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EXPLORING THE LINK BETWEEN OUT-OF-DISTRIBUTION DETECTION AND CONFORMAL PREDICTION WITH ILLUSTRATIONS OF ITS BENEFITS

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Paper under double-blind review

Abstract

Research on Out-Of-Distribution (OOD) detection focuses mainly on building scores that efficiently distinguish OOD data from In Distribution (ID) data. On the other hand, Conformal Prediction (CP) uses non-conformity scores to construct prediction sets with probabilistic coverage guarantees. In other words, the former designs scores, while the latter designs probabilistic guarantees based on scores. Therefore, we claim that these two fields might be naturally intertwined. This work advocates for cross-fertilization between OOD and CP by formalizing their link and emphasizing two benefits of using them jointly. First, we show that in standard OOD benchmark settings, evaluation metrics can be overly optimistic due to the test dataset's finite sample size. Based on the work of Bates et al. (2022), we define new conformal AUROC and conformal FPR@TPR95 metrics, which are corrections that provide probabilistic conservativeness guarantees on the variability of these metrics. We show the effect of these corrections on two reference OOD and anomaly detection benchmarks, OpenOOD Yang et al. (2022) and ADBench Han et al. (2022). Second, we explore using OOD scores as non-conformity scores and show that they can improve the efficiency of the prediction sets obtained with CP.

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1 INTRODUCTION

Even though current Machine Learning (ML) and Deep Learning (DL) models are able to perform several complex tasks that previously only human beings could, we are still a step away from their widespread adoption in safety-critical applications. Indeed, it is difficult to certify an ML component, mainly due to the poor control of the circumstances that may provoke such a ML component to fail. Out-of-Distribution (OOD) detection tries to tackle this problem by identifying data that differs significantly from the data used to train the model at runtime. Besides being recognized as an essential step in the certification of ML systems by multiple certification authorities (see, e.g., Sections 5.3 and 8.4 of Balduzzi et al. (2021) or Section 5.1 of EASA & Daedalean (2024)), OOD detection is a very active branch in machine learning research.

Current OOD detection strategies rely on constructing an OOD score s, a function that assigns a
 scalar to each input example. This score discriminates between in-distribution (ID) data and OOD
 data by assigning lower scores to the former and higher scores to the latter.

When OOD detection is used in a machine learning pipeline to identify examples that differ from
the data the model has been trained on, there is a natural qualitative interpretation of OOD detection
in terms of model uncertainty. For instance, an example with a low OOD score should be one for
which the model can predict with low uncertainty, while an example with a high OOD score should
be linked to a highly uncertain prediction.

Conformal Prediction (CP) is a family of post-hoc methods for Uncertainty Quantification and Uncertainty Representation Caprio et al. (2024), that work as wrappers over machine learning models, transforming point predictions into prediction sets with rigorous probabilistic guarantees based on so-called nonconformity scores. The user pre-specifies a risk level α , and the constructed prediction set is guaranteed to contain the ground truth value with a probability of at least $1 - \alpha$. Since CP is a way of providing rigorous uncertainty quantification guarantees built upon scores, it is natural to apply it to the scores used in OOD detection. **The main purpose of our work is to dig into the**

Conformal Prediction interpretation of OOD detection scores and show some of its advantages for both Conformal Prediction and OOD detection.

To that end, we first follow the work of Bates et al. (2022) on outlier detection and apply their ideas to OOD detection. Bates et al. (2022) cast the OOD detection problem into the statistical framework of hypothesis testing. They show that the p-values, built with a calibration dataset, are provably marginally valid but depend on the choice of the calibration dataset, and so is the False Positive Rate (FPR) derived from these p-values. One of the main contributions of our work is to explore the consequences of this effect for OOD detection and to propose alternative *conformal AUROC* and *conformal FPR@TPR95* metrics.

063 The relevance of the new metrics we propose is best appreciated in the context of safety-critical 064 applications, or in an eventual certification process of an OOD detection component. The true AUROC 065 or FPR metrics are inaccessible for a given OOD score, and we can only provide an approximation 066 obtained from a finite dataset. However, this can introduce fluctuations in our approximation, thus 067 overestimating or underestimating the true metrics. In a certification process, we are mainly interested 068 in guaranteeing that our estimations are conservative with high probability, at the expense of losing 069 some approximation precision EASA (2023), which is precisely what Conformal AUROC and Conformal FPR do. We show the effect of these new metrics on two large reference benchmarks, 071 the OOD benchmark OpenOOD Yang et al. (2022), and the anomaly detection benchmark Han et al. (2022).072

Second, we show that not only can CP contribute to OOD detection, but research in OOD detection can also help CP. Indeed, CP has traditionally focused on constructing prediction sets from nonconformity scores. Still, the scores used are usually simple functions of the softmax scores for classification tasks or classical distances in Euclidean space for regression tasks. Here, we draw inspiration from the OOD detection literature to build more involved nonconformity scores and compare their performance to the traditional nonconformity scores of CP. For the task of classification, we build prediction sets based on multiple different OOD scores and find that some of them, notably Mahalanobis Leys et al. (2018) or KNN Sun et al. (2022), are good candidates as nonconformity scores.

Ultimately, one of the key messages of this work is that since OOD is concerned with designing scores
 and conformal prediction with interpreting these scores, the two fields may be inherently intertwined.
 Highlighting this relationship might offer significant potential for cross-fertilization.

- Our contributions can be summarized as follows:
 - We cast the OOD detection problem into the framework of statistical hypothesis testing and apply the ideas of Bates et al. (2022) to correct OOD scores and propose new conformal AUROC and conformal FPR@TPR95 metrics, which are provably conservative with high probability.
 - We show the effect of conformal AUROC and conformal FPR in the reference benchmarks OpenOOD Yang et al. (2022) and ADBench Han et al. (2022).
 - We build new nonconformity scores for CP based on OOD and perform a comparison between the scores. We find that the Mahalanobis score outperforms the classical CP score.
 - We point out that OOD and CP are two domains that have much to contribute to each other and advocate for further research exploring this link.
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2 BACKGROUND

099 100 101 102 Out-of-Distribution Detection Given n examples, $\{x_1, \ldots, x_n\}$ sampled from a probability 101 distribution \mathcal{P}_{id} on a space \mathcal{X} , and a new data point x_{n+1} , the task of Out-of-Distribution (OOD) 101 detection consists in assessing if x_{n+1} was sampled from \mathcal{P}_{id} - in which case it is considered 102 In-Distribution (ID) - or not - thus considered OOD.

The most common procedure for OOD detection is to construct a score $s : \mathcal{X} \to \mathbb{R}$ and a threshold τ such that:

$$\begin{cases} \boldsymbol{x}_{n+1} \text{ is declared OOD if } s(\boldsymbol{x}_{n+1}) > \tau \\ \boldsymbol{x}_{n+1} \text{ is declared ID if } s(\boldsymbol{x}_{n+1}) \le \tau \end{cases}$$
(1)

We call s an OOD score.

108 **Task-based OOD** This is the most common approach in the literature regarding OOD detection for 109 neural networks. It also encompasses Open-Set Recognition. Let's consider that x_i can be assigned a 110 label y_i so that we can construct a dataset $\{(x_1, y_1), \ldots, (x_n, y_n)\}$ defining some supervised deep 111 learning task. In that case, $\mathcal{P}_{id} := \mathcal{P}_{train}$. Task-based OOD uses representations built by the neural 112 network f throughout its training to design s. Many sophisticated methods follow this approach Yang et al. (2021). A simple example is to take the negative maximum of the output of f (after the softmax) 113 Hendrycks & Gimpel (2018) as an OOD score $(s(\boldsymbol{x}_{n+1}) = -\max(f(\boldsymbol{x}_{n+1})))$ where $\max(\boldsymbol{x})$ is the 114 highest component of the vector \boldsymbol{x} . Another simple idea is to find the distance to the nearest neighbor 115 in some intermediate layer of f Sun et al. (2022). 116

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Task-agnostic OOD This approach encompasses One-Class Classification and Anomaly/Outlier Detection. Let's consider a dataset $\{x_1, \ldots, x_n\}$ in a fully unsupervised way. There is no notion of labels, so we have to approximate \mathcal{P}_{id} somehow or some related quantities from scratch. Examples are GANs or VAEs with *s* defined as reconstruction error. See Yang et al. (2021) for a thorough review.

123 **Conformal Prediction** Few Machine Learning and Deep Learning models provide a notion of 124 uncertainty related to their predictions. Even the models trained for classification tasks providing 125 softmax outputs, which can be interpreted as the probabilities for the input belonging to the different 126 classes, are usually ill-calibrated and overconfident, making the softmax output an incorrect proxy 127 of the true uncertainty of the prediction. Pearce et al. (2021). Conformal Prediction (CP) Vovk et al. (2005); Angelopoulos & Bates (2022) is a series of post-processing uncertainty quantification 128 techniques that are model-agnostic and provide finite-sample guarantees on the model predictions. 129 One of the simplest CP techniques, the split CP, works as a wrapper on a trained model f. It requires 130 a calibration dataset $\{(x_{n+1}, y_{n+1}), \dots, (x_{n+n_{cal}}, y_{n+n_{cal}})\}$ independent of the training data, and a 131 risk (or error rate) α that the user can tolerate. Based on so-called nonconformity scores computed on 132 the calibration dataset, it builds a prediction set $C_{\alpha}(x_{n+n_{cal}+1})$ for a new test sample $x_{n+n_{cal}+1}$ with 133 the following finite sample guarantee 134

$$\mathbb{P}\left(y_{n+n_{\rm cal}+1} \in C_{\alpha}(\boldsymbol{x}_{n+n_{\rm cal}+1})\right) \ge 1 - \alpha.$$
(2)

To obtain the guarantee equation (2), the only assumption required is that the calibration and test data form an exchangeable sequence (a condition weaker than, and therefore automatically satisfied by independence and identical distribution)Shafer & Vovk (2008) and that they are independent of the training data. It is essential to know that the guarantee equation (2) is marginal, i.e. holds in average over both the calibration dataset and the test sample choice. As we shall emphasize, there might be fluctuations due to the finite sample size of the calibration dataset.

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3 Related Works

In this work, we study the potential of using Conformal Prediction as a statistical framework for
 interpreting OOD scores. This idea of casting OOD in a statistical framework has already been
 attempted in different settings.

148 Selective Inference and Testing Selective Inference works on top of an ML predictor by using 149 an additional decision function to decide for each example whether the original model's prediction 150 should be considered. A score equivalent to an OOD score is used to define this decision function. 151 Several approaches exist, for instance, through building a statistical test Haroush et al. (2022) or by 152 training a neural network with an appropriate loss Geifman & El-Yaniv (2017; 2019). However, the 153 framework of Conformal Prediction appears better suited to our goal since it applies to scores in a 154 post-processing manner, does not require assumptions or modifications on the model, and benefits 155 from dynamic development in the ML community.

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157 Conformal OOD and AD Conformal Prediction has been previously applied to Out-of-Distribution 158 and Anomaly Detection. For instance, Liang et al. (2022) have proposed a method based on CP 159 for OOD with labeled outliers, and Kaur et al. (2022) propose to use conformal p-values. CP 160 is one of several frameworks that allow obtaining statistical guarantees for OOD detection. One 161 of the first methods for Anomaly Detection was introduced by Vovk et al. (2003). Since then, 162 several other methods have been proposed by Laxhammar & Falkman (2011); Laxhammar (2014); 162 Balasubramanian et al. (2014), as well as more recently Angelopoulos & Bates (2022); Guan & 163 Tibshirani (2022), where the lengths of the prediction sets as OOD scores. These works all use the 164 standard CP setting, in which basic marginal guarantees are obtained. We go further on this approach 165 by using CP as a probabilistic tool to refine the interpretation and, hence, the usefulness of any OOD 166 score.

