Abstract

Correctly quantifying the robustness of machine learning models is a central aspect in judging their suitability for specific tasks, and thus, ultimately, for generating trust in the models. We show that the widely used concept of adversarial robustness and closely related metrics based on counterfactuals are not necessarily valid metrics for determining the robustness of ML models against perturbations that occur “naturally”, outside specific adversarial attack scenarios. Additionally, we argue that generic robustness metrics in principle are insufficient for determining real-world-robustness. Instead we propose a flexible approach that models possible perturbations in input data individually for each application. This is then combined with a probabilistic approach that computes the likelihood that a real-world perturbation will change a prediction, thus giving quantitative information of the robustness of the trained machine learning model. The method does not require access to the internals of the classifier and thus in principle works for any black-box model. It is, however, based on Monte-Carlo sampling and thus only suited for input spaces with small dimensions. We illustrate our approach on two dataset, as well as on analytically solvable cases. Finally, we discuss ideas on how real-world robustness could be computed or estimated in high-dimensional input spaces.

Keywords: Robustness, Black Box Models, Trustworthy AI, Testing of AI, Reliability

1. Introduction

“Robustness” is a term widely used in the context of machine-learning (ML) and statistics. In ML, it usually refers to how robust a model-prediction is to specific perturbations in the
input data. A widely studied field is adversarial robustness, closely related to adversarial examples (e.g. Szegedy et al., 2014; Goodfellow et al., 2015). Adversarial robustness (first described in Szegedy et al. (2014) for neural networks) deals with the susceptibility of an ML model to perturbations that were specifically crafted to “fool” the model - so called adversarial attacks. Here the threat-model is that an attacker starts from a correctly classified input (e.g. an image), and then modifies the input image with a minimal - often imperceptible - perturbation that still leads to a misclassification. These perturbations typically look random, but they are in fact not random and exploit specific characteristics of the ML model and/or the training data.

While adversarial robustness is an important topic, it only deals with a certain type of perturbations/attack-scenarios. In this paper, we deal with a different question: How can we assess the robustness of a ML-model to perturbations that are not crafted by an adversarial attacker, but that occur by chance and/or accident? We will call these perturbations real-world-perturbations. Such perturbations could occur - among others - from: noise, measurement errors, data-drift and data-processing errors. In this paper we will show that adversarial robustness is not necessary a valid measure for the robustness against such perturbations. Throughout this paper, the term real-world-perturbations will only refer to this type of perturbations.

It is impossible to completely separate our idea of real-world-perturbations from other central aspects in ML, namely generalization and distribution-shift. Additionally, the question of how to acquire a suitable test-set is related, as well as the concept of counterfactuals and the ideas behind data-augmentation (including test-time augmentation (Shanmugam et al., 2020)).

1.1 Contributions

We start our discussion with a different angle of view compared to earlier works and focus on the main question:

Given a trained ML application and a test-dataset, how can we assess the robustness to perturbations that could occur when deploying the model in a real application, but are not represented in the test set?

And more specifically:

How can we assess the robustness of a single test sample?

To answer these questions, in this paper we will

- define real-world-robustness in a mathematical way,
- argue why adversarial robustness and metrics based on counterfactuals are insufficient for determining real-world-robustness,
- show how to compute real-world-robustness for low-dimensional datasets,
- compare adversarial robustness with real-world-robustness in two examples,
- discuss issues surrounding transferring the ideas to high-dimensional problems.
Another major difference compared to earlier work is that our approach is independent (or in other words, completely ignorant) of the training data, and has thus to be differentiated from all related concepts that have something to do with training data (e.g. robustness to noise in training data). Our method starts from a trained classifier, where this classifier comes from does not matter. It could even be a “hand-coded” one (e.g. symbolic AI). Noise tolerance in this sense is for example also an issue of lifelong learning machines (Kudithipudi et al. 2022).

This work is addressed both to the research community and to practitioners in the growing field of testing and certifying AI-applications (Supreme Audit Institutions of Finland, Germany, the Netherlands, Norway and the UK, 2020; Winter et al. 2021). Therefore, this paper also aims to convey an intuitive understanding of the issues surrounding robustness of ML models.

1.2 Taxonomy

We use the term robustness in the above described meaning. It should be noted that sometimes robustness refers to how well a model works in other settings, and then the word reliability is used instead to describe the sensitivity to small changes in the input (e.g. in the NIST draft for a taxonomy of AI risk (NIST, 2021)).

2. Related Concepts and Related Work

In this section we discuss concepts that are related to our problem in the existing literature. A recent review (Huang et al., 2020) also gives a broad overview on safety and trustworthiness of deep neural networks with focus on related topics like verification, testing, adversarial attack and defence, and interpretability.

