Why is the Mahalanobis Distance Effective for Anomaly Detection?

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Abstract
The Mahalanobis distance-based confidence score, a recently proposed anomaly detection method for pre-trained neural classifiers, achieves state-of-the-art performance on both out-of-distribution and adversarial example detection. This work analyzes why this method exhibits such strong performance while imposing an implausible assumption; namely, that class conditional distributions of intermediate features have tied covariance. We reveal that the reason for its effectiveness has been misunderstood. Although this method scores the prediction confidence for the original classification task, our analysis suggests that information critical for classification task does not contribute to state-of-the-art performance on anomaly detection. To support this hypothesis, we demonstrate that a simpler confidence score that does not use class information is as effective as the original method in most cases. Moreover, our experiments show that the confidence scores can exhibit different behavior on other frameworks such as metric learning models, and their detection performance is sensitive to model architecture choice. These findings provide insight into the behavior of neural classifiers when provided with anomalous inputs.

1. Introduction
Modern neural networks classifiers often exhibit unexpected behavior to inputs dissimilar from training data (Gal, 2016; Hendrycks & Gimpel, 2017). Furthermore, it is known that neural classifiers are easily fooled by small adversarial perturbations to inputs (Szegedy et al., 2013; Goodfellow et al., 2015; Nguyen et al., 2015). Since these problems pose a serious threat to the safety of machine learning systems, anomaly detection methods such as out-of-distribution and adversarial example detection have attracted considerable attention (Pimentel et al., 2014; Hendrycks & Gimpel, 2017; Li & Li, 2017). However, anomaly detection for high-dimensional data is a difficult task, and behavior of neural networks towards anomalous inputs is not well understood.

Distance-based methods are a primitive yet popular approach to anomaly detection. Although they have been well studied for low-dimensional data (Pimentel et al., 2014), distance-based methods applied to high-dimensional data suffer from the curse of dimensionality. One way to address this problem is to use a lower dimensional representation of data. Some previous studies on out-of-distribution (Song et al., 2017; Guo et al., 2018; Papernot & Mcdaniel, 2018) and adversarial example detection (Feinman et al., 2017; Ma et al., 2018; Gilmer et al., 2018) use the Euclidean distance of intermediate representations in neural networks. In this line of research, recent work of anomaly detection on intermediate features of pre-trained neural classifiers (Lee et al., 2018) shows that the Mahalanobis distance-based confidence score outperforms methods based on the Euclidean distance. This method achieves state-of-the-art performance in out-of-distribution and adversarial example detection, and

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is regarded as the new standard in anomaly detection on pre-trained neural classifiers (Ren et al., 2019; Rajendran & Levine, 2019; Tardy et al., 2019; Roady et al., 2019; Wang et al., 2019; Maçêdo et al., 2019; Ahuja et al., 2019; Cohen et al., 2019). However, why it works so well has not been sufficiently investigated. In this work, we reveal that the behavior of intermediate features with regard to anomalous inputs has been misunderstood. The Mahalanobis distance-based method by Lee et al. (2018) constructs the prediction confidence for the original classification task, a similar idea to the method by Hendrycks & Gimpel (2017) that uses the output of the softmax function as a confidence score. However, our analysis shows that the information in intermediate features that is not critical for the original classification task is the main contribution to state-of-the-art performance of the method. Namely, the subspace spanned by principal components with small explained variance, which may not be expected to have useful information about the input, contains information critical for anomaly detection.

Our analysis is motivated by an unreasonable assumption; Lee et al. (2018) assumes that class conditional distributions of the final features have tied covariance, and uses the Mahalanobis distances from class means as confidence scores. This assumption is not consistent with observations in previous work. The standard framework of neural classifiers with a softmax function following a fully connected layer evaluates similarity based on inner products. Thus, the final features are radially distributed as the decision rule is largely determined by angular similarity (Wen et al., 2016; Liu et al., 2016) as shown in Figure 1. Ahuja et al. (2019) has already pointed out this problem of the assumption, and proposed usage of more representative class of distributions to estimate class conditional distributions. However, to the best of our knowledge, there is no prior work analyzing why the Mahalanobis distance-based confidence score can detect anomalous samples effectively despite imposing this unrealistic assumption. Our analysis reveals that information on intermediate features that is not critical for the original classification task contributes to its state-of-the-art performance in anomaly detection. We also propose a simpler method named the marginal Mahalanobis distance-based confidence score. This method approximates intermediate feature distribution with a single Gaussian distribution, and uses the Mahalanobis distance from the mean as confidence scores. In most settings of anomaly detection, our method, while not using class information at all, is competitive with the original confidence score based on class conditional distributions.

Furthermore, we evaluate the Mahalanobis distance-based confidence score on representation spaces of distance-based metric learning methods. The representation spaces of metric learning behave differently from these of neural classifiers towards anomalous inputs, and the Mahalanobis distance works poorly in some of these cases. While Lee et al. (2018) suggests that their confidence score is widely applicable to other frameworks such as few-shot learning, our observation implies that this is not the case, as the method may utilize a unique property of ordinary neural classifiers. We also observe that detection performance of the confidence score depends on model architecture choice. Consequently, we note that caution is needed when applying the Mahalanobis distance-based confidence score to new architectures or data sets.

