META-GMVAE: MIXTURE OF GAUSSIAN VAES FOR UNSUPERVISED META-LEARNING

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ABSTRACT

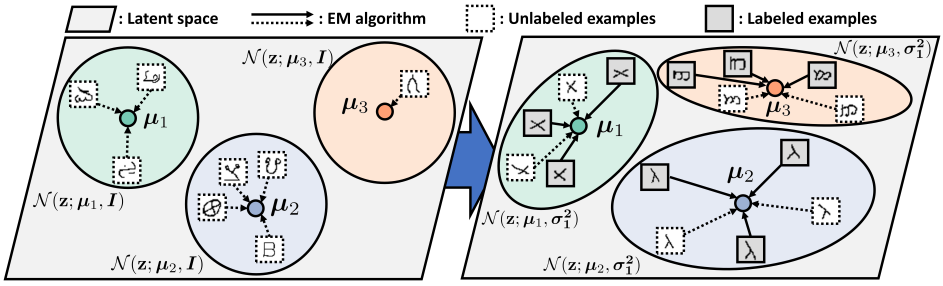
Unsupervised learning aims to learn meaningful representations from unlabeled data which can captures its intrinsic structure, that can be transferred to downstream tasks. Meta-learning, whose objective is to learn to generalize across tasks such that the learned model can rapidly adapt to a novel task, shares the spirit of unsupervised learning in that the both seek to learn more effective and efficient learning procedure than learning from scratch. The fundamental difference of the two is that the most meta-learning approaches are supervised, assuming full access to the labels. However, acquiring labeled dataset for meta-training not only is costly as it requires human efforts in labeling but also limits its applications to pre-defined task distributions. In this paper, we propose a principled unsupervised meta-learning model, namely Meta-GMVAE, based on Variational Autoencoder (VAE) and set-level variational inference. Moreover, we introduce a mixture of Gaussian (GMM) prior, assuming that each modality represents each class-concept in a randomly sampled episode, which we optimize with Expectation-Maximization (EM). Then, the learned model can be used for downstream few-shot classification tasks, where we obtain task-specific parameters by performing semi-supervised EM on the latent representations of the support and query set, and predict labels of the query set by computing aggregated posteriors. We validate our model on Omniglot and Mini-ImageNet datasets by evaluating its performance on downstream few-shot classification tasks. The results show that our model obtain impressive performance gains over existing unsupervised meta-learning baselines, even outperforming supervised MAML on a certain setting.

1 INTRODUCTION

Unsupervised learning is one of the most fundamental and challenging problems in machine learning, due to the absence of target labels to guide the learning process. Thanks to the enormous research efforts, there now exist many unsupervised learning methods that have shown promising results on real-world domains, including image recognition (Le, 2013) and natural language understanding (Ramachandran et al., 2017). The essential goal of unsupervised learning is obtaining meaningful feature representations that best characterize the data, which can be later utilized to improve the performance of the downstream tasks, by training a supervised task-specific model on the top of the learned representations (Reed et al., 2014; Cheung et al., 2015; Chen et al., 2016) or fine-tuning the entire pre-trained models (Erhan et al., 2010).

Meta-learning, whose objective is to learn general knowledge across diverse tasks, such that the learned model can rapidly adapt to novel tasks, shares the spirit of unsupervised learning in that both seek more efficient and effective learning procedure over learning from scratch. However, the essential difference between the two is that most meta-learning approaches have been built on the supervised learning scheme, and require human-crafted task distributions to be applied in few-shot classification. Acquiring labeled dataset for meta-training may require a massive amount of human efforts, and more importantly, meta-learning limits its applications to the pre-defined task distributions (e.g. classification of specific set of classes); thus applying it to a completely new downstream task from an unknown distribution is not straightforward.

To tackle such obstacles in the widespread applications of meta-learning, two recent works have proposed *unsupervised meta-learning* that can bridge the gap between unsupervised learning and



(a) Unsupervised Meta-training (b) Supevised Meta-test

Figure 1: During meta-training, Meta-GMVAE learns multi-modal latent space that can best explain the unlabeled data using EM algorithm. At meta-test time, we use semi-supervised EM to map both the support (labeled data) and queries (unlabeled data) to each mode learned during meta-training.

meta-learning by focusing on constructing supervised tasks with pseudo-labels from the unlabeled data. To do so, CACTUs (Hsu et al., 2019) clusters data in the embedding space learned with several unsupervised learning methods, while UMTRA (Khodadadeh et al., 2019) assumed that each randomly drawn sample represents a different class and augmented each pseudo-class with data augmentation (Cubuk et al., 2018). After constructing the meta-training dataset with such heuristics, they simply apply supervised meta-learning algorithms as usual. Despite the success of the existing unsupervised meta-learning methods, they are fundamentally limited, since 1) they only consider unsupervised learning for heuristic pseudo-labeling of unlabeled data, and 2) the two-stage approach makes it impossible to recover from incorrect pseudo-class assignment when learning the unsupervised representation space.

In this paper, we propose a principled, end-to-end unsupervised meta-learning model based on Variational Autoencoder (VAE) (Kingma & Welling, 2014) and set-level variational inference using self-attention (Vaswani et al., 2017). Moreover, we introduce multi-modal prior distributions, a mixture of Gaussians (GMM), assuming that each modality represents each class-concept in any given tasks. Then the parameter of GMM is optimized by running *Expectation-Maximization* (EM) on the observations sampled from the task-dependent variational posterior, which is inferred by set-encoding a given task (dataset) on to latent space. In this framework, however, there is no guarantee that each modality obtained from EM algorithm corresponds to a label we are interested in. To realize modality as label, we deploy semi-supervised EM algorithm at meta-test time, considering the support set and query set as labeled and unlabeled observations, respectively. We refer to our method as *Meta-Gaussian Mixture Variational Autoencoders* (Meta-GMVAE) (See Figure 1 for high-level concept). While our method can be used as a full generative model for generating the samples (images), the ability to generalize samples may not be necessary for capturing the the meta-knowledge for non-generative downstream tasks. Thus, we propose another version of Meta-GMVAE that reconstructs high-level features instead of generating samples, in the embedding space learned with other powerful unsupervised representation learning approaches (e.g. SimCLR, Chen et al. (2020)).