2.1 Adversarial Examples, Counterfactuals and Adversarial Robustness

Adversarial examples are samples of input for a ML classification system that are very similar to a normal input example, but cause the ML system to make a different classification. A typical example are images that are slightly modified (often so slightly that the difference is invisible by eye) and then lead to a misclassification. The concept is generic and not limited to image recognition systems. Such adversarial examples exploit certain properties of ML classifiers, and are explicitly and purposefully searched with specific algorithms (called adversarial attacks). There is a lot of discussion in the literature on why such examples do exist at all. In Szegedy et al. (2014) the authors suggested that adversarial examples could be of extremely low probability. If this is true, then one would not expect that they occur by chance (i.e. outside an adversarial attack scenario). Goodfellow et al. (2015), however, disputed this low-probability explanation of adversarial examples, and instead argued that they are caused by the local linearity of the neural networks. Other perspectives/explanations have been offered as well (Ilyas et al., 2019; Tanay and Griffin, 2016). There is also literature on “real-world adversarial attacks” that deals with adversarial attacks in real-world scenarios (Kurakin et al., 2017; Eykholt et al., 2018). This has, however, nothing to do with our definition of real-world-robustness, as it still considers the adversarial threat model.
Counterfactuals (also known as counterfactual explanations (Kment, 2006)) are very similar to adversarial examples. The idea is to find, for a given test data point, a different data point with a different classification (either with a different classification of a specified class, or with any classification different than the classification of the test point), under the constraint that this example should be as similar as possible as the original test point. It can thus be used for explaining classifications in a certain sense (“if feature x had a value of b instead of a, then the classification would be different”). Such examples are called counterfactuals. They have been first proposed in order to fulfill the “right to an explanation” in the General Data Protection Regulation (GDPR) (Wachter et al., 2018; Mittelstadt et al., 2019).

Adversarial examples and counterfactual explanations are highly related, up to the point that they are sometimes seen as the same thing with two different names. Undisputed is that both stem from the same mathematical optimization problem, and are thus mathematically the same thing. Whether they are also semantically the same is part of ongoing discussions as well. See Freiesleben (2021); Katz et al. (2017) for a thorough discussion on the topic. Here, we do not attempt to answer that question, but instead use the terms interchangeably, as for our setting the (potential) distinction is not important.

Usually, counterfactuals (and adversarial examples) require a pre-defined distance metric. However, Pawelczyk et al. (2020) proposed a method that learns a suitable distance metric from data. Many different methods for generating counterfactuals and adversarial examples are known. Ten alone are integrated into the CARLA python library (Pawelczyk et al., 2021), and additional ones in the Adversarial Robustness Toolbox (Nicolae et al., 2019). Some methods work only on specific model types, others on black box models (like CERTIFAI (Sharma et al., 2020)).

In our paper, we discuss adversarial examples and counterfactuals agnostic of they way they are be produced - we simply assume that they could somehow be obtained.

Together with the idea of adversarial attacks, the concept of measuring adversarial robustness emerged. This is a measure to quantify how robust (or susceptible) a classifier is to adversarial attacks. Two examples of ways to estimate adversarial robustness are the CLEVER score, which is an attack-agnostic robustness metric for NNs (Weng et al., 2018), and the CERTIFAI-robustness score for black box models, which assigns a robustness score for individual data points based on the distance to the closest counterfactuals using a genetic algorithm (Sharma et al., 2020).

2.2 Perturbation Theory and Interpretability Methods

If small perturbations are introduced to a physical system (e.g. noise, fluctuations, etc.) it is often very helpful to develop a truncated power series expansion in terms of these perturbations in order to find approximate solutions of the system. The perturbed system can then be described as a simpler (ideally mathematical directly solvable) system plus corresponding correction terms, a very common approach in quantum mechanics for example. The mathematical foundation behind is called perturbation theory and the general question of how (small) perturbations are affecting a system of interest is obviously also linked to our discussion here. While a direct assessment of a perturbation theoretic approach is beyond the scope of our paper, at least related concepts have found their way to modern machine
learning literature as well. Investigating the influence of perturbations of input data (Olden and Jackson, 2002) or analyzing machine model behaviour based on power series decomposition (Montavon et al., 2017) have been introduced especially in the field of explainable AI for example. One of the most popular methods to identify the influence of specific input features in the output of a machine learning model (so-called attribution methods) is based on perturbing the input. A description of CAPTUM, an open-source library for interpretability methods containing generic implementations of a number of gradient and perturbation-based attribution algorithms, as well as a set of evaluation metrics for these algorithms, can be found in Kohlikyan et al. (2020). Such approaches usually focus on “faithfulness”, e.g. the ability of a machine learning algorithm to recognize important features, instead of the overall robustness of the model.

2.3 Data Augmentation

Data augmentation are techniques to artificially create new training samples from existing training data. It is widely used in tasks that work with images, as for image recognition it is relatively easy to find modifications that change the image, but in a way that the image still contains the same semantic information. Data augmentation is used to prevent overfitting. Therefore, it is indirectly related to robustness, as the robustness of a classifier also depends on its generalization properties, but it cannot be used as a measure for robustness. Data augmentation is usually used during model training and not when the trained model is evaluated. There is, however, also the idea of test-time data augmentation (Shanmugam et al., 2020). Here “test-time” refers to making predictions with the model after training. This is used because it can help improve the predictions, but it is also only indirectly related to robustness.

2.4 Distribution Shift

Distribution shift (Federici et al., 2021; Bengio et al., 2019; Hendrycks et al., 2021) is the phenomenon when the training data does not completely represent the test data that is encountered in a real world application. A curated benchmark of various datasets reflecting a diverse range of naturally occurring distribution shifts (such as shifts arising from different cameras, hospitals, molecular scaffolds, experiments, demographics, countries, time periods, users, and codebases) can be found in Koh et al. (2021). Robustness against distribution shift (Taori et al., 2020) is closely related to the ability of a ML classifier to generalize to points beyond the training examples and also to overfitting as a counterpart to generalization.