2. Related Work

High-Dimensional Out-of-distribution Detection Although out-of-distribution detection has been well studied for low-dimensional data (Pimentel et al., 2014), recent work has shown that it does not work well for high-dimensional data. For a pre-trained neural classifier, Hendrycks & Gimpel (2017) proposed a method using the output of the softmax function as a confidence score, and Liang et al. (2018) improved upon this. Hendrycks et al. (2019) proposed to use out-of-distribution data during training to improve out-of-distribution detectors. An approach related to this paper is the use of lower dimensional representations in neural networks. Mandelbaum & Weinshall (2017) proposed a confidence score based on local density estimation in the embedding spaces of neural networks. There is some work using intermediate features of autoencoders as well (Sabokrou et al., 2018; Denouden et al., 2018; Perera et al., 2019).

Adversarial Examples Detection Adversarial examples (Szegedy et al., 2013; Goodfellow et al., 2015) are a major concern of modern neural networks. A popular approach to avoid this problem is to make neural networks robust to adversarial attacks with methods such as adversarial training (Goodfellow et al., 2015). Another approach to mitigate adversarial attacks related to this paper is adversarial example detection. Li & Li (2017) proposed usage of a cascade detector on features acquired via principal component analysis (PCA) on intermediate representations. Grosse et al. (2017) examined statistical properties of adversarial examples, and Ma et al. (2018) proposed usage of the Local Intrinsic Dimensionality (LID). However, Carlini & Wagner (2017) has reported that these detection methods can be bypassed relatively easily.

3. Background

In this section, we first describe the Mahalanobis distance-based confidence score by Lee et al. (2018). We then explain the relationship between the Mahalanobis distance and PCA, which motivates our analysis in Section 4.1.
3.1. Mahalanobis Distance-Based Confidence Score

Lee et al. (2018) proposed a confidence score for anomaly detection based on the class-conditional Mahalanobis distance with the assumption of tied covariance. This method is motivated by an induced generative classifier. Here, we consider a generative classifier with the assumption that \( P(t = c) = \beta_c / \sum_{c'} \beta_{c'} \) and class-conditional distributions follow Gaussian distributions with tied covariance \( \mathcal{N}(\mathbf{x} | \mu_c, \Sigma) \). Then, its posterior distribution \( P(t = c | \mathbf{x}) \) can be represented in the following manner:

\[
\frac{\exp(\mu_c^T \Sigma^{-1} \mathbf{x} - \frac{1}{2} \mu_c^T \Sigma^{-1} \mu_c + \log \beta_c)}{\sum_{c'} \exp(\mu_{c'}^T \Sigma^{-1} \mathbf{x} - \frac{1}{2} \mu_{c'}^T \Sigma^{-1} \mu_{c'} + \log \beta_{c'})}. \tag{1}
\]

This posterior distribution is equivalent to a softmax classifier by considering \( \mu_c^T \Sigma^{-1} \mathbf{x} - \frac{1}{2} \mu_c^T \Sigma^{-1} \mu_c + \log \beta_c \) to be the weights and biases. This observation leads to the idea that the final features of pre-trained neural classifier might follow a class-conditional Gaussian distribution, and the Mahalanobis distances from class means represent confidence scores of the classification, which is more informative than the output of the softmax function. Given training data \( \{(\mathbf{x}_1, t_1), \ldots, (\mathbf{x}_n, t_n)\} \), the parameters of the generative classifier can be estimated as follows:

\[
\hat{\mu}_c = \frac{1}{n_c} \sum_{i : t_i = c} f(\mathbf{x}_i), \tag{2}
\]

\[
\hat{\Sigma} = \frac{1}{n} \sum_e \sum_{i : t_i = e} (f(\mathbf{x}_i) - \hat{\mu}_e)(f(\mathbf{x}_i) - \hat{\mu}_e)^T, \tag{3}
\]

where \( f(\cdot) \) denotes the output of the penultimate layer, and \( n_c \) is the number of training examples with label \( c \). The Mahalanobis distance-based score is calculated as the minimum squared Mahalanobis distance from the class means:

\[
M(\mathbf{x}) = \max_e - (f(\mathbf{x}) - \hat{\mu}_e)^T \hat{\Sigma}^{-1} (f(\mathbf{x}) - \hat{\mu}_e). \tag{4}
\]

To improve detection performance, the authors proposed input pre-processing similar to Liang et al. (2018) and a feature ensemble consisting of logistic regression using the confidence scores from all layers.

3.2. Mahalanobis Distance and PCA

The Mahalanobis distance can be alternatively represented by using the eigenvectors \( u_i \) of the covariance matrix \( \Sigma \) (Murphy, 2012):

\[
\Delta^2 = (\mathbf{x} - \mu)^T \Sigma^{-1} (\mathbf{x} - \mu) = \sum_{i=1}^{N} \frac{y_i^2}{\lambda_i} \tag{5}
\]

where \( N \) is the dimension of data, \( \lambda_i \) is the \( i \)-th eigenvalue, and \( y_i = u_i^T (\mathbf{x} - \mu) \). Note that the eigenvectors and eigenvalues of data sets can be interpreted as the principal components and explained variance of principal component analysis, so this formulation shows the relationship between the Mahalanobis distance and PCA. This observation motivates our analysis in Section 4.1.