To investigate the effectiveness of our framework, we experiment it on two benchmark few-shot image classification datasets, namely Omiglot (Lake et al., 2011) and Mini-Imagenet (Ravi & Larochelle, 2017). The experimental results show that our Meta-GMVAE obtains impressive performance gains over the relevant unsupervised meta-learning baselines on both datasets, obtaining even better accuracy than fully supervised MAML (Finn et al., 2017) while utilizing as small as 0.1% of the labeled data on one-shot settings in Omniglot dataset. Moreover, our model can generalize to classification tasks with different number of ways (classes) without loss of accuracy. Our contribution is threefold:

- We propose a novel unsupervised meta-learning model which meta-learns the posterior network of a VAE, which is a principled unsupervised meta-learning method unlike existing unsupervised meta-learning methods that combines heuristic pseudo-labeling with supervised meta-learning.
- We propose to capture multi-modal structure in the given unlabled data as Gaussian mixtures, using EM algorithms at meta-training and semi-supervised EM at meta-test time.
- We show that Meta-GMVAE largely outperforms relevant unsupervised meta-learning baselines on two benchmark datasets, while obtaining even better performance than a supervised meta-learning model under a specific setting. We further show that Meta-GMVAE can generalize to classification tasks with different number of ways (classes).

2 RELATED WORK

Unsupervised learning The framework we propose is in the line with the unsupervised learning (Hastie et al., 2019; Le, 2013), which aims at obtaining transferable feature representations from the given data without any supervision. To obtain better feature representations for downstream tasks, many prior unsupervised learning methods have developed proxy objectives which is either based on reconstruction (Vincent et al., 2010; Higgins et al., 2017), adversarially obtained image fidelity (Radford et al., 2016; Salimans et al., 2016; Donahue et al., 2017; Dumoulin et al., 2017), disentanglement (Bengio et al., 2013; Reed et al., 2014; Cheung et al., 2015; Chen et al., 2016; Mathieu et al., 2016; Denton & Birodkar, 2017; Kim & Mnih, 2018; Ding et al., 2020), clustering (Coates & Ng, 2012; Krähenbühl et al., 2016; Bojanowski & Joulin, 2017; Caron et al., 2018), or instance classification with contrastive learning (Chen et al., 2020). Our work based on variational autoencoders (Kingma & Welling, 2014) which has a reconstruction objective. However, by introducing multi-modal prior distribution in the latent space, it can learn latent representations that are more transferable to the few-shot downstream tasks, compared to those learned with existing methods.

Meta-learning Meta-learning (Thrun & Pratt, 1998) shares the intuition of unsupervised learning in that it aims to improve the model performance on an unseen task by leveraging prior knowledge, rather than learning from scratch. While the literature on meta-learning is vast, we only discuss relevant existing works for few-shot image classification. Metric-based meta-learning (Koch et al., 2015; Vinyals et al., 2016; Snell et al., 2017; Oreshkin et al., 2018; Mishra et al., 2018) is one of the most popular approaches, where it learns to embed the data instances of the same class to be closer in the shared embedding space. One can measure the distance in the embedding space by cosine similarity (Vinyals et al., 2016), or Euclidean distance (Snell et al., 2017). On the other hand, gradient-based meta-learning (Finn et al., 2017; 2018; Li et al., 2017; Lee & Choi, 2018; Ravi & Beatson, 2019; Flennerhag et al., 2020) aims at learning a global initialization of parameters, which can rapidly adapt to a novel task with only a few gradient steps. While all of these works assume supervised learning scenarios where one has access to full labels in meta-training stage, we focus on unsupervised setting in this paper.

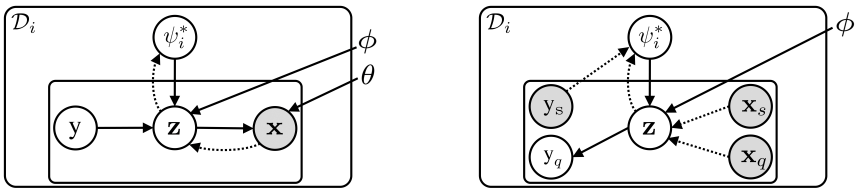
Unsupervised meta-learning One of the main limitation of conventional meta-learning methods is that their application is strictly limited to the tasks from a pre-defined task distribution. A few works (Hsu et al., 2019; Khodadadeh et al., 2019) have been proposed to resolve this issue by combining unsupervised learning with meta-learning. The main idea is to construct meta-training dataset in an unsupervised manner by leveraging existing supervised meta-learning models. CACTUs (Hsu et al., 2019) deploy several deep metric learning (Berthelot et al., 2019; Donahue et al., 2017; Caron et al., 2018; Chen et al., 2016) to episodically cluster the unlabeled dataset, and then train MAML (Finn et al., 2017) and Prototypical Networks (Snell et al., 2017) on the constructed data. UMTRA (Khodadadeh et al., 2019) assumes that each randomly drawn sample is from a different class from others, and use data augmentation (Cubuk et al., 2018) to construct synthetic task distribution for meta-training. Instead of only deploying unsupervised learning for constructing meta-training task distributions, we propose an unsupervised meta-learning model that meta-learns set-level variational posterior by matching the multi-modal prior distribution representing latent classes.

3 UNSUPERVISED META-LEARNING WITH META-GMVAES

In this section, we describe our problem setting with respect to unsupervised meta-learning, and demonstrate our approach. The graphical illustration of our model for unsupervised meta-training and supervised meta-test is depicted in Figure 2.

