Does Your Model Know the Digit 6 Is Not a Cat?
A Less Biased Evaluation of “Outlier” Detectors

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Abstract

In the real world, a learning system could receive an input that looks nothing like anything it has seen during training, and this can lead to unpredictable behaviour. We thus need to know whether any given input belongs to the population distribution of the training data to prevent unpredictable behaviour in deployed systems. A recent surge of interest on this problem has led to the development of sophisticated techniques in the deep learning literature. However, due to the absence of a standardized problem formulation or an exhaustive evaluation, it is not evident if we can rely on these methods in practice. What makes this problem different from a typical supervised learning setting is that we cannot model the diversity of out-of-distribution samples in practice. The distribution of outliers used in training may not be the same as the distribution of outliers encountered in the application. Therefore, classical approaches that learn inliers vs. outliers with only two datasets can yield optimistic results. We introduce OD-test, a three-dataset evaluation scheme as a practical and more reliable strategy to assess progress on this problem. The OD-test benchmark provides a straightforward means of comparison for methods that address the out-of-distribution sample detection problem. We present an exhaustive evaluation of a broad set of methods from related areas on image classification tasks. Furthermore, we show that for realistic applications of high-dimensional images, the existing methods have low accuracy. Our analysis reveals areas of strength and weakness of each method.

1 Introduction

If we pass a natural image of an unknown class to the currently popular deep neural network that is trained to discriminate ImageNet classes, we will get a prediction with a high (softmax) probability of an arbitrary class (see Fig. 1). With English speaking phone assistants, if you talk in another language, it will generate an English sentence that most often is not even remotely similar to what you have said. Optical character recognition (OCR) systems that are only trained with text images fail to detect the absence of text and will continue to generate predictions on irrelevant regions of an image. The silent failure of these systems is due to an implicit assumption: the input to the ImageNet classifier will be from the same ImageNet distribution, the user will be speaking in English, the OCR will be only inquired with text images. However, in practice, any automation pipeline that involves a deep neural network will have a critical challenge:
Can we trust the output of a neural network for a particular input?

A trivial solution is to add a None class to the discriminative models to account for the absence of other classes. However, this approach is not as viable as it may seem at first. The first challenge is defining the None class. For the text-to-speech problem, would None mean all other languages or all other conceivable sounds? The second problem is capturing the diversity of None class with a finite sample set to use for training, which is not trivially possible. Hard-negative mining is an attempt to collect such sample sets for specific models. The third and the most prohibitive problem is that we have to significantly increase the complexity of our models to capture the diversity of the None class. Despite these challenges, we might be able to achieve reasonable results on low dimensional problems such as OCR, but as the input dimension grows, so does the severity of intractability.

The source of our difficulty is the IID assumption. When we assume the samples are independently and identically distributed (IID), we expect the train and test examples to be drawn from a fixed population distribution. However, this condition cannot be easily enforced in deployed applications. The IID assumption is crucial to providing meaningful statistical guarantees [2]. More precisely, measuring the expected risk of a learned model \( \hat{h} \in \mathcal{H} \) through empirical risk over a finite set \( \mathcal{D} = \{(x_i, y_i)\}_{i=1}^m \) sampled from the population distribution \( \mathbb{D} \) and a loss function \( l \) as

\[
E_{(x_i, y_i) \sim \mathbb{D}} [\ell(\hat{h}(x_i), y_i)] \approx R_{\text{emp}}(\hat{h}) = \frac{1}{m} \sum_{i=1}^m \ell(\hat{h}(x_i), y_i),
\]

is a standard practice in supervised learning which entails an IID assumption. When the IID assumption is not satisfied in test data, the expected risk can no longer be reliably related to the empirical risk of the test set through this approximation. This implies that a low error on one distribution cannot provide an estimate of performance on another distribution by itself: without any further assumptions, the outputs on out-of-distribution (OOD) samples can be arbitrarily bad. The OOD samples violate the identically distributed (ID) assumption. Thus, as long as we rely on the empirical risk alone to train and evaluate deep neural networks, the first condition for making
a reliable prediction (with bounded error) on any input would be whether the ID assumption is satisfied. Note that satisfying the ID assumption is not a sufficient condition for a reliable prediction, i.e., samples could come from a fixed distribution, yet, the model could fail in prediction (a test error). When we *a priori* expect to change the effective underlying distribution, the traditional applicable frameworks are transfer learning, multitask learning, and zero-shot learning. In our setting, we only wish to detect out-of-distribution samples.

In real life deployment of products that use complex machinery such as deep neural networks (DNNs), we would have very little control over the input. In the absence of extrapolation guarantees, when the IID assumption is violated, the behaviour of the pipeline may be be unpredictable. From a quality assurance perspective, it is desirable to detect and prevent these scenarios automatically. A reliable pipeline would first determine whether it can process a given sample, then it would use the prediction of the target neural network. The unfortunate incident that mislabeled people as non-human[^1] for instance, is a clear example of OOD extrapolation that could have been prevented by such a decision scheme: the model simply did not know that it did not know. While incidents of similar nature have fueled research on de-biasing the datasets and the deep learning machinery, we still would need to identify the limitations of our models. The application is not limited to fortifying large-scale user-facing products. Successful detection of such violations could also be used in active learning, unsupervised learning, learning with noisy data, or simply be a condition to invoking transfer learning strategies. In this work, we are interested in evaluating mechanisms that detect OOD samples[^2]. We would like to emphasize that any learned complex model for which we have no reliable characterization of the inductive biases (deep neural networks) that is trained to estimate the performance of a target system will also heavily rely on the IID assumption. Therefore, the behaviour of these learned models may be unpredictable on the unseen data as well.

While problems of similar nature have been studied in a variety of domains (to be reviewed in Section 2), there has been a recent surge of interest in specifically OOD sample detection with deep neural networks [8, 9, 10, 11, 12]. Given that the problem is still in its infancy, there is an imminent need to standardize the problem formulation and properly define an evaluation benchmark that is both realistic and principled to compare the previous and future approaches reliably.

