META-LEARNING FOR OUT-OF-DISTRIBUTION DETECTION VIA DENSITY ESTIMATION IN LATENT SPACE

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ABSTRACT
Many neural network-based out-of-distribution (OoD) detection methods have been proposed. However, they require many training data for each target task. We propose a simple yet effective meta-learning method to detect OoD with small in-distribution data in a target task. With the proposed method, the OoD detection is performed by density estimation in a latent space. A neural network shared among all tasks is used to flexibly map instances in the original space to the latent space. The neural network is meta-learned such that the expected OoD detection performance is improved by using various tasks that are different from the target tasks. This meta-learning procedure enables us to obtain appropriate representations in the latent space for OoD detection. For density estimation, we use a Gaussian mixture model (GMM) with full covariance for each class. We can adapt the GMM parameters to in-distribution data in each task in a closed form by maximizing the likelihood. Since the closed form solution is differentiable, we can meta-learn the neural network efficiently with a stochastic gradient descent method by incorporating the solution into the meta-learning objective function. In experiments using six datasets, we demonstrate that the proposed method achieves better performance than existing meta-learning and OoD detection methods.

1 Introduction
Out-of-Distribution (OoD) detection is an important machine learning problem that finds instances that do not belong to training classes [23]. Deep learning models tend to make incorrect predictions with high confidence for instances from unseen classes [39, 27]. By OoD detection, we can safely deploy machine learning models in the open world, where new classes can emerge. OoD detection can also be beneficial for ensuring the quality of the collected data, and finding instances with unusual behavior for data analysts [44]. Many neural network-based OoD detection methods have been proposed [28, 33, 3, 22, 24, 6, 43, 9]. However, these methods require a large number of data for training. In some real-world applications, enough data might be unavailable in target tasks. For example, it is important to detect manufacturing failures that are not categorized in existing failure classes in each factory for improving productivity, but many data are not accumulated in newly operated factories.

We propose a simple yet effective method for improving the OoD detection performance on unseen target tasks by meta-learning from data in tasks different from the target tasks. Even when enough data are unavailable for a newly operated factory, many data for different factories would be available. For the meta-training data, instances with class labels from various tasks are assumed to be given, where classes are different across tasks. For a target task, a small number of instances with class labels are given as in-distribution (ID) data. We want to identify whether test instances are ID or OoD for the target task.

With the proposed method, OoD scores are calculated by density estimation in a latent space. Density estimation has been used for OoD detection [4]. However, ID data can have low likelihoods in extremely high dimensions, and density estimation in the original high dimensional space sometimes fails to detect OoD [7, 29, 13]. To avoid such problems, the proposed method embeds instances into a latent space by a neural network that is shared among all tasks.
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Figure 1: Meta-learning step for the proposed method. For the meta-training data, we are given multiple tasks with different classes. 1) Randomly sample support instances and ID query instances from a task, and sample OoD query instances from another task. 2) Embed sampled instances by a neural network in a latent space. 3) Estimate task-specific Gaussian mixture model parameters based on the maximum likelihood. 4) Calculate the density of the query instances using the estimated GMM parameters. 5) Evaluate the OoD score based on AUC. 6) Backpropagate the AUC to update the neural network parameters.

Meta-learning is formulated as a bilevel optimization problem. In the inner optimization problem, task-specific parameters are adapted to the given task-specific data. In the outer optimization problem, common parameters shared across all tasks are meta-learned to improve the expected test performance when the task-specific parameters adapted in the inner optimization are used. With the proposed method, the inner optimization problem corresponds to fitting a density model to the task-specific data in a latent space. We use a Gaussian mixture model (GMM) for the density model. The GMM parameters, which are the class probability, mean, and covariance for each class, are adapted in a closed form by maximizing the likelihood. In the outer optimization problem, we meta-learns the neural network such that the OoD detection performance improves when the density is estimated with the adapted GMM parameters. By incorporating the closed form solution of the inner optimization problem into the outer optimization problem, we can solve the bilevel optimization problem efficiently by a stochastic gradient descent method.

For each meta-learning step, instances in the meta-training data are randomly selected for ID, and instances in classes different from the ID instances are randomly selected for OoD. By generating ID and OoD data in this way, we can evaluate the OoD detection performance using the meta-training data, which is required for the objective function in the outer optimization problem. The performance is evaluated by the area under the ROC curve (AUC), which is often used in the existing literature [23, 41, 44]. Although data in target tasks are labeled with their classes, only ID instances are given as the task-specific data. Therefore, the inner optimization needs to be performed without OoD instances. The proposed method enables this by defining the inner optimization as density estimation using ID instances. Figure 1 illustrates a meta-learning step of the proposed method.