3.1 PROBLEM STATEMENT

Our goal is to learn unsupervised feature representations which can be transferred to wide range of downstream few-shot classification tasks. As suggested by Hsu et al. (2019); Khodadadeh et al. (2019), we only assume an unlabeled dataset $\mathcal{D}_u = \{\mathbf{x}_u\}_{u=1}^{U}$ in the meta-training stage. We aim toward applying the knowledge learned during unsupervised meta-training stage to novel tasks in meta-test stage, which comes with a modest amount of labeled data (or as few as a single example



(a) Unsupervised Meta-training (b) Supevised Meta-test

Figure 2: The graphical illustration of Meta-GMVAE. The dotted lines denote either variational inference or Expectation Maximization. (a): We introduce the multimodal distribution $p_\psi(\mathbf{z})$ into prior distribution, and its optimal task-specific parameter ψ_i^* is obtained by EM in an episodic manner. (b): For meta-test, we obtain task-specific parameter ψ_i^* by semi-supervised EM using $\mathbf{x}_s, \mathrm{y}_s$, and $\mathbf{x}_q$.

per class) for each task. As with most meta-learning methods, we further assume that the labeled data are drawn from the same distribution as that of the unlabeled data, with a different set of classes. Specifically, the goal of a K-way S-shot classification task $\mathcal{T}$ is to correctly predict the labels of query data points $\mathcal{Q} = \{\mathbf{x}_q\}_{q=1}^{Q}$, using S support data points and labels $\mathcal{S} = \{(\mathbf{x}_s, \mathrm{y}_s)\}_{s=1}^{S}$ per class, where S is relatively small (i.e. between 1 and 50).

3.2 Meta-Level Gaussian Mixture VAE

Unsupervised meta-training We now describe the meta-learning framework for learning unsupervised latent representations that can be transferred to human-designed few-shot image-classification tasks. In particular, we aim toward learning multi-modal latent spaces for Variational Autoencoder (VAE) in an episodic manner. To this end, we randomly draw M data points from the unlabeled dataset $\mathcal{D}_u$, and treat them as the episode-specific dataset $\mathcal{D}_i = \{\mathbf{x}_j\}_{j=1}^{M}$. Then the variational lower bound of marginal likelihood is as follows:

$$\log p_\theta(\mathcal{D}_i) \geq \sum_{j=1}^{M} \left[\mathbb{E}_{\mathbf{z}_j \sim q_\phi(\mathbf{z}_j|\mathbf{x}_j, \mathcal{D}_i)} \left[\log p_\theta(\mathbf{x}_j|\mathbf{z}_j) + \log p_{\psi_i}(\mathbf{z}_j) - \log q_\phi(\mathbf{z}_j|\mathbf{x}_j, \mathcal{D}_i)\right)\right] \tag{1}$$

$$\approx \sum_{j=1}^{M} \frac{1}{N} \sum_{n=1}^{N} \left[\log p_\theta(\mathbf{x}_j|\mathbf{z}_j^{(n)}) + \log p_{\psi_i}(\mathbf{z}_j^{(n)}) - \log q_\phi(\mathbf{z}_j^{(n)}|\mathbf{x}_j, \mathcal{D}_i)\right] \tag{2}$$

$$=: \mathcal{L}(\theta, \phi, \psi_i, \mathcal{D}_i), \quad \mathbf{z}_j^{(n)} \overset{i.i.d}{\sim} q_\phi(\mathbf{z}_j|\mathbf{x}_j, \mathcal{D}_i). \tag{3}$$

Here the lower bound for each datapoint is approximated by Monte Carlo estimation with the sample size N. The difference of our model from original VAE is that we utilize a set-level variational posterior $q_\phi(\mathbf{z}_j|\mathbf{x}_j, \mathcal{D}_i)$, for inferring isotropic Gaussian distribution distribution, to encode characteristics of a given dataset $\mathcal{D}_i$ into the latent representation. Specifically, we utilize self-attention mechanism (Vaswani et al., 2017) on top of a convolutional neural network.

We also introduce another parameter ψ_i which defines a *multi-modal* prior distribution $p_{\psi_i}(\mathbf{z}) = \sum_{k=1}^{K} p_{\psi_i}(\mathrm{y}=k) p_{\psi_i}(\mathbf{z}|\mathrm{y}=k)$. Specifically, we set the prior distribution as a mixture of Gaussian (GMM), where y is a discrete random variable indicating the component of a latent variable $\mathbf{z}$. In our case, the parameter ψ_i of the prior GMM is a task-specific parameter that is characterized by the given dataset $\mathcal{D}_i$. Assuming that the modalities in prior distribution represent class-concepts of any datasets, we propose to locally maximize the lower bound for the given episode dataset $\mathcal{D}_i$ (i.e. Eq 3), with respect to the task-specific prior parameter ψ_i. We then obtain the optimal task-specific parameter ψ_i^* by solving the following optimization problem:

$$\psi_i^* = \arg\max_{\psi_i} \mathcal{L}(\theta, \phi, \psi_i, \mathcal{D}_i) = \arg\max_{\psi_i} \sum_{j,n=1}^{M,N} \log p_\psi(\mathbf{z}_j^{(n)}), \quad \mathbf{z}_j^{(n)} \overset{i.i.d}{\sim} q_\phi(\mathbf{z}_j|\mathbf{x}_j, \mathcal{D}_i), \tag{4}$$

where we only consider the term related to the task-specific parameter ψ_i, and eliminate the normalization term $\frac{1}{N}$ since it does not change the solution of the optimization problem. The above formula implies that the optimal parameter maximizes the log-likelihood of observations which can be drawn from the variational posterior distribution. However, we do not have an analytic solution for Maximum Likelihood Estimation (MLE) of a GMM.