4. Analysis

While Lee et al. (2018)’s Mahalanobis distance-based confidence score imposes the implausible assumption that covariance matrices of class conditional distributions of intermediate features are tied, the method achieves state-of-the-art results on both out-of-distribution and adversarial example detection. Since it is clear that the method is not superior for low-dimensional cases (Figure 1), we hypothesize that it utilizes a property of high-dimensional feature spaces. When a representation space is low-dimensional, all dimensions may be used to represent information critical for classification. However, in high-dimensional cases, a small number of directions will explain almost all variance of training data, and most of directions may not contribute to classification. Therefore, in high-dimensional cases, we hypothesize that the directions which are not important for the original classification task contribute to anomaly detection (Figure 2).

Our hypothesis is supported by observations presented in this section and experiments in Chapter 5.

4.1. Partial Mahalanobis Distance

**Definition** As mentioned in Section 3.2, the squared Mahalanobis distance is equivalent to the squared sum of principal component scores (Equation 5). Here, examine the partial sum:

\[
\Delta_S^2 = \sum_{i \in S} \frac{y_i^2}{\lambda_i}, \quad S \subset \{1, \ldots, N\} \tag{6}
\]

We will refer to this metric as the partial Mahalanobis distance. We use the partial Mahalanobis distance to analyze the Mahalanobis distance-based confidence score. For ac-

![Image](331x144 to 518x249)

**Figure 2.** Visualization of our hypothesis on the structure of intermediate features in neural classifiers. We hypothesize that directions with small explained variance, while containing relatively less information relevant to classification, strongly contribute to anomaly detection.
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Figure 3. PCA on the final features of ResNet trained on CIFAR-10. The corresponding class mean is subtracted from each input. (a) The proportion of variance of training data. The first several principal components explain almost all variances. (b) Variance of the penultimate layers of CIFAR-10 (test data, blue) and SVHN (out-of-distribution, red) on 1st to 30-th principal components. (c) Variance on 370-th to 420-th principal components. SVHN has larger variance even when the explained variance are small.

Table 1. Analysis of out-of-distribution performance of the partial Mahalanobis distance on ResNet trained on CIFAR-10. The out-of-distribution data is SVHN. “All” denotes the original Mahalanobis distance using all features, and “Partial (i − j)” denotes the partial Mahalanobis distance using i-th to j-th principal components. The partial Mahalanobis distance using principal components with small explained variance (Partial (10-512)) works better than that using principal components with large explained variance (Partial (1-9)).

| Method       | TNR at TPR 95% | AUROC | Detection Accuracy | AUPR in | AUPR out |
|--------------|----------------|-------|--------------------|---------|----------|
| All (original) | 91.60          | 93.92 | 89.13              | 91.56   | 95.96    |
| Partial (10-512) | 96.73          | 94.05 | 89.27              | 91.70   | 96.11    |
| Partial (1-9)  | 93.70          | 88.09 | 84.66              | 83.47   | 92.35    |
| Euclidean     | 93.61          | 89.33 | 84.98              | 84.89   | 92.43    |

Experiments Figure 3a shows the proportion of variance when PCA is applied to the in-distribution final features of ResNet trained on CIFAR-10. Here, the corresponding class mean is subtracted from each feature. It shows that the first nine components explain almost all of the variance of the features. We evaluate two partial Mahalanobis distances to analyze behavior of the final features of anomalous inputs. The first one is $\Delta^2_{[1,9]} = \sum_{i=1}^{9} y_i^2 / \lambda_i$ and the second one is $\Delta^2_{[10,512]} = \sum_{i=10}^{512} y_i^2 / \lambda_i$, where the principal components are sorted in descending order with respect to the proportion of variance. Table 1 shows out-of-distribution detection performance using different confidence scores. The results show that $\Delta^2_{[10,512]}$ solely achieves the performance by the original Mahalanobis distance-based confidence score while it uses information on principal components with very small explained variance. On the contrary, the performance of $\Delta^2_{[1,9]}$ is worse and similar to that by the Euclidean distance while it uses principal components explaining most of the variances in training data. This observation suggests that the subspace spanned by principal components with small explained variance contains information critical for anomaly detection.

Figure 3b and c compares variances of the final features of in-distribution data (test data of CIFAR-10) and out-of-distribution data (SVHN) on each principal components. Here, we subtract the nearest class mean in terms of the Mahalanobis distance from each input. Figure 3b shows that out-of-distribution data has large variances on principal components with large explained variance. This is an expected result as the principal components with large explained variance may represent important features of data, so it may capture difference between in-distribution and out-of-distribution inputs. However, note that variance of out-of-distribution data is large even on principal components with small explained variance, which may not be expected to contain useful information about input data (Figure 3c). Li & Li (2017) reported a similar observation for adversarial examples. Our analysis reveals that this phenomenon also occurs towards out-of-distribution data, and the Mahalanobis distance-based confidence score effectively captures this property of anomalous inputs on the intermediate features.