The main contributions of this paper are as follows:

1. We propose a meta-learning method for OoD detection that uses labeled data in various tasks to improve the performance on unseen target tasks that consist of unlabeled data.
2. The proposed method enables an efficient bilevel optimization by modeling the inner optimization with the maximum likelihood of a Gaussian mixture model in a latent space, which gives a closed-form solution for the adaptation to each task.
3. We confirm that the proposed method achieves better performance than existing methods.
The remainder of this paper is organized as follows. In Section 2, we briefly review related work. In Section 3, we formulate our problem, and present our meta-learning method for OoD detection. In Section 4, we demonstrate that the proposed method achieves better performance than existing meta-learning and OoD detection methods. Finally, we present concluding remarks and a discussion of future work in Section 5.

2 Related work

Many meta-learning methods have been proposed [46, 2, 10, 40, 37, 22]. Meta-learning methods learn how to learn from a small amount of labeled data in various tasks, and use the learned knowledge in unseen tasks. However, most of these methods are not designed for OoD detection, and are inapplicable to our problem. A meta-learning method for OoD detection based on model-agnostic meta-learning (MAML) [10] has been proposed [16]. For the inner optimization, MAML requires costly back-propagation through iterative gradient descent steps. On the other hand, the proposed method achieves an efficient inner optimization in a closed form based on density estimation with GMMs. The closed form inner optimization for meta-learning has been successfully used in various methods [3, 14, 37, 11, 12]. However, they define the inner optimization problem as regression or classification, but not as density estimation. An OoD detection method based on Mahalanobis distance assumes a GMM in a latent space [21]. However, it uses a covariance shared among all classes, which has lower expressive power than class-specific covariances. In addition, it requires many training data since it is not a meta-learning method. Anomaly detection is related to OoD detection. Anomaly detection methods usually do not use class labels [5, 19, 11, 45, 35], where class labels indicate categories that ID instances belong to and they are different from ID/OoD labels. On the other hand, the proposed method uses class labels for effectively estimating the density. The better performance of the proposed method compared with these existing methods are demonstrated in our experiments in Section 4.

3 Proposed method

3.1 Problem formulation

In a meta-training phase, meta-training data \( \mathcal{D} = \{(x_{tn}, y_{tn})\}_{n=1}^{N_t} \) are given, where \( T \) is the number of tasks, \( N_t \) is the number of labeled instances in the \( t \)th task, \( x_{tn} \in \mathcal{X} \) is the feature of the \( n \)th instance, \( y_{tn} \in \{c_1, \ldots, c_{K_t}\} \) is its class label, \( c_{tk} \) is the \( k \)th class, and \( K_t \) is the number of classes. In a meta-test phase, labeled support set \( \mathcal{S} = \{(x_n, y_n)\}_{n=1}^{N_s} \) is given in a target task that are different from the training tasks, where \( y_n \in \{c_1, \ldots, c_K\} \), \( K \) is the number of classes in the support set, and the classes in the target task do not overlap with those in the training tasks. Our aim is to identify whether unlabeled instances \( \{x\} \) belong to the classes in the support set \( \{c_1, \ldots, c_K\} \) (in-distribution) or not (out-of-distribution). We assume that feature space \( \mathcal{X} \) is the same across all tasks.

3.2 Model

In this subsection, we present our model to output task-specific OoD score \( u(x \mid \mathcal{S}; \Phi) \) of unlabeled instance \( x \) given superset \( \mathcal{S} = \{(x_n, y_n)\}_{n=1}^{N_s} \), where \( \Phi \) is the set of the common model parameters shared across tasks.

The proposed model uses the following negative log density in a latent space for the OoD score,

\[
-u(x \mid \mathcal{S}; \Phi) = - \log p \left( f(x; \phi) \mid \hat{\Theta}(\mathcal{S}; \Phi) \right),
\]

where \( p \) is the probability density function in the latent space, \( f : \mathcal{X} \rightarrow \mathbb{R}^D \) is a neural network that maps an instance from the original space to the \( D \)-dimensional latent space, \( \phi \in \Phi \) is the neural network parameters that are shared across tasks, and \( \hat{\Theta}(\mathcal{S}; \Phi) \) is the set of the task-specific parameters of the probability density function adapted to support set \( \mathcal{S} \). The negative log likelihood is an natural OoD score since instances with the low probability density can be seen OoD, and it has been used for OoD detection [4]. With neural network \( f \), we can find a latent space that is appropriate for detecting OoD even when the density estimation in the original space does not perform well on OoD detection.