168 **Finding Efficient Scores for Conformal Prediction** We also investigate the benefits of using OOD scores as non-conformity scores in CP. Common ways to build prediction sets for classification, such 169 170 as LAC Sadinle et al. (2019) or APS Romano et al. (2020) and RAPS Angelopoulos et al. (2020) are based on the softmax output of classifiers. However, non-conformity scores also exist for other 171 predictors Vovk et al. (2005), for instance, based on nearest neighbor distance Shafer & Vovk (2008). 172 In this work, we suggest interpreting any OOD score as a potential general replacement for scores 173 in CP, opening a large avenue for CP score crafting. This idea could apply to any ML task, but we 174 demonstrate that on a classification task, to be consistent with the standard OOD benchmark settings 175 we follow in the present paper. 176

OOD SCORES THROUGH THE LENS OF CP 4

179 Let us begin by describing the typical benchmark setup for evaluating an OOD score. First, 180 an OOD detector is fit on $\mathcal{D}_{id}^{train} = \{x_1, \dots, x_n\}$. Then, the OOD score is evaluated on $\mathcal{D}_{id}^{val} = \{x_{n+1}, \dots, x_{n+n_{val}}\}$ and $\mathcal{D}_{ood} = \{\bar{x}_1, \dots, \bar{x}_{n_{val}}\}$, where \mathcal{D}_{ood} is a dataset sampled from a different distribution $\mathcal{P}_{ood} \neq \mathcal{P}_{id}$ (typically, another dataset). We apply s to obtain 182 $\{s(\bar{x}_1), \ldots, s(\bar{x}_{n_{\text{val}}}), s(x_{n+1}), \ldots, s(x_{n+n_{\text{val}}})\}$. Then, we assess the discriminative power of s by evaluating metrics depending on a threshold τ . By considering ID samples as negative and OOD as 185 positive, we can compute: 186

- The Area Under the Receiver Operating Characteristic (AUROC): we compute the False Positive Rate (FPR) and the True Positive Rate (TPR) for $\tau_i = s(\boldsymbol{x}_{n+i}), i \in \{1, \dots, n_{\text{val}}\},\$ and compute the area under the curve with FPR as x-axis and TPR as y-axis.
- FPR@TPR95: The value of the False Positive Rate (FPR) when τ is selected among $\tau_1, \ldots, \tau_{n_{\text{val}}}$ so that the True Positive Rate (TPR) is 0.95. It can be generalized to FPR@TPR β , for any $\beta \in (0, 1)$.

A crucial step in any of these metrics is to compute the FPR. The FPR and its empirical estimation $FPR(\tau)$ are defined as follows:

$$\operatorname{FPR}(\tau) = \mathbb{P}_{\boldsymbol{x} \sim \mathcal{P}_{id}}(s(\boldsymbol{x}) \ge \tau), \qquad \widehat{\operatorname{FPR}}(\tau) = \frac{1}{n_{\operatorname{val}}} \sum_{i=1,\dots,n_{\operatorname{val}}} \mathbf{1}_{s(\boldsymbol{x}_i) \ge \tau}.$$
 (3)

4.1 OOD DETECTION AND P-VALUES

201 Let us now rewrite the problem of OOD detection using the framework of statistical hypothesis 202 testing. This framework allows us to reason in terms of p-values, which have multiple benefits: 203 they have a rigorous mathematical definition and probabilistic interpretation, they can be interpreted 204 equivalently for any score, and used for comparison of different scores. Given a test example x_{test} , 205 we wish to test for $x_{\text{test}} \sim \mathcal{P}_{id}$, i.e. we wish to test the null hypothesis $\mathcal{H}_0 : x_{\text{test}} \sim \mathcal{P}_{id}$ against the 206 alternate hypothesis $\mathcal{H}_1: \boldsymbol{x}_{\text{test}} \not\sim \mathcal{P}_{id}$. The value $P_{\boldsymbol{x} \sim \mathcal{P}_{id}}(s(\boldsymbol{x}) \geq s(\boldsymbol{x}_{\text{test}}))$ is an exact p-value for the 207 null hypothesis \mathcal{H}_0 . Note that this p-value corresponds to $FPR(s(\boldsymbol{x}_{test}))$ as defined in equation (3). 208 Hence, the values $\widehat{\text{FPR}}(\tau_1) = \widehat{\text{FPR}}(s(\boldsymbol{x}_{n+1})), \dots, \widehat{\text{FPR}}(\tau_p) = \widehat{\text{FPR}}(s(\boldsymbol{x}_{n+n_{\text{val}}}))$ used in every OOD 209 detection benchmark to compute the AUROC and FPR@TPR β can be considered as approximate 210 p-values. The relationship between the FPR and the p-values emphasizes the link between OOD 211 detection evaluation and hypothesis testing.

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- 213 4.2 FLUCTUATIONS OF THE P-VALUE
- This is where the framework of Conformal Prediction comes into play. Since we do not have access 215 to the distribution \mathcal{P}_{id} , we approximate the FPRs (so the p-values) by using the validation dataset

216 \mathcal{D}_{id}^{val} , which allows using two results from CP to improve the evaluation of the FPR. Note that \mathcal{D}_{id}^{val} can be related to the calibration dataset used in CP. 217

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4.2.1 MARGINAL VALIDITY OF THE FPR

The first point that CP teaches us is that fluctuations in the scores of the validation dataset can lead to over-confident estimations of the p-value. In order to avoid that, we have to use the correction 222 proposed by Bates et al. (2022) (which can be originally traced to Papadopoulos et al. (2002)): 223

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With this correction, if the x_i are i.i.d and the distribution of s(x) under the ID law is continuous, we obtain marginally valid p-values, that is, p-values that satisfy

 $\widehat{u}^{\text{marg}}(\boldsymbol{x}) = \frac{1}{1+n_{\text{val}}} \left(1 + \sum_{i=1,\dots,n-1} \mathbf{1}_{s(\boldsymbol{x}_i) \ge s(\boldsymbol{x})} \right).$

 $\mathbb{P}_{\boldsymbol{x} \sim \mathcal{P}_{id}} \left(\widehat{u}^{\text{marg}}(\boldsymbol{x}) \leq t \right) \leq t, \quad \text{for all} \quad 0 \leq t \leq 1.$ (5)

(4)

231 By marginally, we are pointing out that the probability in the above formula integrates over both the validation set \mathcal{D}_{id}^{val} and the test point x. This correction directly translates in terms of FPR. We can 232 correct equation (3) to obtain a new estimation that enjoys this property: 233

$$\widehat{\text{FPR}}(\tau) = \frac{1}{1 + n_{\text{val}}} \left(1 + \sum_{i=1...n_{\text{val}}} \mathbf{1}_{s(\boldsymbol{x}_i) \ge \tau} \right).$$
(6)

However, the work of Bates et al. (2022) tells us that the FPR may still be overly confident. We discuss this point in the next section.

4.3 FLUCTUATIONS OF THE FPR

243 In this part, we mainly explain the work of Bates et al. (2022) that emphasizes that the FPR fluctuates 244 depending on \mathcal{D}_{id}^{val} . We illustrate this phenomenon in the context of OOD detection and adapt the 245 corrections proposed in Bates et al. (2022) to this field by defining new conformal AUROC and 246 conformal FPR@TPR β .

247 Note first that the FPR can also be defined using a threshold t applied to the p-values as: 248

$$\operatorname{FPR}(t, \mathcal{D}_{id}^{val}) = \mathbb{P}_{\boldsymbol{x} \sim \mathcal{P}_{id}} \left(\widehat{u}^{\operatorname{marg}}(\boldsymbol{x}) \le t \,|\, \mathcal{D}_{id}^{val} \right), \tag{7}$$

250 where $t \in [0, 1]$. The authors point out that due to the empirical estimation of $\hat{u}^{\text{marg}}(x)$, the quantity 251 $P_{\boldsymbol{x} \sim \mathcal{P}_{id}}\left(\widehat{u}^{\text{marg}}(\boldsymbol{x}) \leq t \mid \mathcal{D}_{id}^{val}\right)$ is a random variable that depends on \mathcal{D}_{id}^{val} . 252

253 As a practical consequence, the FPR will fluctuate depending on which dataset \mathcal{D}_{id}^{val} it is evaluated. The random variable FPR $(t, \mathcal{D}_{id}^{val})$ follows a distribution that is known: it is a Beta distribution that 254 depends on the parameters n_{val} and t: 255

$$FPR(t, \mathcal{D}_{id}^{val}) \sim Beta(\ell, n_{val} + 1 - \ell), \tag{8}$$

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where $\ell = |(n_{val} + 1)t|$ (cf. Bates et al. (2022) or Vovk (2012) for a proof of the result).

4.3.1 Illustration on SVHN 260

261 To illustrate why this phenomenon matters in OOD detection, we leverage the fact that SVHN dataset 262 provides an additional set of 530000 extra test images. It allows the simulation of 53 draws of the 263 random variable $F(t; \mathcal{D}_{id}^{val})$, by splitting the over 530000 examples in the *svhn_extra* dataset into 53 264 different folds of 10000 examples each. For each fold, the 10000 examples are used to constitute the 265 calibration dataset \mathcal{D}_{id}^{val} , whereas the remaining over 520000 examples are used to approximate the 266 computation of F, i.e., given a calibration dataset \mathcal{D}_{id}^{val} , 267

$$F(t; \mathcal{D}_{id}^{val}) \approx \hat{F}(t; \mathcal{D}_{id}^{val}) = \frac{1}{520000} \sum_{i=1...520000} \mathbf{1}_{\hat{u}^{\text{marg}}(\boldsymbol{x}_i) \le t}.$$
(9)

270 Due to the large number of points used in the 271 approximating sum, the 53 values obtained are 272 faithful approximations of the random variables 273 $F(t; \mathcal{D}_{id}^{val})$.

274 We perform this simulation with t = 0.1 and 275 plot the 53 values into a histogram. Addition-276 ally, we fit a Beta distribution to the histogram 277 using the *scikit-learn* library. These plots are 278 found in figure 1. As we can see, the estimated 279 parameters of the fitted beta distribution are very 280 close to those predicted by the theoretical result of equation (8). If the value $\widehat{u}^{\text{marg}}(\boldsymbol{x})$ were a 281 true p-value, the value of $F(t; \mathcal{D}_{id}^{val})$ would be 282 equal to τ , but as we can see from the theoretical 283 result and the experiment above, $F(t; \mathcal{D}_{id}^{val})$ is a 284 random variable that fluctuates around its mean 285 value τ . This phenomenon can be detrimental to 286 safety-critical applications, which are the appli-287 cations of choice for OOD detection. Indeed, it 288 may result in underestimating the FPR, whereas 289 we would like the FPR to be conservative. 290



Figure 1: Histogram of $F(0.1; \mathcal{D}_{id}^{cal})$ for different calibration sets. The histogram is obtained by splitting the dataset *svhn_extra* into disjoint calibration sets of 10000 points each, and approximating the value of F for each calibration set by integrating over the remaining 521131 examples.

4.3.2 PROBABILISTIC GUARANTEES FOR P-VALUES AND THE FPR

To solve this problem, Bates et al. (2022) further corrects the marginal p-values, thus obtaining *calibration-conditional* p-values. Given a user-predefined risk level δ , the calibration-conditional p-values \hat{u}^{cc} will satisfy

$$\mathbb{P}\Big(\mathbb{P}\big(\widehat{u}^{cc}(\boldsymbol{x}) \le t \,|\, \mathcal{D}^{val}_{id}\big) \le t, \,\forall t \in (0,1)\Big) \ge 1 - \delta,\tag{10}$$

where the probability inside is taken over $x \sim \mathcal{P}_{id}$, and the probability outside over the choice of \mathcal{D}_{id}^{val} . Thus, with a probability of at least $1 - \delta$, we can be confident that we have a *good* calibration set, meaning that our p-values will be conservative.