The most prevalent approach for estimating the parameters for the mixture of Gaussian is solving it with Expectation Maximization (EM) algorithm. To this end, we propose to optimize the task-specific parameter of GMM prior distribution using EM algorithm as follows:

$$\begin{aligned}
&\text{(E-step)} \quad Q_{j,n}(k) := p(\mathrm{y}_j^{(n)} = k|\mathbf{z}_j^{(n)}) = \frac{\pi_k \mathcal{N}(\mathbf{z}_j^{(n)}; \boldsymbol{\mu}_k, \boldsymbol{I})}{\sum_k \pi_k \mathcal{N}(\mathbf{z}_j^{(n)}; \boldsymbol{\mu}_k, \boldsymbol{I})} \\
&\text{(M-step)} \quad \boldsymbol{\mu}_k := \frac{\sum_{j,n=1}^{M,N} Q_{j,n}(k)\mathbf{z}_j^{(n)}}{\sum_{j,n=1}^{M,N} Q_{j,n}(k)}, \quad \pi_k := \frac{\sum_{j,n=1}^{M,N} Q_{j,n}(k)}{\sum_{k=1}^{K}\sum_{j,n=1}^{M,N} Q_{j,n}(k)} \\
&\qquad\qquad \psi_i := \{(\boldsymbol{\mu}_k, \boldsymbol{I}, \pi_k)\}_{k=1}^{K},
\end{aligned} \tag{5}$$

where π_k, $\boldsymbol{\mu}_k$, and $\mathcal{N}(\cdot)$ denote the mixing probability of k-th component, mean parameter, and normal distribution, respectively. We assume that the covariance matrix of Gaussian distribution is fixed with the identity matrix $\boldsymbol{I}$, following the assumption of original VAE on the prior distribution. We initialize π_k and $\boldsymbol{\mu}_k$ as $\frac{1}{K}$ and randomly drawn K different points. We can obtain MLE solution for the parameters of GMM, by iteratively performing E-step and M-step until the log-likelihood converges. However, we find that using a fixed number of iterations for the EM algorithm does not degrade the performance, and consider it as a hyperparameter of our framework.

Note that we want to maximize the variational lower bound of the marginal log-likelihood over all the episode datasets $\mathcal{D}_i$ that can be sampled from $\mathcal{D}_u$. We use stochastic gradient ascent with respect to the variational parameter ϕ and the generative parameter θ, to maximize the following objective:

$$\mathcal{L}(\theta, \phi, \{\mathcal{D}_i\}_{i=1}^{B}) := \frac{1}{B}\sum_{i=1}^{B}\left[\max_{\psi_i} \mathcal{L}(\theta, \phi, \psi_i, \mathcal{D}_i)\right] \tag{6}$$

$$= \frac{1}{B}\sum_{i=1}^{B}\sum_{j=1}^{M}\frac{1}{N}\sum_{n=1}^{N}\left[\log p_\theta(\mathbf{x}_j|\mathbf{z}_j^{(n)}) + \log p_{\psi_i^*}(\mathbf{z}_j^{(n)}) - \log q_\phi(\mathbf{z}_j^{(n)}|\mathbf{x}_j, \mathcal{D}_i)\right]. \tag{7}$$

Here we use B mini-batch of episode datasets, where each dataset consists of M datapoints. The task-specific parameter ψ_i^* for each episode dataset $\mathcal{D}_i$ is obtained by EM algorithm in Eq 5.

Supervised meta-test By introducing the multi-modal prior distribution into a generative learning framework, our model learns pseudo-class concepts by clustering latent features with EM algorithm. However, there is no guarantee that each modality obtained by EM algorithm corresponds to the label we are interested in at the meta-test stage. To realize modality as label in downstream few-shot image classification tasks, we deploy semi-supervised EM algorithm instead. Given a task $\mathcal{T}$ that consists of support set $\mathcal{S} = \{(\mathbf{x}_s, \mathrm{y}_s)\}_{s=1}^{S}$ and query set $\mathcal{Q} = \{\mathbf{x}_q\}_{q=1}^{Q}$, we use both the support set and query set as an episode dataset $\mathcal{D}_i = \{\mathbf{x}_s\}_{s=1}^{S} \cup \{\mathbf{x}_q\}_{q=1}^{Q}$ and draw latent variables from the variational posterior $q_\phi(\mathbf{z}_j|\mathbf{x}_j, \mathcal{D}_i)$. We then perform semi-supervised EM algorithm as follows:

$$\begin{aligned}
&\text{(E-step)} \quad Q_{q,n}(k) := p(\mathrm{y}_q^{(n)} = k|\mathbf{z}_q^{(n)}) = \frac{\mathcal{N}(\mathbf{z}_q^{(n)}; \boldsymbol{\mu}_k, \boldsymbol{\sigma}_k^{\mathbf{2}})}{\sum_k \mathcal{N}(\mathbf{z}_q^{(n)}; \boldsymbol{\mu}_k, \boldsymbol{\sigma}_k^{\mathbf{2}})} \\
&\text{(M-step)} \quad \boldsymbol{\mu}_k := \frac{\sum_{s,n=1}^{S,N} \mathbf{1}_{\mathrm{y}_s^{(n)}=\mathrm{k}}\mathbf{z}_s^{(n)} + \sum_{q,n=1}^{Q,N} Q_{q,n}(k)\mathbf{z}_q^{(n)}}{\sum_{s,n=1}^{S,N} \mathbf{1}_{\mathrm{y}_s^{(n)}=\mathrm{k}} + \sum_{q,n=1}^{Q,N} Q_{q,n}(k)}, \\
&\qquad\qquad \boldsymbol{\sigma}_k^{\mathbf{2}} := \frac{\sum_{s,n=1}^{S,N} \mathbf{1}_{\mathrm{y}_s^{(n)}=\mathrm{k}}(\mathbf{z}_s^{(n)} - \boldsymbol{\mu}_k)^2 + \sum_{q,n=1}^{Q,N} Q_{q,n}(k)(\mathbf{z}_q^{(n)} - \boldsymbol{\mu}_k)^2}{\sum_{s,n=1}^{S,N} \mathbf{1}_{\mathrm{y}_s^{(n)}=\mathrm{k}} + \sum_{q,n=1}^{Q,N} Q_{q,n}(k)} \\
&\qquad\qquad \psi_i := \{(\boldsymbol{\mu}_k, \boldsymbol{\sigma}_k^{\mathbf{2}}, \frac{1}{K})\}_{k=1}^{K},
\end{aligned} \tag{8}$$