Our definition of real-world robustness differs from distribution shifts, and it is not true in a general sense that models that generalize well are automatically robust within our real-world-robustness definition. Still, distribution shifts are also a relevant issue when determining real-world-robustness in our approach. We model possible real world distributions, but when the application is put in practice, it might be that the actual occurring perturbations are different - thus representing a distribution shift in the possible perturbations. Yet another similar topic is robustness towards out-of-distribution points (Yang et al., 2021), which focuses on unusual data that was not observed in the training dataset (e.g. a self-driving cat that detects a new object type it has never seen before).
2.5 Certification of Neural Networks

For neural networks (NNs) there is a lot of active research on finding formal guarantees and thus “proofing” that a network is robust to particular perturbations and/or fulfills other properties. This is often referred to as “verification” or “certification” (Singh et al., 2019). For example, it is possible to find robustness guarantees for NNs with defining hypercubes around test points, and then test whether the classification stays the same for all areas within this hypercube. At the moment, this is only possible with strong assumptions and restrictions on the possible perturbations (e.g. (Cohen et al., 2019; Singh et al., 2019)). Huang et al. (2017) proposed a method that can offer high guarantees, but under the restriction that input perturbations need to be discretized.

2.6 Robustness to Noise in Training Data

Sáez et al. (2016b) define robustness as “A robust classification algorithm can build models from noisy data which are more similar to models built from clean data.” This robustness against noise refers to the ability of the training algorithm to deal with noisy training data (noise can be on the features and/or on the labels). The Relative Loss of Accuracy (RLA) score proposed by Sáez et al. (2011) and the Equalized Loss of Accuracy (ELA) score proposed by Sáez et al. (2016a) are ways of measuring this type of robustness (specifically to noise on the class labels). This idea of robustness, however, is fundamentally different from our definition of robustness, which deals with robustness of the trained classifier against noise (and other perturbations) added to test samples. A systematic overview of the impact of noise on classifiers is given in Zhu and Wu (2004), and the effect of label noise on the complexity of classification problems in Garcia et al. (2015).

3. Methods

In this section we formalize our question on how to asses real-world-robustness, show why adversarial samples and counterfactuals are insufficient for that purpose, and discuss how to compute real-world robustness.

3.1 Adversarial Examples and Counterfactuals

Untargeted counterfactuals $x_c$ (or untargeted adversarial examples) with respect to a test point $x$ are defined via the following minimization problem (e.g. Freiesleben (2021)):

\[
\min d(x_c, x) \text{ subject to } f(x_c) \neq f(x),
\]  

where $d$ is a distance function that needs to be pre-defined and $f$ is the corresponding machine learning model.

There is also the concept of targeted counterfactuals or adversarial attacks, in which the goal is not only that the counterfactual has a different predicted label, but a specific different one. In this paper we only speak about untargeted counterfactuals and adversarial examples. For binary classification problems (which will be used in this study as examples), targeted and untargeted counterfactuals are per definition the same. Many different meth-
Real-world-robustness

Formally, our definition of real-world-robustness can be stated in the following way: given a trained machine learning model \( f \), a test-data point \( x_t \) and the accompanying predicted label \( y = f(x_t) \), how can we assess how robust \( y \) is to perturbations \( x' \) of \( x_t \)? We consider \( x' \) not in an abstract way (e.g., a hypersphere), but as originating from real-world processes. These can be, for example, noise or measurement errors.

We will use \( x' \) for the perturbation, and \( \hat{x} \) for the perturbed value, thus

\[
\hat{x} = x_t + x'.
\]

Further, the perturbations \( x' \) are not given in absolute values, but are described probabilistically, leading to a \( N \)-dimensional probability density function \( \hat{p}(x') \), which assigns a probability density to each point \( x \) in the input space of the model. The input space has dimension \( N \), where \( N \) is the number of input features. Additionally, as in the real world we cannot expect that potential perturbations are the same for all data-points, we introduce \( \hat{p} \) as a function dependent on \( x_t \)

\[
\hat{p}(x') \rightarrow \hat{p}(x_t, x').
\]

Thus each test-point \( x_t \) gets assigned a probability-distribution (defined over the input space \( \mathbb{R}^N \)).

To consider the example of measurements from temperature sensors, the noise of the sensors might be different for high and for low temperatures. Or, another example, there could be hard boundaries in some cases (e.g., a percentage range cannot be lower than 0 or higher than 100).

The first challenge is thus to model \( \hat{p}(x_t, x') \). In principle there are two ways to model \( \hat{p}(x_t, x') \): (1) analytically or (2) as a process that generates samples (e.g., via a Monte-Carlo simulation). Both will require expert knowledge, and details of the specific application.

The second challenge is to find out whether our ML-model \( f \) yields different predictions in the region of interest around \( x_t \). Here we intentionally use the vague term **region of interest**, as defining this is one of the main problems, and the approach we choose is part of what distinguishes this work from previous work. One possible ansatz is to define hard boundaries for \( x' \) (and subsequently for \( \hat{x} \)), and then try to find out whether the prediction for \( f \) is the same for the whole region defined in this way, yielding a binary measure (either whole region yields same prediction, or not). This is one of the things that previous work on certifying neural networks are aiming at (e.g., Singh et al. (2019)). This approach would be, however, contrary to our idea of describing possible perturbations as probability distributions. We thus formulate the problem the following way:

How likely is it that the model prediction changes under the assumed perturbations?