4.2. Marginal Mahalanobis Distance

Definition The analysis of partial Mahalanobis distances suggests that principal components of the final features with small explained variance contribute to out-of-distribution detection. However, principal components with small explained variance may not contain information relevant to
Table 2. Out-of-distribution detection performance of the marginal Mahalanobis distance on ResNet trained on CIFAR-10. The out-of-distribution data is SVHN. “Conditional” denotes the original Mahalanobis distance (Lee et al., 2018). “Marginal” represents our marginal Mahalanobis distance, and “Marginal (10-512)” represents the partial Mahalanobis distance using 10-th to 512-th principal components of the marginal Mahalanobis distance. Here, PCA is applied to the original features without subtracting class means. “Euclidean” denotes the Euclidean distance from the mean. “Ensemble” and “Pre-processing” denote features ensemble and input pre-processing proposed. The out-of-distribution detection performance by the marginal Mahalanobis distance is competitive to the original Mahalanobis distance.

| Method       | Ensemble | Pre-processing | TNR at 95% | AUROC | Detection Accuracy | AUPR in | AUPR out |
|--------------|----------|----------------|------------|-------|-------------------|--------|---------|
| Conditional  | o        | o              | 91.45      | 98.37 | 93.55             | 96.43  | 99.35   |
| Marginal     |          |                | 96.42      | 99.14 | 95.75             | 98.26  | 99.60   |
| Marginal (10-512) | o        | o              | 96.01      | 99.10 | 95.54             | 98.14  | 99.60   |

Classification. Motivated by this observation, we propose to use the Mahalanobis distance with the assumption that the marginal distribution is Gaussian, which ignores class information. Here, the model parameters are estimated as follows:

\[
\hat{\mu} = \frac{1}{n} \sum_{i=1}^{n} f(x_i) \quad (7)
\]

\[
\hat{\Sigma} = \frac{1}{n} \sum_{i=1}^{n} (f(x_i) - \hat{\mu})(f(x_i) - \hat{\mu})^T. \quad (8)
\]

Based on the estimated parameters, we use the Mahalanobis distance from \( \hat{\mu} \), the global mean:

\[
M'(x) = -(f(x) - \hat{\mu})^T \hat{\Sigma}^{-1}(f(x) - \hat{\mu}) \quad (9)
\]
as a confidence score instead of using class conditional distributions.

**Experiments** Table 2 shows that the marginal Mahalanobis distance achieves almost the same performance as the original class conditional Mahalanobis distance-based score. Notably, “Mahalanobis (10-512)” effectively detects out-of-distribution inputs while only using principal components with small explained variance. This observation supports our hypothesis that the Mahalanobis distance-based confidence score uses information that is not critical for the original classification task. We also evaluate feature ensemble and input pre-processing proposed by Lee et al. (2018), and show that these techniques are also effective on our marginal Mahalanobis distance score.

Additionally, we conduct a simple experiment to verify the hypothesis that information in the final features that is relatively unimportant for classification contributes to state-of-the-art performance in out-of-distribution detection. We apply PCA to the penultimate features, and evaluate classification using some of the principal components. The logistic regression on the final features of neural classifiers trained on CIFAR-10 achieves 94.11% accuracy when all principal components are used. The classifier using first 9 principal components achieves 94.05%, but that using 10-th to 512-th components only achieves 20.48%. These results suggest that principal components with small explained variance do not contain information critical for classification. However, they contribute to anomaly detection as shown in “Mahalanobis (10-512)” of Table 2. This analysis provides an explanation that the Mahalanobis distance-based confidence score outperforms a method based on the output of the softmax function (Liang et al., 2018) as the softmax function only provides information related to classification. We further evaluate the marginal Mahalanobis distance in Section 5.2.

### 4.3. Analysis of Input Pre-processing

Lee et al. (2018) has proposed the following input pre-processing:

\[
\tilde{x} = x + \epsilon \text{sign}(\nabla_x M(x)) \quad (10)
\]

where \( \epsilon \) is the magnitude of noise. While this considerably improves the detection performance, the mechanism of its contribution has not been analyzed well. This method is similar to the pre-processing by Liang et al. (2018) that takes the gradient of the cross-entropy. For cross-entropy loss, Liang et al. (2018) demonstrated that the norms of the gradients for in-distribution data tend to be larger than those for out-of-distribution data, so the pre-processing increases confidence for in-distribution data more than that for out-of-distribution data. However, in the input pre-processing for the Mahalanobis distance, we observe the opposite behavior. Figure 4a shows that L1 norms of the differences between the original and pre-processed features on the penultimate layer for the class conditional Mahalanobis distance. It shows that L1 norms of SVHN (out-of-distribution data) tend to be
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Figure 4. Analysis of input pre-processing. (a) L1 norm of the difference between the original and pre-processed features ($\varepsilon = 1$) on the penultimate layer. SVHN (out-of-distribution data) has larger norm than CIFAR-10 (in-distribution data). (b) (c) The mean Mahalanobis distance of CIFAR-10 and SVHN on the final features with different levels of input pre-processing. For both of the data sets, the Mahalanobis distances once decrease. However, after they reach the minimum values, the distance on SVHN features increases faster than that on CIFAR-10 as the magnitude increases because the gradients are larger on SVHN. (d) As a result, the detection performance improves after it reaches the minimum value. This observation is opposite to what reported by Liang et al. (2018) for cross-entropy loss.

larger than those for CIFAR-10 (in-distribution data). As a result, the input pre-processing lowers the Mahalanobis distance and increase confidence for out-of-distribution inputs more than for in-distribution data. However, as shown in Figure 4b and c, the mean Mahalanobis distance on the final features of SVHN increase much faster than that of CIFAR-10 as the magnitude increases after it reaches the minimum value. For $\varepsilon = 0.01$, the mean Mahalanobis distance of CIFAR-10 is still lower than that for $\varepsilon = 0$, while that of SVHN is much larger than the original value. As a result, the detection performance is improved from 98.37 to 99.14 in AUROC. These results and Figure 4d suggest that a proper magnitude that increases the Mahalanobis distances of out-of-distribution inputs more than those of in-distribution data, the detection performance will be improved. We provide further experimental results in the appendix.