We (i) introduce OD-test, a new formulation of the task that reduces the problem to its core, thus enabling a clear vision of applicable methods. We also (ii) establish a new benchmark to evaluate the existing techniques for OOD detection exhaustively and reliably. We (iii) study the performance of several previously proposed methods under OD-test and highlight shortcomings and potential future directions for research. Furthermore, we demonstrate that the performance of current techniques quickly approaches the random prediction baseline as we make a transition to realistic high-dimensional images, highlighting the gap between the current state-of-art and what is needed in practice. To speed up progress on the presented problem, we also (iv) release our PyTorch[^3] implementation to easily replicate all the results[^3].

[^1]: [https://www.wired.com/story/when-it-comes-to-gorillas-google-photos-remains-blind/](https://www.wired.com/story/when-it-comes-to-gorillas-google-photos-remains-blind/)
[^2]: By OOD samples we mean the samples that are unlikely to come from the same distribution as the train set.
[^3]: Available at [https://github.com/ashafaei/OD-test](https://github.com/ashafaei/OD-test)
2 Related Work

The violation of the ID assumption is not the only way to wreak havoc on deep learning pipelines. Adversarial example [14] attacks are adversarially crafted signals in otherwise innocent-looking images that fool the neural networks into misclassification. These perturbations can be constructed in such a way that they break a variety of architectures trained on different datasets, with a high probability [15]. While the OOD sample detection is a model-independent problem, adversarial images specifically exploit the inductive bias in the model families. We limit our attention to the OOD sample detection problem.

2.1 Previous Work on Related Problems

By stretching the definition of OOD sample detection in different directions, we can end up exploring different areas of artificial intelligence. While each field brings a unique angle of this problem to light, none captures the exact issue at hand in its entirety. In this section, we provide a brief overview of these closely related domains. Most of the recent attempts by the deep learning community could be interpreted under one of these paradigms. Thus, we cover the other domains first, then move on to the recent deep learning literature in Section 2.2 and connect the approaches to the previous work.

The Uncertainty View. A commonly invoked strategy in addressing similar problems is to characterize a notion of uncertainty. The assumption is that if we are not certain about a prediction, then it must be the case that we do not know the prediction. Such a mechanism could be easily adapted to reject OOD samples as we would expect the uncertainty to be high on such inputs. It is usually the case that we do not have access to the groundtruth uncertainty; therefore, we often cannot predict it directly and must rely on alternative approaches. The literature distinguishes aleatoric uncertainty, the uncertainty inherent to the process (the known unknowns, like flipping a coin), from epistemic uncertainty, the uncertainty that can be eliminated with more information (the unknown unknowns). The Bayesian approach to epistemic uncertainty estimation is to measure the degree of disagreement among the potentially viable models (the posterior). For instance, if $h_1$ and $h_2$ are reasonable candidates (likely in the posterior), then the disagreement between $h_1(x)$ and $h_2(x)$ would imply an epistemic uncertainty regarding the actual label for $x$. For this interpretation to be reliable in our problem, we need the $h_1(x)$ and $h_2(x)$ to not be correlated on OOD samples. If all the $h_i$’s are biased, either through the inductive bias imposed by the family $H$ or the bias in the training data, the uncertainty estimate will subsequently suffer. Furthermore, the reliability of such uncertainty measure is closely tied to how well the underlying model learns the target distribution [16]. The MC-Dropout [17] approach is often advertised as a feasible method to estimate uncertainty for a variety of applications [16,17,18]. Similarly, we can adopt a non-Bayesian approach by training independent models and then measuring the disagreement. Lakshminarayanan et al. [12] show an ensemble of five neural networks (DeepEnsemble) that are trained with an adversarial-sample-augmented strategy is sufficient to provide a non-Bayesian alternative to capturing predictive uncertainty. We evaluate DeepEnsemble and MC-Dropout.

The Abstention View. If we change the learning problem to give our models the choice of abstaining from prediction at the cost of a penalty, we end up with the abstention view in learning theory. The purpose of abstention is to incur a lower cost than the cost of misclassification when
possible. The pair \((h, r)\) consists of the predictive hypothesis \(h \in \mathcal{H} : \mathcal{X} \rightarrow \mathcal{Y}\) and a reject function \(r : \mathcal{X} \rightarrow \{0, 1\}\). The reject function makes the abstention choice and could simply be a threshold on the magnitude of the prediction, \(i.e. r(x) = |h(x)| > \tau\) or chosen from a reject hypothesis set \(\mathcal{R}\). The learning problem is then choosing an appropriate pair \((h, r)\) that minimizes an abstention-augmented loss and provides generalization guarantees. The abstention view aims to detect when \(h\) would make a wrong prediction through \(r \in \mathcal{R}\). In that respect, the abstention methods are essentially the binary counterparts of uncertainty estimation methods. While the binary version of the problem gives us more flexibility on the choice of the reject class \(\mathcal{R}\) compared to the continuous uncertainty setting\(^4\), the reliability of \(r\) itself still is contingent on the evaluation on a fixed distribution. That is, if we encounter an OOD sample, we do not know \textit{apriori} if \(r\) would reject it. Our problem formulation is inspired by the abstention view with key differences that we will discuss in Section 3. We show that all the prior work on detecting OOD samples can be reduced to an abstract problem of learning a reject function within a specific reject-hypothesis set \(\mathcal{R}\).

