Adaptive Distribution Calibration for Few-Shot Learning with Hierarchical Optimal Transport

Dandan Guo [1], Long Tian[2], He Zhao [3], Mingyuan Zhou[4], Hongyuan Zha[1,5]
[1]The Chinese University of Hong Kong, Shenzhen [2]Xidian University
[3]CSIRO's Data61 [4]The University of Texas at Austin
[5] School of Data Science, Shenzhen Institute of Artificial Intelligence and Robotics for Society
`guodandan@cuhk.edu.cn` `tianlong@xidian.edu.cn` `he.zhao@ieee.org`
`mingyuan.zhou@mccombs.utexas.edu` `zhahy@cuhk.edu.cn`

Abstract

Few-shot classification aims to learn a classifier to recognize unseen classes during training, where the learned model can easily become over-fitted based on the biased distribution formed by only a few training examples. A recent solution to this problem is calibrating the distribution of these few sample classes by transferring statistics from the base classes with sufficient examples, where how to decide the transfer weights from base classes to novel classes is the key. However, principled approaches for learning the transfer weights have not been carefully studied. To this end, we propose a novel distribution calibration method by learning the adaptive weight matrix between novel samples and base classes, which is built upon a hierarchical Optimal Transport (H-OT) framework. By minimizing the high-level OT distance between novel samples and base classes, we can view the learned transport plan as the adaptive weight information for transferring the statistics of base classes. The learning of the cost function between a base class and novel class in the high-level OT leads to the introduction of the low-level OT, which considers the weights of all the data samples in the base class. Experimental results on standard benchmarks demonstrate that our proposed plug-and-play model outperforms competing approaches and owns desired cross-domain generalization ability, indicating the effectiveness of the learned adaptive weights.

1 Introduction

Deep learning models have become the regular ingredients for numerous computer vision tasks such as image classification [1, 2] and achieve state-of-the-art performance. However, the strong performance of deep neural networks typically relies on abundant labeled instances for training [3]. Considering the high cost of collecting and annotating a large amount of data, a major research effort is being dedicated to fields such as transfer learning [4] and domain adaptation [5]. As a trending research subject in the low data regime, few-shot classification aims to learn a model on the data from the base classes, so that the model can generalize well on the tasks sampled from the novel classes. Several lines of works have been proposed such as those based on meta-learning paradigms [3, 6–11] and those directly predicting the weights of the classifiers for novel classes [12, 13]. Recently, methods based on distribution calibration have gained increasing attention. As a representative example, Yang et al. [14] calibrate the feature distribution of the few-sample classes by transferring the statistics from the base classes and then utilize the sampled data to train a classifier for novel classes. A unique advantage of distribution calibration methods over others is that they build on top of off-the-shelf pretrained feature extractors and do not finetune/re-train the feature extractor.

36th Conference on Neural Information Processing Systems (NeurIPS 2022).

The key of distribution calibration methods is to select the corresponding base classes and transfer their statistics for the labeled samples in a novel task. Existing approaches in this line usually do so with heuristic or less adaptive solutions. Specifically, Yang et al. [14] use the average features of the samples as the representation of a base class and select the top-k (e.g., $k = 2$) closest base classes based on the Euclidean distance between the features of a novel sample and a base class. Despite the effectiveness of Yang et al. [14], it is questionable whether the Euclidean distance is the proper metric to measure the closeness between a base class and a novel sample since viewing a novel sample and a base class as points in the same space may not be the best solution. Moreover, it is less sound to characterize a base class only by the unweighted average over all its samples, when measuring its closeness with the novel sample. Representing a base class in this way would completely ignore the fact that each sample of a base class may contribute to the classification boundary differently. Finally, it may also be less effective to treat each of the top-k base classes equally as their contributions can also be different, not to mention the omission of the other base classes.