4.4. Applicability and Limitations

Lee et al. (2018) has suggested that their confidence score may be applied to other architectures such as few-shot learning. Our experiments in Section 5.3 show that the situation is not that simple; the method does not always work effectively on metric learning. This observation suggests that the Mahalanobis distance-based confidence score utilizes a unique property of ordinary neural classifiers, so caution is needed when applying the method to other architectures.

5. Experiments

We show further experimental results supporting our hypothesis that the Mahalanobis distance-based score utilizes information that is not critical for the original classification.

5.1. Settings

Evaluation We evaluate confidence scores on threshold-based detectors of test data and out-of-distribution data. We measure the following metrics: the true negative rate (TNR) at 95% true positive rate (TPR), the area under the receiver operating characteristic curve (AUROC), the area under the precision-recall curve (AUPR), and the detection accuracy.

Neural Classifiers For experiments on intermediate features of ResNet (He et al., 2016) and DenseNet (Huang et al., 2017), we use the implementation by Lee et al. (2018)¹. We evaluate the networks on several data sets: CIFAR-10, CIFAR-100 (Krizhevsky, 2009), SVHN (Netzer et al., 2011), TinyImageNet (Chrabaszcz et al., 2017; Deng et al., 2009), and LSUN (Yu et al., 2016). For adversarial example detection, we evaluate on four types of attacks: FGSM (Goodfellow et al., 2015), BIM (Kurakin et al., 2017), DeepFool (Moosavi-Dezfooli et al., 2016), and CW (Carlini & Wagner, 2017). We use both input pre-processing and feature ensemble. The results of the baseline method are slightly different from what are reported in Lee et al. (2018) since we re-evaluated them. We also compare adversarial examples performance with local intrinsic dimensional (LID) (Ma et al., 2018) implemented by Lee et al. (2018).

Distance-Based Metric Learning We use the implementation by Chen et al. (2019)². We evaluate two types of distance-based metric learning: Prototypical Networks (Snell et al., 2017) and Matching Networks (Vinyals et al., 2016) with four-layer convolutional networks (Conv-4) and a simplified ResNet (Conv-4 and ResNet-10 in Chen et al. (2019)). In this experiment, we use two pairs of data

¹https://github.com/pokaxpoka/deep_Mahalanobis_detector
²https://github.com/wyharveychen/CloserLookFewShot
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Table 3. Out-of-distribution detection on neural classifiers using the marginal Mahalanobis distance-based confidence scores (marginal) and the Mahalanobis distance-based confidence scores by Lee et al. (2018) (class conditional).“Validation on adversarial samples” is out-of-distribution performance of detector trained on samples generated by FGSM (Goodfellow et al., 2015). Our marginal confidence scores which does not use class information performs almost as well as the original scores which are based on class conditional distributions.

| In-dist          | OOD                | Validation on OOD samples | Validation on adversarial samples |
|------------------|--------------------|----------------------------|----------------------------------|
|                  |                    | TNR | AUROC | Detection | TNR | AUROC | Detection |
|                  |                    | class conditional / marginal (ours) | class conditional / marginal (ours) |
| CIFAR-10 (Densenet) | SVHN               | 90.2/76.6 | 98.18/78.4 | 93.7/96.3 | 84.8/84.8 | 96.10/96.6 | 91.10/90.9 |
|                  | TinyImageNet       | 95.2/76.1 | 98.9/78.9 | 95.1/95.7 | 95.2/92.7 | 98.9/98.3 | 95.1/95.5 |
|                  | LSUN               | 97.0/98.0 | 99.2/98.4 | 96.2/96.9 | 97.2/95.1 | 99.3/98.9 | 96.3/95.5 |
| CIFAR-100 (Densenet) | SVHN               | 92.7/77.7 | 99.0/78.6 | 91.2/90.0 | 46.3/39.2 | 87.17/86.5 | 80.17/92.5 |
|                  | TinyImageNet       | 86.9/87.5 | 97.4/87.5 | 92.2/92.0 | 87.4/87.0 | 97.0/97.2 | 91.9/91.7 |
|                  | LSUN               | 91.8/90.9 | 98.0/98.0 | 93.9/93.6 | 91.8/90.3 | 98.0/97.8 | 93.9/93.3 |
| SVHN (Densenet)  | CIFAR-10           | 96.8/94.5 | 99.9/98.5 | 96.0/95.7 | 95.8/82.9 | 98.6/94.2 | 95.6/90.3 |
|                  | TinyImageNet       | 99.9/99.9 | 99.9/99.9 | 99.8/98.9 | 100.0/99.3 | 99.9/99.5 | 98.9/98.3 |
|                  | LSUN               | 100.0/99.9 | 99.9/99.9 | 99.3/99.2 | 100.0/99.9 | 99.9/99.8 | 99.2/98.8 |
| CIFAR-10 (ResNet) | SVHN               | 96.4/76.0 | 99.1/99.1 | 85.0/95.5 | 87.2/86.5 | 96.0/97.3 | 91.9/91.7 |
|                  | TinyImageNet       | 97.1/76.0 | 99.5/99.5 | 96.3/96.4 | 87.7/94.0 | 96.3/98.5 | 91.8/91.7 |
|                  | LSUN               | 98.9/99.0 | 99.7/99.8 | 97.7/97.8 | 93.9/97.2 | 97.9/99.2 | 94.0/96.3 |
| CIFAR-100 (ResNet) | SVHN               | 91.9/98.7 | 98.4/97.6 | 93.7/92.6 | 44.2/44.1 | 85.8/88.0 | 78.0/81.1 |
|                  | TinyImageNet       | 90.9/91.9 | 98.2/98.3 | 93.3/93.6 | 44.1/61.9 | 66.4/76.1 | 71.9/79.0 |
|                  | LSUN               | 90.9/93.3 | 98.2/98.4 | 93.6/94.3 | 26.7/46.7 | 52.8/66.2 | 63.3/72.4 |
| SVHN (ResNet)    | CIFAR-10           | 98.4/98.3 | 99.3/99.2 | 96.9/96.8 | 95.7/95.2 | 98.4/98.2 | 95.4/95.2 |
|                  | TinyImageNet       | 99.9/99.9 | 99.9/99.9 | 99.1/99.1 | 99.4/99.4 | 99.4/99.4 | 98.9/98.9 |
|                  | LSUN               | 99.9/99.9 | 99.9/99.9 | 99.5/99.5 | 100.0/100.0 | 99.9/99.9 | 99.5/99.5 |