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1. We omit a vector notation for simplicity, all variables with \( x \) in our discussion are typically vectors with dimension of the input space of the machine-learning model \( f \).
In mathematical terms, we want to know the probability that \( f(\hat{p}(x_t, x')) \) returns a prediction label different from \( f(x_t) \). For this we can define a binary function that returns one if the prediction is different than the one for the original data point, and zero otherwise:

\[
f'(x_t, x') = \begin{cases} 
0 & f(x_t + x') = f(x_t) \\
1 & f(x_t + x') \neq f(x_t) 
\end{cases}
\] (2)

Then we can, in principle, integrate \( f'(\hat{p}(x_t + x')) \) over the whole input space and thus obtain the probability for a different prediction compared to the unperturbed data point:

\[
P(f(\hat{x}) \neq f(x_t)) = \int_{\mathbb{R}^N} f'(x_t, x') \, dx'.
\] (3)

In order to define a robustness measure we can compute

\[
P_r = 1 - P
\]

This is what from now we will refer to as real-world-robustness.

An important thing to realize is that there are many possible ways that \( P \) could exceed a certain value: there could be a region on the other side of the decision boundary (thus in a region where the predicted label is different) that is small but has high probability, but equally well there can be situations where the density of \( \hat{p} \) is relatively small on the other side of the decision boundary, but that the region is actually large. In the first situation, there are not many different possible points around \( x_t \) that could cause a wrong prediction, but those points are not very unlikely. In the second situation, the points that would cause a wrong prediction are all relatively unlikely, but there are many of them, thus making the probability of getting one of them in a real setting is actually equally high as in the first situation. This is illustrated in fig. 1 for a binary classifier. For simplicity, we will show only illustrations of classifiers with a single decision boundary - all the principles here also apply to more complicated settings were the decision boundary consists of multiple unconnected pieces.

### 3.3 Why Counterfactuals are not Enough

The above discussed principle - that there are many different situations that can lead to the same probability of misclassification for a given uncertainty distribution around the data point - shows something important, namely that the shortest distance to the decision boundary alone is not enough for determining the robustness of a prediction. To revisit fig. 1: The right data point is much closer to the decision boundary than the left one, and still both have the same robustness in our sense. This insight leads us to the first conclusion of this paper: The distance to the closest counterfactuals (or adversarial examples), as for example suggested in Sharma et al. (2020), is not sufficient for determining robustness to perturbations that could occur by chance in the real world. In fig. 1, the closest counterfactual to the left data point would be much further away than the closest counterfactual for the right data-point - thus suggesting a different robustness - but in fact we have demonstrated above that both points have the same robustness. This stems from the different shapes of the decision boundary in the vicinity of the two points. Another
Figure 1: Example of a binary classifier with two-dimensional feature space. Two data-points (black dots) with uncertainty around them - here an elliptical distribution, the ellipses are lines of equal likelyhood. The purple line is the decision boundary of a binary classifier. The left point shows a situation where all possibilities of a misclassification are not very likely (all in regions of the elliptical distribution with low probability), but these regions summed together are in fact quite large, thus the probability of misclassification is not that low (indicated by the green area). In other words, one needs to get relatively far away from the original data point to get a misclassification, but this can happen in many different directions. The right data-point illustrates a different scenario: here only in a small range of directions a misclassification is possible, but in those directions a misclassification is happening in regions of high likelyhood.
example is given in fig. 2a): Here we have two data points (for simplicity again with both data points having the same uncertainty), and the distance to their closest counterfactuals (indicated as yellow dots) is the same for both points. Therefore, the distance would indicate that they have the same robustness. However, due to the different shapes of the decision boundary, the left point actually is less robust than the right one. This is the case for all types of classifier that have curved decision boundaries (thus all non-linear classifiers). For completeness we point out that for linear classifiers (e.g. logistic regression), the distance to the closest counterfactual does not suffer from the above mentioned problems (but the issues discussed below are still relevant even for linear classifiers).

Another reason why the distance to the closest counterfactual is not enough is depicted in fig. 2b). Here we have three data points, all with the same distance to the decision boundary, and thus the same distance to the closest counterfactual (orange points). In this example, also the shape of the decision boundary is very similar in the vicinity of all three data points. However, the uncertainty of the data points is not the same. All points have elliptical uncertainty distributions, but with different orientation with respect to the decision boundary. Therefore, their robustness against real-world perturbations is not the same - the leftmost point is more robust than the others. At a first thought, one might be tempted to think that the latter problem might be solved the following way: Given the density distribution \( p(x_t) \), we could compute the density at the location of the counterfactual and use this as a robustness measure. In the example in fig. 2b) this would indeed yield the desired result: The leftmost point would be rated more robust then the two other points. However, if we return to the example in fig. 2a), then this approach would immediately fail: Here both points would be rated equally robust - as the counterfactuals lie on the same probability lines - but indeed we had shown above that in terms of real-world-robustness, the left point is less robust than the right one. The opposite would be the case in the example in fig. 1: Here the density at the location of the closest counterfactual would be higher for the right than for the left point - but indeed the real-world robustness is the same for both points.

We can thus draw our first conclusion:

For determining robustness against real-world perturbations, counterfactuals/adversarial examples are insufficient.

This does of course not mean that counterfactuals/adversarial examples are useless in that respect - it only means that they do not cover the whole picture.