where $\mathbf{1}$ denotes an indicator function. We fix the mixing probability as $\frac{1}{K}$ since the labels in each task $\mathcal{T}$ are uniformly distributed. Moreover, we utilize diagonal covariance $\boldsymbol{\sigma}_k^{\mathbf{2}}$ to obtain more accurate statistics for the inference. We initialize $\boldsymbol{\mu}_k$ as the average value of support latent representation

and $\boldsymbol{\sigma}_k^2$ as $\boldsymbol{I}$. We then obtain the MLE solution for the parameters of GMM, by iteratively performing E-step and M-step in Eq 8. Finally, we infer the labels of query set using the obtained parameters ψ_i^* as follows:

$$p(\mathrm{y}_q|\mathbf{x}_q, \mathcal{D}_i) = \mathbb{E}_{q_\phi(\mathbf{z}_q|\mathbf{x}_q,\mathcal{D}_i)}\left[p_{\psi_i^*}(\mathrm{y}_q|\mathbf{z}_q)\right] \approx \frac{1}{N}\sum_{n=1}^{N} p_{\psi_i^*}(\mathrm{y}_q|\mathbf{z}_q^{(n)}), \quad \mathbf{z}_q^{(n)} \overset{i.i.d}{\sim} q_\phi(\mathbf{z}_q|\mathbf{x}_q, \mathcal{D}_i). \tag{9}$$

Here we compute $p_{\psi_i^*}(\mathrm{y}_q|\mathbf{z}_q^{(n)})$ with Bayes rule, and we reuse N different Monte Carlo samples that is drawn for Eq 8 to compute the aggregated posterior.

Visual feature reconstruction While our method is a generative model that can generate samples from output distribution, the ability to generate samples may not be necessary for discriminative downstream tasks (Chen et al., 2020). Moreover, it is known to be challenging to train generative models in high-dimensional data (e.g. Mini-ImageNet). In preliminary experiments, we found that VAE almost fails to learn in Mini-ImageNet dataset with the architecturally limited constraints of the meta-learning literature. Thus, we propose a high-level feature reconstruction objective instead for Mini-ImageNet dataset. We experimentally find that the recently proposed constrastive learning framework, namely SimCLR (Chen et al., 2020), is the most effective for our settings. Specifically, SimCLR learns high-level representation by performing a constrastive prediction task on pairs of augmented examples derived from a minibatch. We train SimCLR on the unsupervised dataset $\mathcal{D}_u = \{\mathbf{x}_u\}_{u=1}^{U}$, and use high-level features extracted by SimCLR as an input for our framework. We also refer the reader to Chen et al. (2020) for more details.

4 EXPERIMENT

In this section, we now validate the effectiveness of our Meta-GMVAE on several downstream few-shot classification tasks.

4.1 EXPERIMENTAL SETUPS

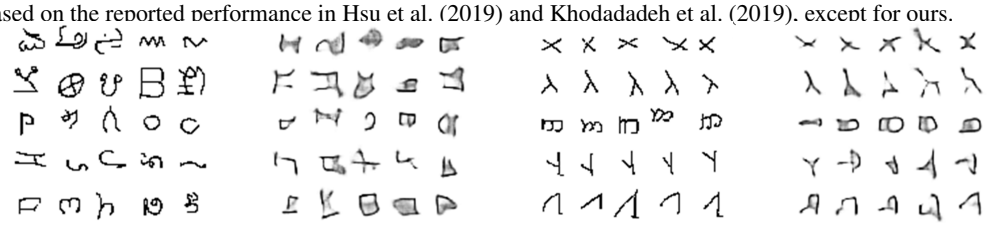
Baselines and ours We now describe two supervised meta-learning approaches which we consider as "oracles", unsupervised meta-learning baselines, and the proposed Meta-GMVAE. **1) MAML (oracle)**: Model Agnostic Meta Learning by Finn et al. (2017). We compare against its performance reported in Hsu et al. (2019). **2) ProtoNets (oracle)**: Euclidean distance-based meta-learning approach by Snell et al. (2017). We also compare against it using its performance reported in Hsu et al. (2019). **3) CACTUs**: Clustering to Automatically Construct Tasks for Unsupervised meta-learning by Hsu et al. (2019). It automatically constructs tasks by clustering the unsupervised dataset in embedding space learned by ACAI (Berthelot et al., 2019), BiGAN (Donahue et al., 2017), and DeepCluster (Caron et al., 2018). Then they train either MAML or ProtoNets using the cluster indices as pseudo-labels. **4) UMTRA**: Unsupervised Meta-learning with Tasks constructed by Random sampling and Augmentation by Khodadadeh et al. (2019). For constructing a K-way 1-shot task, it randomly samples K-way datapoints from unsupervised dataset and augments each datapoint. Then MAML is trained on the constructed tasks. **5) Meta-GMVAE**: Our proposed Meta-level Gaussian Mixture VAE. It learns a latent representation by matching set-level amortized variational posterior and task-specific multimodal prior optimized by EM algorithm.