The probability density function parameters \( \Theta \) is adapted to support set \( \mathcal{S} \) by maximizing the log likelihood,

\[
\hat{\Theta}(\mathcal{S}; \Phi) = \arg \max_{\Theta} \log p(\mathcal{S} \mid \Theta; \Phi) = \arg \max_{\Theta} \sum_{(x, y) \in \mathcal{S}} \log p(x \mid y, \Theta; \Phi).
\]
The proposed model assumes a Gaussian mixture model (GMM) in the latent space,

\[
p(f(x; \phi) \mid \Theta) = \sum_{k=1}^{K} \gamma_k \mathcal{N}(f(x; \phi) \mid \mu_k, \Sigma_k)
\]

\[
= \sum_{k=1}^{K} \gamma_k (2\pi)^{-\frac{D}{2}} |\Sigma_k|^{-\frac{1}{2}} \exp \left(-\frac{1}{2}(f(x; \phi) - \mu_k)^T \Sigma_k^{-1}(f(x; \phi) - \mu_k)\right),
\]

where \(\gamma_k \in [0, 1]\) is the class probability of the \(k\)th class, \(\mathcal{N}(\cdot \mid \mu, \Sigma)\) is the Gaussian distribution with mean \(\mu \in \mathbb{R}^D\) and covariance \(\Sigma \in \mathbb{R}^{D \times D}\), and \(\Theta = \{\gamma_k, \mu_k, \Sigma_k\}_{k=1}^{K}\) is the set of the task-specific GMM parameters. Since the class label is given for each support instance, we can obtain the adapted parameters in a closed form using the GMM by solving Eq. (4) as follows,

\[
\hat{\gamma}_k(S) = \frac{1}{|S_k|}, \quad \hat{\mu}_k(S) = \frac{1}{|S_k|} \sum_{x \in S_k} f(x; \phi),
\]

\[
\hat{\Sigma}_k(S) = \frac{1}{|S_k|} \left( \sum_{x \in S_k} (f(x; \phi) - \hat{\mu}_k(S))(f(x; \phi) - \hat{\mu}_k(S))^T + \beta I \right),
\]

where \(S_k = \{x \mid (x, y) \in S, y = k\}\) is the set of instances with label \(k\) in the support set, \(|S_k|\) is its size, \(\beta \in \mathbb{R}_{>0}\) is the parameter, and \(\Theta(S; \Phi) = \{\hat{\gamma}_k(S), \hat{\mu}_k(S), \hat{\Sigma}_k(S)\}_{k=1}^{K}\). By parameter \(\beta\), the covariance is regularized, and is guaranteed to be positive definite, which is necessary to compute the inverse of the covariance stably. The inverse is required to calculate the likelihood in Eq. (3).

### 3.3 Meta-training

The common parameters to be meta-learned are \(\Phi = \{\phi, \beta\}\), where \(\phi\) is the set of the neural network parameters, and \(\beta\) is the regularization parameter for covariance estimation. Let \(Q_1 = \{x_1^n\}_{n=1}^{N_1}\) be a query set of instances that are ID of the support set, and \(Q_O = \{x_{O,n}\}_{n=1}^{N_O}\) be a query set of instances that are OoD of the support set. Each meta-training task contains support set \(S\) and query set \(Q = \{Q_1, Q_O\}\). We want to improve the expected AUC over tasks,

\[
\Phi = \arg \max_{\Phi} \mathbb{E}_{t \in \{1, \ldots, T\}} \left[ \mathbb{E}_{S, \hat{Q} \subset \mathcal{D}_t} \left[ \text{AUC}(Q \mid \hat{\Theta}(S; \Phi), \Phi) \right] \right],
\]

where \(\mathbb{E}\) represents the expectation, and \(\text{AUC}(Q \mid \hat{\Theta}, \Phi)\) is the AUC on query set \(Q\) calculated using task-specific parameters \(\hat{\Theta}\) and common parameters \(\Phi\), and \(\hat{\Theta}(S; \Phi)\) is a task-specific parameters adapted to support set \(S\) by maximizing the log likelihood in Eq. (2). It is a bilevel optimization problem where Eq. (2) is the inner problem, and Eq. (5) is the outer problem. Since the inner problem is solved in a closed form as shown in Eq. (4), the bilevel optimization can be efficiently solved by incorporating the inner solution into the outer problem. The objective functions of the inner and outer problems are the likelihood and AUC, respectively, and they are different. It is because while only ID data are given in the inner problem, which is the same setting with the meta-test phase, both of the ID and OoD data are given in the outer problem.