Likewise, we can correct the FPR directly. Bates et al. (2022) propose a correction of the empirical FPR that satisfies the following:

$$\mathbb{P}\left[\operatorname{FPR}(\tau) \le \widehat{\operatorname{FPR}}^+(\tau), \forall \tau \in \mathbb{R}\right] \ge 1 - \delta,\tag{11}$$

where $\widehat{\text{FPR}}^+(\tau)$ is a correction version of the empirical $\widehat{\text{FPR}}(\tau)$. The corrected FPR is obtained by applying a correction function *h* to the empirical FPR, i.e. $\widehat{\text{FPR}}^+(\tau) = h \circ \widehat{\text{FPR}}(\tau)$. In the following, we refer to the quantity $\widehat{\text{FPR}}^+(\tau) = h \circ \widehat{\text{FPR}}(\tau)$ as *conformal* FPR.

Four different correction functions h are proposed by Bates et al. (2022), the Simes, DKWM, Asymptotic and Monte Carlo corrections. The Simes, DKWM and Monte Carlo corrections all provide the finite sample guarantees of equation (10) and equation (11), while the Asymptotic correction provides only an asymptotic guarantee, that is, when the number of calibration points goes to infinity. Between the three corrections providing the finite sample guarantee, we find the Monte Carlo one to give tighter bounds (please see Appendix A for more details on how the Simes and Monte Carlo corrections are defined).

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4.4 CONFORMAL METRICS FOR OOD

Based on the previously defined conformal FPR (already defined in Bates et al. (2022), we define
 conformal AUROC and *conformal* FPR@TPR95. These two quantities are obtained similarly as their
 classical versions, but using the conformal FPR:

• Conformal AUROC: we compute the *conformal* FPR for $\tau_i = s(\boldsymbol{x}_{n+i}), i \in \{1, \dots, n_{\text{val}}\}$ and the True Positive Rate (TPR) for each of these values. We then compute the area under the curve with *conformal* FPR as x-axis and TPR as y-axis.



Figure 2: Different zoom levels of the ROC curves. The TPR is calculated by using all the points in the "Cifar10" dataset for the three curves. As for the TPR, the blue curve is obtained by using all data points in the "svhn_extra" dataset, the orange curve is an approximation of the blue curve using 1000 calibration points, whereas the green curve is obtained by correcting the FPR via the conformal AUROC method.

• Conformal FPR@TPR95: We select τ among $\tau_1, \ldots, \tau_{n_{val}}$ so that the True Positive Rate (TPR) is 0.95. We then compute the corresponding *conformal* FPR. It can be generalized to FPR@TPR β , for any $\beta \in (0, 1)$.

The computations are performed by considering the ID validation dataset as the calibration dataset. We would like to insist on the fact that Conformal FPR, AUROC, and FPR@TPR95 are not necessarily better approximations of the real FPR, AUROC and FPR@TPR95 values. Nonetheless, they are guaranteed to use conservative estimates of the FPR with a user-defined miscalibration tolerance δ , which is an essential property in many safety-critical applications or certification processes Sellke et al. (2001). The effect of the correction on the ROC curve is illustrated in Figure 2 using the SVHN dataset as ID and Cifar-10 as OOD.

Remark 4.1 (Conformal metrics do not require extra validation data). Computing the conformal FPR only requires a correction to the estimated FPR. It does not require extra validation data. This is not like in CP, where we need a calibration dataset to find a threshold based on nonconformity scores obtained on calibration data, which is subsequently used to provide CP confidence intervals. Here, there are no confidence prediction intervals; we only use CP theory to obtain probabilistic guarantees of the FPR.

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4.5 SAFER BENCHMARKS FOR OOD

AUROC and (to a lesser extent) FPR@TPR95 are two metrics that OOD and AD practitioners
intensively use to benchmark and evaluate the performances of different OOD detection algorithms.
However, as we saw in the previous sections, the evaluation can be overly optimistic, which can
be detrimental to algorithms designed for safety-critical applications. In this section, we reevaluate
various OOD baselines included in the very furnished OpenOOD Yang et al. (2022), and ADBench
Han et al. (2022) benchmarks and illustrate the trade-off between performances and probabilistic
guarantees. All our experiments can be easily carried out on a standard laptop CPU.

365 366 4.5.1 OPENOOD

367 OpenOOD Yang et al. (2022) is an extensive benchmark for task-based OOD, i.e. for OOD methods 368 that assess if some test data resembles some trained backbone's training data. Usually, backbones 369 trained on CIFAR-10, CIFAR-100, Imagenet200, and Imagenet are considered. In our case, we consider a ResNet18 trained on the first three datasets only since we are not evaluating a new baseline 370 but only investigating a new metric for the benchmark. We evaluate the AUROC of several baselines 371 with various OOD datasets gathered into two groups, Near OOD and Far OOD, following OpenOOD's 372 guidelines. We then compute the correction for the AUROC, with $\delta = 0.01$. The results are displayed 373 in Table 1. We also run the benchmark for $\delta = 0.05$ and FPR-95, which we defer to Appendix C. 374

Table 1 shows that after the correction, the conformal AUROC is lower than the classical AUROC, by often more than 1 percent. On the one hand, this is significant, especially for such benchmarks where the State-of-the-art often holds by a fraction of a percentage. On the other hand, the correction is not *so* severe, and the best baselines still get very good AUROC despite the correction. In other

		CIFA	R-10			CIFA	R-100		ImageNet-200			
OOD type	Near	OOD	Far (OOD	Near	OOD	Far (DOD	Near	OOD	Far (DOD
	class.	conf.	class.	conf.	class.	conf.	class.	conf.	class.	conf.	class.	conf.
OpenMax Bendale & Boult (2015)	87.2	85.95	89.53	88.3	76.66	74.95	79.12	77.52	80.4	78.82	90.41	88.77
MSP Hendrycks & Gimpel (2018)	87.68	86.56	91.0	89.98	80.42	78.93	77.58	76.0	83.3	81.85	90.2	88.83
TempScale Guo et al. (2017)	87.65	86.55	91.27	90.3	80.98	79.51	78.51	76.95	83.66	82.21	90.91	89.53
ODIN Liang et al. (2018)	80.25	79.04	87.21	86.26	79.8	78.3	79.44	77.92	80.32	78.85	91.89	90.59
MDS Lee et al. (2018)	86.72	85.49	90.2	89.09	58.79	56.85	70.06	68.31	62.51	60.68	74.94	73.09
MDSEns Lee et al. (2018)	60.46	58.69	74.07	72.72	45.98	43.97	66.03	64.43	54.58	52.76	70.08	68.35
Gram Sastry & Oore (2020)	52.63	50.69	69.74	68.11	50.69	48.69	73.97	72.63	68.36	66.74	70.94	69.3
EBO Liu et al. (2020)	86.93	85.9	91.74	90.9	80.84	79.36	79.71	78.19	82.57	81.1	91.12	89.71
GradNorm Huang et al. (2021)	53.77	51.92	58.55	56.76	69.73	68.11	68.82	67.19	73.33	71.85	85.29	83.99
ReAct Sun et al. (2021)	86.47	85.41	91.02	90.12	80.7	79.23	79.84	78.32	80.48	79.0	93.1	91.79
MLS Hendrycks et al. (2022)	86.86	85.81	91.61	90.74	81.04	79.58	79.6	78.07	82.96	81.5	91.34	89.94
KLM Hendrycks et al. (2022)	78.8	77.58	82.76	81.63	76.9	75.38	76.03	74.52	80.69	79.14	88.41	86.74
VIM Wang et al. (2022)	88.51	87.42	93.14	92.25	74.83	73.17	82.11	80.69	78.81	77.2	91.52	90.05
KNN Sun et al. (2022)	90.7	89.69	93.1	92.19	80.25	78.79	82.32	80.93	81.75	80.27	93.47	92.25
DICE Sun & Li (2022)	77.79	76.44	85.41	84.37	79.15	77.61	79.84	78.33	81.97	80.5	91.19	89.84
RankFeat Song et al. (2022)	76.33	74.76	70.15	68.39	62.22	60.33	67.74	65.9	58.57	57.0	38.97	37.09
ASH Djurisic et al. (2022)	74.11	72.71	78.36	77.02	78.39	76.89	79.7	78.23	82.12	80.72	94.23	93.11
SHE Zhang et al. (2023)	80.84	79.64	86.55	85.55	78.72	77.18	77.35	75.8	80.46	79.0	90.48	89.17

Table 1: Classical AUROC (class.) vs Conformal AUROC (conf.) obtained with the Monte Carlo method and $\delta = 0.01$ for several baselines from OpenOOD benchmark.

words, the correction is large enough to manifest its importance but low enough to still be useable in practice: it costs only roughly 1 or 2 percent in AUROC to be 99% sure that the FPR involved in the AUROC calculation is not overestimated.

4.5.2 ADBENCH

We perform the same procedure as OpenOOD with ADBench Han et al. (2022), which gathers many task-agnostic OOD baselines – considered Anomaly Detection (AD), hence the benchmark's name. We conduct the experiments with "unsupervised AD" baselines, i.e. baselines that do not leverage labeled anomalies. We apply the correction with $\delta = 0.05$ and summarize the results in Figure 3. The complete results are deferred to Appendix D.



Figure 3: Results for ADBench benchmark. (left) Scatter plot with mean classical AUROC and mean AUROC correction over different methods for each dataset as y-axis and x-axis, respectively. (right) Mean AUROC and AUROC correction over different datasets for each AD method.

Figure 3 (left) shows a scatter plot with mean classical AUROC and mean AUROC correction over different methods for each dataset as y-axis and x-axis, respectively. The variability and magnitude of the correction are higher than for OpenOOD since the number of points in the test set changes depending on the dataset and is generally way lower. This observation is important because it illustrates the brittleness of the conclusions that can be drawn from AD benchmarks and supports the increasingly commonly accepted fact that no method is provably better than others in AD – one of the key conclusions of ADBench's paper itself Han et al. (2022). Figure 3 (right) shows the mean classical and conformal AUROC for each baseline over the datasets. The correction is more stable, demonstrating that the correction affects all baselines similarly.

5 OOD SCORES AS NONCONFORMITY SCORES FOR CP

In the previous sections, we have mostly emphasized that practitioners of OOD detection should look at CP as an additional building block for correctly interpreting the scores that all the OOD methods rely on. In this section, we advocate that the link between OOD and CP goes even deeper and that both fields could benefit from each other.