Datasets We validate all models on two benchmark datasets for few-shot classification. **1) Omniglot**: This is a collection of 28 $\times$ 28 gray-scale hand-written characters that describe 1623 different alphabets, each of which contains 20 instances. Following the experimental setup of Hsu et al. (2019), we use 1200 classes for unsupervised meta-training, 100 classes for meta-validation and the remaining 323 classes for meta-test. We further augment each class by rotating the images 90, 180, and 270 degrees, such that the total number of classes is 1623 $\times$ 4, following the convention. **2) Mini-ImageNet.**: This is a subset of ILSVRC-2012 (Deng et al., 2009) introduced by Ravi & Larochelle (2017), consisting of 100 classes that comes with 600 images of size 84 $\times$ 84 that describe different instances. We use 64 classes for unsupervised meta-training, 16 classes for meta-validation, and the remaining 20 classes for meta-test, following the standard protocol.

Implementation details We now introduce the specific implementation details of Meta-GMVAE on the two benchmark datasets. **1) Variational posterior network** $q_\phi(\mathbf{z}|\mathbf{x}, \mathcal{D}_i)$: we use the standard

		Omniglot (way, shot)				Mini-ImagNet (way, shot)			
Method	**Clustering**	**(5,1)**	**(5,5)**	**(20,1)**	**(20,5)**	**(5,1)**	**(5,5)**	**(5,20)**	**(5,50)**
Training from Scratch	N/A	52.50	74.78	24.91	47.62	27.59	38.48	51.53	59.63
CACTUs-MAML	BiGAN	58.18	78.66	35.56	58.62	36.24	51.28	61.33	66.91
CACTUs-ProtoNets	BiGAN	54.74	71.69	33.40	50.62	36.24	50.16	59.56	63.27
CACTUs-MAML	ACAI/DC	68.84	87.78	48.09	73.36	39.90	53.97	63.84	69.64
CACTUs-ProtoNets	ACAI/DC	68.12	83.58	47.75	66.27	38.18	53.36	61.54	63.55
UMTRA	N/A	83.80	95.43	74.25	**92.12**	39.93	50.73	61.11	67.15
Meta-GMVAE (ours)	N/A	**94.92**	**97.09**	**82.21**	90.61	**42.82**	**55.73**	**63.14**	**68.26**
MAML (oracle)	N/A	94.46	98.83	84.60	96.29	46.81	62.13	71.03	75.54
ProtoNets (oracle)	N/A	98.35	99.58	95.31	98.81	46.56	62.29	70.05	72.04

Table 1: The few-shot classification results (way, shot) on the Omniglot and Mini-ImageNet datasets. DC denotes DeepCluster. We report the average of accuracies evaluated over 1000 episodes. All the values are based on the reported performance in Hsu et al. (2019) and Khodadadeh et al. (2019), except for ours.



(a) Meta-train (Real) (b) Meta-train (Generated) (c) Meta-test (Real) (d) Meta-test (Generated)

Figure 3: The samples obtained and generated for each mode at unsupervised meta-training and supervised meta-test step of Meta-GMVAE. Samples in each row are in the same modality obtained by EM.

Conv4 architecture on Omniglot dataset for a fair comparison against relevant baselines. On top of the Conv4 architecture, we stack two multi-head attention layers and an affine transformation layer to predict the mean and log-variance of Gaussian distribution. For Mini-ImageNet dataset, we only utilize two Transformer encoder layers and an affine transformation layer since the input used for Mini-ImageNet is already a high-level visual representation extracted from the Conv5 architecture trained with SimCLR. For both datasets, we set the dimensionality of the latent variable to 64. **Generative network** $p_\theta(\mathbf{x}|\mathbf{z})$: For Omniglot dataset, the architecture of generative network is symmetric to the Conv4 architecture of variational posterior network. The last layer predicts the parameter of output Bernoulli distribution. For Mini-ImageNet dataset, we use 3-layer MLP with ReLU activation to predict the mean of output Gaussian distribution. The variance of output Gaussian distribution is obtained as suggested in Rybkin et al. (2020). **Other details**: we utilize Adam optimizer (Kingma & Ba, 2015) with a constant learning rate of 0.0001 to optimize the generative and variational parameters. We set the number of iterations for EM algorithm as 5 for all the experiments. For the more detailed training procedure and network architecture, please see the Appendix.

4.2 Experimental Results

Table 1 shows the few-shot classification results obtained by supervised meta-learning baselines (oracle), the two unsupervised meta-learning baselines, and our Meta-GMVAE. The Meta-GMVAE outperforms all the baselines that only utilize unsupervised-learning for constructing meta-training tasks, except for the UMTRA on the Omniglot dataset 20-shot 5-shot classification. This shows that meta-learning the posterior network that can capture the multi-modal distribution of any given tasks with Meta-GMVAE, is indeed more effective over unsupervised meta-learning baselines which simply trains supervised meta-learning models with pseudo-labels obtained from unlabeled data. Moreover, our Meta-GMVAE obtains better performance than supervised MAML on Omniglot 5-way 1-shot classification, while utilizing as small as 0.1% of the labeled data. This matches the observation in Chen et al. (2020) that well-calibrated unsupervised learning approaches with a modest amount of labels can obtain a performance comparable to or even better than supervised approaches.

To better understand how our Meta-GMVAE learns and realizes class-concepts in few-shot classification tasks, we visualize the actual samples in an episode and ones generated by generative network $p_\theta(\mathbf{x}|\mathbf{z})$, during unsupervised meta-training and supervised meta-testing. Specifically, for a given episode dataset $\mathcal{D}_i$, we obtain the task-specific parameter ψ_i^* using either Eq 5 or Eq 8. Then we classify the actual samples using Eq 9, and generate samples by feeding each latent representation

Method	Ep	O	M
Training From Scratch		24.91	27.59
SimCLR + Logistic Regression		N/A	40.11
Vanilla VAE + EM		69.68	38.40
Meta-GMM w/o **Set**, $\boldsymbol{\sigma^2}$	✓	78.64	40.51
Meta-GMM w/o $\boldsymbol{\sigma^2}$	✓	81.65	41.13
Meta-GMM w/o **Set**	✓	80.94	40.92
Meta-GMM	✓	**82.21**	**42.82**
MAML (oracle)	✓	84.60	46.81
ProtoNets (oracle)	✓	95.31	46.56

