Contrastive Out-of-Distribution Detection for Pretrained Transformers

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Abstract

Pretrained transformers achieve remarkable performance when the test data follows the same distribution as the training data. However, in real-world NLU tasks, the model often faces out-of-distribution (OoD) instances. Such instances can cause the severe semantic shift problem to inference, hence they are supposed to be identified and rejected by the model. In this paper, we study the OoD detection problem for pretrained transformers using only in-distribution data in training. We observe that such instances can be found using the Mahalanobis distance in the penultimate layer. We further propose a contrastive loss that improves the compactness of representations, such that OoD instances can be better differentiated from in-distribution ones. Experiments on the GLUE benchmark demonstrate the effectiveness of the proposed methods.

1 Introduction

Many natural language understanding models are developed based on a closed-world assumption, i.e., the training and test data are sampled from the same distribution. While in real-world scenarios, out-of-distribution (OoD) instances (e.g., data from new categories or annotated for dissimilar tasks) can often be present in inference phases. Such instances may come from categories or tasks that are not known to the model, severely causing the semantic shift problem to the model (Hsu et al., 2020). Hence, in those scenarios, the model needs to detect and reject such OoD instances. Although the state-of-the-art pretrained transformers (Devlin et al., 2019; Liu et al., 2019) achieve remarkable results when being intrinsically evaluated on in-distribution data, recent work (Hendrycks et al., 2020) shows that many of them fail short of detecting OoD instances. For instances belonging to new categories, models will still assign them to existing categories with high confidence. Therefore, developing a method for accurately identifying OoD input instances is a critical support for learning systems to make reliable inference, and importantly leads to more practical real-world decision making.

Despite the importance, the problem of detecting OoD instances has not been well attempted for NLP tasks. For example, some prior studies propose techniques (Hendrycks et al., 2018; Larson et al., 2019) to train a model on both the in-distribution and OoD data, and regularizes the model to give lower confidence on OoD inferences than in-distribution ones. However, as the OoD instances reside in an unbounded feature space and the distribution of them during inference is usually unknown, it is hard to decide which OoD instances should be used in training. Another practiced method for OoD detection is to use the maximum class probability as an indicator (Shu et al., 2017; Hendrycks et al., 2020), in which case smaller values indicate OoD instances. Though simple, previous studies (Dhamija et al., 2018; Liang et al., 2018) show that OoD samples can also get high class probability and thus hard to be distinguished.

In this paper, we aim at training an NLU classifier that is capable of detecting OoD instances in testing without losing performance on the in-distribution data. For practicality purposes, we tackle the problem for transformer-based pretrained transformers that have been the backbone of many recent NLP systems, and only use in-distribution data in training. We observe that although the in-distribution instances cannot be well distinguished from OoD in the softmax layer of transformers, their representations in the penultimate layer can be approximated by a class-conditional multivariate Gaussian distribution, and identified during testing using the Mahalanobis distance (Lee et al., 2018b). Based on this observation, we further propose a contrastive loss to increase the compactness of in-distribution instances. For instances from the same class, we regularize their distance to be as small as possible. For those from different classes, we reg-
ularize their distance to be larger than that of any pair of instances in the same class. Experiments on the GLUE (Wang et al., 2018) benchmark show that our method significantly improves the OoD detection performance of pretrained transformers.

2 Background

Determining whether an instance is OoD is critical for the safe deployment of machine learning systems in the real world (Amodei et al., 2016). Recently, this problem has received a lot of research attention in the computer vision community. The main challenge of OoD detection is that the distribution of OoD data is hard to know a priori. Based on the availability of OoD data, recent methods can be grouped into the following categories:

**Supervised methods** train models on both the in-distribution and OoD data, where the models are expected to output a uniform distribution over known classes on OoD data (Lee et al., 2018a; Dhamija et al., 2018; Hendrycks et al., 2018). Though effective, it is hard to assume the presence of a large dataset providing comprehensive coverage for OoD instances in practice.