The Anomaly View. Anomaly or outlier detection in data mining is another lens through which we can approach the OOD sample detection. The assumptions in this domain are the closest to our setting. Density estimation-based techniques assume the samples that have a low probability are outliers and should be discarded. Given that density estimation in high-dimensional spaces is challenging in both sample complexity and computational complexity, the approaches tend to work well mostly within low-dimensional or simple distributions. PixelCNN++\(^{22}\) is a recent auto-regressive model based on PixelCNN\(^{23}\) with a tractable likelihood that could be used within a density estimation scheme. We evaluate the performance of PixelCNN++ in our work. Note that the problem of density estimation is not equivalent to the binary OOD detection problem: a perfect density estimator can solve the outlier detection problem, but a perfect outlier detection method does not necessarily have the information needed to solve the density estimation problem. Proximity-based methods rely on a distance measure within the train data to establish what is an anomaly. A simple strategy within this domain is to make a decision based on the K-nearest neighbours of a given input. We call this method K-NNSVM. Clustering methods reject points that do not conform to any of the previously identified clusters. The popular one-class SVM\(^{24}\) with a radial basis function learns a conservative region that covers the train data. In the biggest comparison of outlier detection methods\(^{25}\), the proximity-based approaches are demonstrated to be the most effective strategy. Reconstruction-based methods learn to reconstruct the train data first, then try to reconstruct each given sample. The samples that cannot be reconstructed well are then discarded as anomalies. The reconstruction procedure could be through linear subspaces such as PCA\(^{26}\), or non-linear methods such as autoencoders. We use an autoencoder with a reconstruction threshold to test this idea (AEThreshold).

The Novelty View. Open-set recognition and novelty detection in computer vision study the detection of anomalies at a semantic level. As a result, these methods are typically concerned with recognition of unseen classes, \(e.g.\), new objects in the scene. This is a special case of OOD sample detection where the OOD samples differ by the semantic content. An unseen viewpoint of a target object violates the ID assumption, but it does not necessarily constitute a novelty. The notion of a novelty is often underspecified in practice and results are limited to particular assumptions and problem formulations. In this work, we take the broader statistical perspective, the OOD detection, which imposes a strict condition that is grounded in the learning assumptions. Bendale

\(^{4}\)It subsumes the class of functions that can be used for uncertainty estimation by adding a threshold.
and Boult [11] present OpenMax, a replacement for the softmax layer that also detects unknown classes through evaluation against a representative neural activation of each class. Liu et al. [27] provide theoretical analysis for open-set recognition in a special setting where they wish to identify alien samples in a fixed mixture of distributions. We evaluate the OpenMax algorithm.

2.2 Deep Learning Literature

The previous related work in deep learning can be categorized into two broad groups based on the underlying assumptions: (i) in-distribution techniques, and (ii) out-of-distribution techniques.

In-Distribution. These methods focus primarily on the performance of the network on the in-distribution inputs to either calibrate the predictions or abstain from prediction. Guo et al. [28] observed that modern neural networks tend to be overconfident in their predictions. They show that temperature scaling in the softmax operator, also known as Platt scaling, can be used to calibrate the output probabilities of a neural network to empirically align the accuracy of a prediction with its probability. Their efforts fall under the uncertainty estimation approaches. Geifman and El-Yaniv [29] present a framework for selective classification with deep neural networks that follows the abstention view. A selection function decides whether to make a prediction or not. For the choice of selection function, they experiment with MC-Dropout and the softmax output. They provide an analytical trade-off between risk and coverage within their formulation.

Out-of-Distribution. Hendrycks and Gimpel [8] investigate OOD sample detection within computer vision, natural language processing, and speech recognition. They demonstrate that it is possible to detect OOD samples by simply thresholding the output softmax probabilities. We call this method PbThreshold. More recently, Liang et al. [9] present ODIN, a method based on (i) temperature rescaling and (ii) input perturbation to detect OOD samples. Temperature rescaling, in light of the previous work [28], provides the means of confidence calibration. They further posit that the predictive function, as represented by the deep neural network, would have a different behaviour around the in-distribution samples as opposed to OOD samples. Therefore, the input perturbation serves as a way to assess how the network would behave nearby the given input. When the temperature is 1 and the perturbation step is 0 we simply recover the PbThreshold method. ODIN, the state-of-the-art at the time of this writing, is reported to outperform the previous work [8] by a significant margin. We also assess the performance of ODIN in our work.

Wang et al. [30] present an alternative “safe” classification paradigm based on generative adversarial networks (GANs) [31]. The idea is to train an independent generator per class, and then, during the test, find the best approximate input to all the generators and use the distance of the generated samples from the input as a measure for prediction and also its uncertainty. There are also other ideas that rely on GANs [10, 32, 33, 34] to detect anomalies or novelty in the data. These methods provide an abstract idea which depends on the successful training of GANs. To the best of our knowledge, training GANs is itself an active area of research, and it is not apparent what design decisions would be appropriate to implement these ideas in practice. Furthermore, some of these ideas are prohibitively expensive to execute at the time of this writing. We are therefore unable to evaluate these ideas fairly at this time.

5Note that some of the most recent work are not yet peer reviewed.
Figure 2: The OD-test procedure for OOD sample detection methods can be visualized as follows: a.1) A set of distributions represented as shapes within the input space $\mathcal{X}$. Our source distribution $D_s$ is identified in the image; everything else is outlier. a.2) We pick one validation distribution $D_v$ and use the method to learn a binary reject function $r$ that partitions the space $\mathcal{X}$ based on $D_s$ and $D_v$ only. a.3) We then evaluate the partition function $r$ on the other distributions, now identified as $D_t$, and measure accuracy. b) Demonstrates how we use the dataset splits for each step.

All the previous work that directly addresses the OOD sample detection focus on small-scale MNIST [35], SVHN [36], and CIFAR [37] datasets. In our work, we exhaustively evaluate several previously proposed solutions in controlled experiments on a variety of problems with varying complexity. We demonstrate that, in such low-dimensional spaces, simple data mining strategies tend to work as well or even better, therefore stressing that a more comprehensive evaluation must be undertaken for realistic assessments of the current and future work.