sets: CUB-200-2011 (Wah et al., 2011) vs. mini-ImageNet (Vinyals et al., 2016; Chen et al., 2019; Ravi & Larochelle, 2017), and Omniglot vs. EMNIST (Cohen et al., 2017). For both of the pairs, the models are trained on “base” data, and anomaly detection is evaluated on “novel” data of training and out-of-distribution data. How the data sets are split are explained in Chen et al. (2019). For comparison, we evaluate neural classifiers using the same architectures and cross entropy as a loss function.

5.2. Neural Classifiers

We perform the same experiments as in Lee et al. (2018) and demonstrate that our method is as effective as the original method in most of the cases.

Out-of-distribution Detection Table 3 shows performance of out-of-distribution detection on intermediate features of neural classifiers. “Validation on OOD samples” is the out-of-distribution detectors trained on the corresponding out-of-distribution data, and “Validation on adversarial samples” is evaluation of the robustness, which shows outlier detection performance of detectors trained on adversarial samples generated by FGSM (Goodfellow et al., 2015). In both settings, out-of-distribution detection with our marginal Mahalanobis distance-based confidence score performs as well as the original score by Lee et al. (2018).

Adversarial Examples Detection Table 4 shows adversarial detection performance. Our Mahalanobis distance-based confidence score is as effective as the class conditional method by Lee et al. (2018) in most cases. “Detection of unknown attack” evaluates a detector trained on FGSM, and shows that our confidence score also generalizes well to other types of attacks. However, our model is slightly worse than the original class conditional method for some cases (e.g. CIFAR-10 on DenseNet, CIFAR-100 on ResNet), so some class conditional information may be useful in adversarial examples detection. However, we note that our method marginally outperforms LID (Ma et al., 2018) and also achieves state-of-the-art performance.

5.3. Distance-Based Metric Learning

Table 5 shows out-of-distribution detection performance of the Mahalanobis distance-based confidence score evaluated on distance-based metric learning architectures. We only use the final features, without using feature ensembles nor input pre-processing. Since in-distribution data sets evaluated here have too many labels, we only evaluate our marginal method. For CUB vs. mini-ImageNet, it seems that neural classifiers and metric learning models exhibit similar out-of-distribution behavior on the final features; the Mahalanobis distance outperforms the Euclidean distance. However, metric learning models exhibit unexpected behaviors for Omniglot vs. EMNIST; the detection performance of the Euclidean distance is better on the metric learning models for this pair of data sets. Our experimental results suggest that the intermediate features of distance-based metric learning models do not always have the property that principal components with small explained variance provide informa-
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Table 4. AUROC for adversarial example detection on neural classifiers using LID (Ma et al., 2018), the class conditional Mahalanobis distance-based score by Lee et al. (2018) (Conditional), and our marginal Mahalanobis distance-based score (Marginal). Our confidence score achieves competitive performance when compared to the original method for many cases.