To this end, this work develops a more adaptive distribution calibration method leveraging optimal transport (OT), which is a powerful tool for measuring the cost in transporting the mass in one distribution to match another given a specific point-to-point cost function. First, we formulate a distribution P over the base classes and a distribution Q over the labeled samples from the novel classes. With such formulation, how to transfer the statistics from the base classes to the novel samples can be viewed as the OT problem between two distributions, denoted as the high-level OT. By solving the high-level OT, the learned transport plan can be used as the similarity or closeness between novel samples and base classes. Since the high-level OT requires specifying the cost function between one base class and one novel sample, we further introduce a low-level OT problem to learn this cost automatically, where we formulate a base class as a distribution over its samples. In this way, the similarity between a novel sample and a base class is no longer representing a base class by the unweighted average over all its samples and then using the Euclidean distance. In our method, the weights of the samples are considered in a principled way. In summary, the statistics of base classes can be better transferred to the novel samples for providing a more effective way to measure the similarity between them. Notably, even in the challenging cross-domain few-shot learning, our H-OT can still effectively transfer the statistics from the source domain to the target domain.

We can refer to this adaptive distribution calibration method as a novel hierarchical OT method (H-OT) for few-shot learning, which is applicable to a range of semi-supervised and supervised tasks, such as few-shot classification [9] and domain adaptation [5]. Our contributions are summarized as follows: (1) We develop a new distribution calibration method for few-shot learning, which can be built on top of an arbitrary pre-trained feature extractor for being implemented over the feature-level, without further costly fine-tuning. (2) We formulate the task of transferring statistics from base classes to novel classes in distribution calibration as the H-OT problem and tackle the task with a principled solution. (3) We apply our method to few-shot classification and also explore the cross-domain generalization ability. Experiments on standardized benchmarks demonstrate that introducing the H-OT into distribution calibration methods can learn adaptive weight matrix, paving a new way to transfer the statistics of base classes to novel samples.

2 Background

2.1 Optimal Transport Theory

Optimal Transport (OT) is a powerful tool for the comparison of probability distributions, which has been widely used in various machine learning problems, such as generative models [15], text analysis [16, 17], adversarial robustness [18], and imbalanced classification [19]. Here we limit our discussion to OT for discrete distributions and refer the reader to Peyré and Cuturi [20] for more details. Denote $p = \sum_{i=1}^{n} a_i \delta_{x_i}$ and $q = \sum_{j=1}^{m} b_j \delta_{y_j}$ as two n and m dimensional discrete probability distributions, respectively. In this case, $\boldsymbol{a} \in \Delta^n$ and $\boldsymbol{b} \in \Delta^m$, where Δ^m denotes the probability simplex of $\mathbb{R}^m$. The OT distance between p and q is defined as

$$\text{OT}(p, q) = \min_{\mathbf{T} \in \Pi(p,q)} \langle \mathbf{T}, \mathbf{C} \rangle, \tag{1}$$

where $\langle \cdot, \cdot \rangle$ denotes the Frobenius dot-product; $\mathbf{C} \in \mathbb{R}_{\geq 0}^{n \times m}$ is the transport cost function with element $C_{ij} = C(x_i, y_j)$; $\mathbf{T} \in \mathbb{R}_{>0}^{n \times m}$ denotes the doubly stochastic transport probability matrix such that $\Pi(p, q) := \{\mathbf{T} \mid \sum_i^n T_{ij} = b_j, \sum_j^m T_{ij} = a_i\}$, meaning that $\mathbf{T}$ has to be one of the joint distribution

of p and q. As directly optimising Equation (1) can be time-consuming for large-scale problems, the entropic regularization, $H = -\sum_{ij} T_{ij} \ln T_{ij}$, is introduced in Cuturi [21], resulting in the widely-used Sinkhorn algorithm for discrete OT problems with reduced complexity.

2.2 Few-Shot Classification

Following a typical few-shot learning problem, we divide the whole dataset with labeled examples into a base dataset $\mathbf{D}_{\text{base}}$ with B base classes and a novel dataset $\mathbf{D}_{\text{novel}}$ with N_{all} novel classes, each with a disjoint set of classes. To build a commonly-used N-way-K-shot task [8, 14], we randomly sample N classes from N_{all} novel classes, and in each class, we only pick K (*e.g.*, 1 or 5) samples for the support set $\mathcal{S} = \{(x_i, y_i)\}_{i=1}^{N \times K}$ to train or fine-tune the model and sample q instances for the query set $\mathcal{Q} = \{(x_i, y_i)\}_{i=N \times K+1}^{N \times K + N \times q}$ to evaluate the model. By averaging the accuracy on the query set of multiple tasks from the novel dataset, we can evaluate the performance of a model.