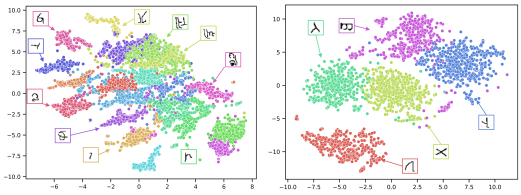
	Training (way, shot)			
Test way	**(5, 1)**	**(5, 5)**	**(20, 1)**	**(20, 5)**
2-way	98.26	98.00	98.36	98.23
5-way	94.92	94.57	93.93	94.01
10-way	89.87	89.99	89.10	89.30
15-way	85.11	85.12	85.36	85.33
20-way	81.38	81.11	82.21	81.98
30-way	77.80	77.42	78.40	77.24
40-way	73.76	73.15	74.03	73.56
50-way	70.92	70.85	69.86	70.02

Table 2: **Left**: The results of the ablation study on Meta-GMVAE (**O**: 20-way 1-shot classification on Omniglot, **M**: 5-way 1-shot classification on Mini-ImageNet). **Right**: The results of cross-way 1-shot experiments on Omniglot. The values in the parenthesis indicate that a model is trained based on the (way, shot) setting.

drawn from $p_{\psi_i^*}(\mathbf{z}|\mathrm{y}=k)$ into generative network $p_\theta(\mathbf{x}|\mathbf{z})$. Then we visualize the actual samples and generated ones that have a same modality in a same row. In Figure 3-**Left**, we can observe that our Meta-GMVAE captures the similar visual structure in each modality during meta-training, but the modalities are not the class-concepts. However, as shown Figure 3-**Right**, our Meta-GMVAE easily realizes each modality as each class-concept with only few examples at meta-test time.

Furthermore, we compare the performance of our model variants by eliminating each of the most important components for our model. We describe the each variant as follows: **1) SimCLR + Logistic Regression**: This performs the logistic regression using support set base on SimCLR. **2) Vanilla VAE + EM**: We train Vanilla VAE on $\mathcal{D}_u$ and predict labels using semi-supervised EM with fixed identity covariance $\boldsymbol{I}$. **3) Ep** Meta-GMVAE with an episodic training with task specific parameter ψ_i^* obtained by EM. **4) Set**: Meta-GMM whether having set-level variational posterior (i.e. $q_\phi(\mathbf{z}|\mathbf{x},\mathcal{D}_i)$) or not (i.e. $q_\phi(\mathbf{z}|\mathbf{x})$). **5) $\boldsymbol{\sigma^2}$**: Meta-GMM performs semi-supervised EM algorithm whether using diagonal covariance matrix or fixing it with identity matrix $\boldsymbol{I}$. Table 2-**Left** shows that all the components we consider are critical for the performance on the few-shot classification tasks as expected. The best performance gain comes from **Ep**, which supports our proposal on meta-learning the set-level variational posterior by matching it with the multi-modal prior, where the task-specific parameter is obtained with EM.

We then experiment our Meta-GMVAE by varying the number of way (between 2 and 50) and fixing the number of shot as 1. Table 2-**Right** shows that the difference in the number of way used for training and test does not significantly affect the performance, which demonstrates the robustness of Meta-GMVAE on varying number of way at test time. We also visualize the latent space for the cross-shot experiment using t-SNE (Rauber et al., 2016), in Figure 4, which shows that Meta-GMVAE trained with 20-way can cluster 5-way meta-test task.



(a) 20-way Meta-training (b) 5-way Meta-test

Figure 4: The visualization of the latent space for the cross-shot generalization experiment.

5 Conclusion

We proposed a novel unsupervised meta-learning model, namely Meta-GMVAE, which can generate a task-dependent posterior for a given unseen task with multi-modal Gaussian Mixture priors. Given a random episode that consists of samples from diverse classes, we optimize the task-specific parameter of the mixture of Gaussian prior with Expectation-Maximization algorithm, such that each mode can capture intrinsic groupings in the given data. We meta-train the variational posterior network over such data-driven prior obtained over large number of episodes. Then, at the meta-test step, we realize each modality with a label by deploying semi-supervised EM algorithm with both the support and the query set. We validate our method on two few-shot image classification benchmark datasets, and show that Meta-GMVAE largely outperforms the relevant unsupervised meta-learning baselines, even achieving better performance than supervised MAML on Omniglot 5-way 1-shot experiments. We further show that Meta-GMVAE can generalize across classification tasks with different number of ways (classes). As future work, we plan to extend our model to the zero-shot generation to unseen class-concepts.

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A Omniglot Experiments

A.1 Training Procedure

Omniglot is a collection of 28 $\times$ 28 gray-scale hand-written characters that describe 1623 different alphabets, each of which contains 20 instances. Following the experimental setup of Hsu et al. (2019), we use 1200 classes for unsupervised meta-training, 100 classes for meta-validation and the remaining 323 classes for meta-test. We further augment each class by rotating the images 90, 180, and 270 degrees, such that the total number of classes is 1623 $\times$ 4, following the convention. We evaluate the trained model uisng 1000 randomly selected tasks from test set. During evaluation, $K \times S$ data instances are used as support inputs and $K \times 15$ data instances are used as query inputs. We use the Adam (Kingma & Ba, 2015) optimizer with a constant learning rate of 0.0001 to train all models. All models are trained for 60,000 iterations. For the 5-way experiments (i.e. $K = 5$), we set the mini-batch size, the number of datapoints, and Monte Carlo sample size as 4, 200, and 32, respectively (i.e. $B = 4, M = 200$, and $N = 32$). For the 20-way experiments (i.e. $K = 20$), we set them as 4, 300, and 32 (i.e. $B = 4, M = 300$, and $N = 32$). We set the number of EM iterations as 5.