The AUC is calculated by the ratio that the OoD score of the OoD query instances is higher than that of the ID query instances,

\[
\text{AUC}(Q \mid \hat{\Theta}(S; \Phi), \Phi) = \frac{1}{N_O N_1} \sum_{x^O \in Q_O} \sum_{x^I \in Q_1} I \left( u(x^O \mid S; \Phi) > u(x^I \mid S; \Phi) \right),
\]

where \(I\) is the indicator function, i.e., \(I(A) = 1\) if \(A\) is true, and \(I(A) = 0\) otherwise. To make the AUC differentiable, we use the following smooth approximation of the AUC,

\[
\widehat{\text{AUC}}(Q \mid \hat{\Theta}(S; \Phi), \Phi) = \frac{1}{N_O N_1} \sum_{x^O \in Q_O} \sum_{x^I \in Q_1} \sigma \left( u(x^O \mid S; \Phi) - u(x^I \mid S; \Phi) \right),
\]

where \(\sigma(x) = \frac{1}{1 + \exp(-x)}\) is the sigmoid function which is used for the smooth approximation of the indicator function [15].

Algorithm 1 shows the meta-learning procedures of the proposed model. The expectation in Eq. (5) is calculated by the Monte Carlo method, where support and query sets are randomly sampled from the meta-training data in Lines 3–6.

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**Algorithm 1:** Meta-learning for Out-of-Distribution Detection via Density Estimation in Latent Space

1. **Meta-training**
   - **Input:** \(Q_1, Q_O, S\)
   - **Output:** \(\Phi\)
   - **Initialization:** \(\Theta = \{\gamma_k, \mu_k, \Sigma_k\}_{k=1}^{K}\)
   - **for** \(t \in \{1, \ldots, T\}\) **do**
     - \(\Theta_t = \hat{\Theta}(S; \Phi)\)
     - \(\Phi_t = \arg \max_{\Phi} \mathbb{E}_{S, \hat{Q} \subset \mathcal{D}_t} \left[ \text{AUC}(Q \mid \Theta_t, \Phi) \right]\)
   - **end for**

2. **Meta-test**
   - **Input:** \(Q_1, Q_O\)
   - **for** \(t \in \{1, \ldots, T\}\) **do**
     - \(\Phi_t = \text{AUC}(Q_1, Q_O)\)
   - **end for**

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4
When the latent space dimensionality is larger than the number of instances, \( D > N \) with uniform class probability, we can reduce the complexity to \( O(\sum_k N_k^2 D) \). Therefore, when class probability \( N \) is the number of support instances per class, and \( D \) is the latent space dimensionality. The complexity to calculate the OoD score is \( O(\sum_k N_k^3) \), where the complexity of the inverse of the covariance matrix is the cubic of the matrix size. When the latent space dimensionality is larger than the number of instances, \( D > N \), we can reduce the complexity to \( O(\sum_k N_k^3) \) using the Woodbury formula \([32]\). The complexity to calculate the smooth AUC is \( O(\sum_k N_k N_t) \) since it is a summation over \( N_t \) OoD query instances and \( N_t \) ID query instances.

### 3.4 Relation to existing methods

A OoD detection method based on Mahalanobis distance \([21]\) assumes a GMM with a full covariance matrix shared by all classes,

\[
p_M(f(\mathbf{x}; \phi) \mid \Theta) = \sum_{k=1}^{K} \gamma_k N(\mathbf{x}; \mu_k, \Sigma).
\]

The negative OoD score is calculated by the minimum of the Mahalanobis distance over classes,

\[
u_M(\mathbf{x} \mid S; \Phi) = \min_k [(f(\mathbf{x}; \phi) - \hat{\mu_k})^\top \Sigma_{\phi}^{-1} (f(\mathbf{x}; \phi) - \hat{\mu_k})]
\]

\[= \max_k \log N(f(\mathbf{x}; \phi) \mid \hat{\mu_k}, \Sigma_{\phi})
\]

\[
\approx - \log \sum_k N(f(\mathbf{x}; \phi) \mid \hat{\mu_k}, \Sigma_{\phi}),
\]

where we used the fact that the LogSumExp is a smooth approximation of the maximum, \( \log \sum_k \exp(\cdot) \approx \max_k \cdot \). Therefore, when class probability \( \gamma_k \) are the same for all classes, the Mahalanobis distance-based method can be seen that it uses log likelihood in a latent space as the OoD score as with the proposed method.