**Unsupervised methods** utilize only the in-distribution data for OoD detection. Most methods estimate for each instance an OoD detection score and assume that in-distribution data will have a lower score than OoD, where the score can be calculated based on the softmax probability (Bendale and Boult, 2016; Hendrycks and Gimpel, 2017; Liang et al., 2018), cosine similarity (Techapanurak et al., 2020), energy scores (Shu et al., 2017; Liu et al., 2020), or Mahalanobis distances (Lee et al., 2018b). One advantage is that the calculation of OoD detection scores does not depend on the training process, such that these methods can be applied to trained classifiers. Other methods (Lawson et al., 2017; Deecke et al., 2018) learn a reconstruction model and assumes that in-distribution data have lower reconstruction loss than OoD. All these methods require comparing the OoD detection scores with a threshold that can be determined solely from the in-distribution data or additional OoD validation data.

**Self-supervised methods** apply some modification techniques to change some properties of data (e.g., rotation of an image) and simultaneously learn an auxiliary model to predict the property changes (e.g., the rotation angle). Such an auxiliary model is expected to have worse generalization on OoD instances, therefore, it can be used to identify such instances where a higher generalization loss is posed (Bergman and Hoshen, 2020; Tack et al., 2020). These methods have shown SOTA performance on image classification tasks. However, it is hard to define such transformations for NLP tasks.

Though extensively studied in computer vision, OoD detection has yet raised less attention in NLP. It is unclear whether the emerging techniques can be effectively applied to SOTA pretrained transformers. Hendrycks et al. (2020) show that pretrained transformers exhibit better OoD detection performance than models such as LSTM (Hochreiter and Schmidhuber, 1997) when using the maximum softmax probability as the detection score, while the performance is still imperfect.

3 Method

3.1 Overview

In this paper, we aim at improving the OoD detection performance of natural language classifiers that are based on pretrained transformers utilizing only the in-distribution data. Specifically, given a natural language classification task (e.g., sentence classification, NLI, relation extraction, etc.), for an instance $x$ to be classified in the main task, our goal is to develop an auxiliary OoD detection function $f(x) : X \rightarrow \mathbb{R}$. This function should return low for an in-distribution $x \in X_{\text{train}}$, otherwise high for an OoD $x \in X_{\text{ood}}$. After calculating the OoD detection score, we can make the decision by:

$$x \sim \begin{cases} X_{\text{train}} & \text{if } f(x) \leq \theta, \\ X_{\text{ood}} & \text{if } f(x) > \theta, \end{cases}$$

where $\theta$ is a threshold.

OoD can be further divided into semantic shift and non-semantic shift (Hsu et al., 2020). Semantic shift thereof refers to the shift between groups of instances that belong to different sets of labels. More specifically, instances with semantic shift may come from unseen categories or a different task. Non-semantic shift, on the other hand, refers to the change in the forms, e.g., style of the text. Specifically, semantic shift can be especially hazardous to model inference (Hsu et al., 2020). This is due to that failing to detect corresponding instances will always lead to incorrect predictions on them, and drastically hinder the reliability of decision making by the model. On the contrary, tasks...
with non-semantic shift may still be supported by a well-trained model (Wang and Deng, 2018). In this paper, we focus on OoD caused by semantic shift while leaving non-semantic shift as future work. Meanwhile, we also expect that the OoD detection auxiliary should be performed without negatively interfering with the performance of the main task on in-distribution data.

To identify OoD instances, we expect that there exists a space in which the distribution of the representations of in-distribution data and OoD data are well separated. Accordingly, we need another function to determine which distribution a data instance comes from. This process is equivalent to decomposing the OoD detection function as \( f(x) = g \circ h(x) \), where the representation function \( h: \mathcal{X} \rightarrow \mathbb{R}^d \) maps the input text into a (high-dimensional) representations, and the scoring function \( g: \mathbb{R}^d \rightarrow \mathbb{R} \) maps the representations to OoD detection scores. For most unsupervised OoD detection methods, they only define \( g \) without modeling a specific form of \( h \). Using this decomposition, we can use different combinations of \( h \) and \( g \). We present our design for \( h \) in 3.2, and then study different functions for \( g \) in 3.3.