		LAC			APS			RAPS	
α	0.005	0.01	0.05	0.005	0.01	0.05	0.005	0.01	0.05
Cifar10									
Gram	9.57	8.34	1.89	9.60 ± 0.10	1.93 ± 0.06	8.66 ± 0.13	9.56 ± 0.13	8.7 ± 0.16	1.89 ± 0.03
ReAct	3.75	1.98	1.03	4.47 ± 0.16	1.97 ± 0.09	3.62 ± 0.17	4.46 ± 0.15	3.67 ± 0.19	2.02 ± 0.09
ODIN	7.15	5.82	1.14	7.42 ± 0.17	1.53 ± 0.06	5.14 ± 0.08	7.45 ± 0.16	5.1 ± 0.10	1.57 ± 0.08
KNN	2.57	1.48	1.01	3.62 ± 0.15	1.09 ± 0.03	2.71 ± 0.11	3.69 ± 0.11	2.77 ± 0.09	1.08 ± 0.02
Mahalanobis	1.85	1.47	1.04	1.89 ± 0.07	1.04 ± 0.01	$\textbf{1.49} \pm 0.04$	1.92 ± 0.05	$\textbf{1.49} \pm 0.05$	1.04 ± 0.01
CP (Softmax)	2.44	1.73	1.03	3.92 ± 0.26	1.1 ± 0.01	$\underline{2.16} \pm 0.13$	3.81 ± 0.24	$\underline{2.17} \pm 0.11$	1.09 ± 0.01
Cifar100									
ReAct	52.41	29.77	10.06	53.02 ± 0.27	32.02 ± 0.11	10.45 ± 0.15	53.12 ± 0.26	32.12 ± 0.13	10.43 ± 0.15
ODIN	66.54	45.25	16.25	65.46 ± 0.3	45.56 ± 0.14	17.49 ± 0.13	65.61 ± 0.25	45.51 ± 0.27	17.6 ± 0.14
KNN	41.64	27.74	8.62	39.45 ± 0.35	29.81 ± 0.24	9.80 ± 0.11	39.63 ± 0.21	29.74 ± 0.29	9.81 ± 0.10
Mahalanobis	31.29	24.76	7.57	$\overline{31.07} \pm 0.07$	24.77 ± 0.20	$\overline{8.47} \pm 0.29$	$\overline{31.15} \pm 0.07$	$\overline{24.82} \pm 0.19$	8.48 ± 0.21
CP (Softmax)	31.96	27.21	5.73	46.55 ± 1.47	36.82 ± 0.39	17.59 ± 0.41	45.64 ± 1.19	36.83 ± 0.79	17.12 ± 0.74

Table 2: Efficiency (mean \pm std. dev. for APS and RAPS) of the prediction sets for different scores for CP classification on CIFAR-10 and CIFAR-100. The best is bolded, the second is underlined.

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So far, we have shown how OOD can use CP, but we argue that CP could also use OOD. Indeed, CP 454 is about interpreting scores to provide probabilistic results. But CP works regardless of the given 455 score. Indeed, all scores will have the same guarantee, but better scores will give tighter prediction 456 sets, and worse scores will give very large and uninformative prediction sets. For CP to provide 457 powerful probabilistic guarantees, the scores have to be informative, hence the common practice of 458 relying on scores derived from the softmax values of a neural network Sadinle et al. (2019). It turns 459 out that the maximum softmax is also a score used in OOD detection Hendrycks & Gimpel (2018), 460 which suggests that OOD scores and CP scores might be related in some way. In this section, we 461 explore using different OOD scores to perform CP. We consider two ResNet18 trained on CIFAR-10 462 and CIFAR-100 and build conformal prediction sets following the procedure described in section 2. 463 To build these prediction sets, we use scores based on ReAct Sun et al. (2021), Gram Sastry & Oore (2020), KNN Sun et al. (2022), Mahalanobis Lee et al. (2018), and ODIN Liang et al. (2018). Note 464 that we had to adapt those scores to make them class-dependent since the score used in CP is defined 465 as $s_{cp}(x, y)$. We did so following a procedure that we describe in detail in Appendix B. Then, given 466 the OOD score $s(\boldsymbol{x}, y_i)$, we construct softmax-like scores $\hat{s}(\boldsymbol{x}, y_i) = \exp s(\boldsymbol{x}, y_i) / \sum_i \exp s(\boldsymbol{x}, y_i)$, 467 and use it for CP. 468

469 For each defined score, we perform the calibration step on $n_{cal} = 2000$ points following the classical Least-Ambiguous set classifiers (LAC) procedure Sadinle et al. (2019), and the more recent 470 Adaptive Prediction Set (APS) Romano et al. (2020) and Regularized Adaptive Prediction Set (RAPS) 471 Angelopoulos et al. (2020) methods. For all methods, we construct the prediction sets for each 472 of the remaining $n_{val} - n_{cal} = 8000$ points, and for coverages $1 - \alpha \in \{0.005, 0.01, 0.05\}$. We 473 assess the mean efficiency of the prediction sets for each score, including LAC, APS, and RAPS 474 based on softmax, as classically done in CP in Table 5). Since APS and RAPS involve sampling a 475 uniform random variable, we report the mean and the standard deviation of the mean efficiency for 476 10 evaluations. 477

Table 5 shows that all OOD scores are inefficient for CP. For example, Gram performs very poorly (hence, we only run it on CIFAR-10). However, in some instances, some scores, like KNN or Mahalanobis, perform better than classical CP scores. This suggests that OOD scores may be good candidates as nonconformity scores.

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6 LIMITATIONS

485 While we believe that OOD detection and CP have much to gain from each other, we acknowledge that our paper has limitations: *Data availability*. Computing conformal AUROC and conformal

FPR requires an extra calibration dataset, which might be a drawback in applications with low data availability. *Extra compute resources*. The extra calibration step requires additional calibration resources. However, these resources are negligible compared to those needed for training and fine-tuning a neural network.

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7 CONCLUSION & DISCUSSION

493 In conclusion, our work highlights the inherent randomness of OOD metrics and demonstrates how 494 Conformal Prediction (CP) can effectively correct these metrics. We have also shown that recent 495 advancements in CP allow for uniform conservativeness guarantees on OOD metrics, providing more 496 reliable evaluations. Furthermore, our analysis reveals that the correction introduced by CP does not 497 significantly impact the performance of the best OOD baselines. On the other hand, we also showed 498 that we could use OOD to improve existing CP techniques by using OOD scores as nonconformity scores. We found that some of them, especially Mahalanobis and KNN, are good candidates for 499 nonconformity scores, unlocking a whole avenue for crafting CP nonconformity scores based on the 500 plethora of existing post-hoc OOD scores. 501

502 By integrating CP with OOD, we have demonstrated the fruitful synergy between the two fields. OOD 503 detection focuses on developing scores that accurately discriminate between OOD and ID, while CP 504 specializes in interpreting scores to provide probabilistic guarantees. This interplay between OOD and CP presents opportunities for mutual advancement: advancements in CP research can enhance 505 OOD by offering more refined probabilistic interpretations of OOD scores, which is particularly 506 crucial in safety-critical applications. Conversely, progress in OOD research can benefit CP by 507 providing scores that improve the efficiency of prediction sets. This suggests that further exploration 508 and collaboration between the two fields hold great potential. 509

In summary, our findings underscore the intertwined nature of OOD and CP, emphasizing the need
 for continued investigation and cross-fertilization to advance both disciplines.

- 513 REFERENCES 514
- Anastasios Angelopoulos, Stephen Bates, Jitendra Malik, and Michael I Jordan. Uncertainty sets for
 image classifiers using conformal prediction. *arXiv preprint arXiv:2009.14193*, 2020.
- Anastasios N. Angelopoulos and Stephen Bates. A gentle introduction to conformal prediction and distribution-free uncertainty quantification, 2022.
- Vineeth Balasubramanian, Shen-Shyang Ho, and Vladimir Vovk. *Conformal prediction for reliable machine learning: theory, adaptations and applications*. Newnes, 2014.
- Giovanni Balduzzi, Martino Ferrari Bravo, Anna Chernova, Calin Cruceru, Luuk van Dijk, Peter de Lange, Juan Jerez, Nathanaël Koehler, Mathias Koerner, Corentin Perret-Gentil, et al. Neural network based runway landing guidance for general aviation autoland. Technical report, United States. Department of Transportation. Federal Aviation Administration ..., 2021.
 - Stephen Bates, Emmanuel Candès, Lihua Lei, Yaniv Romano, and Matteo Sesia. Testing for Outliers with Conformal p-values, May 2022. URL http://arxiv.org/abs/2104.08279.
 - Abhijit Bendale and Terrance E. Boult. Towards Open Set Deep Networks. *CoRR*, abs/1511.06233, 2015. URL http://arxiv.org/abs/1511.06233.
- Michele Caprio, Souradeep Dutta, Kuk Jin Jang, Vivian Lin, Radoslav Ivanov, Oleg Sokolsky, and Insup Lee. Credal bayesian deep learning, 2024. URL https://arxiv.org/abs/2302. 09656.
- Andrija Djurisic, Nebojsa Bozanic, Arjun Ashok, and Rosanne Liu. Extremely Simple Activation Shaping for Out-of-distribution Detection. *CoRR*, abs/2209.09858, 2022. doi: 10.48550/ARXIV. 2209.09858. URL https://doi.org/10.48550/arXiv.2209.09858.
- 538EASA.Easa artificial intelligence concept paper, 2023.URL539https://www.easa.europa.eu/en/newsroom-and-events/news/
easa-artificial-intelligence-concept-paper-proposed-issue-2-open.URL

EASA and Daedalean. Concepts of design assurance for neural networks (codann) ii with appendix b. 541 Technical report, EASA and Daedalean, 1 2024. 542 Yonatan Geifman and Ran El-Yaniv. Selective classification for deep neural networks. Advances in 543 neural information processing systems, 30, 2017. 544 Yonatan Geifman and Ran El-Yaniv. SelectiveNet: A deep neural network with an integrated 546 reject option. In Kamalika Chaudhuri and Ruslan Salakhutdinov (eds.), Proceedings of the 36th 547 International Conference on Machine Learning, volume 97 of Proceedings of Machine Learning Research, pp. 2151-2159. PMLR, 09-15 Jun 2019. URL https://proceedings.mlr. 548 press/v97/geifman19a.html. 549 550 Leying Guan and Robert Tibshirani. Prediction and outlier detection in classification problems. 551 Journal of the Royal Statistical Society Series B: Statistical Methodology, 84(2):524–546, 2022. 552 Chuan Guo, Geoff Pleiss, Yu Sun, and Kilian Q. Weinberger. On Calibration of Modern Neural 553 Networks. CoRR, abs/1706.04599, 2017. URL http://arxiv.org/abs/1706.04599. 554 Songqiao Han, Xiyang Hu, Hailiang Huang, Minqi Jiang, and Yue Zhao. Adbench: Anomaly 556 detection benchmark. Advances in Neural Information Processing Systems, 35:32142–32159, 2022. 558 Matan Haroush, Tzviel Frostig, Ruth Heller, and Daniel Soudry. A statistical framework for efficient 559 out of distribution detection in deep neural networks, March 2022. URL http://arxiv.org/ abs/2102.12967. 561 562 Dan Hendrycks and Kevin Gimpel. A Baseline for Detecting Misclassified and Out-of-distribution 563 Examples in Neural Networks. CoRR, abs/1610.02136, 2016. URL http://arxiv.org/ abs/1610.02136. 564 565 Dan Hendrycks and Kevin Gimpel. A Baseline for Detecting Misclassified and Out-of-Distribution Ex-566 amples in Neural Networks, October 2018. URL http://arxiv.org/abs/1610.02136. 567 568 Dan Hendrycks, Steven Basart, Mantas Mazeika, Andy Zou, Joseph Kwon, Mohammadreza Mostajabi, Jacob Steinhardt, and Dawn Song. Scaling Out-of-distribution Detection for Real-world 569 Settings. In Kamalika Chaudhuri, Stefanie Jegelka, Le Song, Csaba Szepesvári, Gang Niu, and 570 Sivan Sabato (eds.), International Conference on Machine Learning, ICML 2022, 17-23 July 2022, 571 Baltimore, Maryland, USA, volume 162 of Proceedings of Machine Learning Research, pp. 8759-572 8773. PMLR, 2022. URL https://proceedings.mlr.press/v162/hendrycks22a. 573 html. 574 575 Rui Huang, Andrew Geng, and Yixuan Li. On the Importance of Gradients for Detecting Distributional Shifts in the Wild. CoRR, abs/2110.00218, 2021. URL https://arxiv.org/abs/2110. 576 00218. 577 578 Ramneet Kaur, Susmit Jha, Anirban Roy, Sangdon Park, Edgar Dobriban, Oleg Sokolsky, and 579 Insup Lee. iDECODe: In-Distribution Equivariance for Conformal Out-of-Distribution Detection. 580 Proceedings of the AAAI Conference on Artificial Intelligence, 36(7):7104–7114, June 2022. ISSN 581 2374-3468, 2159-5399. doi: 10.1609/aaai.v36i7.20670. URL https://ojs.aaai.org/ 582 index.php/AAAI/article/view/20670. 583 Rikard Laxhammar. Conformal anomaly detection. Skövde, Sweden: University of Skövde, 2, 2014. 584 585 Rikard Laxhammar and Göran Falkman. Sequential conformal anomaly detection in trajectories 586 based on hausdorff distance. In 14th international conference on information fusion, pp. 1–8. IEEE, 2011. 588 Kimin Lee, Kibok Lee, Honglak Lee, and Jinwoo Shin. A Simple Unified Framework for Detecting Out-of-distribution Samples and Adversarial Attacks. CoRR, abs/1807.03888, 2018. URL http: 590 //arxiv.org/abs/1807.03888. Christophe Levs, Olivier Klein, Yves Dominicy, and Christophe Ley. Detecting multivariate outliers: 592 Use a robust variant of the Mahalanobis distance. Journal of Experimental Social Psychology, 2018.