The prototypical network is a meta-learning method for classification \([31]\), and it assumes the following Gaussian mixture model with a spherical covariance in a latent space,

\[
p_T(f(\mathbf{x}; \phi) \mid \Theta) = \sum_{k=1}^{K} \gamma_k N(f(\mathbf{x}; \phi) \mid \mu_k, \tau I),
\]

with uniform class probability \( \gamma_k = \frac{1}{K} \). Mean vectors \( \{\mu_k\}_{k=1}^{K} \) are obtained by maximizing the log likelihood of the support set. The proposed model can express more complicated distributions by adapting a full covariance matrix for each class. When parameter \( \beta \) in Eq. \( (\ref{eq:mix_model}) \) is large, the proposed model becomes similar to a GMM with a fixed spherical covariance as with the prototypical network. By meta-learning \( \beta \) such that the OoD detection performance is improved, the proposed method can estimate the density flexibly while avoiding overfitting. Different from the proposed method, the objective function of the outer optimization problem of the prototypical network is the classification cross-entropy loss, where the posterior class probability is calculated by

\[
p(k \mid \mathbf{x}) = \frac{\exp(-\frac{1}{2\tau} \| f(\mathbf{x}; \phi) - \hat{\mu_k}(S) \|^2)}{\sum_{k'=1}^{K} \exp(-\frac{1}{2\tau} \| f(\mathbf{x}; \phi) - \hat{\mu_{k'}}(S) \|^2)}.
\]
With classifier-based OoD detection methods [23], the negative OoD score is calculated by the maximum of the posterior class probability,

$$u_P(x \mid S; \Phi) = - \max_k p(k \mid x) \propto - \max_k N(f(x; \phi) \mid \mu_k, \tau I),$$  

(12)

which is also related to the density estimation in a latent space.

Temperature scaling is used for OoD detection [23], where $\tau$ is the temperature in Eq. (11), and the temperature scaling controls the covariance. Since the proposed method adapts the covariance for each class to the support set, the proposed method is related to the temperature scaling that adapt to each task.

4 Experiments

4.1 Data

We evaluated the proposed method with the following six datasets: Omniglot, Miniimagenet, CIFAR10, SVHN, Patent, and Dmoz.

The Omniglot dataset [20] consisted of hand-written images of 964 characters from 50 alphabets (real and fictional). There were 20 images for each character category. Each image was represented by gray-scale with $28 \times 28$ pixels. The number of instances, attributes, and categories were 19280, 784, and 964, respectively.

The Miniimagenet dataset consisted of images from 100 categories [40]. Each image was represented by RGB with $84 \times 84$ pixels. The number of instances, attributes, and categories were 60000, 21168, and 100, respectively.

The CIFAR10 dataset consisted of images from 10 categories [18]. Each image was represented by RGB with $32 \times 32$ pixels. The number of instances, attributes, and categories were 60000, 3072, and 10, respectively.

The SVHN dataset consisted of digit images obtained from house numbers in Google street view [30]. Each image was represented by RGB with $32 \times 32$ pixels. The number of instances, attributes, and categories were 73257, 3072, and 10, respectively.

The Patent dataset consisted of patents published in Japan from January to March in 2004, which were categorized by International Patent Classification. Each patent was represented by bag-of-words. We omitted words that occurred in fewer than 100 patents, omitted patents with fewer than 100 unique words, and omitted categories with fewer than ten patents. The number of instances, attributes, and categories were 5714, 3201, and 285, respectively.

The Dmoz dataset consisted of webpages crawled in 2006 from the Open Directory Project [25]. Each webpage was categorized in a web directory, and represented by bag-of-words. We omitted words that occurred in fewer than 300 webpages, omitted webpages with fewer than 300 unique words, and omitted categories with fewer than ten webpages. The number of instances, attributes, and categories were 15159, 17659, and 354, respectively.

For each of the Omniglot, Miniimagenet, Patent, and Dmoz datasets, we randomly used 60% of the categories for training, 20% for validation, and the remaining categories for testing. For each of the CIFAR10 and SVHN datasets, since their number of classes was small, the Miniimagenet dataset was used for the training and validation, where we rescaled images in the Miniimagenet dataset to $32 \times 32$ pixels. For the test of the CIFAR10 dataset, CIFAR10 images were used for the ID, and SVHN images were used for the OoD. For the test of the SVHN dataset, SVHN images were used for the ID, and CIFAR10 images were used for the OoD. It is known that when a neural network-based density model is trained on the CIFAR10 images, the likelihood of the SVHN images is likely to be higher than that of the CIFAR10 images [29]. For all datasets, we generated 64 tasks for each validation and test data. For each task in the validation and test data, we first randomly selected five categories for ID, and one category for OoD. Then, we randomly selected five support instances from each of the ID categories, and five query instances from each of the ID and OoD categories. We performed five experiments with different data splits for each dataset.

