails to capture the ground truth for the points that fall into untrustworthy regions in the data set.

To also perform the experiments on a real-world data set, we next used the DCC data set with a similar procedure. The results are shown in Figure 7j and 7k and they follow the same course as the previous experiment.

We repeated the experiments with 5 classification algorithms including, Logistic Regression (LR), K-Nearest-Neighbor (k-NN),
Neural Networks (NN), Random Forest (RF), and SVM. All the classifiers underwent a hyper-parameter tuning procedure to achieve optimal prediction performance. We confirm that we obtained similar results in all cases and that all models failed to perform satisfactorily for query points that have a high distrust value. Hence, we provide the results for the NN model, the more advanced and powerful model. Depending on the results of the classification, we chose the most appropriate performance measures that indicated the behavior of the model. For example, if the results were dominated by TPs and TNs, accuracy is the measure that best describes the model, otherwise, F1 might be a better choice. Depending on the number of FPs and FNs and the balance between them, the same rule applies to FPR and FNR measures.

Validation on Regression: In this experiment, we study the effectiveness of our distrust measures in the regression tasks. Accordingly, we used RN and HS data sets and computed SDT and WDT distrust values for all the query points in the uniform sample. Thereafter, we repeated the bucketization process as we did in the last experiment, and having trained a regression model over the data set, we evaluate the model’s prediction over the tuples from each bucket. The results are presented in Figures 7l, 7m, 7n and 7o. As the distrust value increases, the RSS of the regression model follows the same trend denoting that the model fails to perform for tuples with a high distrust value. We repeated the experiments with 3 different regression algorithms including ElasticNet, DT, and k-NN, all three with tuned hyper-parameters. Regardless of the regression model, the outcome was similar and therefore we only report the results for the k-NN regressor.

Summary of Proof of Concept: In short, experiments consistently demonstrate that as the distrust values grow, the ML models fail more to capture the truth for the corresponding regions. Consequently, when distrust values for a query point in a data set are high, one should discard or at least not rely on the outcome of the model constructed on it for critical decisions.

6.3 Comparison with the Existing Work
We used synthetic data with three labels to conduct experiments with the existing work. To do so, we trained a probabilistic classifier (Gaussian Naive Bayes) on it. Figure 8a shows the WDT values, while Figures 8b and 8c show the prediction labels and prediction probabilities for the class orange, respectively. From the results, the probabilities show a confident prediction for the query point q that is not well-represented in D. Similarly, conformal predictions (Figure 8d) provide a single label (confident prediction) for q. However, this is only valid if the true decision boundary is identical to the one estimated by the base classifier and as previously discussed in section 4.1, this may not always be the case if the distribution between training data and production data vary. Therefore, model-centric techniques such as conformal prediction and prediction probabilities fail to detect such points as not-reliable. On the other hand, as reflected in [67] data coverage failed on detecting uncertain regions. Besides it only returned a binary value sensitive to the choice of parameters.

6.4 Performance Evaluations
After demonstrating the effectiveness of the distrust measures, we now focus on the performance of our algorithms. In this section, we use the DCC and RN data sets to evaluate the time efficiency of algorithms. We obtained similar results with almost identical plots for both classification and regression tasks. In the following, we present the results for classification tasks using DCC data set with different settings, while extensive experiment results (for other data sets, tasks, and parameters) are provided in the appendix.

6.4.1 Query Time. The query time consists of (i) the time to find the k-vicinity of the query point q and identifying the tuple in k-vicinity that has the maximum distance from q, and (ii) the time to apply binary search on the sorted multi-sets.

Varying n: To study the impact of the number of tuples n on the performance of the query time, we gradually increase the size of the data set from 50 to 100K. The results are provided in Figure 9a. The total query time is dominated by the first bottleneck, and the time to binary search the lists are negligible compared to it. In our experiments, the query time did not (meaningfully) change as the data set size increased, showing the scalability of our algorithm to the very large settings.

Varying d: We next study the impact of the number of attributes d by varying it from 2 to 20. The results in Figure 9b verify the scalability of our algorithms with respect to the number of dimensions.

6.4.2 Preprocessing Time. Our preprocessing time consists of two parts. The first is the time to build the k-NN data structure, identifying the k-vicinity radius (in Algorithm 1) and computing uncertainty (in Algorithm 2) for each tuple in the data set. The second one is the time to construct the sorted multi-sets of k-vicinity radii and uncertainty values. We use the exact k-vicinity radii and entropy values in this experiment.

Varying n: In this experiment, we study the impact of the number of tuples n in the data set on the preprocessing time by gradually increasing the size of the data set from 50 to 100K. We then measure the time to build the k-NN data structure and construct the sorted multi-sets. The results are provided in Figure 9c. The total preprocessing time is dominated by the time to build the k-NN data structure and the time to build the multi-sets is almost negligible compared to it. Nevertheless, the cumulative preprocessing time was small enough that the algorithm could scale to larger settings, finishing in less than a second for n=100K.