| Model | Dataset | Score | Detection of known attack | Detection of unknown attack |
|-------|---------|-------|---------------------------|----------------------------|
|       |         |       | FGSM | BIM | DeepFool | CW | BIM | DeepFool | CW |
| DenseNet | CIFAR-10 | LID | 98.3 | 99.7 | 85.1 | 80.3 | 94.0 | 70.4 | 68.8 |
|         |         | Conditional | 99.9 | 99.8 | 83.4 | 84.9 | 99.5 | 83.2 | 85.7 |
|         |         | Marginal (ours) | 99.9 | 99.8 | 81.1 | 82.4 | 99.2 | 79.3 | 81.2 |
|         | CIFAR-100 | LID | 99.3 | 98.1 | 69.8 | 89.6 | 78.7 | 68.2 | 68.8 |
|         |         | Conditional | 99.9 | 99.3 | 77.6 | 82.7 | 98.7 | 77.0 | 80.2 |
|         |         | Marginal (ours) | 99.9 | 99.2 | 76.9 | 81.6 | 98.1 | 74.3 | 78.7 |
|         | SVHN | LID | 99.3 | 94.8 | 91.9 | 94.1 | 92.0 | 80.1 | 81.2 |
|         |         | Conditional | 99.9 | 99.3 | 95.1 | 96.5 | 99.2 | 94.2 | 96.4 |
|         |         | Marginal (ours) | 99.9 | 99.0 | 92.2 | 95.0 | 98.8 | 90.2 | 93.4 |
| ResNet | CIFAR-10 | LID | 99.7 | 96.6 | 88.5 | 83.0 | 94.0 | 73.6 | 78.1 |
|         |         | Conditional | 100.0 | 99.6 | 91.4 | 95.9 | 99.0 | 80.6 | 94.3 |
|         |         | Marginal (ours) | 100.0 | 99.6 | 91.0 | 95.8 | 99.5 | 86.2 | 95.6 |
|         | CIFAR-100 | LID | 98.4 | 97.0 | 71.8 | 78.4 | 59.8 | 65.1 | 76.2 |
|         |         | Conditional | 99.8 | 96.7 | 85.3 | 92.0 | 96.4 | 81.9 | 91.1 |
|         |         | Marginal (ours) | 99.8 | 97.7 | 73.5 | 90.4 | 97.1 | 69.8 | 87.6 |
|         | SVHN | LID | 97.9 | 90.6 | 92.2 | 88.3 | 82.2 | 68.5 | 75.1 |
|         |         | Conditional | 99.6 | 97.1 | 95.7 | 92.2 | 95.8 | 73.9 | 87.9 |
|         |         | Marginal (ours) | 99.6 | 97.2 | 95.2 | 91.9 | 95.3 | 70.2 | 86.2 |

Table 5. Marginal Mahalanobis distance-based out-of-distribution detection on distance-based metric learning models. We evaluate Prototypical Networks (ProtoNet), Matching Networks (MatchNet), and ordinary neural classifiers (Classifier). “Conv” and “ResNet” denote Conv-4 and ResNet-10 in Chen et al. (2019). “Maha” and “Eucl” denote the Mahalanobis and Euclidean distance.

| Model | Method | Score | TNR at TPR 95% | AUROC | Detection Accuracy | AUPR in | AUPR out |
|-------|--------|-------|-----------------|-------|--------------------|--------|---------|
| Conv  | (Classifier) | Maha | 98.27 | 80.65 | 75.65 | 31.81 | 96.14 |
|       | (Classifier) | Eucl | 95.77 | 47.48 | 58.83 | 13.37 | 87.62 |
|       | ProtoNet | Maha | 97.80 | 80.34 | 72.84 | 38.66 | 95.63 |
|       | ProtoNet | Eucl | 98.05 | 84.71 | 76.85 | 50.53 | 96.58 |
|       | MatchNet | Maha | 96.02 | 57.47 | 60.04 | 16.20 | 89.93 |
|       | MatchNet | Eucl | 98.35 | 72.43 | 75.09 | 22.46 | 94.73 |
| Conv  | (Classifier) | Maha | 9.34 | 60.21 | 75.69 | 95.11 | 11.1 |
|       | (Classifier) | Eucl | 8.57 | 52.73 | 52.38 | 93.62 | 8.37 |
|       | ProtoNet | Maha | 32.93 | 61.97 | 58.92 | 86.15 | 26.97 |
|       | ProtoNet | Eucl | 16.22 | 55.68 | 54.94 | 82.59 | 21.95 |
|       | MatchNet | Maha | 25.31 | 64.07 | 61.69 | 88.12 | 26.21 |
|       | MatchNet | Eucl | 12.50 | 53.46 | 54.17 | 83.83 | 20.23 |
| ResNet | (Classifier) | Maha | 14.10 | 51.60 | 54.20 | 83.29 | 19.43 |
|       | (Classifier) | Eucl | 20.87 | 50.50 | 51.01 | 80.93 | 20.31 |
|       | ProtoNet | Maha | 21.07 | 61.39 | 59.99 | 87.35 | 24.85 |
|       | ProtoNet | Eucl | 19.58 | 46.49 | 50.10 | 77.74 | 18.83 |
|       | MatchNet | Maha | 35.51 | 67.59 | 63.67 | 90.05 | 29.31 |
|       | MatchNet | Eucl | 21.36 | 52.07 | 52.43 | 82.41 | 20.86 |

for anomaly detection. This observation suggests that the Mahalanobis distance-based confidence score utilizes the unique property of ordinary neural classifiers, and its performance may depend on model architecture along with the choice of in-distribution and out-of-distribution data.

Furthermore, for CUB vs. ImageNet, Table 5 shows that detection performance on the neural classifier and Matching Networks is influenced by model architecture. For neural classifiers, Table 3 and 4 also suggest sensitivity of detection performance to model architecture choice. In conclusion, caution is required when applying the Mahalanobis distance-based confidence score to new architectures or data sets.