### 3.2 Contrastive Representation Learning

We hereby discuss the design for the representation function \( h \). For better OoD detection performance, \( h \) is supposed to minimize the overlap of the representations of in-distribution and OoD. It is easy to design \( h \) for supervised OoD detection methods. For example, Dhamija et al. (2018) trains the neural model on both in-distribution and OoD, and defines an objectosphere loss where the features of OoD instances are regularized to have a smaller magnitude than in-distribution:

\[
\mathcal{L}_{os} = \begin{cases} 
\max (\xi - \|h(x)\|, 0)^2 & \text{if } x \in \mathcal{X}_{\text{train}}, \\
\|h(x)\|^2 & \text{if } x \in \mathcal{X}_{\text{ood}}, 
\end{cases}
\]

where \( \xi \) is a positive hyper-parameter. This loss enforces the OoD instances to form a compact cluster at \( 0 \), such that they are not likely to overlap with in-distribution data.

However, as we do not use OoD data in training, we need further modification on this loss term to make it applicable to our problem setting. Accordingly, given each class in the in-distribution data, the instances within the class are determined to be in-distribution, while any data that do not belong to the class can be considered as OoD (Vyas et al., 2018). Follow this strategy, we expect \( h \) to let data within the same class form their own isolated clusters, and clusters of other classes are placed apart beyond a certain margin. In this way, while the model can learn to differentiate between instances of different classes by clusters, instances that pose as “background representations” (i.e., that are far from all clusters) are considered OoD.

We formulate this strategy as a contrastive loss. Specifically, given a training dataset \( \{(x_i, y_i)\}_{i=1}^N \), where \( x_i \) in the input text, \( y_i \) is the corresponding class, the contrastive loss can be defined as:

\[
\begin{align*}
\mathcal{L}_1 &= \mathbb{E}_{y_a=y_b} ||h(x_a) - h(x_b)||^2, \\
\mathcal{L}_2 &= \mathbb{E}_{y_a \neq y_b} \max(\xi - ||h(x_a) - h(x_b)||^2, 0), \\
\mathcal{L}_{\text{con}} &= \mathcal{L}_1 + \mathcal{L}_2,
\end{align*}
\]

where \( 1 \leq a < b \leq N \). We train the contrastive loss in a batched manner, where the within-class and between-class instances are determined based on a batch \( \mathcal{B} \). Moreover, for avoiding introducing a new hyperparameter, we use an adaptive \( \xi \) for each instance, which is defined as the maximum distance from the instance to others of the same class in a batch:

\[
\xi_a = \max_{x_b \in \mathcal{B}, y_a = y_b} ||h(x_a) - h(x_b)||.
\]

In experiments, we set \( h \) as the penultimate layer representation of the pretrained transformer. In training, the model is jointly trained to optimize the main-task supervision loss \( \mathcal{L}_{\text{sup}} \) and \( \mathcal{L}_{\text{con}} \):

\[
\mathcal{L} = \mathcal{L}_{\text{sup}} + \lambda \mathcal{L}_{\text{con}},
\]

where \( \lambda \) is a hyperparameter. We can tune \( \lambda \) based on the contrastive loss during training and the classification performance on the in-distribution validation set, where a good value for \( \lambda \) should achieve smaller contrastive loss while maintaining the classification performance on the validation set.

### 3.3 Scoring Functions

Next, we introduce the considered scoring function \( g \) in our experiments. The goal of the scoring function \( g \) is to map the representations to OoD detection scores, where higher scores indicate higher likelihoods for OoD. All of these functions are calculated based on the penultimate layer of \( h(x) \).