594 595 596	Shiyu Liang, Yixuan Li, and R. Srikant. Enhancing The Reliability of Out-of-distribution Image Detection in Neural Networks. In 6th International Conference on Learning Representations, ICLR 2018, Vancouver, BC, Canada, April 30 - May 3, 2018, Conference Track Proceedings.
597	OpenReview.net , 2018. URL https://openreview.net/forum?id=H1VGkIxRZ.
598 599	Ziyi Liang, Matteo Sesia, and Wenguang Sun. Integrative conformal p-values for powerful out- of-distribution testing with labeled outliers, August 2022. URL http://arxiv.org/abs/
600 601	2208.11111.
602 603	Weitang Liu, Xiaoyun Wang, John D. Owens, and Yixuan Li. Energy-based Out-of-distribution Detection. <i>CoRR</i> , abs/2010.03759, 2020. URL https://arxiv.org/abs/2010.03759.
605 606 607 608	Harris Papadopoulos, Kostas Proedrou, Volodya Vovk, and Alex Gammerman. Inductive confidence machines for regression. In <i>Machine Learning: ECML 2002: 13th European Conference on Machine Learning Helsinki, Finland, August 19–23, 2002 Proceedings 13</i> , pp. 345–356. Springer, 2002.
609 610	Tim Pearce, Alexandra Brintrup, and Jun Zhu. Understanding softmax confidence and uncertainty. <i>arXiv preprint arXiv:2106.04972</i> , 2021.
611 612 613	Yaniv Romano, Matteo Sesia, and Emmanuel Candes. Classification with valid and adaptive coverage. Advances in Neural Information Processing Systems, 33:3581–3591, 2020.
614 615	Mauricio Sadinle, Jing Lei, and Larry Wasserman. Least ambiguous set-valued classifiers with bounded error levels. <i>Journal of the American Statistical Association</i> , 114(525):223–234, 2019.
616 617 618 619 620	Chandramouli Shama Sastry and Sageev Oore. Detecting Out-of-distribution Examples with Gram Matrices. In Proceedings of the 37th International Conference on Machine Learning, ICML 2020, 13-18 July 2020, Virtual Event, volume 119 of Proceedings of Machine Learning Research, pp. 8491–8501. PMLR, 2020. URL http://proceedings.mlr.press/v119/sastry20a. html.
621 622 623	Thomas M. Sellke, Maria J. Bayarri, and James O. Berger. Calibration of <i>ρ</i> values for testing precise null hypotheses. <i>The American Statistician</i> , 55:62 – 71, 2001. URL https://api.semanticscholar.org/CorpusID:396772.
625 626	Glenn Shafer and Vladimir Vovk. A tutorial on conformal prediction. <i>Journal of Machine Learning Research</i> , 9(3), 2008.
627 628 629	Yue Song, Nicu Sebe, and Wei Wang. RankFeat: Rank-1 Feature Removal for Out-of-distribution Detection. <i>CoRR</i> , abs/2209.08590, 2022. doi: 10.48550/ARXIV.2209.08590. URL https://doi.org/10.48550/arXiv.2209.08590.
630 631 632 633 634 635	Yiyou Sun and Yixuan Li. DICE: Leveraging Sparsification for Out-of-distribution Detection. In Shai Avidan, Gabriel J. Brostow, Moustapha Cissé, Giovanni Maria Farinella, and Tal Hassner (eds.), <i>Computer Vision - ECCV 2022: 17th European Conference, Tel Aviv, Israel, October 23-27, 2022, Proceedings, Part XXIV</i> , volume 13684 of <i>Lecture Notes in Computer Science</i> , pp. 691–708. Springer, 2022. doi: 10.1007/978-3-031-20053-3_40. URL https://doi.org/10.1007/978-3-031-20053-3_40.
636 637 638	Yiyou Sun, Chuan Guo, and Yixuan Li. ReAct: Out-of-distribution Detection With Rectified Activations. CoRR, abs/2111.12797, 2021. URL https://arxiv.org/abs/2111.12797.
639 640 641	Yiyou Sun, Yifei Ming, Xiaojin Zhu, and Yixuan Li. Out-of-distribution Detection with Deep Nearest Neighbors. <i>CoRR</i> , abs/2204.06507, 2022. doi: 10.48550/ARXIV.2204.06507. URL https://doi.org/10.48550/arXiv.2204.06507.
642 643 644 645	Vladimir Vovk. Conditional Validity of Inductive Conformal Predictors. In <i>Proceedings of the</i> <i>Asian Conference on Machine Learning</i> , pp. 475–490. PMLR, November 2012. URL https: //proceedings.mlr.press/v25/vovk12.html.
646 647	Vladimir Vovk, Ilia Nouretdinov, and Alexander Gammerman. Testing exchangeability on-line. In <i>Proceedings of the 20th International Conference on Machine Learning (ICML-03)</i> , pp. 768–775, 2003.

- Vladimir Vovk, Alexander Gammerman, and Glenn Shafer. Algorithmic learning in a random world, volume 29. Springer, 2005.
- Haoqi Wang, Zhizhong Li, Litong Feng, and Wayne Zhang. ViM: Out-Of-distribution with Virtual-logit Matching. CoRR, abs/2203.10807, 2022. doi: 10.48550/ARXIV.2203.10807. URL https: //doi.org/10.48550/arXiv.2203.10807.
- Jingkang Yang, Kaiyang Zhou, Yixuan Li, and Ziwei Liu. Generalized Out-of-distribution Detection: A Survey. CoRR, abs/2110.11334, 2021. URL https://arxiv.org/abs/2110.11334.
 - Jingkang Yang, Pengyun Wang, Dejian Zou, Zitang Zhou, Kunyuan Ding, Wenxuan Peng, Haoqi Wang, Guangyao Chen, Bo Li, Yiyou Sun, et al. Openood: Benchmarking generalized out-ofdistribution detection. Advances in Neural Information Processing Systems, 35:32598–32611, 2022.
 - Jinsong Zhang, Qiang Fu, Xu Chen, Lun Du, Zelin Li, Gang Wang, Xiaoguang Liu, Shi Han, and Dongmei Zhang. Out-of-distribution Detection based on In-distribution Data Patterns Memorization with Modern Hopfield Energy. In The Eleventh International Conference on Learning Representations, ICLR 2023, Kigali, Rwanda, May 1-5, 2023. OpenReview.net, 2023. URL https://openreview.net/pdf?id=KkazG4lgKL.

APPENDIX: SIMES AND MONTE CARLO CORRECTIONS А

In our work we use two of the corrections proposed by Bates et al. (2022), Simes and Monte Carlo Correction. In this section, we introduce these corrections for the sake of completeness, as well as two other corrections that we do not use for reasons to be detailed.

Simes Correction Generally, we are interested in small p-values and the Simes correction focuses on those, that is by adding a smaller correction to the smaller p-values than the larger ones.

$$b_{n+1-i}^{s} = 1 - \delta^{2/n} \left(\frac{i \cdots (i - n/2 + 1)}{n \cdots (n - n/2 + 1)} \right)^{2/n}, \quad i = 1, \dots, n$$
(12)

DKWM The former approach may be compared to the classical uniform concentration DKWM result, where the b are defined as

$$b_i^{\rm d} = \min\{(i/n) + \sqrt{\log(2/\delta)/2n}, 1\};$$
 (13)

However, DKWM tends to provide much larger bounds than Simes.

Asymptotic Correction The previous approach brought finite sample guarantees but at the cost of a large correction. In order to produce a tighter bound, for a more powerful test, we look into a correction that is correct asymptotically.

$$c_n(\delta) := \left(\sqrt{2\log\log n}\right)^{-1} \left(-\log\left[-\log(1-\delta)\right] + 2\log\log n + \frac{(1/2)\log\log \log n}{(1+2\log\log n)}\right)$$
(14)

$$+2\log\log n + (1/2)\log\log\log n - (1/2)\log \pi$$
.

$$b_i^{a} = \min\left\{\frac{i}{n} + c_n(\delta)\frac{\sqrt{i(n-i)}}{n\sqrt{n}}, 1\right\}, \quad i = 1, \dots, n$$
 (15)

This bound is quite similar to Simes for small values, but quite tighter for the remaining ones.

Monte Carlo Correction The Monter Carlo Correction offers advantages of both the Simes and Asymptotic methods. It provides a finite-sample guarantee, mimics Simes for small p-values and remains closer to the asymptotic correction for larger ones.

$$h^{\mathrm{m},\hat{\delta}}(t) = \min\left\{h^{\mathrm{s}}(t), h^{\mathrm{a},\hat{\delta}}(t)\right\}, \quad t \in [0,1].$$

$$(16)$$

B APPENDIX: DESIGNING CLASS-DEPENDENT OOD SCORES FOR CP

Let's consider a classification task with a classifier f trained to fit a dataset $\{(x_1, y_1), ..., (x_n, y_n)\}$, where $x_i \in \mathcal{X}$ and $y_i \in \{1, ..., C\}$ for all $i \in \{1, ..., n\}$. In OOD, the score function $s : \mathcal{X} \to \mathbb{R}$, whereas in CP, the non-conformity score $s_{cp} : \mathcal{X} \times \mathbb{R} \to \mathbb{R}$. Hence, in order to construct a nonconformity score out of s, we have to make it class-dependent. In this section, we describe how to construct class-dependent OOD scores out of classical OOD scores for appropriate usage in CP.

B.1 REACT

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712ReAct method Sun et al. (2021) gets the quantiles of f's penultimate layer's activation values and
then clips the activation values for a new input data point. The output softmax are then used for OOD
scoring. Therefore, making the score class-dependent is straightforward: one only has to get the class
softmax.713softmax.

B.2 ODIN

The idea of ODIN Liang et al. (2018) is also to tweak the network so that the softmax becomes more informative for OOD detection. Similarly to ReAct, one only has to get each class's softmax to make the score class-dependent.