A.2 Network Architecture

We summarize the network architecture in the following Table 3, and 4. We assume that the output follows Bernoulli distribution, therefore, the output of generative network $p_\theta(\mathbf{x}|\mathbf{z})$ is the mean parameter.

Set-level variational posterior network $q_\phi(\mathbf{z}|\mathbf{x}, \mathcal{D}_i)$

Output Size	**Layers**
$1 \times 28 \times 28$	Input Images
$64 \times 14 \times 14$	conv2d(3×3, stride 1, padding 1), BatchNorm2D, ReLU, Maxpool(2×2, stride 2)
$64 \times 7 \times 7$	conv2d(3×3, stride 1, padding 1), BatchNorm2D, ReLU, Maxpool(2×2, stride 2)
$64 \times 4 \times 4$	conv2d(3×3, stride 1, padding 1), BatchNorm2D, ReLU, Maxpool(2×2, stride 2)
$64 \times 2 \times 2$	conv2d(3×3, stride 1, padding 1), BatchNorm2D, ReLU, Maxpool(2×2, stride 2)
256	Flatten
256	MultiheadAttention($d_{\text{model}} = 256, h = 4$, ELU, LayerNorm = False)
256	MultiheadAttention($d_{\text{model}} = 256, h = 4$, ELU, LayerNorm = False)
64×2	Linear(256, 64×2)

Table 3: Set-level variational posterior network used for Omniglot dataset. We refer the hyperparameter notation of MultiheadAttention to Vaswani et al. (2017).

Generative network $p_\theta(\mathbf{x}|\mathbf{z})$

Output Size	**Layers**
64	Latent code
256	Linear(64,256), ELU
256	Linear(256, 256), ELU
256	Linear(256, 256), ELU
$64 \times 2 \times 2$	Unflatten
$64 \times 4 \times 4$	deconv2d(4×4, stride 2, padding 1), BatchNorm2D, ReLU
$64 \times 7 \times 7$	deconv2d(3×3, stride 2, padding 1), BatchNorm2D, ReLU
$64 \times 14 \times 14$	deconv2d(4×4, stride 2, padding 1), BatchNorm2D, ReLU
$1 \times 28 \times 28$	deconv2d(4×4, stride 2, padding 1), Sigmoid

Table 4: Generative Network for $p_\theta(\mathbf{x}|\mathbf{z})$ for Omniglot dataset.

B MINI-IMAGENET EXPERIMENTS

B.1 TRAINING PROCEDURE

Mini-ImageNet is a subset of ILSVRC-2012 (Deng et al., 2009) introduced by Ravi & Larochelle (2017), consisting of 100 classes that comes with 600 images of size 84×84 that describe different instances. We first train Conv5 feature extractor using SimCLR objective with temperature term $\tau = 0.5$, on Mini-ImageNet unsupervised meta-training dataset. We train the feature extractor using Adam optimizer with learning rate of 0.0001 for 400 epochs. We use 64 classes for unsupervised meta-training, 16 classes for meta-validation, and the remaining 20 classes for meta-test, following the standard protocol. We evaluate the trained model using 1000 randomly selected tasks from test set. During evaluation, $5 \times S$ data instances are used as support inputs and 5×15 data instances are used as query inputs. For all the experiments, we use the Adam (Kingma & Ba, 2015) optimizer with a constant learning rate of 0.0001, and set the mini-batch size, the number of datapoints, and Monte Carlo sample size as 4, 5, and 32, respectively (i.e. $B = 4, M = 5$, and $N = 32$). For the 1, 5, 20, 50-shot experiments (i.e. $S = 1, 5$), we train the models for 3K, 20K, 25K, and 30K, respectively. We set the number of EM iterations as 5.

B.2 NETWORK ARCHITECTURE

We summarize the network architecture in the following Table 5, 6, and 7. We assume that the output follows Gaussian distribution, therefore, the output of generative network $p_\theta(\mathbf{x}|\mathbf{z})$ is the mean parameter. Moreover, the variance of output Gaussian distribution is obtained as suggested in Rybkin et al. (2020).

Feature Extractor for SimCLR

Output Size	**Layers**
$3 \times 84 \times 84$	Input Images
$64 \times 42 \times 42$	conv2d(3×3, stride 1, padding 1), BatchNorm2D, ReLU, Maxpool(2×2, stride 2)
$64 \times 21 \times 21$	conv2d(3×3, stride 1, padding 1), BatchNorm2D, ReLU, Maxpool(2×2, stride 2)
$64 \times 10 \times 10$	conv2d(3×3, stride 1, padding 1), BatchNorm2D, ReLU, Maxpool(2×2, stride 2)
$64 \times 5 \times 5$	conv2d(3×3, stride 1, padding 1), BatchNorm2D, ReLU, Maxpool(2×2, stride 2)
$64 \times 2 \times 2$	conv2d(3×3, stride 1, padding 1), BatchNorm2D, ReLU, Maxpool(2×2, stride 2)
256	Flatten

Table 5: Feature Extractor trained on Mini-ImageNet dataset using SimCLR objective.

Set-level variational posterior network $q_\phi(\mathbf{z}|\mathbf{x}, \mathcal{D}_i)$

Output Size	**Layers**
256	Input Features
256	MultiheadAttention($d_{\text{model}} = 256, h = 4$, ReLU, LayerNorm = False)
256	MultiheadAttention($d_{\text{model}} = 256, h = 4$, ReLU, LayerNorm = False)
64×2	Linear(256, 64×2)

Table 6: Set-level variational posterior network used for Mini-ImageNet dataset. We refer the hyperparameter notation of MultiheadAttention to Vaswani et al. (2017).

Generative network $p_\theta(\mathbf{x}|\mathbf{z})$

Output Size	**Layers**
64	Latent code
512	Linear(64, 512), ReLU
512	Linear(512, 512), ReLU
256	Linear(512, 256), ReLU

Table 7: Generative Network for $p_\theta(\mathbf{x}|\mathbf{z})$ for Mini-ImageNet dataset.