#### Maximum Softmax Probability (MSP)

(Hendrycks and Gimpel, 2017) use the maximum output from the softmax layer as an OoD
Table 1: Performance of the four OoD detection methods. For each dataset, we use all datasets from different tasks as OoD data and report the macro average of AUROC and FAR95.

| AUROC↑ / FAR95↓ | MRPC | RTE | SST-2 | CoLA | MNLI | QNLI | QQP |
|-----------------|------|-----|-------|------|------|------|-----|
| w/o $\mathcal{L}_{\text{con}} +$ MSP | 62.8 / 96.3 | 78.5 / 79.8 | 90.8 / 56.6 | 63.0 / 95.2 | 74.7 / 85.8 | 86.1 / 64.4 | 52.4 / 95.3 |
| w/o $\mathcal{L}_{\text{con}} +$ Maha | 82.9 / 78.0 | 82.0 / 59.8 | 98.5 / 0.07 | 64.1 / 94.5 | 85.1 / 42.2 | 94.8 / 20.5 | 89.0 / 47.4 |
| w/ $\mathcal{L}_{\text{con}} +$ MSP | 55.4 / 97.3 | 85.7 / 64.6 | 88.2 / 59.6 | 67.8 / 95.3 | 75.0 / 90.8 | 87.0 / 68.4 | 51.0 / 95.6 |
| w/ $\mathcal{L}_{\text{con}} +$ Maha | 92.1 / 42.6 | 92.5 / 27.9 | 99.6 / 0.05 | 71.3 / 90.2 | 86.6 / 40.4 | 93.2 / 26.1 | 90.3 / 43.6 |

Table: Performance of the four OoD detection methods. For each dataset, we use all datasets from different tasks as OoD data and report the macro average of AUROC and FAR95.

indicator:

\[
p = \text{softmax}(W_{\text{cls}} h(x)),
\]

\[
g(x) = 1 - \frac{1}{C} \max_{j=1}^{C} p_j,
\]

where $W_{\text{cls}}$ is the weights of the classifier, $C$ is the number of classes. This method has been widely adopted as a baseline for OoD detection.

**Mahalanobis Distance (Maha)** (Lee et al., 2018b) fits class-conditional multivariate Gaussian distributions on the $h(x)$, and then calculate the OoD detection score by the minimum Mahalanobis distance among classes:

\[
\mu_j = \mathbb{E}_{y_i = j} [h(x_i)], j = 1, ..., C
\]

\[
\Sigma = \mathbb{E} [h(x_i) - \mu_{y_i}](h(x_i) - \mu_{y_i})^\top,
\]

\[
g(x) = - \min_{j=1}^{C} (h(x) - \mu_{y_j})^\top \Sigma^{-1} (h(x) - \mu_{y_j}),
\]

where $C$ is the number of classes. The parameters can be fit on an in-distribution validation set.

4 Experiments

4.1 Experimental Setup

**Datasets.** We evaluate our method on the GLUE benchmark (Wang et al., 2018), which consists of different tasks including natural language inference (RTE (Dagan et al., 2005; Bar-Haim et al., 2006; Giampiccolo et al., 2007; Bentivogli et al., 2009), MNLI (Williams et al., 2018), QNLI (Rajpurkar et al., 2016)), sentence-pair similarity (MRPC (Dolan and Brockett, 2005), QQP), sentiment analysis (SST-2 (Socher et al., 2013)), and linguistic acceptability (CoLA (Warstadt et al., 2019)). From each task, we use its training set to train the model, then use its test set as in-distribution instances and test sets from other tasks as OoD instances.

**Evaluation Metrics.** We adopt two metrics that are commonly used for OoD detection (Hendrycks and Gimpel, 2017; Lee et al., 2018b): (1) AUROC is the area under the receiver operating characteristic curve, which plots the true positive rate (TPR) against the negative positive rate (FPR). A higher AUROC value indicates better OoD detection performance, and a random guessing detector corresponds to an AUROC score of 50%. (2) FAR95 is the probability that a negative example (OoD) is mistakenly classified as positive (in-distribution) when the TPR is 95%, in which case a lower value indicates better OoD detection performance.