3.4 Analytical Solutions

For combinations of certain types of classifiers and assumed uncertainties it is possible to find analytical solutions to Eq. (3). In the Appendix this is shown for two examples: 1) A linear classifier and 2) a non-linear rule-based model, where for both the uncertainty of the test-points is assumed to be a multivariate Gaussian distribution.
3.5 Assessing Real-World Robustness with MC Sampling

In this section we describe a brute-force approach based on Monte-Carlo sampling that in principle can approximate the real-world robustness of any black box classifier, on a test-point by test-point basis:

1. Build a function that returns discrete samples from \( \hat{p} \).
2. Draw \( N \) samples from that function.
3. Test the black box function \( f \) with the new data points, and compute the fraction that leads to a different classification than the original data point.

For \( N \to \infty \) this method should converge to the exact solution of Eq. (4).

The challenge now lies in accurately describing the uncertainty \( \hat{p} \). This needs to be done on an application-by-application basis and will require expert knowledge. Here we only outline some basic approaches that could be taken, in order to help practitioners.

### 3.5.1 Continuous Features

For continuous features, if appropriate for the application, the easiest approach would be to define \( \hat{p} \) as a multivariate normal distribution. For \( n \) features, this can be defined via a covariance matrix of shape \( n \times n \). This can account for both uncorrelated and correlated uncertainty of the individual features.

### 3.5.2 Categorical Features

For categorical features one can work with transition matrices that describe transition probabilities. If we have single categorical feature with \( m \) possible values this would result in a (symmetric) \( m \times m \) matrix. Each row (and each column) describes the transition probability of one categorical value to all other categorical values.
3.5.3 Regression Problems

The discussion in this paper focuses on classification problems - as does most of the literature on robustness of machine learning algorithms. It is, however, possible to adapt our approach to regression problems as well. In this case, Eq. (2) would need to be adjusted with a threshold $\gamma$. If the difference between the regression output of the perturbed testpoint and the original testpoint is smaller than the threshold, then the output is considered unchanged, otherwise it is considered as changed:

$$f'(x_t, x) = \begin{cases} 0 & |f(x) - f(x_t)| < \gamma \\ 1 & |f(x) - f(x_t)| > \gamma \end{cases}$$

The rest remains the same as for classification problems.

3.6 Assessing Real-World-Robustness in High-Dimensional Datasets

The above described brute-force approach is bound to fail in settings with high-dimensional feature spaces due to the curse of dimensionality. In order to explore the whole area of interest around a test-point, a very huge number of samples would need to be drawn from $\hat{p}$, which is unfeasible. Finding solutions to (part) of this problem is actually the topic of all work on certification and formal verification of neural networks mentioned in the introduction. However, to the best of our knowledge, no complete solution is known at the moment. Instead, the literature focuses only on providing guarantees for certain aspects of input perturbations. Work on adversarial robustness of course also deals with these issues and partly provides solutions. However, as outlined in this paper, adversarial robustness is not necessarily the same thing as robustness to real-world-perturbations. One interesting line of research would be to rephrase the question behind formal guarantees of neural networks: Instead of trying to find bounds within which perturbations do not change the prediction, one could attempt to formally guarantee that the probability of misclassification under a given (high-dimensional) perturbation strategy is below a certain probability threshold - thus finding an upper bound for $P$ in Eq. (3)

For certain applications, one could also use dimensionality-reduction to reduce the problem. The number of input features in the input space does not always have to the actual dimensionality of the input data, as features can be (highly) correlated. It could be that in some use-cases real-world-perturbations occur only - or at least mainly - along certain directions in feature space, which could coincide with the directions along which most variance occurs in the training or test data. Methods for dimensionality reduction - such as Principal Component Analysis (PCA) - could thus help in exploring the relevant space around test points. This would be possible through modelling real-world-perturbations not on the full input space, but on the leading principal components, or on feature found with stochastic games Wicker et al. (2018). This will, however, never work generically. For example, in some applications white noise will be a potential real world perturbation, but this will not be represented at all in the leading principal components.

Other potential approaches:
• Try to use multiple different adversarial examples (e.g. not only the example closest to the original point, but the \( n \) closest ones) as guidance towards the "interesting" direction(s) in feature space.

• For classifiers where the gradient of the output is available (e.g. for neural networks), it would be possible to compare the direction of the largest absolute gradient at the testpoint with the direction of highest probability in the assumed perturbation distribution around the test point. If the two directions are similar, then the robustness is lower. This could for example be based on the approach used in the CLEVER score of Weng et al. (2018). Such an approach would be, however, closer to an extension of adversarial robustness with information on perturbation distributions than a solution for finding real-world-robustness in our definition.

4. Examples

In this section we compare adversarial robustness with real-world robustness on classifiers trained on two datasets: The Iris flower dataset (Anderson, 1936) and the Ionosphere dataset (Sigillito et al., 1989), both available in the UCI repository (Dua and Graff, 2017). The experiments we conduct are mainly for illustration purposes. On both datasets, a classifier is trained, and then robustness is estimated with different assumptions on how real-world perturbations could look like. We simply use two approaches as illustrations of the concept, they do not necessarily correspond to what would be real-world perturbations in applications that use classifiers based on these datasets.