## 3 OD-test: A Less Biased Evaluation of Outlier Detectors

Let us define the source distribution $D_s$ to be our input distribution. The objective is to decide whether a given sample belongs to $D_s$. Similar to the learning theory literature, we define a reject function $r : \mathcal{X} \rightarrow \{0, 1\}$ that makes this binary decision. Note that this decision can be made independently from the ultimate prediction task. While in learning theory and applications we reject the samples that the final predictive hypothesis $h$ is likely to mislabel, here we reject the samples that do not belong to the source distribution $D_s$, hence decoupling the reject function $r$ and the predictive hypothesis $h$.

If the reject function $r$ flags an input, it would mean that the given sample does not belong to the source distribution; thus, the output of the predictive pipeline may not be reliable. On the other hand, if the function accepts a given input, we can safely continue the pipeline with the ID assumption. This perspective on rejection is more relaxed than the previous formulations. In addition to the previously proposed methods, we can study new approaches that operate in the input space directly (e.g. K-NNSVM, or AEThreshold).

The $r$ function is a binary classifier; the classes are in-distribution vs. out-of-distribution. To learn the classifier, we might adopt the supervised learning assumptions and use a dataset $D_v$ as a representative of the OOD samples. This strategy is sometimes called supervised outlier detection. Unfortunately, this approach may be misleading because the learned models can be biased by $D_v$. A

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high accuracy in this scenario may not yield an accurate model for practice in many settings where the outlier may not look like samples from $D_v$. The actual OOD samples are beyond our direct reach and our models can easily overfit in distinguishing $D_s$ from $D_v$ (we verify this empirically). We present a less optimistic evaluation framework that prevents scoring high through overfitting.

Specifically, we introduce a third “target” distribution $D_t$ to measure whether a method can actually detect outliers that are not only outside of $D_s$ but that also might be outside of $D_v$. The idea is to treat the problem as a binary classification between three different datasets. Similar to the supervised outlier detection, we begin by training our reject function to distinguish $D_s$ from $D_v$. But, to evaluate our method, we use a third unseen distribution $D_t$ instead of $D_v$ (see Fig. 2). $D_t$ represents OOD examples that were not encountered during training – a more realistic evaluation setting for uncontrolled situations. As we see later, the spectrum of choices for $D_s$, $D_v$, and $D_t$ allows for a rigorous evaluation of the $r$ functions. The pseudocode of the evaluation procedure is outlined in Alg. 1.

**Algorithm 1: OD-test – the evaluation procedure for a supervised method $M$.**

```plaintext
begin
A ←− {}
/* Generate a rejection hypothesis class $R$ using $D_s^{\text{train}}$. */
$R$ ←− $M(D_s^{\text{train}})$
for $D_v$ ∈ $D$ do
    /* Find the best binary classifier in $R$. */
    $r$ ←− train($R$, $\{D_v^{\text{valid}} : 0, D_v : 1\}$)
    for $D_t$ ∈ $D \setminus \{D_v\}$ do
        /* Evaluate accuracy of $r$. */
        acc ←− eval($r$, $\{D_t^{\text{test}} : 0, D_t : 1\}$)
        add acc to $A$
return mean($A$)
```

When $D_v = D_t$, we simply recover the evaluation protocols of the previous work in the deep learning literature \[8, 9\]. However, in our evaluation, we specifically require $D_v \neq D_t$, to ensure the evaluation is not biased by $D_v$. Analogous to supervised learning, $D_v$ is acting like a validation set (we do not care about our performance at this task) and $D_t$ is acting like the test set (we care about our performance at this task).

As an example, let us walk through the stages of evaluation for **PbThreshold**, the method that thresholds the maximum probability of a discriminative neural network. We need a trained deep neural network and a threshold for the maximum probability that would reject the outliers. Given our source dataset $D_s$, and a collection of datasets that are compatible with $D_s$, we first train a deep neural network on $D_s$ to discriminate the image classes (line 3). The hypothesis class $R$ returned on line 3 will have a single free parameter $\tau$, the threshold to use on the underlying classifier. We must learn the optimal threshold $\tau$ in the next step. On line 5 we pick the best threshold $\tau$ to discriminate between $D_s$ and $D_v$. After finding the best threshold $\tau$ on line 5, we evaluate the learned reject function on $D_s$ and $D_t$. For unsupervised OOD detection methods the learning on line 5 is skipped and evaluation amounts to a single loop over $D_t$ (see Appendix A.1).

If the method $M$ successfully learns a density function for $D_s$, it would be capable of scoring very
high in this evaluation. With a density function, we only would have to pick a single threshold to reject OOD samples. We could also follow the same recipe for methods that generate a confidence measure. Furthermore, a typical binary classification method is also not sufficient to score high on this benchmark since we change the second distribution during the test stage. In the results section, we demonstrate how a traditional binary classifier would fall short. The methods that learn conservative boundaries around $D_s$ will have a higher chance of success. All the existing approaches can be implemented within this framework (see appendices for more information).

While in the original intractable density estimation problem the only important factor is the intrinsic complexity of $D_s$, our formulation adds flexibility by introducing new factors that control the difficulty of the problem. The critical observation is that some notion of similarity between $D_s$, $D_v$, and $D_t$ would control the difficulty of the problem. If $D_s$ and $D_v$, the source and the validation, are too similar in distribution, a high accuracy would require learning more complex boundaries; therefore it would be a more difficult problem. Through this observation, we can control the difficulty of the evaluation. We can gradually make the problem harder and harder and improve our methods until they are satisfyingly accurate. For instance, we expect that it would be easier to separate a random noise distribution from the ImageNet samples, whereas separating a new breed of dog from ImageNet would not be straightforward. Note that we can empirically assess the difficulty of separation without having an explicit notion of similarity. What we empirically observe is that separating low-level statistics is much easier than separating high-level concepts. If $D_v$ and $D_t$, the validation and the target, are too similar, the learned reject function $r$ could yield good results due to overfitting. Hence, we must exhaustively evaluate over a combination of datasets to be able to measure performance reliably. We cycle through mutually exclusive datasets in our evaluation and aggregate the results.