2.3 Distribution Calibration for Few-Shot Classification

Distribution calibration [14] uses the statistics of base classes to estimate the statistics of novel samples in the support set and generate more samples. Specifically, for the bth base class, its samples are assumed to be generated from a Gaussian distribution, whose mean and covariance matrix are:

$$\mu_b = \frac{1}{J_b} \sum_{j=1}^{J_b} \boldsymbol{x}_j, \quad \boldsymbol{\Sigma}_b = \frac{1}{J_b - 1} \sum_{j=1}^{J_b} (\boldsymbol{x}_j - \boldsymbol{\mu}_b)(\boldsymbol{x}_j - \boldsymbol{\mu}_b)^{\mathrm{T}}, \tag{2}$$

where $b \in [1, B]$, $\boldsymbol{x}_j \in \mathbb{R}^V$ is the V-dimensional feature of sample j extracted from the pre-trained feature encoder, J_b the number of samples in class b, and $\{\mu_b, \boldsymbol{\Sigma}_b\}$ are the statistics of base class b.

The samples of a novel class are also assumed to be generated from a Gaussian distribution with mean $\boldsymbol{\mu}'$ and covariance $\boldsymbol{\Sigma}'$. As the novel class only has one or a few labeled samples, it is hard to accurately estimate $\boldsymbol{\mu}'$ and $\boldsymbol{\Sigma}'$. Thus, the key idea is to transfer the statistics of the base classes to calibrate the novel class's distribution. Once the distribution of the novel class is calibrated, we can generate more samples from it, which are useful for training a good classifier. As a result, how to effectively transfer the statistics from the base classes is critical to the success of distribution calibration-based methods for few-shot learning. Accordingly, Free-Lunch [14] designs a heuristic approach that calibrates the Gaussian parameters of a novel distribution with one data sample $\boldsymbol{x}$:

$$\boldsymbol{\mu}' = \frac{\sum_{i \in \text{topk}(\mathbb{S}_d)} \boldsymbol{\mu}_i + \tilde{\boldsymbol{x}}}{k+1}, \quad \boldsymbol{\Sigma}' = \frac{\sum_{i \in \text{topk}(\mathbb{S}_d)} \boldsymbol{\Sigma}_i}{k} + \alpha, \tag{3}$$

where: 1) $\tilde{\boldsymbol{x}}$ is the transformed data by Tukey's Ladder of Powers transformation (TLPT) [22], *i.e.*, $\tilde{\boldsymbol{x}} = \boldsymbol{x}^\lambda$ if $\lambda \neq 0$ and $\tilde{\boldsymbol{x}} = \log(\boldsymbol{x})$ if $\lambda = 0$, for reducing the skewness of distributions and make distributions more Gaussian-like. 2) $\mathbb{S}_d = \left\{ -\|\boldsymbol{\mu}_b - \tilde{\boldsymbol{x}}\|^2 \mid b = [1, B] \right\}$ is a distance set defined by the Euclidean distance between the transformed feature $\tilde{\boldsymbol{x}}$ of a novel sample in support set and the mean $\boldsymbol{\mu}_b$ of the base class b. 3) $\text{topk}(\mathbb{S}_d)$ is the operation that selects the top-k closest base classes from the set $\mathbb{S}_d$. 4) α determines the degree of dispersion of features sampled from the calibrated distribution.

Although effective, Free-Lunch represents a base class by the unweighted average over all its samples when computing its closeness with a novel sample, which ignores the fact that each sample of a base class may contribute to the classification boundary differently. In addition, the Euclidean distance in the feature space may not well capture the relations between a base class and a novel sample. Moreover, each selected top-k base class has an equal weight (*i.e.*, $1/k$), which may not reflect the different contributions of the base classes and omit useful information in unselected base classes.