For both datasets, we describe the expected uncertainty around the test-point as multivariate normal distributions, which are the same for each point (we thus assume that the uncertainty of input features is independent of their value). The multivariate normal distribution is described by a covariance matrix normalized to a trace of 1, and an overall perturbation scale, which in our example is a scalar. We use two types of covariance matrices, an identity matrix (no covariance terms, all diagonal terms 1) and random covariance matrices (normalized to a trace of 1). The random covariance matrices are generated the following way:

\[
C_r = A^T A,
\]

where \( A \) is a matrix whose entries are all independently drawn from a normal distribution with zero mean and unit variance. Eq. (5) ensures that \( C_r \) is a proper covariance matrix (symmetric and positive semi-definite).

Real-world-robustness in our definition is a probability, and therefore contained in \([0, 1]\). The typical way of using adversarial examples as robustness measure is the distance \( d_i \) between the test point \( x_i \) and the closest adversarial example. This is a metric in \((0, \infty)\) (in contrast to real-world-robustness, the distance cannot be zero, therefore the interval has an open lower bound). In order to allow a better comparison, we rescale the distance to the range \((0, 1]\), thus we define adversarial robustness as

\[
r_i = \frac{d_i}{\max (d_{1,2,\ldots,N})}.
\]

For each test point, \( N = 10000 \) samples from the perturbation distribution around the test point are drawn for computing real-world-robustness.
4.1 Iris Dataset

As a very simple example we reduced the dataset to two classes (to make it binary). This results in an easy classification task. The data is normalized to unite variance, then a random forest classifier with 10 trees and a max-depth of 3 is fitted on the training data (2/3 of dataset). Robustness computed on remaining 1/3 test points. To compute the real-world robustness we use the covariance matrices described above, whereas different perturbation scales are tested. CF/adversarial-examples are computed with the CEML library (Artelt, 2019).

4.2 Ionosphere Dataset

The ionosphere dataset has 34 features (2 categorical and 32 continuous), of which we removed the 2 categorical features. The task is binary classification. As model we use a neural network with 2 hidden layers with 256 neurons each and relu-activation functions. As the CEML library had - in contrast to on the Iris dataset - convergence problems on this higher dimensional dataset, for the Ionosphere dataset we use the Brendel&Bethge method as implemented in the Adversarial Robustness Toolbox (Nicolae et al., 2019) to compute CFs/adversarial-examples.

4.3 Results

Figures 3 and 4 show the results with identity covariance matrix for Iris and Ionosphere dataset, respectively. The scatter plots (a,b) show two particular real world perturbation scales, panel c shows correlation between adversarial robustness and real-world-robustness for different assumed real world perturbation scales. The two robustness measures clearly yield different results, showing that they are not measuring the same thing. The crucial thing is not that the correlation is not 1, but that the order of the test points - and therefore their ranking in terms or robustness - is partly different. Another notable aspect is that the distribution of the two measures is different. Real-world-robustness, in contrast to the distance to the closest counterfactual, is dense close to a robustness of 1 (meaning
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Figure 4: Example on Ionosphere dataset, comparing adversarial robustness and real-world robustness. a,b: comparison between adversarial robustness and real-world robustness with two different assumed scales of real world perturbations. c: correlation between adversarial robustness and real-world robustness for different real world perturbation scales.

The probability of change in classification close to zero). This reflects the fact that if the test-point is already far away from the decision boundary, then it does not make a large difference for real-world-robustness it it would be even farther away. This is not correctly reflected by the distance to the closest counterfactual.

The perturbation scale where the correlation is highest indicates the scale of real perturbations (with the given cross-correlation across the features) at which the adversarial robustness measure works best in estimating real-world-robustness - but still it does not represent real-world-robustness completely. Furthermore, it is unlikely that in a real application the expected perturbations correspond to exactly that scale, since the scale occurring in reality would be determined by the application, in contrast to the optimal scale, which is determined by the classifier.

To test whether the Monte Carlo approach for the computation of real-world-robustness has converged, for both datasets, the procedure has been repeated 20 times, and the correlation between the real-world-robustness obtained between all 20 runs computed. The correlation was larger than 0.999 for all pairs of runs, showing that it has converged (not shown).

Finally a comparison between using identity matrices and random covariance matrices for real-world-robustness is show in fig. 5. For the ionosphere dataset, the results are very similar, but for the Iris dataset, assuming different perturbation distributions around the test-points leads to different robustness estimations. This shows that knowledge of the exact expected perturbations in the real-world is important for accurately estimating robustness not only from a theoretical example, but also far a real trained classifier.

5. Discussion

One of the shortcomings when using CFs for approximating real-world-robustness in our definition is that real-world-perturbations are not necessary equally likely along all directions of the input space. This could at least partly be adopted into CFs via an adaption of the distance function in eq. 1. This would, however, not alleviate the problem that the
classification boundary might have a different distance to the test point in different directions, and thus suffers from the same shortcomings as the approach of using the density of the input perturbations at the location of the CF mentioned in sec. 3.3.

Methods for finding counterfactuals only approximately solve the minimization problem in 1. In our discussion of the short-comings, we assumed perfect CFs. However, CFs actually found by CF methods will deviate from perfect CFs, and thus are even less suited for approximating real-world-robustness.