4.2 Comparing methods

We compared our proposed method (Ours) with ablation of the proposed method (Ours-C), three types of prototypical networks [37] (Proto-C, Proto-A, and Proto-O), three types of model-agnostic meta-learning [10] (MAML-C, MAML-A, and MAML-O), OoD-MAML [16], learnable class boundary networks [41] (LCBO), Mahalanobis distance-based method [21] (Mahalanobis), deep support vector data description (SVDD) [34], density estimation with a single Gaussian model (Gaussian), and kernel density estimation (KDE) in a latent space. All methods use neural networks to...
map instances from the original space to a latent space. ‘C’ in the method names indicates that the method is meta-learned by minimizing the expected test classification cross-entropy loss, ‘A’ indicates that the method is meta-learned by maximizing the AUC of OoD detection, and ‘O’ indicates that the method is based on out-of-distribution detector for neural networks (ODIN) [23].

The methods based on prototypical networks (Proto-C, Proto-A, and Proto-O) assume a Gaussian mixture model with a unit spherical covariance in a latent space, and the class probability is calculated based on the Bayes rule. The methods based on model-agnostic meta-learning [10] (MAML-C, MAML-A, and MAML-O) model the class probability by a softmaxed linear projection from the latent space. With the methods based on ODIN (Proto-O and MAML-O), the temperature of the class probability is meta-learned, and small perturbations are added to the input to the direction that maximizes the maximum class probability. The neural network is meta-learned by minimizing the expected test classification cross-entropy loss. With prototypical network-based and MAML-based methods, the negative OoD score is calculated by the likelihood in the latent space. Except for Ours-C, Proto-C, MAML-C, Proto-O, and MAML-O, the negative OoD score is calculated by the minimum Mahalanobis distance to the class mean in the latent space. With Gaussian and KDE, the OoD score is modeled by a neural network that takes the mean for each class and the instance in the latent space as input. With Mahalanobis, SVDD, Gaussian, and KDE do not use class label information in the support set. With SVDD [34], the OoD score is calculated by the distance from the mean of the support instances in the latent space. With Gaussian and KDE, the OoD score is calculated based on the Bayes rule. The methods learned by minimizing the expected test classification cross-entropy loss, ‘A’ indicates that the method is meta-learned by maximizing the AUC of OoD detection.

### Table 1: Average test AUC for OoD detection and its standard error. Values in bold are not statistically significantly different at the 5% level from the best performing method in each column according to a paired t-test.

| Method       | Omniglot | Minimagenet | CIFAR10 | SVHN  | Patent | Dmoz |
|--------------|----------|-------------|---------|-------|--------|------|
| Ours         | 0.992±0.001 | 0.673±0.005 | 0.619±0.017 | 0.989±0.001 | 0.873±0.006 | 0.828±0.005 |
| Ours-C       | 0.999±0.001 | 0.621±0.006 | 0.471±0.034 | 0.989±0.000 | 0.824±0.009 | 0.785±0.006 |
| Proto-C      | 0.888±0.007 | 0.577±0.006 | 0.565±0.012 | 0.369±0.008 | 0.737±0.009 | 0.705±0.006 |
| Proto-A      | 0.980±0.002 | 0.185±0.014 | 0.351±0.022 | 0.274±0.034 | 0.827±0.010 | 0.783±0.006 |
| Proto-O      | 0.768±0.012 | 0.567±0.005 | 0.799±0.010 | 0.199±0.013 | 0.163±0.012 | 0.072±0.005 |
| MAML-C       | 0.935±0.004 | 0.592±0.003 | 0.605±0.007 | 0.350±0.013 | 0.623±0.010 | 0.563±0.005 |
| MAML-A       | 0.521±0.009 | 0.498±0.006 | 0.636±0.022 | 0.309±0.040 | 0.487±0.014 | 0.464±0.005 |
| MAML-O       | 0.498±0.011 | 0.504±0.005 | 0.634±0.023 | 0.466±0.010 | 0.511±0.008 | 0.003±0.001 |
| OoD-MAML     | 0.982±0.003 | 0.672±0.003 | 0.669±0.025 | 0.656±0.024 | 0.810±0.006 | 0.767±0.007 |
| LCBO         | 0.559±0.005 | 0.522±0.007 | 0.481±0.012 | 0.541±0.032 | 0.573±0.008 | 0.564±0.006 |
| Mahalanobis  | 0.989±0.002 | 0.520±0.006 | 0.623±0.011 | 0.988±0.001 | 0.875±0.007 | 0.826±0.007 |
| SVDD         | 0.832±0.003 | 0.528±0.003 | 0.462±0.033 | 0.718±0.050 | 0.693±0.009 | 0.619±0.005 |
| Gaussian     | 0.989±0.000 | 0.539±0.002 | 0.626±0.011 | 0.984±0.002 | 0.878±0.007 | 0.828±0.007 |
| KDE          | 0.858±0.006 | 0.511±0.015 | 0.421±0.029 | 0.706±0.032 | 0.733±0.008 | 0.655±0.016 |