3 Our Proposed Model

3.1 Overall Method

In this work, we propose a novel adaptive distribution calibration framework, a holistic method for few-shot classification. Compared to the novel classes, which only have a limited number of labeled samples, the base classes typically have a sufficient amount of data, allowing their statistics to be estimated more accurately. Due to the correlation between novel and base classes, it is reasonable

to use the statistics of base classes to revise the distribution of the novel sample. Therefore, the key is how to transfer the statistics from the base classes to a novel class to achieve the best calibration results, which is the focus of this paper. Here, we develop the H-OT to learn the *Transport Plan* matrix between base classes and novel samples, where each element of the transport plan measures the importance of each base class for each novel sample and more relevant classes usually have a larger transport probability. Computing the high-level OT requires the specification of the cost function between one base class and one novel class, which leads to the introduction of a low-level OT problem. By viewing the learned transport plan as the adaptive weight matrix, we provide an elegant and principled way to transfer the statistics from the base classes to novel classes.

3.2 Hierarchical OT for Few-Shot Learning

Moving beyond the Free-Lunch method [14], which uses the Euclidean distance between a novel sample and a base class to decide their similarity and endow the chosen base classes with the equal importance, we aim to capture the correlations between the base class and novel samples at multiple levels and transfer the related statistics from base classes to novel samples. We learn the similarity by minimizing a high-level OT distance between base and novel classes and build the cost function used in high-level OT by further introducing a low-level OT distance. To formulate the task as the high-level OT problem, we model P as a following discrete uniform distribution over B base classes:

$$P = \sum_{b=1}^{B} \frac{1}{B} \delta_{R_b}, \tag{4}$$

where R_b represents the base class b in the V-dimensional feature space, which will be introduced later. Taking the N-way-1-shot task as the example, where each novel class has one labeled sample $\boldsymbol{x}$, we represent Q as a discrete uniform distribution over N novel classes from support set:

$$Q = \sum_{n=1}^{N} \frac{1}{N} \delta_{\tilde{\boldsymbol{x}}_n}, \tilde{\boldsymbol{x}}_n \in \mathbb{R}^{V \times 1}, \tag{5}$$

where $\tilde{\boldsymbol{x}}_n$ is the transformed feature from $\boldsymbol{x}$ following Yang et al. [14] and detailed below Equation 3. The OT distance between P and Q is thus defined as $\mathrm{OT}(P,Q) = \min_{\mathbf{T} \in \Pi(P,Q)} \langle \mathbf{T}, \mathbf{C} \rangle$. We adopt a regularised OT distance with an entropic constraint [21] and express the optimisation problem as:

$$\mathrm{OT}_\epsilon(P,Q) \stackrel{\text{def.}}{=} \sum_{b,n}^{B,N} C_{bn} T_{bn} - \epsilon \sum_{b,n}^{B,N} -T_{bn} \ln T_{bn}, \tag{6}$$

where $\epsilon > 0$, $\mathbf{C} \in \mathbb{R}_{\geq 0}^{B \times N}$ is the transport cost matrix, and C_{bn} indicates the cost between base class b and novel sample n. Importantly, the transport probability matrix $\mathbf{T} \in \mathbb{R}_{>0}^{B \times N}$ should satisfy $\Pi(P,Q) := \left\{ \sum_n^N T_{bn} = \frac{1}{B}, \sum_b^B T_{bn} = \frac{1}{N} \right\}$ with element $T_{bn} = T(R_b, \tilde{\boldsymbol{x}}_n)$, which denotes the transport probability between the bth base class and the nth novel sample and is an upper-bounded positive metric. Therefore, T_{bn} provides a natural way to weight the importance of each base class which can be used as the class similarity matrix when calibrating the novel distribution. Hence, the transport plan is the main thing that we want to learn from the data.