6. Conclusion

In this paper we discussed how to assess robustness of machine learning classifiers to real world perturbations. We defined real world perturbations as perturbations that can occur “naturally” in a given real world application, for example through noise or measurement errors. This differentiates it from adversarial attack scenarios, in which the threat scenario is that an adversary modifies input data of the classifier in order to change its classification. Additionally, we differentiated it from robustness against distribution shifts, formal certification of neural networks and the problem of testing sets that correspond to testing “in the wild”. We defined real-world-robustness in a mathematical way, and showed theoretically that measures for adversarial robustness are not necessarily a valid measure for real-world-robustness, as they measure something different than our definition of real-world-robustness. We further proposed that real-world robustness can - at least for low to medium dimensional problems - be estimated with Monte Carlo sampling, which requires careful modeling of perturbations that are expected for a certain application. This can only be done with expert knowledge.

We empirically tested our approach on classifiers trained on two widely used ML-datasets (the Iris flower dataset and the Ionosphere dataset) and compared the results to robustness.
estimated with adversarial examples. The results were different, showing that the two approaches do indeed measure two distinct things.

This shows that claims that robustness scores based on adversarial examples / counterfactuals are generic robustness scores (such as in Sharma et al. (2020)) are not completely true.

An inherent limitation in our proposed way for estimating real-world-robustness is that it works only if the dimensionality of the input space is not too high. We discussed several ideas on how this could be dealt with. For certain problems, it should be possible to use dimensionality reduction techniques, but for general problems we cannot offer any solution yet. We suspect that the research fields of adversarial robustness and formal guarantees for neural networks can provide valuable input to this point. Future research should therefore, in addition to adversarial attack scenarios, also focus on how to determine real-world-robustness for high-dimensional problems.

Finally, in this paper, we mainly dealt with black-box classifiers (except in the section on analytical solutions). In cases where the classifier is known, and more specifically the decision boundary(s) is known (such as in decision trees), it would also be possible to use numerical integration to compute real-world-robustness (eq. 3). That would be done via numerically integrating $p$ over the region(s) where the classification is the same as for the test point, and should in principle also work for high-dimensional datasets. This possibility was not explored in this paper.

7. Code and Data Availability

The datasets we used are publicly available at the UCI repository https://archive.ics.uci.edu/ml/index.php. All code developed for this study and links to the datasets are available in the accompanying repository (repository will be published with the camera-ready version of this paper).

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Appendix A. Analytical solutions

The analytical solution of real-world-robustness is presented here for two simple cases: A linear decision boundary, and a simple rule based model. Both are binary classifiers with 2-dimensional feature space.

A.1 Linear decision boundary

A linear decision boundary in 2-dimensional feature space can be described as

\[ y(x_1, x_2) = w_1 x_1 + w_2 x_2 + b, \]

with the corresponding binary classifier function

\[ f(x_1, x_2) = \begin{cases} 0 & y < 1/2 \\ 1 & y > 1/2 \end{cases} \]

For this classifier we can compute analytical solutions both for the distance to the closest counterfactual as well as for our definition of real-world-robustness.

The closest counterfactual for a test-point \((x_1, x_2)\) is obtained by minimizing the distance from \((x_1, x_2)\) to the decision boundary \(1/2 = w_1 x_1 + w_2 x_2 + b\). If we use euclidean distance, this results in

\[ x_{cf1} = -\frac{2w_2 x_2 + 2b + x_1 - 1}{2w_1 - 1} \]
\[ x_{cf2} = -\frac{2w_1 x_1 + 2b + x_2 - 1}{2w_2 - 1} \]

The distance \(d_{cf}\) to the counterfactual is given by

\[ d_{cf} = \sqrt{(x_1 - x_{cf1}) + (x_2 - x_{cf2})}. \]

We assume multivariate Gaussian uncertainty \(p(x_1, x_2, x'_1, x'_2)\) with covariance matrix \(\Sigma = \begin{pmatrix} \sigma_1^2 & 0 \\ 0 & \sigma_2^2 \end{pmatrix}\) given by

\[ p(x_1, x_2, x'_1, x'_2) = \frac{1}{2\sigma_1\sigma_2} \exp \left[ -\frac{(x'_1 - x_1)^2}{2\sigma_1^2} - \frac{(x'_2 - x_2)^2}{2\sigma_2^2} \right]. \tag{6} \]

The real-world-robustness \(P_r\), given by Eq. (3) in the main paper, can then be computed as \(1 - P\), where \(P\) is obtained by integrating \(p\) over the region of \(\mathbb{R}^2\) where \(f(x + x') \neq f(x)\). Alternatively, \(P_r\) can be directly computed via \(p\) over the region of \(\mathbb{R}^2\) where \(f(x + x') = f(x)\):

\[ P_r (x_1, x_2) = \int \int_{f(x + x') = f(x)} p(x_1, x_2, x'_1, x'_2) \, dx'_2 dx'_1. \tag{7} \]

This equation can be solved via a rotation of the coordinate system such that one of the rotated coordinate axes is parallel to the decision boundary.
Figure A.1: Analytical solution of real-world-robustness (left) and distance to closest counterfactual (right) for a 2-dimensional linear decision boundary with $w_1 = 0, w_2 = 1, b = 0$ and Gaussian test-point uncertainty with $\sigma = 1$. Here the distance to the closest counterfactual is not normalized.

For illustration purposes here we assume a classifier with $w_1 = 0$ and $b = 0$, in which case the decision boundary is parallel to the $x_1$-axis.