#### 4.3 Setting

In image datasets (Omniglot, Minimagenet, CIFAR10, and SVHN), we used a four-layered convolutional neural network of filter size 32, kernel size three, and padding size one for $f$ with all methods. In text datasets (Patent and Dmoz), we used a three-layered feed-forward neural network with 256 hidden and output units for $f$. The instances in a latent space were normalized by dividing by the standard deviation of the support set. For the activation function, we used rectified linear unit $\text{ReLU}(x) = \max(0, x)$. We optimized using Adam [17] with learning rate $10^{-3}$, and dropout rate $10^{-1}$ [38]. For MAML-based method, we used three inner epochs. The validation data were used for early stopping, for which the maximum number of training epochs was 5,000. Our implementation was based on PyTorch [31].

#### 4.4 Results

Table 1 shows the test AUC. Our proposed method achieved high AUC with all datasets. With the CIFAR10 dataset, the AUC by the proposed method was lower than that by Proto-O. However, the AUC by Proto-O with the SVHN dataset was very low. It indicates that Proto-O estimated that the CIFAR10 images were ID and the SVHN images were OoD by meta-learning with the Minimagenet dataset. By meta-learning a neural network for density estimation in a latent space, the proposed method achieves a relatively high AUC on both of the CIFAR10 and SVHN datasets.
The proposed method meta-trained by maximizing the OoD detection performance (Ours) was better than that by minimizing the classification loss (Ours-C). This result indicates that the directly maximizing the OoD detection performance is important.

The prototypical network-based methods performed worse than the proposed method. This result demonstrates the effectiveness of density estimation by full covariance GMMs in a latent space. The MAML-based methods adapt the whole neural network to the support set. On the other hand, the proposed method adapts only a GMM in a latent space to the support set. The better performance of the proposed method than the MAML-based methods indicates that the GMM in a latent space is effective for OoD detection when the number of instances in the support set is small. OoD-MAML improved the AUC compared with the other MAML-based methods by generating fake OoD instances. However, since it is difficult to generate a wide variety of OoD instances for each task, it was worse than the proposed method. The proposed method detects OoD by density estimation using only ID instances without OoD instances, and it does not need to generate fake OoD instances.

With LCBO, the OoD score is calculated by a neural network that takes the support set as input. Therefore, the OoD score of the support set is not necessarily high. In contrast, with the proposed method, the density-based OoD score of the support set is high since we maximize the likelihood of the support set. Therefore, the proposed method can flexibly adapt to a given support set even when it does not appear in the meta-training dataset, and it led to better performance of the proposed method. While Mahalanobis achieved good performance, it was worse than the proposed method on the Omniglot and Miniimagenet datasets. This result indicates the effectiveness to model class-specific full covariances in GMMs. The AUC by the methods that do not use class label information was lower than the proposed method. This result shows the usefulness of the class label information for OoD detection.

Figure 2 shows a visualization of density estimation in a two-dimensional latent space by the proposed method on the Omniglot dataset. We additionally used a three-layered feed-forward neural network for the two-dimensional embedding after the convolutional neural network. By the neural network, ID instances were embedded in a high-density area, and OoD instances were embedded in a low-density area. By the GMMs, the task-specific density function was modeled flexibly in the latent space depending on the support set.

Figure 3 shows the test AUC with different numbers of meta-training classes by the proposed method on the Omniglot dataset. The test AUC increased as the number of meta-training classes increased. This result indicates that the proposed method can increase the performance by collecting meta-training data from many classes.

Figure 4 shows the test AUC with different latent space dimensionality by the proposed method on the Omniglot dataset. When the latent space dimensionality was small, the test AUC was low. It is because in a low-dimensional space representing complicated instances is difficult, and the density estimated with GMMs does not have enough expressive power.

Table 2 shows the test classification accuracy of class labels. Since the proposed method (Ours) is not meta-learned to improve the classification performance, it was worse than the proposed method that is meta-learned by minimizing the classification loss (Ours-C). Since we focus on improving OoD detection performance in this paper, we use the AUC on OoD detection as the objective function. When we also want to improve classification performance, we can add the classification cross-entropy loss in the objective function. The classification accuracy by Ours-C was almost the same with that by Proto-C. In contrast, the AUC for OoD detection by Ours was better than Proto-A. This result indicates that
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Figure 3: Average test AUC for OoD detection with different numbers of meta-training classes by the proposed method on the Omniglot dataset. The bar shows standard error.