Varying d: To study the impact of the number of attributes d of the data set on the preprocessing time, we gradually change d from 2 to 20. The results are brought in Figure 9d. Like the previous settings, the total preprocessing time is dominated by the time to build the k-NN data structure and the algorithm linearly scales to larger settings, finishing in less than 3 seconds for d=20.

6.4.3 Training Regression Models for No Data Access. In this experiment, we study the efficiency of the training process for building the regression models to estimate the values of k-vicinity radius and entropy. As explained in §5.3, we apply exponential sampling to generate the right amount of data such that the trained models satisfy the user-specified error. As a heuristic, we generate a
fraction of samples uniformly and the others from the underlying distribution of the training data using GAN methods or Gaussian copula distribution functions [58]. Figure 7p illustrates the monotonic drop in the error of both regression models trained to predict the entropy and $k$-vicinity radii of query points (as discussed in section 5.3), as the number of synthetic i.i.d samples increases. Since both entropy and $k$-vicinity radii values are in the range of [0,1], selecting a sufficiently small (RMSE) error threshold (e.g. $10^{-3}$ or $0.01\%$ average difference between the actual and predicted values) guarantees not going overboard with generating too many samples (affecting preprocessing time) while achieving good prediction accuracy.

7 CONCLUSION
Towards addressing the need for trustworthy AI, in this paper, we proposed distrust measures as the warning signals that limit datasets’ scope of use for predicting future query points. These measures are valuable alongside other techniques for trustworthy AI. We proposed novel ideas for the effective implementation of distrust measures and designed efficient algorithms that scale to very large, high-dimensional data. Our comprehensive experiments on real-world and synthetic data sets validated our proposal and verified the scalability of our algorithms with sub-second run times.
\[ T_{c,k} = \frac{\mu_{\text{out}}(c,k) - \mu_{\text{in}}(c,k)}{\sqrt{|cn|^{-1} (\sigma^2_{\text{out}}(c,k) + \sigma^2_{\text{in}}(c,k))}} \]

If \( c \) is known, it is enough to find \( k^*_c = \arg \max_k T_{c,k} \) that maximizes the standardized difference between the outliers and inliers for the corresponding \( c \). Otherwise, we assume that \( k \)-vicinity radii form a random sample following a Normal distribution with the mean \( \mu_{\text{out}}(c,k) \) and variance \( \sigma^2_{\text{out}}(c,k) \) for outliers, and one with mean \( \mu_{\text{in}}(c,k) \) and variance \( \sigma^2_{\text{in}}(c,k) \) for the inliers. Then given a value of \( c \), \( T_{c,k} \) approximately follows a non-central \( t \) distribution with degrees of freedom \( df_c = 2 |cn| - 2 \) and the non-centrality parameter:

\[ ncp_c = \frac{\mu_{\text{out}}(c,k) - \mu_{\text{in}}(c,k)}{\sqrt{|cn|^{-1} (\sigma^2_{\text{out}}(c,k) + \sigma^2_{\text{in}}(c,k))}} \]

We cannot directly compare the largest standardized difference \( T_{c,k}^* \) across different values of \( c \) because \( T_{c,k} \) follows different non-central \( t \) distributions depending on \( c \). Instead, we can compare the quantiles that correspond to \( T_{c,k}^* \) in each respective non-central distribution so that the comparison is on the same scale. To do so, we define \( c_{opt} = \arg \max_c \mathbb{P}(z < T_{c,k}^*; df_c; ncp_c) \), where the random variable \( z \) follows a non-central \( t \) distribution with \( df_c \) degrees of freedom and \( ncp_c \) non-centrality parameter. \( c_{opt} \) is where \( T_{c,k}^* \) is the largest quantile in the corresponding \( t \) distribution as compared to the others.
A.0.2 Tuning Uncertainty Ratio Parameter. The next parameter we need to tune is the uncertainty ratio $u$, which estimates what percentage of data belongs to uncertain regions. Similar to the outliers ratios that help us transform the $k$-vicinity radii to probabilities, the expected uncertainty ratio $u$ helps us transform an uncertainty value in a $k$-vicinity to a probability. We consider the distribution of uncertainty values within the $k$-vicinity of tuples in $D$ for identifying $u$. To explain the intuition behind this choice, let us consider a classification task. While the uncertainty for the tuples far from the decision boundary should be low, the uncertainty suddenly increases as one gets close to the boundary. As a result, looking at the distribution of uncertainty values, one should be able to identify an estimation of $u$ by finding the sharp slope in the distribution of uncertainty values. Following this intuition, we calculate the $k$-vicinity uncertainty for each tuple in $D$, and create the reverse cumulative distribution $V : [0, 1] \rightarrow \mathbb{R}$ such that, for every value $r$, the ratio of tuples in $D$ with an uncertainty value larger than $V(r)$ is $r$. For example, $V(0.1)$ returns the value $u_{0.1}$ such that the uncertainty for 10% of tuples is larger than it. We then identify the knee of this function (the sharp decrease in $V(r)$) as the estimated uncertainty ratio. As a rule of thumb in our experiments, we observe that the knee falls around 10-15%.

