CAN CONFORMAL PREDICTION OBTAIN MEANINGFUL GUARANTEES FOR ML MODELS AT HIGH SAFETY LEVELS?

Anonymous authors
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ABSTRACT

Conformal Prediction (CP) has been recently proposed as a methodology to calibrate the predictions of Machine Learning (ML) models, so that they can output rigorous quantifications of their uncertainties. For example, one can calibrate the predictions of an ML model into prediction sets, that guarantee to cover the ground truth class with a probability larger than a specified threshold. In this short paper, we want to explore whether CP can provide such guarantees at high Safety integrity levels (SIL) that would be required in safety-critical applications, which doesn't seem to have been much explored. Surprisingly, we find that even state-of-the-art (SOTA) models fail to provide meaningful guarantees (e.g. containing only a small, non-trivial fraction of all possible classes) on the ImageNet dataset. We corroborate our results by deriving a simple connection between the CP prediction sets and top-k accuracy.

1 INTRODUCTION & RELATED WORK

Deep Neural Networks (DNNs) have recently shown remarkable performance in a large series of tasks including image and speech recognition Krizhevsky et al. (2017); Graves et al. (2013), language Brown et al. (2020), or game playing Silver et al. (2018). But despite that, it is well known that predictions made by DNNs are heuristic, and cannot offer us a notion of their uncertainties.

Recently, Conformal Prediction (CP) Angelopoulos & Bates (2021) has been proposed as a method to build statistically rigorous uncertainty sets for DNN predictions. This is done by calibrating the DNN predictions into prediction sets, in such a way that the latter satisfy some statistical guarantees, such as for example that they contain the correct class with probability at least 90%. Conformal Prediction has been applied to a series of ML problems, such as classification, regression, image segmentation and more Angelopoulos & Bates (2021).

In this work, we focus on the standard setting of classification prediction sets, and ask the following question: what is the efficiency of the guarantees obtained - e.g. the prediction set sizes - as we increase the required confidence levels from 90% to 99% or 99.9%? What happens as confidence levels move into higher SILs Smith & Simpson (2020) that would be necessary for safety-critical domains? This question doesn't seem to have been addressed in the literature, where the focus is lies more on the methodology side.

In order to answer this, we evaluate several SOTA models, based on Convolutional Neural Nets (CNN) or Transformers (ViT) Dosovitskiy et al. (2020) on the ImageNet Deng et al. (2009) dataset. The results show that, at high safety levels, the guaranteed prediction sets become trivial, and essentially include almost all classes of the dataset. This shows that even SOTA DNNs struggle to obtain any meaningful CP guarantees at high safety levels, which may have interesting implications for safety-critical domains such as Autonomous Driving or Medical Imaging.

Finally, we investigate this phenomenon theoretically, and demonstrate a simple connection between CP prediction sets and the top-k accuracy of a model, that holds regardless of the CP variant used. Essentially, we find that a DNN can obtain non-trivial prediction set sizes only if it's top-k accuracy is sufficiently high. This shows that, independently of statistical wrappers such as CP, highly accurate models are necessary in order to obtain reasonable safety guarantees at high SIL levels.

Table 1: Average prediction set size $|C(\hat{y})|$ for each risk level a

Model / a	$a = 10\%$	$a = 5\%$	$a = 1\%$	$a = 0.5\%$	$a = 0.1\%$	$a = 0.05\%$	$a = 0.01\%$
ResNet-152	3.05	4.22	36.81	80.12	266.74	368.46	829.47
WideResNet-102	3.33	4.47	34.62	76.79	249.19	384.19	716.52
ConvNext (large)	3.59	6.31	16.47	39.57	265.43	452.15	878.70
ViT (large, 16 bit)	3.03	5.14	43.39	127.24	714.30	847.68	991.79

2 METHODOLOGY & RESULTS

In order to answer the question posed in the introduction, we evaluate various SOTA models on the ImageNet dataset. We evaluate the following models: a ResNet-152 He et al. (2016), a WideResNet-102 Zagoruyko & Komodakis (2016), a ConvNext (large) Liu et al. (2022) and a ViT (large, 16 bit) Dosovitskiy et al. (2020). We split the ImageNet validation data into a calibration set of 480000 images, where we apply CP, and a test set of 2000 images, where we evaluate the resulting prediction set sizes. We use the Regularized Adaptive Prediction Sets (RAPS) CP methodology from Brown et al. (2020), which is an improvement of the Adaptive Prediction Sets (APS) method Brown et al. (2020) that guarantees much smaller prediction sets. We apply the split in calibration and test test 10 times, and report the average set sizes. The results can be seen in Table 1.