6. Conclusion

The Mahalanobis distance-based confidence score, an anomaly detection method proposed by Lee et al. (2018), achieves state-of-the-art performance. This paper is the first
work analyzing why this method can detect anomalous inputs effectively while imposing the implausible assumption that class conditional distributions have tied covariance. We demonstrate that the subspace spanned by principal components with small explained variance contain information critical for anomaly detection, and our method that is not using class information achieves competitive performance with the original method. This observation suggests that it does not use information that is critical for the original classification task although the method by Lee et al. (2018) scores the prediction confidence for the original classification task, so it reveals that the reason for its effectiveness has been misunderstood. We also reveal misunderstandings in input pre-processing, a technique that significantly improves the performance and the applicability of the method. This work provides critical insight into the new standard anomaly detection method and the behavior of neural networks towards anomalous inputs.

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A. Input Pre-Processing

We provide further experimental results analyzing input pre-processing by Lee et al. (2018). Figure 5 to 22 show that input pre-processing does not always improve detection performance. When L1 norms of input pre-processing for out-of-distribution inputs on the final features are sufficiently larger than these for in-distribution inputs, detection performance will be improved as mentioned in the main part (Figure 5, 8, 17). However, in some cases, input pre-processing does not improve performance as it does not make the Mahalanobis distance of out-of-distribution inputs sufficiently large. When L1 norms of in-distribution inputs are larger than these of out-of-distribution inputs, i.e. the situation corresponding to what is discussed in Liang et al. (2018), detection performance does not improve (Figure 15, 16, 18, 19). To sum up, our experiments show that the effect of input pre-processing depends on the network architecture and choice of data set.

B. Mahalanobis Distance on Autoencoders

Settings We evaluate autoencoders trained on MNIST (LeCun et al., 1998) and CIFAR-10. We use Fashion-MNIST (Xiao et al., 2017) and SVHN as out-of-distribution data, respectively. Our implementation is based on a code from the Keras blog 3. We use training data from MNIST and CIFAR-10 to calculate parameters for the Mahalanobis distances, and evaluate out-of-distribution detectors on test data from in-distribution and out-of-distribution data sets. In this experiment, we only use the final features, and do not apply input processing nor feature ensemble.

Experiments Table 6 shows that the Mahalanobis distance-based confidence score effectively detects out-of-distribution inputs on the representation space of the autoencoders in our settings. For CIFAR-10 vs SVHN, even the Euclidean distance is enough to effectively detect out-of-distribution data. For MNIST vs. Fashion-MNIST, intermediate features of autoencoders exhibit similar properties to those of neural classifiers. The marginal Mahalanobis distance achieves almost the same performance as the original Mahalanobis distance, even when the partial Mahalanobis distance using principal components with small explained variance is used. The performance of the above three methods outperforms the Euclidean distance and the partial Mahalanobis distance using principal components with large explained variance, which is consistent with the behavior of features of neural classifiers. However, as these confidence scores are sensitive to the choice of architecture and data set for metric learning models, caution is needed when applying the method to other architectures and data sets.

| Method  | type  | in-dist | out-dist | TNR at TPR 95% | AUROC | Detection Accuracy | AUPR in | AUPR out |
|---------|-------|---------|----------|----------------|--------|--------------------|--------|---------|
| Maha    | Class | MNIST   | Fashion  | 95.15          | 99.62  | 97.23              | 99.67  | 99.59   |
| Maha    | Marg  | MNIST   | Fashion  | 95.07          | 99.55  | 96.91              | 99.52  | 99.60   |
| Maha(20-128) | Marg  | MNIST   | Fashion  | 95.08          | 99.48  | 96.54              | 99.44  | 99.54   |
| Maha(1-20) | Marg  | MNIST   | Fashion  | 94.53          | 97.85  | 92.62              | 98.21  | 97.30   |
| Eucl    | Class | MNIST   | Fashion  | 94.24          | 97.05  | 90.96              | 97.39  | 96.87   |
| Maha    | Marg  | CIFAR-10| SVHN     | 27.75          | 100.0  | 100.0              | 100.0  | 100.0   |
| Maha(20-128) | Marg  | CIFAR-10| SVHN     | 27.75          | 100.0  | 100.0              | 100.0  | 100.0   |
| Eucl    | Marg  | CIFAR-10| SVHN     | 88.68          | 100.0  | 100.0              | 100.0  | 100.0   |

3https://blog.keras.io/building-autoencoders-in-keras.html
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Figure 5. ResNet CIFAR-10 SVHN

Figure 6. ResNet CIFAR-10 ImageNet

Figure 7. ResNet CIFAR-10 LSUN

Figure 8. ResNet CIFAR-100 SVHN
Why is the Mahalanobis Distance Effective for Anomaly Detection?

Figure 9. ResNet CIFAR-100 ImageNet

Figure 10. ResNet CIFAR-100 LSUN

Figure 11. ResNet SVHN CIFAR-10

Figure 12. ResNet SVHN ImageNet
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Figure 13. ResNet SVHN LSUN

Figure 14. DenseNet CIFAR-10 SVHN

Figure 15. DenseNet CIFAR-10 ImageNet

Figure 16. DenseNet CIFAR-10 LSUN
Why is the Mahalanobis Distance Effective for Anomaly Detection?

Figure 17. DenseNet CIFAR-100 SVHN

Figure 18. DenseNet CIFAR-100 ImageNet

Figure 19. DenseNet CIFAR-100 LSUN

Figure 20. DenseNet SVHN CIFAR-10
Why is the Mahalanobis Distance Effective for Anomaly Detection?

Figure 21. DenseNet SVHN ImageNet

Figure 22. DenseNet SVHN LSUN