4 Evaluation

The evaluation metrics in the previous work [8, 9] include (i) false-positive rate at 95% true-positive rate, (ii) optimal detection error, (iii) area under the ROC curve, and (iv) area under the PR curve. These measures, in conjunction with the possible combination of the evaluation datasets, lead to large tables that make the interpretation and fair comparison of the results difficult. A common pattern in this literature is to claim state-of-the-art results on one measure in a limited context. Measuring progress under such circumstances could be misleading and overly optimistic. To simplify the evaluation procedure, we equalize the binary classes and only measure accuracy. Furthermore, through the restriction imposed by $r$, we require the methods to pick the optimal parameters such as the threshold. This simplification allows straightforward aggregation and analysis of the results and provides a simple baseline of random prediction. Furthermore, we can meaningfully average over multiple experiments and robustly compare methods in a variety of conditions.

We may also wish to incorporate the prior knowledge on abundance and the risk associated with the OOD samples into the learning objective. We can incorporate such application-driven requirements by modifying the implicit learning objectives on line 5 and 7 similar to the traditional supervised learning settings. We leave the proper choice of application dependent objectives to the practitioner and only focus on assessing the discriminative power of the methods in the fixed 50/50 scenario without any prior knowledge. Through this constraint we ensure that the methods that rely on the
prior likelihood cannot perform better than random prediction.

Datasets. We extend the previous work [8, 9] by evaluating over a broader set of datasets with varying levels of complexity. The variation in complexity allows for a fine-grained evaluation of the techniques. Since OOD detection is closely related to the problem of density estimation, the dimensionality of the input image will be of vital importance in practical assessments. As the input dimensionality increases, we expect the task to become much more difficult. Therefore, to provide a more accurate picture of performance, it is crucial to evaluate the methods on high dimensional data. Table 1 summarizes the datasets that we use. Omitted from the table, we also evaluate with Uniform([0, 1]) and \(\mathcal{N}(\mu = 0.5, \sigma = 0.25)\) samples for outliers.

For a given \(D_s\) we spatially resize the outliers and filter out the conflicting classes during evaluation. We use the original split of the dataset when available; otherwise, we split the data as indicated in Tab. 1. Finally, for training (line 5) and evaluation (line 7) we ensure the classes are balanced by trimming the datasets in a consistent manner.

Summary of Methods. We evaluate the following methods:

- BinClass. A binary classifier that is directly trained on \(D_s\) vs. \(D_v\).
- PbThreshold [8]. A threshold on the softmax output.
- ScoreSVM. A generalization of PbThreshold is to train an SVM [40] classifier on the logits.
- LogisticSVM. Similar to ScoreSVM, but the classifier is trained with logistic regression loss.
- ODIN [9]. A threshold on the scaled softmax outputs of the perturbed input.
- K-NNSVM. A linear SVM on the sorted Euclidean distance between the input and the k-nearest training samples. Note that a threshold on the average distance is a special case of K-NNSVM.
- AEThreshold. A threshold on the autoencoder reconstruction error of the given input. We train an autoencoder with binary cross-entropy (BCE) and mean squared error (MSE).
- K-MNNSVM, K-BNNSVM. A K-NNSVM applied on the learned hidden representations of an autoencoder with MSE or BCE.

\[\text{Tables}\]
• K-VNNSVM. Similar to the previous, except we use the learned representation of a variational autoencoder [41].
• MC-Dropout [16]. A threshold on the entropy of average prediction of 7 evaluations per input.
• DeepEnsemble [12]. Similar to MC-Dropout, except we average over the predictions of 5 networks that are trained independently with adversarial data augmentation.
• PixelCNN++ [22]. A threshold on the log-likelihood of each input.
• OpenMax [11]. Similar to ScoreSVM, but we use the calibrated output of the OpenMax module that also includes a probability for an unknown class.

For the methods that rely on the output of discriminative neural networks, we use two generic architectures: VGG-16 [5] and Resnet-50 [4] and reuse the same networks for all the methods to provide a fair and meaningful comparison. We train these architectures with a cross-entropy loss (CE), and a k-way logistic regression loss (KL). CE loss is the typical choice for k-way classification tasks – it enforces mutual exclusion in the predictions. KL loss is the typical choice for attribute prediction tasks – it does not enforce mutual exclusivity of the predictions. We test these two loss functions to see if the exclusivity assumption of CE has an adverse effect on the ability to predict OOD samples. CE loss cannot make a None prediction without an explicitly defined None class, but KL loss can make None predictions through low activations of all the classes.

Note that our formulation of the problem separates the target task from the OOD sample detection. Thus, it is plausible to use, for OOD detection, a different predictive model from the actual predictive model of the target problem if there is an advantage. We tune the hyper-parameters of these methods following the best practices and the published guidelines in the respective articles. The implementation details, a discussion of evaluation cost, and the performance statistics of the above methods are in Appendix A.2. The PyTorch implementation with the pre-trained models is available on https://github.com/ashafaei/OD-test.

5 Results and Discussion

We evaluate the performance of the competing techniques in a strictly controlled regime against the datasets in Tab. 1. We run a total of 10,000 experiments over all the combinations of $D_s$, $D_v$, and $D_t$. First we analyze the aggregated results for each method, then we look at the breakdown of the accuracy per each source dataset. Figure 3 shows the average accuracy of all the discussed methods. Each method is evaluated over the same set of 308 experiments consisting of all compatible triplet of datasets.

BinClass, the method that directly learns a binary classifier between the two datasets, achieves a near-perfect accuracy on the train and validation splits of the same datasets, however, once tested on a third dataset that it has not seen before, the average accuracy drops to 68% for both VGG and Resnet. This example demonstrates why we need to adopt a different evaluation framework for this task. The classifier overfits to the two distributions ($D_s$ and $D_v$) effortlessly, but it cannot distinguish a third distribution ($D_t$). Because of the innumerable diversity in the OOD samples, no matter how large $D_v$ gets, we can always encounter new samples that we have not seen before.