B EXPERIMENTS

B.1 Data Sets

B.1.1 Regression Real Data Sets. In this section we discuss the details of the regression data sets used in the experiments:

3D Road Network (RN) Data set [40] is a benchmark data set for regression that was constructed by adding elevation information to a 2D road network in North Jutland, Denmark. It includes 434,874 records with attributes Latitude, Longitude, and Altitude. We took 30 samples of size 10000 from RN data set and generated 30 data sets and repeated each experiment 30 times, using different data sets. To address the evaluation challenge for RN data set, we generated a uniform sample of 6400 points $(x_1, x_2)$ in the range $[0, 1]$. We then transform the uniform samples back to the same space as the points in RN. Then, we used an off-the-shelf APP that given every coordinate (Latitude, Longitude) in the data space, it yields the corresponding Altitude as the oracle to obtain the ground truth values.

House Sales in King County (HS) Data set [34] is a regression data set for house sale prices for King County (Seattle). It includes houses sold between May 2014 and May 2015. It includes 21614 records having 21 attributes with 2 categorical and 16 continuous types. Given attributes such as no. of bedrooms, square footage, floors, etc. the task is to predict the price of the house. We took 30 samples of size 10000 from HS data set and generated 30 data sets and repeated each experiment 30 times, using different data sets. To address the evaluation challenge for HS data set, for each sample, we removed the outliers and then split the data set into train and test sets, and then added the outliers back to the test set. Although with HS we can not measure the distrust values for the whole query space, we believe the findings can still confirm the effectiveness of our measures.

Diamond (DI) Data set [6] is a regression data set for predicting the price of diamond given some visual properties. This data set has 53941 records with 14 attributes, 6 of which are continuous and 3 categorical. We used a similar approach to HS data set for utilizing DI in our experiments.

B.1.2 Classification Real Data Sets. In this section we discuss the details of the classification data sets used in the experiments:

Default of Credit Card Clients (DCC) Data set [81] is a data set for classification that was constructed from payment data in October 2005 from an important bank in Taiwan and the targets are the credit card holders of the bank. The data set is binary class with - default payment (Yes = 1, No = 0), as the response variable. Among the 30000 records, 6636 (22.12%) are the cardholders with default payment. The data set has 23 features (9 categorical and 14 continuous) including credit line, age, gender, education, history of payment, amount of bill statement, amount of the previous statement, etc. Since it was not feasible for us to devise a function that can produce the ground truth for DCC, we took a sample of size 15000 from the data set and then split it into two sets of train (5000 tuples) and test (10000 tuples) and used the test set as a substitute for the uniform sample over the query space. Following the same procedure, we generated 30 data sets and repeated each experiment 30 times, using different data sets. Similar to HS, we can not measure the distrust values for the whole query space in DCC, yet the findings can still confirm the effectiveness of our measures.

Adult (AD) Data set [44] is a well-known benchmark data set for classification tasks predicting whether income exceeds $50K annually based on census data. This data set has 32561 records with 14 attributes, 6 of which are continuous and 8 categorical. We used a similar approach to HS data set for utilizing AD in our experiments.

B.2 Additional Proof of Concept Experiments

We extended our experiments to two other data sets, AD and DI, and repeated the experiments with identical settings as before. The results are shown in Figures 10a, 10b, 10c and 10d, verifying our findings in the main experiment section. For tuples with high distrust values, models tend to fail more to perform well. Next, we repeated the experiments on the aforementioned data sets, using Deep Learning models. Both models went through a parameter-tuning process. For DI we built a regression model with four hidden layers of size 128, 64, 32, and 16 respectively. For AD, we trained a classification model with two hidden layers of size 64 and 32 units respectively. The results are illustrated in Figures 10e, 10f, 10g, 10h and are compliant with our previous experiments, showing that even with the choice of more complex models, they still fail for query points with high distrust values.

B.3 Conformal Prediction: A Case Study

In this section, we perform a case study using conformal prediction (CP), and through experiments, we demonstrate that model-centric techniques may fall short for some query points. Consider data set $D$ as shown in Figure 11a created with three Gaussian distributions representing classes red, blue, orange. An arbitrary classification model (e.g. Gaussian Naïve Bayes classifier) is trained on $D$ and the predicted results are depicted in Figure 11b. Next, we employ the CP framework with confidence level $\alpha$ of 0.2, 0.1, and 0.05 and softmax
Therefore, although $q$ is in an uncertain region, CP fails to capture the distrust associated with $q$ as it is an outlier, yet does not belong to an uncertain region.