In that case Eq. (7) simplifies to

$$
Pr(x_1, x_2) = \begin{cases} 
\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} p(x_1, x_2, x'_1, x'_2) \, dx'_2 \, dx'_1 & x_2 > \frac{1}{2w_2} \\
\int_{-\infty}^{1} \int_{-\infty}^{\infty} p(x_1, x_2, x'_1, x'_2) \, dx'_2 \, dx'_1 & x_2 < \frac{1}{2w_2} 
\end{cases}
$$

with the analytical solution

$$
Pr(x_1, x_2) = \begin{cases} 
\frac{1}{2} \text{erf} \left( \frac{2\sqrt{2}w_2x_2 - \sqrt{2}}{4\sigma_2w_2} \right) + \frac{1}{2} & x_2 > \frac{1}{2w_2} \\
-\frac{1}{2} \text{erf} \left( \frac{2\sqrt{2}w_2x_2 - \sqrt{2}}{4\sigma_2w_2} \right) + \frac{1}{2} & x_2 < \frac{1}{2w_2} 
\end{cases}
$$

(8)

where erf is the error function. Example plots for both robustness metrics are shown in fig. A.1. Both are independent of $x_1$, and decline steadily with larger distance along $x_2$ from the decision boundary along. Distance to the closest counterfactual declines linear with distance (per definition of the used distance metric), real-world-robustness declines exponentially (because gaussian uncertainty is assumed).

A.2 Non-linear decision boundary

As an example of a non-linear classifier for which both robustness metrics can be analytically computed we use the following decision function
\[ f(x_1, x_2) = \begin{cases} 1 & x_1 > a_1 \text{ and } x_2 > a_2 \\ 0 & \text{else} \end{cases} \]

which forms a decision boundary in 2d that looks like a right angle, where the tip of the edge is at \((a_1, a_2)\). This could for example originate from a simple rule-based model, or a decision tree with depth 2.

Distance to the closest counterfactual (i.e. distance to the decision boundary) is given by

\[
d_{cf}(x_1, x_2) = \begin{cases} 
\min \left( \sqrt{(x_1 - a_1)^2}, \sqrt{(x_2 - a_2)^2} \right) & x_1 > a_1 \text{ and } x_2 > a_2 \\
\sqrt{(x_2 - a_2)^2} & x_1 > a_1 \text{ and } x_2 < a_2 \\
\sqrt{(x_1 - a_1)^2} & x_1 < a_1 \text{ and } x_2 > a_2 \\
\sqrt{(x_1 - a_1)^2} + (x_2 - a_2)^2 & x_1 < a_1 \text{ and } x_2 < a_2 
\end{cases}
\]

The real-world-robustness thus follows as

\[
P_r(x_1, x_2) = \begin{cases} 
\int_{a_2}^{\infty} \int_{a_1}^{\infty} p(x_1, x_2, x_1', x_2') \, dx_1' \, dx_2' & x_1 > a_1 \text{ and } x_2 > a_2 \\
\int_{-\infty}^{a_2} \int_{a_1}^{\infty} p(x_1, x_2, x_1', x_2') \, dx_1' \, dx_2' \quad \text{else} \\
\int_{-\infty}^{a_2} \int_{-\infty}^{a_1} p(x_1, x_2, x_1', x_2') \, dx_1' \, dx_2'
\end{cases}
\]

For uncertainty around the test points we use the same assumption as in the linear case (Eq. 6). With this, \(P_r\) can be solved analytically again and yields

\[
P_r(x_1, x_2) = \begin{cases} 
\frac{1}{4} \left( \text{erf} \left( \frac{\sqrt{2} x_1 - \sqrt{2}}{2 \sigma_1} \right) + 1 \right) \text{erf} \left( \frac{\sqrt{2} x_2 - 2 \sqrt{2}}{2 \sigma_2} \right) & x_1 > a_1 \text{ and } x_2 > a_2 \\
+ \frac{1}{4} \text{erf} \left( \frac{\sqrt{2} x_1 - \sqrt{2}}{2 \sigma_1} \right) + \frac{1}{4} & \text{else} \\
- \frac{1}{4} \left( \text{erf} \left( \frac{\sqrt{2} x_1 - \sqrt{2}}{2 \sigma_1} \right) + 1 \right) \text{erf} \left( \frac{\sqrt{2} x_2 - 2 \sqrt{2}}{2 \sigma_2} \right) \\
- \frac{1}{4} \text{erf} \left( \frac{\sqrt{2} x_1 - \sqrt{2}}{2 \sigma_1} \right) + \frac{3}{4} & \text{else}
\end{cases}
\]

Example plots for both robustness metrics are shown in fig. A.2.

Far away from the corner the information of both metrics is similar. However, close the corner, they diverge. The distance to the closest counterfactual is only dependent on the smallest distance (be it along \(x_1\) or \(x_2\)). How much larger the distance along the other axis
Figure A.2: Analytical solution of real-world-robustness (left) and distance to closest counterfactual (right) for a 2-dimensional linear decision boundary with \( w_1 = 0, w_2 = 1, b = 0 \) and Gaussian test-point uncertainty with \( \sigma = 1 \). Here the distance to the closest counterfactual is not normalized.

is does not matter in this case. This is in contrast to our definition of real-world-robustness, where it does matter: In close vicinity to the edges the decision boundary is close in both directions, making the prediction less robust, as it can change from perturbations along both axes. This is not correctly reflected when using the distance to the closest counterfactual as robustness metric.

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