MC-Dropout and DeepEnsemble, the two uncertainty prediction techniques, do not seem to provide
Figure 3: The average test accuracy of the OOD detection methods over 308 experiments per method. The error bars are 95% confidence level. /VGG or /Res indicates the backing network architecture. #-NN./ is the number of nearest neighbours. A random prediction would have an accuracy of 0.5.

a strong enough signal to make the distinction between the two classes compared to the simpler ScoreSVM. Interestingly, MC-Dropout has a higher accuracy than DeepEnsemble. The lower accuracy of DeepEnsemble might be attributed to the regularization effect of the adversarial training procedure that was advised in Lakshminarayanan et al. [12]. Considering the training cost of DeepEnsemble, MC-Dropout is clearly a more favourable choice.

VGG-backed and Resnet-backed methods significantly differ in accuracy. The gap indicates the sensitivity of the methods to the underlying networks. PbThreshold, ScoreSVM, and ODIN all prefer VGG over Resnet even though Resnet networks outperform the VGG variants in the underlying image classification on average. This means that the image classification accuracy may not be the only relevant factor in performance of these methods. ODIN is less sensitive to the underlying network. Despite not enforcing mutual exclusivity, training the networks with KL loss instead of CE loss consistently reduces the accuracy of OOD detection methods on average. ScoreSVM/VGG and ScoreSVM/Res both outperform LogisticSVM/VGG, and LogisticSVM/Res respectively. Similarly, the autoencoders that were trained with BCE loss (AEThre./BCE) outperform the ones trained with MSE loss (AEThre./MSE). Note that we are comparing identical network architectures.

Within the nearest-neighbour methods, #-NNSVM, #-BNNSVM, #-MNNSVM, and #-VNNSVM, the number of the nearest neighbours does not significantly impact the accuracy on average. However, performing the nearest-neighbour in the input space directly outperforms nearest-neighbour in the learned representations of autoencoders (BNNSVM, and MNNSVM) and VAE (VNNSVM). Interestingly, 1-NNSVM has a higher accuracy than thresholding the probability (PbThresh) and DeepEnsemble on average. For #-NNSVM, if the reference set of samples fit the GPU memory, a naive implementation could be faster than a forward pass on the predictive neural networks of large datasets such as TinyImagenet. PixelCNN++, the method that estimates the log-likelihood, has a surprisingly low accuracy on
Figure 4: The average test accuracy over 50 experiments per bar. The error bars indicate the 95% confidence level. The figure is best viewed in color.

this problem on average. We suspect the auto-regressive nature of the model, specifically when coupled with the IID assumption, may be the reason for its failure. The network approximates the log-likelihood only in the vicinity of the training data. If we evaluate the model on points that are far from the training data, the estimates are not reliable anymore. This explanation is consistent with the quality of the generated samples of PixelCNN++: the sampling process is directed by the model towards the areas of the input space where it has learned an estimate.

5.1 Evaluation Breakdown by the Source Dataset $D_s$

While the average accuracy across multiple datasets is informative, we expect some of these methods such as K-NNSVM to fail on more difficult, diverse, and high-dimensional datasets. Next, we break down the performance and study these methods on each individual $D_s$. Figure [4] shows the breakdown of test accuracy across each source dataset $D_s$ for some of the methods. For the full figure, see Appendix B. As indicated in the figure, our quantification of performance shows that all the methods have a much lower accuracy on high-dimensional data than the low-dimensional data.

In low-dimensional datasets, K-NNSVM performs similarly or better than the other methods. In the high-dimensional case, however, the accuracy approaches the random prediction baseline quickly. Interestingly, K-NNSVM performs better on STL10 ($96 \times 96$) than TinyImagenet ($64 \times 64$) which might be due to the higher diversity in TinyImagenet compared to STL10. Given the relatively high accuracy of K-NNSVM in $784$ dimensions, it might be feasible to learn an embedding for high-dimensional data, or learn a kernel function, to replace the original image space and enjoy a high accuracy. Going from CIFAR10 to CIFAR100, the dimensionality and the data size remains the same, the only changing factor is the diversity of the data and that seems to make the problem as difficult as the higher dimensional datasets. Except for K-NNSVM, the accuracy of other methods drops significantly in this transition.

AEThreshold has a near perfect accuracy on MNIST, however, the performance drops quickly on complex datasets. AEThreshold also outperforms the density estimation method PixelCNN++ on all datasets. We did not explore autoencoder architectures – more research on better architectures or
reconstruction constraints for AEThreshold may potentially have a high pay-off. The top-performing method, ODIN, is influenced by the number of classes in the dataset. Similar to PbThreshold, ODIN depends on the maximum signal in the class predictions, therefore the increased number of classes would directly affect both of the methods. Furthermore, neither of them consistently prefers VGG over Resnet within all datasets. Overall, ODIN consistently outperforms others in high-dimensional settings, but all the methods have a relatively low average accuracy in the 60%-78% range.

We can summarize the main observations as follows:

i. Outlier detection with two datasets yielded overly optimistic results with VGG and Resnet.

ii. MC-Dropout and DeepEnsemble uncertainty prediction techniques were not reliable enough for OOD detection.

iii. A more accurate image classifier did not lead to a more accurate outlier detector on average.

iv. KL loss did not yield a better-calibrated model than CE loss for OOD detection.

v. The autoencoders worked better with BCE loss than MSE loss for OOD detection.

vi. The nearest neighbour methods were competitive in low-dimensional settings, both in computational cost and accuracy.

vii. The learned latent representations of vanilla (variational)-autoencoders were not useful for this task when combined with nearest neighbour methods.

viii. The method with the state-of-the-art auto-regressive density estimation had a surprisingly low accuracy, performing worse than the random prediction baseline in some settings.

ix. The number of the classes in a dataset (a proxy to diversity) affected the accuracy more than the dimensionality of the data in our experiments.

x. Although ODIN outperforms other methods in realistic high-dimensional settings, its average accuracy is still below 80%.