B.4 Prediction Probabilities: A Case Study

In this section, we perform a case study on the prediction probabilities generated by probabilistic classification models and demonstrate their failure for query points that are not represented by data. To do so, we employ data set $\mathcal{D}$ (Figure 11a) and train an arbitrary probabilistic classifier such as Gaussian Naive Bayes on it (remember that we can use any classifier, however, if the model is not intrinsically probabilistic, we need to make sure that the probabilistic outcomes are calibrated). Figures 12a, 12b, and 12c show the prediction probabilities assigned to either of the classes red, blue and orange. As it can be observed, prediction probabilities fail to capture query points that belong to unrepresented regions and assign a negligible chance of belonging to any other class but the one determined by the decision boundary, however, this is only true if the true decision boundary is identical to the one estimated by the base classifier and as previously discussed in section 4.1, this may not always be the case if the distribution between training data and production data vary.

B.5 Data Coverage: A Case Study

In this section, we conduct a case study on the capacity of data coverage techniques to create proper warnings and demonstrate their failure for query points that are in uncertain regions. To this end, using the continuous notion of data coverage [11] and tuned parameters of $k = 50$ and $\rho = 0.08$, we identify the uncovered region on data set $\mathcal{D}$ as illustrated in Figure 13. While the uncovered region can raise warning signals for the unreliability of underrepresented query points, it fails to capture the unreliability associated with the uncertain regions (regions close to the decision boundary in the case of data set $\mathcal{D}$). Furthermore, even for the query points in underrepresented regions, data coverage creates a binary value that is sensitive to the choice of parameters such as the radius $\rho$. This issue gets further highlighted considering the sharp transition from uncovered to covered, specified by the uncovered region’s decision boundary. As a result, while two points close to each other, where one is inside and the other outside of the decision boundary, are almost equally miss-presented, for one the output signal is covered (no warning at all) while the other is uncovered (maximum warning).

B.6 Studying the Impact of Distance Measures on The Distrust Values

In this experiment, we study the effect of the distance metric chosen to determine the neighborhood of a data point (in the $k$-NN component) on the distrust values. To do so, we employ data set $\mathcal{D}$ (Figure 7a) and calculate the distrust values for the entire query space with respect to six distance measures of braycurtis, canberra, chebyshev;
(a) The data set \( \mathcal{D} \) created using three Gaussian distributions.

(b) Predicted labels by a Gaussian Naive Bayes classifier.

(c) number of labels for \( \alpha = 0.2 \), softmax conformal score: null prediction sets for uncertain regions.

(d) number of labels for \( \alpha = 0.1 \), softmax conformal score.

(e) number of labels for \( \alpha = 0.05 \), softmax conformal score.

(f) number of labels for \( \alpha = 0.2 \), cumulative softmax conformal score.

(g) number of labels for \( \alpha = 0.1 \), cumulative softmax conformal score.

(h) number of labels for \( \alpha = 0.05 \), cumulative softmax conformal score: wide prediction sets for uncertain regions.

(i) Query space colored based on SDT values with regards to \( \mathcal{D} \).

(j) Query space colored based on WDT values with regards to \( \mathcal{D} \).

Figure 11: A case study on how CP techniques fail for certain query points.

cityblock, manhattan and euclidean. Although the distance metric is expected as an input in our implementation, however, the results as depicted in Figures 14a-14l, show general consistency across different measures.

**B.7 Performance Evaluations**

**B.7.1 Preprocessing Time.** We continue the preprocessing performance experiments as followed:

Varying \( k \): To study the impact of neighborhood size \( k \) on the preprocessing time, we vary \( k \) from 1 to 50. The results can be seen in Figure 15a. Similarly, the total preprocessing time in this experiment is also dominated by the time to build the \( k \)-NN data structure and the algorithm was efficient in all settings, finishing in less than a fraction of a second for \( k = 50 \).

**B.7.2 Query Time.** We continue the query performance experiments as followed:

Varying \( k \): Next, we vary the neighborhood size \( k \) from 1 to 50. The results in Figure 15b suggest that the query time is (almost) independent from the \( k \).

Varying \( c \): In our final experiment, we change \( c \) from 0.05 to 0.25. The results are brought in Figure 15c. Results verify that the query time is independent from the \( c \).
Figure 12: a case study on how prediction probabilities of classifiers trained on $\mathcal{D}$ in Figure 11a fail for certain query points.

Figure 13: a case study on how data coverage on data set $\mathcal{D}$ in Figure 11a fails for query points in uncertain regions.
Figure 14: query space colored based on WDT and SDT values with regards to $D$ in Fig. 7a subject to different distance metrics.

Figure 15: preprocessing performance evaluation results