**Compared Methods.** We evaluate all combinations of representation function $h$ and the scoring function $g$. Those include four settings composed of two alternative $h$ (w/ and w/o $\mathcal{L}_{\text{con}}$), and two alternatives of $g$ (MSP or Maha). For all compared methods, we use the RoBERTa-large (Liu et al., 2019) as the backbone.

4.2 Results

We report the OoD performance of different methods in Table 1. We observe that models under settings with the Mahalanobis distance always outperform MSP, and the gain usually increases when incorporated with the contrastive loss. We also notice that improvements are larger on small datasets such as MRPC and RTE. Particularly, w/ $\mathcal{L}_{\text{con}} +$ Maha achieves over 90% AUROC on all datasets except for CoLA and MNLI. However, the OoD detection performance is lesser on CoLA. Also, when using QNLI (pair of a question and an answer) as in-distribution and QQP (pair of questions) as OoD, the best method can only achieve an AUROC of 78.9%, though the tasks are completely different.

5 Conclusion

This work proposes an OoD detection method for pretrained transformers that requires only learning on in-distribution data. An OoD detection score defined based on the Mahalanobis distance is calculated on the basis of the penultimate layer representations of the transformer. On top of that, a contrastive loss is further incorporated to improve the compactness of representations. Experiments on the GLUE benchmark prove the effectiveness of the proposed method.
References

Dario Amodei, Christopher Olah, J. Steinhardt, P. F. Christiano, John Schulman, and Dandelion Mané. 2016. Concrete problems in ai safety. ArXiv, abs/1606.06565.

Roy Bar-Haim, Ido Dagan, B. Dolan, L. Ferro, Danilo Giampiccolo, and B. Magnini. 2006. The second pascal recognising textual entailment challenge. In TAC.

Abhijit Bendale and T. Boult. 2016. Towards open set deep networks. 2016 IEEE Conference on Computer Vision and Pattern Recognition (CVPR), pages 1563–1572.

L. Bentivogli, Peter Clark, Ido Dagan, and Danilo Giampiccolo. 2009. The sixth pascal recognising textual entailment challenge. In MLCW.

Lucas Deecke, Robert A. Vandermeulen, Lukas Ruff, S. Mandt, and M. Kloft. 2018. Image anomaly detection with generative adversarial networks. In ECML/PKDD.

Jacob Devlin, Ming-Wei Chang, Kenton Lee, and Kristina Toutanova. 2019. BERT: Pre-training of deep bidirectional transformers for language understanding. In Proceedings of the 2019 Conference of the North American Chapter of the Association for Computational Linguistics: Human Language Technologies, Volume 1 (Long and Short Papers), pages 4171–4186, Minneapolis, Minnesota. Association for Computational Linguistics.

A. Dhamija, Manuel Günther, and T. Boult. 2018. Reducing network agnostophobia. In NeurIPS.

W. Dolan and Chris Brockett. 2005. Automatically constructing a corpus of sentential paraphrases. In IWP@IJCNLP.

Dan Hendrycks and Kevin Gimpel. 2017. A baseline for detecting misclassified and out-of-distribution examples in neural networks. International Conference on Learning Representations.

Dan Hendrycks, Xiaoyuan Liu, Eric Wallace, Adam Dziedzic, Rishabh Krishnan, and Dawn Song. 2020. Pretrained transformers improve out-of-distribution robustness. In Proceedings of the 58th Annual Meeting of the Association for Computational Linguistics, pages 2744–2751, Online. Association for Computational Linguistics.

Dan Hendrycks, Mantas Mazeika, and Thomas Dietterich. 2018. Deep anomaly detection with outlier exposure. In International Conference on Learning Representations.

S. Hochreiter and J. Schmidhuber. 1997. Long short-term memory. Neural Computation, 9:1735–1780.

Yen-Chang Hsu, Yilin Shen, Hongxia Jin, and Z. Kira. 2020. Generalized odin: Detecting out-of-distribution image without learning from out-of-distribution data. 2020 IEEE/CVF Conference on Computer Vision and Pattern Recognition (CVPR), pages 10948–10957.