To compute the OT in Equation 6, we need to define the cost function $\mathbf{C}$, which is the main parameter defining the transport distance between probability distributions and thus plays the paramount role in learning the optimal transport plan. In terms of the transport cost matrix, a naive method is to specify the $\mathbf{C}$ with Euclidean distance or cosine similarity between the feature space of the novel sample and mean of the features from the base classes, such as $C_{bn} = 1 - \cos(\tilde{\boldsymbol{x}}_n, \boldsymbol{\mu}_b)$. However, these manually chosen cost functions might have the limited ability to measure the transport cost between a base class and a novel sample. Besides, representing the base class only with the average of all features in class b might ignore the contributions of different samples for this class. Hence the optimal transport plan for these cost functions might be inaccurate. To this end, we further introduce a low-level OT optimization problem to automatically learn the transport cost function $\mathbf{C}$ in (6). Specifically, we further treat each base class b as an empirical distribution R_b over the features within this class:

$$R_b = \sum_{j=1}^{J_b} p_j^b \delta_{\boldsymbol{x}_j^b}, \quad \boldsymbol{x}_j^b \in \mathbb{R}^V, \tag{7}$$

where p_j^b is the weight of data $\boldsymbol{x}_j^b$ to base class b and captures the importance of this sample and will be described in short order. Specifically, we train a classifier parameterized by ϕ with the samples in

the base classes, which predicts which base class a sample is in. The predicted probability of sample j belonging to the base class b is denoted by s_j^b and then $[p_1^b, \ldots, p_{J_b}^b]$ is obtained by normalizing the vector $[s_1^b, \ldots, s_{J_b}^b]$ with the Softmax function. We further define the low-level OT distance between each distribution R_b and distributions Q with an entropic constraint as

$$\text{OT}_\epsilon(R_b, Q) \overset{\text{def.}}{=} \sum_{n,j}^{N, J_b} D_{jn}^b M_{jn}^b - \epsilon \sum_{n,j}^{N,J} -M_{jn}^b \ln M_{jn}^b, \tag{8}$$

where the transport probability matrix $\mathbf{M}^b \in \mathbb{R}_{>0}^{J_b \times N}$ should satisfy $\Pi(R_b, Q) := \left\{ \sum_j^{J_b} M_{jn}^b p_j^b = \frac{1}{N}, \sum_n^N M_{jn}^b \frac{1}{N} = p_j^b \right\}$. The element D_{jn}^b of cost function $\mathbf{D}^b \in \mathbb{R}_{>0}^{J_b \times N}$ is the distance between the n-th novel sample and the j-th sample from base class b, where we naturally use the distance between their features, i.e., $\tilde{\boldsymbol{x}}_n$ and $\boldsymbol{x}_j^b$. Empirically, we find that the cosine similarity $D_{jn}^b = 1 - \cos(\tilde{\boldsymbol{x}}_n, \boldsymbol{x}_j^b)$ works well in practice, although other choices are possible.

Minimizing the low-level OT loss in Equation (8) can learn an optimal transport probability matrix $\mathbf{M}^b$ for $b \in B$, where M_{jn}^b tells us the transport weight between the nth novel class and jth sample in b base class. Back to the cost function C_{bn} for the high-level OT, instead of using the manually chose cost functions, we further adopt the learned total transport cost between novel sample $\boldsymbol{x}_n$ and all samples from base class b in the low-level OT to represent the cost function C_{bn} in high-level OT:

$$C_{bn} = \sum_{j=1}^{J_b} D_{jn}^b M_{jn}^b, \tag{9}$$

where C_{bn} is fed into (6) for learning the transport plan between base classes and novel samples. Defined in this way C_{bn} is an adaptive cost between base class b and novel sample n in support set, taking full advantage of all samples in a base class. With the proposed low-level OT distance, the distance between a novel sample and a base class is no longer representing a base class by the unweighted average over all its samples and then using the Euclidean distance. In our method, the weights of the samples are considered in a principled way.

3.3 Calibrating Distribution and Training Classifier

Once we obtain the transport plan matrix by minimizing the OT problem in (6), we can compute the statistics of novel samples by following Yang et al. [14]. For the n-th transformed feature $\tilde{\boldsymbol{x}}_n$ in the support set, we calibrate its mean and covariance as follows:

$$\boldsymbol{\mu}_n' = \frac{N \sum_{b \in B} T_{bn} \mu_b + \tilde{\boldsymbol{x}}_n}{B + 1}, \quad \boldsymbol{\Sigma}_n' = \frac{N \sum_{i \in B} T_{bn} \boldsymbol{\Sigma}_b}{B} + \alpha, \tag{10}$$

where μ_b and $\boldsymbol{\Sigma}_b$ are the statistics of base class b by (2), respectively; T_{bn} provides an adaptive way to weight the importance of base class b for novel sample n; N is used to scale T_{bn} since $\sum_{b \in B} T_{bn} = 1/N$; α is a hyper-parameter explained in Equation (3).