6 Conclusion

By detecting OOD samples, we can ensure the deep learning pipelines operate as expected. While similar problems are studied in various domains of artificial intelligence, none of them adequately address this problem. We introduced OD-test, a new formulation of the problem that provides a realistic assessment of the OOD detection methods. We further presented a new benchmark for OOD sample detection within image classification pipelines. We showed that the traditional supervised learning approach to OOD detection does not always yield reliable results – the previous assessments of the OOD detectors are potentially too optimistic to be practical in many scenarios. We presented a comprehensive evaluation of a diverse set of approaches across a wide variety of datasets for the OOD detection problem. Furthermore, we showed that none of the methods is suitable out-of-the-box for high-dimensional images. We believe any progress on this problem could influence other areas such as active learning or unsupervised learning. We will release the open-source PyTorch project to replicate all the results and invite the machine learning community to tackle the challenges outlined in this work.
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A Appendix: Formulation and Evaluation

A.1 Evaluation of Unsupervised Techniques

Algorithm 2: OD-test – the evaluation procedure for an unsupervised method \( \mathcal{M} \).

input: \( \mathcal{D}_s = (\mathcal{D}_{s\text{train}}, \mathcal{D}_{s\text{valid}}, \mathcal{D}_{s\text{test}}) \) the three-way split of the source dataset.

input: \( \mathcal{D} = \{\mathcal{D}_i\} \) a \( \mathcal{D}_s \)-compatible dataset set.

input: \( \mathcal{M}: \mathcal{D} \rightarrow r \) the method under evaluation.

1: \( A \leftarrow \{} \)
2: \( /* \) Generate a rejection hypothesis \( r \) using \( \mathcal{D}_{s\text{train}} \). \( */ \)
3: \( r \leftarrow \mathcal{M}(\mathcal{D}_{s\text{train}}) \)
4: \( \text{for } \mathcal{D}_t \in \mathcal{D} \text{ do} \)
5: \( /* \) Evaluate the accuracy of \( r \). \( */ \)
6: \( \text{acc} \leftarrow \text{eval}(r, \{\mathcal{D}_{s\text{test}} : 0, \mathcal{D}_t : 1\}) \)
7: \( \text{add acc to } A \)
8: \( \text{return mean}(A) \)

Algorithm 2 outlines the steps of evaluation for an unsupervised method \( \mathcal{M} \). Note that in this setting \( \mathcal{M} \) returns a single binary classifier \( r \). To make the performance of supervised and unsupervised methods comparable, we use the same splits of the datasets to guarantee fairness of evaluation. In this work, we do not evaluate any unsupervised method. This additional information is provided for clarity and completeness.

A.2 Implementation Details

For each training procedure, we randomly separate 80\% and 20\% of the (sub-)data for training and testing respectively. We return the model that has the highest performance on the test (sub-)subset. For classification tasks, we measure the performance by classification accuracy while for other tasks such as AEThreshold we measure the performance through the respective loss value on the test set.

VGG, Resnet. We train two generic classifier architectures VGG-16 and Resnet-50 on \( \mathcal{D}_{s\text{train}} \) to perform the corresponding classification task within the datasets. The network architectures slightly differ across datasets to account for the change in the spatial size or the number of classes. We apply our modifications to the reference implementations available in PyTorch’s torchvision package. These trained networks are subsequently used in PbThreshold, ScoreSVM, ODIN, Log.SVM, and DeepEnsemble. For MC-Dropout we only use the VGG variant, as the Resnet variants do not have dropouts. Table 2 shows the summary of the networks’ classification accuracies on the entire \( \mathcal{D}_{s\text{train}} \) set.

Data Augmentation. We only allow mirroring of the images for data augmentation. We apply data augmentation on all the datasets except MNIST for which mirror augmentation does not make sense. We explicitly instantiate mirrored samples, as opposed to implicit on-air augmentation, to ensure methods such as K-NNSVM are not at disadvantage. We do not apply any other data augmentation.
Table 2: The classification accuracy of the trained networks on $D_{\text{train}}$ using cross-entropy (CE) and K-way Logistic (KL) loss functions. In both scenarios, the prediction is the maximum activation. Note that because of the difference in training data, this table is not comparable to the state-of-the-art performance on the respective datasets.

| Dataset      | CE-Accuracy | KL-Accuracy | Size  | CE-Accuracy | KL-Accuracy | Size  |
|--------------|-------------|-------------|-------|-------------|-------------|-------|
| MNIST [35]  | 99.89%      | 99.91%      | 19MB  | 99.89%      | 99.91%      | 70MB  |
| FashionMNIST [38] | 98.82%    | 98.36%      | 19MB  | 98.75%      | 98.73%      | 70MB  |
| CIFAR10 [37] | 97.63%      | 97.34%      | 159.8MB | 97.75%      | 97.51%      | 94.3MB |
| CIFAR100 [37] | 91.40%      | 91.87%      | 161.3MB | 92.05%      | 91.82%      | 95.1MB |
| TinyImagenet 9 | 69.71%      | 72.23%      | 162.9MB | 89.59%      | 65.95%      | 95.9MB |
| STL10 [39]  | 93.62%      | 95.18%      | 201.7MB | 92.32%      | 93.34%      | 94.3MB |
| Mean        | 91.84%      | 92.48%      | 95.05% | 91.21%      |             |       |

We initially experimented with no data augmentation. Without any augmentation, the performance of all the methods reduces by 3 – 4%, but the relative ranking stays the same.