B.3 KNN

For each $\{x_1, ..., x_n\}$ from the training set, consider $H = \{h(x_1), ..., h(x_n)\}$ where $h : \mathcal{X} \to \mathbb{R}^p$ is defined such that $h(x_i)$ is the activation vector of x_i of f's penultimate layer. Let $N_H : \mathbb{R}^p \to \mathbb{R}^p$ be the nearest neighbor map such that N(h) is the nearest neighbor of h among H. KNN Sun et al. (2022) builds the score s as

$$s(\boldsymbol{x}_{n+1}) = \|h(\boldsymbol{x}_{n+1}) - N_{\boldsymbol{H}}(h(\boldsymbol{x}_{n+1}))\|_{\boldsymbol{X}}$$

To make this score class-dependent, one can build C maps $\{N_{H_1}, ..., N_{H_C}\}$ where $H_k = \{h(x_i)|f(x_i) = k\}$ and then define a new score

$$s(x_{n+1}, y) = \|h(x_{n+1}) - N_{H_y}(h(x_{n+1}))\|$$

B.4 MAHALANOBIS

⁷³⁶ Let consider the map h as in KNN. For each $k \in \{1, ..., C\}$, Mahalanobis distance method Lee et al. ⁷³⁷ (2018) computes Σ_k and μ_k , which are the empirical covariance matrix and mean vectors of each set ⁷³⁸ of points $\{h(x_i)\}_{i|f(x_i)=k}$. Then, the score s is computed as:

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$$s(\boldsymbol{x}_{n+1}) = \sqrt{(\boldsymbol{x}_{n+1} - \mu_{f(\boldsymbol{x}_{n+1})})^T \Sigma^{-1} (\boldsymbol{x}_{n+1} - \mu_{f(\boldsymbol{x}_{n+1})})}$$

where $\Sigma = \frac{1}{C} \sum_{k \in \{1,...,C\}} \Sigma_k$. To make the score class-dependent, one simply has to define

$$s(\boldsymbol{x}_{n+1}, y) = \sqrt{(\boldsymbol{x}_{n+1} - \mu_y)^T \Sigma_y^{-1} (\boldsymbol{x}_{n+1} - \mu_y)}.$$

B.5 GRAM

T48 Let f be a classifier of depth L. Gram method Sastry & Oore (2020) builds a statistic $\delta : \mathcal{X} \to \mathbb{R}^L$ that 749 outputs the channel-wise correlation of the activation maps for each layer. First, $\{\delta(\boldsymbol{x}_1), ..., \delta(\boldsymbol{x}_n)\}$ 750 are computed. Then, a multi-dimensional statistic $\{d_{l,k}\}_{l \in \{1,...,L\},k \in \{1,...,C\}}$ is computed for each 751 layer after a class-wise aggregation.

For a new test point x_{n+1} , $\delta(x_{n+1})$ is computed, along with $f(x_{n+1})$. The score is built out of a weighted mean of the layer-wise deviation:

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$$s(\boldsymbol{x}_{n+1}) = \sum_{l \in \{1, \dots, L\}} w_l |\delta(\boldsymbol{x}_{n+1})_l - d_{l, f(\boldsymbol{x}_{n+1})}|,$$

where $\{w_l\}_{l \in \{1,...,L\}}$ are some normalization weights computed with the training data. It is quite straightforward to make this OOD score class-dependent by defining

$$s(\boldsymbol{x}_{n+1}, y) = \sum_{l \in \{1, \dots, L\}} w_l |\delta(\boldsymbol{x}_{n+1})_l - d_{l,y}|.$$

APPENDIX: COMPLEMENTARY RESULTS ON OPENOOD BENCHMARK С

In this section, we present the full results of benchmarks on OpenOOD. The results displayed are AUROC with $\delta = 0.05$ in Table 3, FPR@TPR95 with $\delta = 0.05$ in Table 5 and FPR@TPR95 with $\delta = 0.01$ in Table 4.

		CIFA	R-10			CIFA	R-100		ImageNet-200			
OOD type	Ne	ar	F	ar	Ne	ear	F	ar	Ne	ear	F	ar
	marg.	conf.	marg.	conf.	marg.	conf.	marg.	conf.	marg.	conf.	marg.	conf.
OpenMax Bendale & Boult (2015)	87.2	86.18	89.53	88.52	76.66	75.26	79.12	77.81	80.4	79.2	90.41	89.49
MSP Hendrycks & Gimpel (2016)	87.68	86.76	91.0	90.17	80.42	79.2	77.58	76.29	83.3	82.2	90.2	89.36
TempScale Guo et al. (2017)	87.65	86.75	91.27	90.48	80.98	79.78	78.51	77.24	83.66	82.58	90.91	90.11
ODIN Liang et al. (2018)	80.25	79.26	87.21	86.43	79.8	78.57	79.44	78.2	80.32	79.19	91.89	91.17
MDS Lee et al. (2018)	86.72	85.71	90.2	89.29	58.79	57.2	70.06	68.63	62.51	60.96	74.94	73.6
MDSEns Lee et al. (2018)	60.46	59.01	74.07	72.96	45.98	44.34	66.03	64.72	54.58	52.99	70.08	68.76
Gram Sastry & Oore (2020)	52.63	51.04	69.74	68.41	50.69	49.06	73.97	72.87	68.36	67.0	70.94	69.69
EBO Liu et al. (2020)	86.93	86.08	91.74	91.05	80.84	79.63	79.71	78.47	82.57	81.47	91.12	90.33
GradNorm Huang et al. (2021)	53.77	52.26	58.55	57.09	69.73	68.41	68.82	67.48	73.33	72.12	85.29	84.45
ReAct Sun et al. (2021)	86.47	85.6	91.02	90.28	80.7	79.5	79.84	78.6	80.48	79.35	93.1	92.4
MLS Hendrycks et al. (2022)	86.86	86.0	91.61	90.9	81.04	79.84	79.6	78.35	82.96	81.88	91.34	90.56
KLM Hendrycks et al. (2022)	78.8	77.8	82.76	81.83	76.9	75.65	76.03	74.8	80.69	79.54	88.41	87.44
VIM Wang et al. (2022)	88.51	87.62	93.14	92.41	74.83	73.47	82.11	80.95	78.81	77.57	91.52	90.7
KNN Sun et al. (2022)	90.7	89.87	93.1	92.35	80.25	79.05	82.32	81.19	81.75	80.63	93.47	92.83
DICE Sun & Li (2022)	77.79	76.68	85.41	84.56	79.15	77.89	79.84	78.61	81.97	80.86	91.19	90.43
RankFeat Song et al. (2022)	76.33	75.05	70.15	68.71	62.22	60.67	67.74	66.24	58.57	57.06	38.97	37.43
ASH Djurisic et al. (2022)	74.11	72.96	78.36	77.27	78.39	77.16	79.7	78.5	82.12	81.07	94.23	93.66
SHE Zhang et al. (2023)	80.84	79.86	86.55	85.73	78.72	77.46	77.35	76.08	80.46	79.34	90.48	89.72

Table 3: Classical AUROC (marg.) vs Conformal AUROC (conf.) obtained with the Monte Carlo method and $\delta = 0.05$ for several baselines from OpenOOD benchmark.

		CIFA	R-10			CIFA	R-100			Imagel	Net-200	
OOD type	Ne	ear	F	ar	Ne	ear	F	ar	Near		Far	
	marg.	conf.	marg.	con								
OpenMax Bendale & Boult (2015)	46.77	48.98	29.48	31.48	55.57	57.8	54.77	57.0	63.32	65.75	32.29	35.3
MSP Hendrycks & Gimpel (2016)	53.57	55.8	31.44	33.45	54.73	56.96	59.08	61.31	55.25	57.69	35.44	38.2
TempScale Guo et al. (2017)	56.85	59.08	33.36	35.38	54.77	56.99	58.24	60.47	55.03	57.5	34.11	37.0
ODIN Liang et al. (2018)	84.55	86.78	60.9	62.97	58.44	60.67	57.75	59.98	66.38	68.8	33.66	36.7
MDS Lee et al. (2018)	46.22	48.44	30.3	32.3	82.75	84.98	70.46	72.68	79.34	81.52	61.26	63.8
MDSEns Lee et al. (2018)	92.06	94.29	61.09	62.87	95.84	98.07	66.97	68.85	91.69	93.8	80.43	82.8
Gram Sastry & Oore (2020)	93.52	95.75	69.29	71.48	92.48	94.71	63.1	65.2	85.43	87.63	84.95	87.4
EBO Liu et al. (2020)	67.54	69.77	40.55	42.58	55.49	57.72	56.41	58.64	59.46	61.93	34.0	37.0
GradNorm Huang et al. (2021)	95.37	97.6	89.34	91.52	86.13	88.36	82.79	85.02	83.07	85.33	66.78	69.0
ReAct Sun et al. (2021)	71.56	73.78	42.43	44.52	56.74	58.97	56.32	58.55	65.37	67.8	27.21	30.2
MLS Hendrycks et al. (2022)	67.54	69.77	40.53	42.56	55.48	57.71	56.53	58.76	58.94	61.44	33.59	36.0
KLM Hendrycks et al. (2022)	86.41	88.63	76.42	78.65	79.52	81.75	70.16	72.39	69.42	71.91	39.57	42.5
VIM Wang et al. (2022)	48.07	50.29	25.77	27.65	62.96	65.19	49.72	51.95	59.91	62.32	26.86	29.8
KNN Sun et al. (2022)	34.54	36.65	23.88	25.77	61.32	63.54	54.04	56.27	60.42	62.9	26.49	29.0
DICE Sun & Li (2022)	80.15	82.38	53.93	56.06	58.1	60.33	55.95	58.17	60.98	63.46	35.93	39.0
RankFeat Song et al. (2022)	67.38	09.01	68.24	70.47	/9.94	82.17	68.89	71.11	92.02	93.91	98.48	99.5
ASH Djurisic et al. (2022)	89.03	91.26	76.66	78.89	66.14	68.37	62.67	64.89	65.95	68.44	26.26	29.4
SHE Zhang et al. (2023)	84.49	86.72	63.26	65.41	59.32	61.54	62.74	64.97	65.92	68.31	41.5	44.0

Table 4: Classical FPR@TPR95 (marg.) vs Conformal FPR@TPR95 (conf.) obtained with the Monte Carlo method and $\delta = 0.01$ for several baselines from OpenOOD benchmark.

		CIFA	R-10			CIFA	R-100		ImageNet-200			
OOD type	N	ear	F	ar	Ne	ear	F	ar	N	ear	Far	
	marg.	conf.	marg.	conf.	marg.	conf.	marg.	conf.	marg.	conf.	marg.	conf.
OpenMax Bendale & Boult (2015)	46.77	48.58	29.48	31.11	55.57	57.39	54.77	56.59	63.32	65.14	32.29	33.98
MSP Hendrycks & Gimpel (2016)	53.57	55.39	31.44	33.08	54.73	56.55	59.08	60.9	55.25	57.06	35.44	37.10
TempScale Guo et al. (2017)	56.85	58.67	33.36	35.01	54.77	56.59	58.24	60.06	55.03	56.85	34.11	35.8
ODIN Liang et al. (2018)	84.55	86.37	60.9	62.59	58.44	60.26	57.75	59.57	66.38	68.2	33.66	35.34
MDS Lee et al. (2018)	46.22	48.03	30.3	31.94	82.75	84.57	70.46	72.28	79.34	81.16	61.26	63.08
MDSEns Lee et al. (2018)	92.06	93.88	61.09	62.54	95.84	97.66	66.97	68.5	91.69	93.51	80.43	82.2
Gram Sastry & Oore (2020)	93.52	95.34	69.29	71.08	92.48	94.3	63.1	64.81	85.43	87.25	84.95	86.7
EBO Liu et al. (2020)	67.54	69.36	40.55	42.21	55.49	57.31	56.41	58.23	59.46	61.28	34.0	35.7
GradNorm Huang et al. (2021)	95.37	97.19	89.34	91.16	86.13	87.95	82.79	84.61	83.07	84.89	66.78	68.0
ReAct Sun et al. (2021)	71.56	73.38	42.43	44.14	56.74	58.56	56.32	58.14	65.37	67.19	27.21	28.8
MLS Hendrycks et al. (2022)	67.54	69.36	40.53	42.19	55.48	57.3	56.53	58.35	58.94	60.76	33.59	35.2
KLM Hendrycks et al. (2022)	86.41	88.23	76.42	78.24	79.52	81.34	70.16	71.98	69.42	71.24	39.57	41.3
VIM Wang et al. (2022)	48.07	49.88	25.77	27.3	62.96	64.78	49.72	51.54	59.91	61.72	26.86	28.4
KNN Sun et al. (2022)	34.54	36.27	23.88	25.42	61.32	63.14	54.04	55.86	60.42	62.23	26.49	28.0
DICE Sun & Li (2022)	80.15	81.97	53.93	55.67	58.1	59.92	55.95	57.77	60.98	62.8	35.93	37.6
RankFeat Song et al. (2022)	67.38	69.2	68.24	70.06	79.94	81.76	68.89	70.71	92.02	93.84	98.48	99.5
ASH Djurisic et al. (2022)	89.03	90.85	76.66	78.48	66.14	67.96	62.67	64.49	65.95	67.77	26.26	27.8
SHE Zhang et al. (2023)	84.49	86.31	63.26	65.02	59.32	61.14	62.74	64.56	65.92	67.74	41.5	43.2

Table 5: Classical FPR@TPR95 (marg.) vs Conformal FPR@TPR95 (conf.) obtained with the Monte Carlo method and $\delta = 0.05$ for several baselines from OpenOOD benchmark.