For N-way-K-shot task with $K > 1$, the N in aforementioned Equations (6) and (8) should be replaced with $N * K$, and the distribution calibration in Equation (10) should be undertaken K times for each novel class. Notably, this way can potentially achieve more diverse and accurate distribution estimation for avoiding the bias provided by one specific sample. Thus, for a class $y \in N$ in novel task, we denote the calibrated distribution with a set of statistics as

$$\mathbb{S}_y = \left\{ \left(\boldsymbol{\mu}_{n1}', \boldsymbol{\Sigma}_{n1}' \right), \ldots, \left(\boldsymbol{\mu}_{nK}', \boldsymbol{\Sigma}_{nK}' \right) \right\}. \tag{11}$$

Based on set $\mathbb{S}_y$ for novel class y, we can sample from the calibrated Gaussian distributions to generate a set of feature vectors with label y: $\mathbb{D}_y = \{(x, y) \mid x \sim \mathcal{N}(\mu, \Sigma), \forall (\mu, \Sigma) \in \mathbb{S}^y\}$. Given the transformed support set $\tilde{\mathcal{S}}$ with TLPT and the generated features $\mathbb{D}_y$, we only need to train the classifier for a task $\mathcal{T}$ (under, N-way-K-shot) by minimizing the cross-entropy loss:

$$\ell = \sum_{(\boldsymbol{x}, y) \sim \tilde{\mathcal{S}} \cup \mathbb{D}_y, y \in \mathcal{Y}^{\mathcal{T}}} -\log \Pr(y \mid x; \theta), \tag{12}$$

where $\mathcal{Y}^{\mathcal{T}}$ is the set of classes for the task $\mathcal{T}$ and the classifier is parameterized by θ. We describe our proposed framework in Algorithm 1.

Algorithm 1 Workflow about our adaptive distribution calibration on few-shot learning.

Require: Datasets $\mathbf{D}_{\text{base}}$, $\mathbf{D}_{\text{novel}}$, pretrained feature extractor $f(\cdot)$, classifier ϕ, classifier θ, hyperparameters

Extract the features of $\mathbf{D}_{\text{base}}$ and $\mathbf{D}_{\text{novel}}$ with $f(\cdot)$; compute $\{\mu_i, \mathbf{\Sigma}_i\}_{i=1}^{B}$ by (2);

Train a classifier ϕ with $\mathbf{D}_{\text{base}}$ to compute p_j^b; Represent base class b as R_b with (7);

for t in number of tasks **do**

    Randomly choose N-way-K-shot task;

    Learn $\mathbf{M}$ with (8) and compute cost C_{bn} with (9);

    Learn the transport plan matrix $\mathbf{T}$ with (6);

    Calibrate the statistics with (10) and generate the samples from (11);

    Train the N-way classifier θ with (12) and test the query set on classifier θ.

end for

---

4 Related Work

Recently, many efforts have been devoted to exploring the idea of learning to learn or meta-learning to alleviate the few-shot challenge. One approach to this problem is the optimization-based meta-learning algorithms [6, 7], which aim to learn a single set of model parameters that can be adapted to individual tasks with a small number of gradient update steps. Some simple but effective algorithms based on metric learning are also developed, with the goal of "learning to compare." For example, MatchingNet [8] and ProtoNet [9] learned to classify samples by comparing the distance to the representatives of each class. Another line of algorithms is to compensate for the insufficient samples by learning to augment. Most methods augment the training set using Generative Adversarial Networks (GANs) [23] or autoencoders [24] to generate samples [25–27] or features [28, 29].