Stefan Larson, Anish Mahendran, Joseph J. Peper, Christopher Clarke, Andrew Lee, Parker Hill, Jonathan K Kummerfeld, Kevin Leach, Michael A Laurennzano, Lingjia Tang, et al. 2019. An evaluation dataset for intent classification and out-of-scope prediction. In Proceedings of the 2019 Conference on Empirical Methods in Natural Language Processing and the 9th International Joint Conference on Natural Language Processing (EMNLP-IJCNLP), pages 1311–1316.

W. Lawson, Esube Bekele, and Keith Sullivan. 2017. Finding anomalies with generative adversarial networks for a patrolbot. 2017 IEEE Conference on Computer Vision and Pattern Recognition Workshops (CVPRW), pages 484–485.

Kimin Lee, Honglak Lee, Kibok Lee, and Jinwoo Shin. 2018a. Training confidence-calibrated classifiers for detecting out-of-distribution samples. In International Conference on Learning Representations.

Kimin Lee, Kibok Lee, Honglak Lee, and Jinwoo Shin. 2018b. A simple unified framework for detecting out-of-distribution samples and adversarial attacks. In Proceedings of the 32nd International Conference on Neural Information Processing Systems, pages 7167–7177.

Shiyu Liang, Yixuan Li, and R Srikant. 2018. Enhancing the reliability of out-of-distribution image detection in neural networks. In International Conference on Learning Representations.

Weitang Liu, Xiaoyun Wang, John Owens, and Yixuan Li. 2020. Energy-based out-of-distribution detection. volume 33.

Yinhan Liu, Myle Ott, Naman Goyal, Jingfei Du, Mandar Joshi, Danqi Chen, Omer Levy, Mike Lewis, Luke Zettlemoyer, and Veselin Stoyanov. 2019. Roberta: A robustly optimized bert pretraining approach. arXiv preprint arXiv:1907.11692.

Pranav Rajpurkar, Jian Zhang, Konstantin Lopyrev, and Percy Liang. 2016. Squad: 100, 000+ questions for machine comprehension of text. In EMNLP.

Lei Shu, Hu Xu, and Bing Liu. 2017. Doc: Deep open classification of text documents. In Proceedings of the 2017 Conference on Empirical Methods in Natural Language Processing, pages 2911–2916.
R. Socher, Alex Perelygin, J. Wu, Jason Chuang, Christopher D. Manning, A. Ng, and Christopher Potts. 2013. Recursive deep models for semantic compositionality over a sentiment treebank. In EMNLP.

Jihoon Tack, Sangwoo Mo, Jongheon Jeong, and Jin-woo Shin. 2020. Csi: Novelty detection via contrastive learning on distributionally shifted instances. In 34th Conference on Neural Information Processing Systems (NeurIPS) 2020. Neural Information Processing Systems.

Engkarat Techapanurak, Masanori Suganuma, and Takayuki Okatani. 2020. Hyperparameter-free out-of-distribution detection using cosine similarity. In Proceedings of the Asian Conference on Computer Vision.

Apoorv Vyas, Nataraj Jammalamadaka, Xia Zhu, Dipsankar Das, Bharat Kaul, and Theodore L Willke. 2018. Out-of-distribution detection using an ensemble of self supervised leave-out classifiers. In Proceedings of the European Conference on Computer Vision (ECCV), pages 550–564.

Alex Wang, Amanpreet Singh, Julian Michael, Felix Hill, Omer Levy, and Samuel R. Bowman. 2018. Glue: A multi-task benchmark and analysis platform for natural language understanding. In BlackboxNLP@EMNLP.

Mei Wang and Weihong Deng. 2018. Deep visual domain adaptation: A survey. Neurocomputing, 312:135–153.

Alex Warstadt, Amanpreet Singh, and Samuel R. Bowman. 2019. Neural network acceptability judgments. Transactions of the Association for Computational Linguistics, 7:625–641.

Adina Williams, Nikita Nangia, and Samuel R. Bowman. 2018. A broad-coverage challenge corpus for sentence understanding through inference. In NAACL-HLT.