D APPENDIX: FULL RESULTS FOR ADBENCH

In this section, we present the full results of the ADBench benchmark. Table 6 displays classical AUROC, Table 7 displays conformal AUROC, and Table 8 displays the difference between the two (AUROC correction), all with $\delta = 0.05$.

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873		IForest	OCSVM	CBLOF	COF	COPOD	ECOD	HBOS	KNN	LOF	PCA	SOD	DeepSVDD	DAGMM
874	cover	0.87	0.93	0.89	0.77	0.89	0.92	0.80	0.86	0.85	0.94	0.74	0.46	0.90
875	donors	0.78	0.72	0.62	0.71	0.82	0.89	0.78	0.82	0.59	0.83	0.56	0.36	0.71
070	fault	0.57	0.48	0.64	0.62	0.44	0.45	0.51	0.73	0.59	0.46	0.68	0.52	0.46
876	fraud	0.90	0.91	0.88	0.96	0.88	0.89	0.90	0.93	0.96	0.90	0.95	0.73	0.90
877	glass	0.77	0.35	0.83	0.72	0.72	0.66	0.77	0.82	0.69	0.66	0.73	0.47	0.76
0	Ionosphere	0.70	0.08	0.00	0.41	0.82	0.73	0.80	0.55	0.58	0.76	0.08	0.52	0.55
878	landsat	0.84	0.70	0.91	0.87	0.79	0.75	0.02	0.88	0.51	0.79	0.80	0.51	0.73
879	ALOI	0.57	0.56	0.55	0.65	0.54	0.56	0.53	0.61	0.67	0.57	0.61	0.51	0.52
	letter	0.61	0.46	0.76	0.80	0.54	0.56	0.60	0.86	0.84	0.50	0.84	0.56	0.50
880	20news 0	0.64	0.63	0.71	0.71	0.61	0.61	0.62	0.73	0.80	0.64	0.73	0.50	0.63
881	20news 1	0.51	0.53	0.52	0.58	0.52	0.54	0.53	0.57	0.61	0.54	0.58	0.48	0.54
	20news 2	0.50	0.51	0.47	0.53	0.50	0.52	0.51	0.51	0.54	0.51	0.50	0.49	0.53
882	20news 3	0.75	0.72	0.83	0.81	0.75	0.75	0.74	0.79	0.71	0.73	0.70	0.67	0.54
883	20news 4	0.48	0.51	0.45	0.57	0.48	0.51	0.50	0.48	0.51	0.51	0.53	0.53	0.48
000	Lymphography	1.00	1.00	1.00	0.30	0.48	1.00	0.49	0.46	0.55	1.00	0.48	0.49	0.34
884	magic gamma	0.73	0.61	0.75	0.51	0.55	0.64	0.71	0.82	0.50	0.67	0.75	0.54	0.59
885	musk	1.00	0.81	1.00	0.39	0.94	0.95	1.00	0.70	0.41	1.00	0.74	0.56	0.77
000	PageBlocks	0.90	0.89	0.85	0.73	0.88	0.92	0.81	0.82	0.76	0.91	0.78	0.59	0.90
886	pendigits	0.95	0.94	0.90	0.45	0.91	0.93	0.93	0.73	0.48	0.94	0.66	0.42	0.64
887	Pima	0.73	0.67	0.71	0.61	0.69	0.63	0.71	0.73	0.66	0.71	0.61	0.51	0.56
001	annthyroid	0.82	0.57	0.62	0.66	0.77	0.79	0.60	0.72	0.70	0.66	0.77	0.77	0.57
888	satellite	0.70	0.59	0.71	0.55	0.63	0.58	0.75	0.65	0.56	0.60	0.64	0.55	0.62
889	saumage-2	1.00	0.97	0.83	0.57	0.97	0.96	0.98	0.95	0.47	0.98	0.85	0.49	0.96
005	smtn	0.86	0.37	0.85	0.52	0.99	0.99	0.55	0.70	0.57	0.99	0.70	0.49	0.98
890	speech	0.51	0.50	0.51	0.56	0.53	0.51	0.50	0.51	0.52	0.51	0.56	0.54	0.53
801	Stamps	0.91	0.84	0.68	0.54	0.93	0.88	0.91	0.69	0.51	0.91	0.73	0.56	0.89
001	thyroid	0.98	0.88	0.95	0.91	0.94	0.98	0.96	0.96	0.87	0.96	0.93	0.49	0.80
892	vertebral	0.37	0.38	0.41	0.49	0.26	0.41	0.29	0.34	0.49	0.37	0.40	0.37	0.53
803	vowels	0.75	0.63	0.90	0.95	0.55	0.62	0.73	0.97	0.93	0.67	0.92	0.56	0.61
000	Waveform	0.71	0.56	0.72	0.73	0.75	0.62	0.69	0.74	0.73	0.65	0.69	0.56	0.49
894	WDBC Wilt	0.99	0.99	0.99	0.96	0.99	0.97	0.99	0.92	0.89	0.99	0.92	0.62	0.77
895	wine	0.42	0.31	0.35	0.30	0.35	0.30	0.32	0.46	0.31	0.20	0.55	0.40	0.67
000	WPBC	0.47	0.45	0.45	0.46	0.49	0.47	0.51	0.47	0.41	0.46	0.51	0.50	0.48
896	veast	0.38	0.41	0.45	0.44	0.37	0.44	0.40	0.39	0.45	0.41	0.42	0.48	0.41
897	campaign	0.73	0.67	0.64	0.58	0.78	0.77	0.79	0.73	0.59	0.73	0.69	0.53	0.58
001	cardio	0.93	0.94	0.90	0.71	0.92	0.94	0.85	0.77	0.66	0.96	0.73	0.58	0.75
898	Cardiotocography	0.68	0.78	0.65	0.54	0.67	0.78	0.61	0.56	0.60	0.75	0.52	0.53	0.62
800	celeba	0.70	0.71	0.74	0.39	0.76	0.76	0.76	0.60	0.39	0.79	0.48	0.54	0.45
000	CIFAR10.0	0.73	0.68	0.70	0.70	0.69	0.70	0.70	0.74	0.74	0.70	0.71	0.56	0.53
900	CIFAR101 CIFAR102	0.55	0.59	0.01	0.05	0.40	0.51	0.44	0.00	0.72	0.00	0.02	0.50	0.58
001	CIFAR10.3	0.50	0.58	0.50	0.56	0.50	0.57	0.54	0.00	0.60	0.56	0.59	0.50	0.56
501	CIFAR105	0.50	0.58	0.58	0.57	0.47	0.52	0.47	0.54	0.60	0.57	0.54	0.46	0.59
902	CIFAR106	0.64	0.65	0.68	0.69	0.65	0.66	0.65	0.72	0.72	0.68	0.69	0.57	0.50
903	CIFAR107	0.54	0.59	0.56	0.57	0.52	0.55	0.50	0.54	0.60	0.57	0.56	0.62	0.61
505	agnews 0	0.50	0.47	0.54	0.61	0.49	0.47	0.48	0.58	0.63	0.47	0.56	0.35	0.48
904	agnews 1	0.58	0.54	0.58	0.71	0.51	0.54	0.55	0.62	0.74	0.55	0.61	0.37	0.56
905	agnews 2	0.65	0.61	0.71	0.73	0.61	0.59	0.61	0.75	0.79	0.61	0.73	0.50	0.53
505	agnews 5 amazon	0.54	0.55	0.57	0.70	0.51	0.55	0.51	0.62	0.70	0.55	0.51	0.50	0.51
906	imdb	0.50	0.45	0.50	0.49	0.50	0.45	0.48	0.48	0.49	0.46	0.50	0.52	0.42
907	yelp	0.61	0.59	0.64	0.68	0.60	0.57	0.59	0.68	0.66	0.59	0.66	0.50	0.55

Table 6: Full results for ADBench: classical AUROC.