Figure 4: Average test AUC for OoD detection with different latent space dimensionality by the proposed method on the Omniglot dataset. The bar shows standard error.

although GMMs with a common spherical covariance are sufficient for classification, GMMs with full covariance for each class are needed for OoD detection.

Table 3 shows the average computational time for meta-training and meta-testing with a GTX 1080Ti GPU. The computational time for the MAML-based methods was much longer than the other methods. It was because MAML-based methods required iterative gradient descent steps for the inner optimization. Also, the ODIN-based methods took a long time since they required to perturb the input for the query instances.

5 Conclusion

We proposed a meta-learning method for OoD detection. Our proposed method trains a neural network such that density-based OoD scores perform well when a Gaussian mixture model in the latent space is adapted to given in-distribution data for each task. Experiments on six datasets confirmed that our proposed method had better OoD detection performance than existing methods did. For future work, we will use other density estimation methods in a latent space in our framework. Also, we want to improve the performance by additionally using OoD techniques such as input perturbations and the use of representations in multiple layers [21].

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Table 2: Average test classification accuracy of class labels and its standard error. Values in bold are not statistically significantly different at the 5% level from the best performing method in each column according to a paired t-test. Since LCBO, SVDD, Gauss, and KDE did not output the class label, we omit them.

|            | Omniglot | Miniimagenet | CIFAR10 | SVHN | Patent | Dmoz |
|------------|----------|--------------|---------|------|--------|------|
| Ours       | 0.995 ± 0.000 | 0.555 ± 0.006 | 0.497 ± 0.006 | 0.276 ± 0.006 | 0.880 ± 0.003 | 0.816 ± 0.005 |
| Ours-C     | 0.994 ± 0.001 | 0.602 ± 0.005 | 0.505 ± 0.007 | 0.269 ± 0.004 | 0.868 ± 0.004 | 0.822 ± 0.001 |
| Proto-C    | 0.994 ± 0.000 | 0.590 ± 0.004 | 0.489 ± 0.010 | 0.270 ± 0.004 | 0.887 ± 0.002 | 0.823 ± 0.005 |
| Proto-A    | 0.995 ± 0.000 | 0.293 ± 0.012 | 0.267 ± 0.009 | 0.198 ± 0.002 | 0.879 ± 0.001 | 0.825 ± 0.004 |
| Proto-O    | 0.991 ± 0.001 | 0.589 ± 0.006 | 0.475 ± 0.009 | 0.251 ± 0.008 | 0.883 ± 0.002 | 0.821 ± 0.003 |
| MAML-C     | 0.990 ± 0.001 | 0.576 ± 0.006 | 0.489 ± 0.006 | 0.239 ± 0.003 | 0.754 ± 0.005 | 0.692 ± 0.007 |
| MAML-A     | 0.197 ± 0.003 | 0.200 ± 0.001 | 0.198 ± 0.002 | 0.201 ± 0.001 | 0.205 ± 0.004 | 0.208 ± 0.004 |
| MAML-O     | 0.678 ± 0.071 | 0.522 ± 0.008 | 0.433 ± 0.020 | 0.219 ± 0.004 | 0.239 ± 0.016 | 0.658 ± 0.020 |
| OoD-MAML   | 0.988 ± 0.002 | 0.563 ± 0.010 | 0.443 ± 0.007 | 0.223 ± 0.004 | 0.765 ± 0.006 | 0.724 ± 0.008 |
| Mahalanobis| **0.994 ± 0.001** | 0.319 ± 0.005 | 0.491 ± 0.007 | **0.275 ± 0.006** | **0.905 ± 0.002** | **0.839 ± 0.006** |

Table 3: Average meta-training and meta-testing computational time in seconds on the Omniglot dataset.

|            | Train | Test |
|------------|-------|------|
| Ours       | 16619.6 | 0.416 |
| Ours-C     | 15230.5 | 0.329 |
| Proto-C    | 13381.7 | 0.325 |
| Proto-A    | 12846.6 | 0.345 |
| Proto-O    | 25299.8 | 0.827 |
| MAML-C     | 57677.4 | 0.960 |
| MAML-A     | 55057.0 | 1.191 |
| MAML-O     | 177137.1 | 1.727 |
| OoD-MAML   | 47581.7 | 0.928 |
| LCBO       | 10673.2 | 0.198 |
| Mahalanobis| 15169.2 | 0.283 |
| SVDD       | 10370.6 | 0.259 |
| Gauss      | 15056.3 | 0.294 |
| KDE        | 11922.2 | 0.299 |
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