**BinClass.** A binary classifier that is directly trained on $D_s$ and $D_v$. We use the reference ResNet or VGG architectures with an additional linear layer to transform the output of the network to a one-dimensional activation. We train the network with a binary cross-entropy loss on ($D_{\text{train}}$+$D_{\text{valid}}$,$D_v$) to ensure the method has access to the same data as the other methods. The networks typically achieve near-perfect accuracy after only a few epochs.

**PbThreshold** [8]. One threshold parameter on top of the maximum of softmax output. The cost of the evaluation is a single forward pass on the network. We reuse the trained reference VGG or ResNet architectures for this.

**ScoreSVM.** A natural generalization of PbThreshold is to train an SVM [40] classifier on the pre-softmax activations. The cost of evaluation is a single forward pass on the network with the additional SVM layer. We reuse the trained reference VGG or ResNet architectures for this. We set the weight-decay regularization to $\frac{1}{m}$, where $m$ is the size of the training set.

**ODIN** [9]. A threshold on the softmax outputs of the perturbed input. The cost of the evaluation is two forward passes and one backward pass. We do a grid search over the $\epsilon$, the perturbation step size, and $\gamma$, the temperature of the softmax operation. The range for grid search is the same as the suggested range in Liang et al. [9]. We reuse the trained reference VGG or ResNet architectures for this.

**K-NNSVM.** A linear SVM on the sorted Euclidean distance between the input and the k-nearest training samples. Note that a threshold on the average distance is a special case of K-NNSVM. The cost of the evaluation is finding the k-nearest neighbours in the training data. We use the $D_{\text{train}}$ as the reference set, and tune the parameters with ($D_{\text{valid}}$, $D_v$).

**K-MNNSVM, K-BNNSVM, K-VNNSVM.** The same as K-NNSVM, except we use the low dimensional representations of an autoencoder trained with MSE, BCE, or the VAE.
**AEThreshold.** A threshold on the autoencoder reconstruction error of the given input. The evaluation cost is a single forward pass on the autoencoder. We train the autoencoder on $D^\text{train}_s$ and train the threshold parameters with $(D^\text{valid}_s, D_v)$. We use the binary cross-entropy loss with continuous target or mean squared error to train and measure the reconstruction error of a given input. The bottleneck dimensionality varies between 32 and 1024. Our decision rule given a reconstruction error $e_x$ for an input $x$ is $r(x) = (e_x - \mu)^2 > \tau$, where $\tau$ is the threshold and $\mu$ is the center around which we are thresholding with $\tau$. If we set $\mu = 0$, this decision function reduces to a basic threshold operator. We found that this simple decision rule improves the final accuracy of the model. The reconstruction errors of the in-distribution samples tend to stay more or less similar, whereas the reconstruction error for OOD samples could either be too low or too high. This decision rule is meant to utilize this observation. The network architectures are procedurally generated. See [https://github.com/ashafaei/OD-test/blob/master/models/autoencoders.py](https://github.com/ashafaei/OD-test/blob/master/models/autoencoders.py) for the models.

**MC-Dropout.** A threshold on the entropy of average predictions of 7 evaluations per input. The dropout probability is $p = 0.5$. This approach follows the work of Lakshminarayanan *et al.* [12] and Kendall and Gal [16]. We did not evaluate this approach on Resnet because the original structure does not have a dropout; therefore, it is not trivial to identify where the dropouts should be located without sabotaging the performance of Resnet. We reuse the trained reference VGG architecture for this.

**DeepEnsemble.** Similar to MC-Dropout, except we average over the predictions of 5 networks that are trained independently with the adversarial strategy of Lakshminarayanan *et al.* [12]. In this approach, we augment the original loss function with a similar loss function on the adversarially-generated examples of the same batch. The adversarially-generated samples are generated through the fast gradient-sign method (FGSM) [42].

**PixelCNN++.** We use the implementation from [https://github.com/pclucas14/pixel-cnn-pp](https://github.com/pclucas14/pixel-cnn-pp). We train the models using $D_s$ until plateau on the test (sub-)subset, then learn a threshold parameter with $D_v$. Our models achieve a 0.89 BPD for MNIST, 2.65 BPD for FashionMNIST, 2.98 BPD for CIFAR10, 3.01 BPD for CIFAR100, 2.70 BPD for TinyImagenet, and 3.59 BPD for STL10 on the test (sub-)subset. Because of the auto-regressive nature, these models are prohibitively expensive to train. The PixelCNN++ authors note that they have used 8 Titan X GPUs for five days to achieve state-of-the-art performance for CIFAR10 [11] (2.92 BPD). For TinyImagenet, and STL10 we process a downsampled version to 32-pixel width to be able to train and evaluate the models. Our experiments with AEThreshold indicate that the downsampled versions of TinyImagenet, and STL10 are easier problems. However, even with this simplification, the PixelCNN++ does not perform up to expectations. Figure 5 shows some of the generated samples.

**OpenMax.** This method is a replacement for the softmax layer after the training has finished. It fits a Weibull distribution on the distances of logits from the representatives of each class to reweight the logits and provide probabilities for encountering an unknown class. The output of the OpenMax is similar to softmax, except with the addition of the probability for an unknown class. We learn the MAV vectors and the Weibull distribution on the $D_s$. We use the $D_v$ to learn the reject function on the calibrated probability outputs.

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**References:**

10. See [http://pytorch.org/docs/0.3.1/nn.html#bcewithlogitsloss](http://pytorch.org/docs/0.3.1/nn.html#bcewithlogitsloss).

11. See [https://github.com/openai/pixel-cnn](https://github.com/openai/pixel-cnn).
Figure 5: Samples of the learned PixelCNN++ model.

B Appendix: More Results

Figure 6 shows the average performance of all the methods per source dataset $D_s$. 

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Figure 6: The average test accuracy over 50 experiments per bar. The error bars indicate the 95% confidence level. The figure is best viewed in color.