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0.0	91	8

927		IForest	OCSVM	CBLOF	COF	COPOD	ECOD	HBOS	KNN	LOF	PCA	SOD	DeepSVDD	DAGMM
928	cover	0.75	0.83	0.79	0.64	0.78	0.82	0.74	0.74	0.73	0.84	0.60	0.30	0.79
929	donors	0.72	0.66	0.54	0.64	0.77	0.85	0.72	0.76	0.53	0.78	0.50	0.31	0.65
000	fault	0.48	0.40	0.55	0.53	0.35	0.37	0.43	0.65	0.50	0.37	0.59	0.43	0.37
930	fraud	0.77	0.63	0.63	0.82	0.62	0.64	0.86	0.68	0.79	0.66	0.69	0.51	0.64
931	glass Hepatitis	0.65 0.54	0.31 0.52	0.73 0.52	0.60 0.23	0.60 0.70	0.53 0.61	0.64 0.66	0.72 0.26	0.58 0.22	0.54 0.62	0.63 0.54	0.38 0.38	0.66 0.40
932	Ionosphere	0.77	0.68	0.85	0.80	0.70	0.63	0.50	0.83	0.85	0.71	0.80	0.38	0.64
022	landsat	0.42	0.30	0.58	0.48	0.35	0.30	0.49	0.52	0.48	0.30	0.54	0.58	0.39
900	letter	0.49	0.40	0.45	0.55	0.45	0.40	0.40	0.32	0.38	0.47	0.52	0.41	0.42
934	20news 0	0.51	0.30	0.57	0.60	0.30	0.35	0.42	0.62	0.72	0.55	0.61	0.40	0.49
005	20news 1	0.36	0.39	0.37	0.00	0.40	0.39	0.37	0.02	0.07	0.39	0.01	0.33	0.39
935	20news 2	0.34	0.36	0.34	0.39	0.34	0.36	0.35	0.36	0.38	0.36	0.34	0.32	0.38
936	20news 3	0.65	0.61	0.73	0.71	0.63	0.64	0.64	0.69	0.58	0.62	0.59	0.54	0.45
000	20news 4	0.28	0.31	0.27	0.39	0.27	0.32	0.30	0.30	0.34	0.31	0.35	0.35	0.30
937	20news 5	0.34	0.32	0.29	0.30	0.30	0.31	0.32	0.29	0.35	0.32	0.28	0.31	0.35
029	Lymphography	0.95	0.95	0.95	0.83	0.95	0.95	0.95	0.45	0.81	0.96	0.62	0.25	0.62
930	magic.gamma	0.70	0.57	0.72	0.63	0.65	0.60	0.68	0.79	0.65	0.64	0.72	0.56	0.55
939	musk	0.57	0.65	0.22	0.21	0.83	0.85	0.58	0.53	0.22	0.32	0.59	0.42	0.64
0.40	PageBlocks	0.84	0.83	0.79	0.67	0.82	0.86	0.74	0.76	0.70	0.85	0.71	0.52	0.84
940	pendigits	0.87	0.86	0.82	0.33	0.82	0.85	0.85	0.60	0.35	0.86	0.53	0.29	0.52
941	Pima	0.63	0.57	0.62	0.51	0.59	0.54	0.62	0.64	0.55	0.61	0.52	0.40	0.45
041	annthyroid	0.76	0.49	0.55	0.59	0.70	0.72	0.53	0.65	0.63	0.59	0.71	0.71	0.49
942	satellite	0.67	0.55	0.67	0.50	0.59	0.54	0.71	0.61	0.51	0.56	0.59	0.50	0.58
0/2	satimage-2	0.51	0.71	0.45	0.41	0.74	0.80	0.77	0.79	0.34	0.70	0.68	0.31	0.84
943	snuttle	0.94	0.87	0.74	0.46	0.89	0.94	0.94	0.65	0.52	0.85	0.63	0.42	0.91
944	smp	0.81	0.00	0.38	0.39	0.38	0.08	0.45	0.70	0.48	0.72	0.32	0.00	0.60
0.45	Stamps	0.51	0.51	0.51	0.37	0.54	0.52	0.51	0.51	0.35	0.52	0.55	0.34	0.54
945	thyroid	0.04	0.75	0.57	0.42	0.87	0.80	0.85	0.37	0.39	0.85	0.02	0.42	0.69
946	vertebral	0.23	0.26	0.80	0.37	0.00	0.29	0.17	0.20	0.37	0.00	0.04	0.33	0.40
	vowels	0.57	0.45	0.73	0.76	0.35	0.45	0.54	0.77	0.74	0.49	0.75	0.35	0.43
947	Waveform	0.56	0.42	0.59	0.58	0.60	0.47	0.53	0.59	0.59	0.50	0.54	0.39	0.34
0/18	WDBC	0.95	0.95	0.95	0.91	0.95	0.92	0.96	0.86	0.81	0.95	0.85	0.50	0.67
340	Wilt	0.29	0.20	0.21	0.37	0.20	0.24	0.19	0.35	0.38	0.12	0.42	0.34	0.26
949	wine	0.70	0.63	0.12	0.31	0.80	0.67	0.84	0.33	0.26	0.75	0.32	0.48	0.48
050	WPBC	0.33	0.32	0.32	0.33	0.36	0.33	0.38	0.32	0.29	0.33	0.39	0.38	0.35
900	yeast	0.29	0.31	0.35	0.35	0.28	0.34	0.31	0.30	0.36	0.31	0.32	0.38	0.31
951	campaign	0.68	0.62	0.59	0.52	0.74	0.72	0.75	0.68	0.53	0.68	0.64	0.48	0.52
050	cardio Cardiotocography	0.84	0.85	0.80	0.60	0.83	0.84	0.75	0.67	0.53	0.86	0.62	0.47	0.64
952	celeba	0.59	0.70	0.57	0.45	0.58	0.70	0.52	0.48	0.31	0.00	0.45	0.45	0.33
953	CIFAR10.0	0.63	0.59	0.60	0.50	0.59	0.60	0.60	0.20	0.50	0.61	0.50	0.46	0.42
0.54	CIFAR101	0.43	0.48	0.50	0.52	0.35	0.39	0.33	0.49	0.62	0.49	0.51	0.39	0.48
954	CIFAR102	0.45	0.48	0.47	0.50	0.44	0.45	0.43	0.49	0.55	0.47	0.48	0.48	0.40
955	CIFAR103	0.44	0.48	0.49	0.46	0.40	0.42	0.39	0.47	0.50	0.46	0.46	0.49	0.45
000	CIFAR105	0.38	0.48	0.47	0.46	0.35	0.40	0.34	0.42	0.49	0.46	0.42	0.34	0.49
956	CIFAR106	0.54	0.55	0.58	0.59	0.54	0.55	0.54	0.61	0.62	0.58	0.59	0.47	0.39
057	CIFAR107	0.43	0.48	0.45	0.46	0.41	0.44	0.39	0.44	0.50	0.46	0.46	0.51	0.50
301	agnews 0	0.41	0.39	0.45	0.53	0.40	0.38	0.39	0.49	0.56	0.39	0.48	0.27	0.40
958	agnews 1	0.50	0.46	0.50	0.64	0.42	0.45	0.46	0.54	0.67	0.47	0.53	0.28	0.48
050	agnews 2	0.57	0.53	0.63	0.66	0.52	0.51	0.52	0.68	0.73	0.53	0.66	0.42	0.45
959	agnews 3	0.45	0.46	0.49	0.63	0.43	0.44	0.43	0.54	0.64	0.46	0.53	0.42	0.42
960	amazon	0.48	0.45	0.50	0.49	0.48	0.46	0.47	0.50	0.48	0.46	0.50	0.37	0.43
500	imdb	0.41	0.36	0.41	0.40	0.42	0.36	0.40	0.39	0.40	0.37	0.41	0.44	0.34
961	yeip	0.52	0.50	0.55	0.60	0.52	0.49	0.51	0.60	0.59	0.51	0.58	0.42	0.47

Table 7: Full results for ADBench: conformal AUROC.

 yelp

978														
979														
980														
981		IForest	OCSVM	CBLOF	COF	COPOD	ECOD	HBOS	KNN	LOF	PCA	SOD	DeepSVDD	DAGMM
982	cover	0.12	0.10	0.11	0.13	0.11	0.10	0.07	0.12	0.12	0.10	0.14	0.15	0.11
983	fault	0.00	0.07	0.08	0.07	0.03	0.04	0.00	0.00	0.00	0.03	0.00	0.03	0.00
000	fraud	0.13	0.28	0.25	0.14	0.26	0.25	0.04	0.26	0.16	0.25	0.26	0.22	0.26
984	glass	0.12	0.05	0.10	0.12	0.12	0.13	0.13	0.10	0.11	0.13	0.10	0.09	0.10
985	Hepatitis	0.16	0.15	0.14	0.18	0.12	0.14	0.13	0.27	0.16	0.14	0.14	0.14	0.14
096	landsat	0.08	0.08	0.00	0.07	0.09	0.10	0.12	0.05	0.05	0.08	0.00	0.15	0.09
900	ALOI	0.07	0.10	0.10	0.09	0.10	0.10	0.06	0.09	0.08	0.10	0.09	0.10	0.10
987	letter	0.17	0.16	0.15	0.14	0.19	0.17	0.18	0.13	0.13	0.17	0.13	0.15	0.15
988	20news 0	0.14	0.14	0.13	0.11	0.14	0.15	0.14	0.11	0.11	0.14	0.12	0.13	0.14
000	20news 1 20news 2	0.15	0.15	0.15	0.14	0.15	0.15	0.16	0.13	0.14	0.15	0.14	0.14	0.15
989	20news 3	0.10	0.13	0.14	0.13	0.10	0.10	0.10	0.13	0.10	0.13	0.13	0.10	0.15
990	20news 4	0.20	0.20	0.17	0.18	0.21	0.19	0.20	0.18	0.16	0.20	0.17	0.18	0.18
001	20news 5	0.17	0.17	0.18	0.20	0.18	0.15	0.17	0.19	0.20	0.16	0.20	0.18	0.19
991	Lymphography	0.05	0.05	0.05	0.08	0.04	0.05	0.05	0.11	0.09	0.04	0.11	0.09	0.11
992	magic.gamma	0.03	0.04	0.03	0.04	0.03	0.04	0.03	0.03	0.04	0.03	0.03	0.04	0.04
993	PageBlocks	0.45	0.15	0.78	0.18	0.06	0.06	0.42	0.17	0.19	0.08	0.10	0.06	0.15
000	pendigits	0.08	0.08	0.09	0.12	0.08	0.08	0.08	0.13	0.13	0.08	0.13	0.13	0.12
994	Pima	0.10	0.10	0.10	0.10	0.10	0.09	0.09	0.10	0.10	0.09	0.10	0.11	0.11
995	annthyroid	0.06	0.08	0.07	0.07	0.07	0.06	0.07	0.07	0.07	0.07	0.06	0.06	0.08
006	satemage_?	0.04	0.04	0.04	0.05	0.04	0.04	0.04	0.05	0.05	0.04	0.05	0.05	0.04
990	shuttle	0.06	0.10	0.09	0.06	0.25	0.05	0.05	0.04	0.05	0.13	0.06	0.07	0.12
997	smtp	0.05	0.12	0.12	0.10	0.12	0.11	0.10	0.09	0.09	0.11	0.08	0.12	0.11
998	speech	0.19	0.19	0.19	0.19	0.19	0.19	0.19	0.20	0.19	0.19	0.21	0.21	0.18
000	Stamps	0.07	0.09	0.11	0.11	0.06	0.08	0.07	0.12	0.12	0.07	0.11	0.14	0.07
999	tnyroid vertebral	0.08	0.10	0.09	0.10	0.08	0.08	0.04	0.09	0.10	0.08	0.09	0.16	0.11
1000	vowels	0.14	0.12	0.17	0.12	0.12	0.12	0.12	0.20	0.19	0.12	0.17	0.21	0.19
1001	Waveform	0.15	0.15	0.14	0.15	0.15	0.15	0.15	0.14	0.14	0.16	0.15	0.16	0.16
1001	WDBC	0.04	0.04	0.04	0.06	0.04	0.05	0.04	0.06	0.08	0.04	0.07	0.12	0.10
1002	Wilt	0.13	0.11	0.12	0.12	0.13	0.12	0.14	0.13	0.13	0.08	0.12	0.12	0.11
1003	WPRC	0.10	0.10	0.14	0.14	0.09	0.11	0.08	0.12	0.11	0.10	0.13	0.11	0.13
1000	veast	0.09	0.10	0.10	0.10	0.09	0.09	0.09	0.09	0.10	0.10	0.11	0.10	0.10
1004	campaign	0.05	0.05	0.05	0.06	0.05	0.05	0.04	0.05	0.06	0.05	0.06	0.05	0.06
1005	cardio	0.09	0.09	0.10	0.12	0.09	0.09	0.10	0.10	0.14	0.10	0.11	0.11	0.11
1006	Cardiotocography	0.09	0.08	0.08	0.09	0.09	0.08	0.08	0.08	0.09	0.09	0.08	0.08	0.09
1000	CIFAR10.0	0.00	0.00	0.05	0.09	0.05	0.05	0.05	0.31	0.09	0.05	0.10	0.00	0.08
1007	CIFAR101	0.12	0.11	0.11	0.11	0.11	0.12	0.11	0.11	0.10	0.11	0.10	0.10	0.11
1008	CIFAR102	0.11	0.11	0.11	0.11	0.11	0.11	0.11	0.11	0.11	0.11	0.11	0.10	0.11
1000	CIFAR103	0.11	0.11	0.10	0.10	0.11	0.11	0.11	0.10	0.10	0.11	0.10	0.11	0.11
1009	CIFAR105 CIFAR106	0.12	0.10	0.11	0.11	0.12	0.12	0.12	0.12	0.11	0.11	0.12	0.12	0.10
1010	CIFAR107	0.11	0.11	0.10	0.10	0.11	0.11	0.11	0.10	0.10	0.10	0.10	0.11	0.11
1011	agnews 0	0.09	0.09	0.08	0.08	0.09	0.09	0.09	0.08	0.08	0.09	0.08	0.09	0.09
1011	agnews 1	0.09	0.09	0.08	0.07	0.09	0.09	0.09	0.08	0.07	0.09	0.08	0.09	0.09
1012	agnews 2	0.08	0.08	0.08	0.07	0.08	0.09	0.08	0.07	0.06	0.08	0.07	0.08	0.08
1013	agnews 3	0.09	0.09	0.08	0.07	0.09	0.09	0.09	0.08	0.07	0.09	0.08	0.08	0.08
	amazon	0.08	0.00	0.00	0.00	0.00	0.00	0.00	0.09	0.09	0.08	0.09	0.00	0.08

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Table 8: Full results for ADBench: AUROC correction (difference between conformal and classical

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972 973

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1022 1023 1024

1014

1015 1016

AUROC).

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0.09

imdb

yelp

1025

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0.08

0.08