From Table 1, we observe that as the risk level a approaches smaller values, the prediction set sizes become trivial, and start to include almost all possible class in the dataset (ImageNet has 1000 classes in total). It seems reasonable that there is a connection between the prediction set sizes, and the model's accuracy. Indeed, we can easily demonstrate the following:

Proposition 1 (CP vs top-k): Let $f_\theta : \mathbb{R}^n \to [K]$ be a model mapping inputs $\mathbf{x} \in \mathbb{R}^n$ into K classes, and let $1 \leq k \leq K$ be an integer. Suppose that a CP method augmenting model predictions $\hat{y} = f_\theta(\mathbf{x})$ into prediction sets $C(\hat{y})$ of size at most k achieves coverage of at least $1-a$ ($a \in (0,1)$) on a distribution $(\mathbf{x}, y) \sim D$. Then, f_θ has top-k accuracy of at lest $1-a$ on D.

Proof: Note that any CP method (e.g. APS or RAPS) will short the output logits of f_θ from largest to smallest, and will include the corresponding class labels in a prediction set $C(\hat{y})$ using that ordering. If sets $C(\hat{y})$ have coverage at least $1-a$, and the size $|C(\hat{y})|$ is at most k, that means that the true class y will lie among the top-k classes with probability at least $1-a$. But that means that the model's top-k accuracy is at least $1-a$. This holds regardless of the specific CP methodology used. □

In order to examine the implications of Proposition 1, let us go through the following example: **Example 1**: Suppose that we have an ImageNet model, and we want that our prediction sets have size at most $k = 10$ (we consider this size reasonable, since it represents no more than 1% of the total $K = 1000$ classes in ImageNet). Further, suppose we require that the methodology has a risk level at most $a = 0.01\%$ (which represents a SIL level of 3). Then, the model's top-k accuracy should be at least: $acc_{10} \geq 1 - a = 0.9999 = 99.99\%$. According to our knowledge, no such model exists. □

Thus, although statistical wrappers such as CP can offer us sound statistical guarantees on a DNN's outputs, at higher SIL levels such guarantees will reduce to trivial, unless the underlying model has sufficient predictive accuracy.

3 CONCLUSION

In this work, we evaluated the efficiency of CP methods at high SIL levels, on SOTA DNNs for the ImageNet dataset. We find, both experimentally and theoretically, that the guarantees obtained become degenerate (essentially covering all possible cases), unless the models' accuracies are high enough. For higher SIL levels, the required accuracy levels would largely exceed what has been currently achieved in the SOTA. This may have implications on safety-critical domains such as Autonomous Driving or Healthcare that are worthwhile to be considered.

URM STATEMENT

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REFERENCES

Anastasios N Angelopoulos and Stephen Bates. A gentle introduction to conformal prediction and distribution-free uncertainty quantification. *arXiv preprint arXiv:2107.07511*, 2021.

Tom Brown, Benjamin Mann, Nick Ryder, Melanie Subbiah, Jared D Kaplan, Prafulla Dhariwal, Arvind Neelakantan, Pranav Shyam, Girish Sastry, Amanda Askell, et al. Language models are few-shot learners. *Advances in neural information processing systems*, 33:1877–1901, 2020.

Jia Deng, Wei Dong, Richard Socher, Li-Jia Li, Kai Li, and Li Fei-Fei. Imagenet: A large-scale hierarchical image database. In *2009 IEEE conference on computer vision and pattern recognition*, pp. 248–255. Ieee, 2009.

Alexey Dosovitskiy, Lucas Beyer, Alexander Kolesnikov, Dirk Weissenborn, Xiaohua Zhai, Thomas Unterthiner, Mostafa Dehghani, Matthias Minderer, Georg Heigold, Sylvain Gelly, et al. An image is worth 16x16 words: Transformers for image recognition at scale. *arXiv preprint arXiv:2010.11929*, 2020.

Alex Graves, Abdel-rahman Mohamed, and Geoffrey Hinton. Speech recognition with deep recurrent neural networks. In *2013 IEEE international conference on acoustics, speech and signal processing*, pp. 6645–6649. Ieee, 2013.

Kaiming He, Xiangyu Zhang, Shaoqing Ren, and Jian Sun. Deep residual learning for image recognition. In *Proceedings of the IEEE conference on computer vision and pattern recognition*, pp. 770–778, 2016.

Alex Krizhevsky, Ilya Sutskever, and Geoffrey E Hinton. Imagenet classification with deep convolutional neural networks. *Communications of the ACM*, 60(6):84–90, 2017.

Zhuang Liu, Hanzi Mao, Chao-Yuan Wu, Christoph Feichtenhofer, Trevor Darrell, and Saining Xie. A convnet for the 2020s. In *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pp. 11976–11986, 2022.

David Silver, Thomas Hubert, Julian Schrittwieser, Ioannis Antonoglou, Matthew Lai, Arthur Guez, Marc Lanctot, Laurent Sifre, Dharshan Kumaran, Thore Graepel, et al. A general reinforcement learning algorithm that masters chess, shogi, and go through self-play. *Science*, 362(6419):1140–1144, 2018.

David J Smith and Kenneth GL Simpson. *The Safety Critical Systems Handbook: A Straightforward Guide to Functional Safety: IEC 61508 (2010 Edition), IEC 61511 (2015 Edition) and Related Guidance*. Butterworth-Heinemann, 2020.

Sergey Zagoruyko and Nikos Komodakis. Wide residual networks. *arXiv preprint arXiv:1605.07146*, 2016.