Recently, Free-Lunch [14] is proposed to calibrate the distribution of the novel samples using the statistics from base classes and augment the data from the calibrated distribution. Although distribution calibration belongs to the scope of data augmentation, it does not need to build any complex generative models or fine-tune the backbone. Therefore, distribution calibration can be considered as a new promising line, where both Free-Lunch and our model fall into. Different from Free-Lunch which adopts a heuristic method to choose base classes for novel samples, we develop a novel hierarchical OT to learn the cost function and similarity (transport plan) between base classes and novel samples, providing a general and adaptive distribution calibration framework for few-shot learning. A recent metric-based work of connecting few-shot learning with OT is DeepEMD [30], which decomposes an image into a set of local features and uses the optimal matching cost between two images to represent their similarity. Besides, the authors of [31] introduce a prototype-oriented OT (POT) framework for set-structured data and apply it to metric-based few-shot classification. However, we directly minimize the OT between base classes and novel samples to learn the transport plan, which serves as the adaptive weight matrix in distribution calibration. Although both using OT for few-shot learning, DeepEMD, POT and ours are totally different methods. The hierarchical topic transport distance (HOTT) [32] is developed to measure the distance between documents, where documents are modeled as distributions over topics (solved by a high-level OT), and topics are further modeled as distributions over words (solved by a low-level OT). Different from HOTT which captures the semantic difference between documents by leveraging OT, topic modeling, and word embeddings, we develop the H-OT to learn the adaptive weight matrix for improving distribution calibration in few-shot learning, a task distinct from document representation.

5 Experiments

5.1 Experimental Setup

Datasets We evaluate our proposed method on several standard few-shot classification datasets with different levels of granularity, including miniImageNet [33], tieredImageNet [34], CUB [35], and CIFAR-FS [36]. Here, miniImageNet, tieredImageNet, and CIFAR-FS have a broad range of classes including various animals and objects while CUB is a more fine-grained dataset that includes various species of birds. The **miniImageNet**, which is randomly chosen from ILSVRC-12 dataset [37], contains 100 diverse classes with 600 samples per class. The image size is $84 \times 84 \times 3$. Following

Table 1: Classification accuracy (%) on miniImageNet, tieredImagenet and CUB with 95% confidence intervals. ○ indicates the results reported by authors and ⋆ is our implementation of Free-Lunch with their released code.

Methods	Backbone	miniImageNet		tieredImagenet		CUB	
		5way1shot	5way5shot	5way1shot	5way5shot	5way1shot	5way5shot
E3BM° [41]	ResNet25	64.3 ± n/a	81.0 ± n/a	70.0± n/a	85.0± n/a	-	-
LEO° [42]	WRN28	61.76 ± 0.08	77.59 ± 0.12	66.33 ± 0.05	81.44 ± 0.09	-	-
MAML [6] by [3]	ResNet18	49.61± 0.92	65.72 ± 0.77	-	-	69.96 ±1.01	82.70±0.65
Baseline++ ° [3]	ResNet18	51.87 ± 0.77	75.68 ± 0.63	-	-	67.02±0.90	83.58±0.54
Negative-Cosine° [43]	ResNet12	63.85 ± 0.81	81.57 ± 0.56	-	-	72.66±0.85	89.40±0.34
DeepEMD° [30]	ResNet12	65.91 ± 0.82	82.41 ± 0.56	71.16 ± 0.87	86.03 ±0.58	75.65±0.83	88.69±0.50
MatchNet [8] by [30]	ResNet12	63.08 ± 0.80	75.99 ± 0.60	68.50 ± 0.92	80.60 ± 0.71	71.87±0.85	85.08±0.57
MatchNet [8] by [31]	ResNet34	-	68.32 ± 0.66	-	-	-	84.66±0.55
MatchNet +POT by [31]	ResNet34	-	68.51 ± 0.64	-	-	-	85.50±0.66
ProtoNet [9] by [30]	ResNet12	60.37 ± 0.83	78.02 ± 0.57	65.65±0.92	83.40±0.65	66.09±0.92	82.50±0.58
ProtoNet [8] by [31]	ResNet34	-	73.99 ± 0.64	-	-	-	87.33±0.48
ProtoNet +POT by [31]	ResNet34	-	75.15 ± 0.63	-	-	-	88.34±0.46
Free-Lunch⋆ [14]	ResNet12	64.73± 0.44	81.15±0.42	71.40±0.31	85.56±0.40	74.13±0.86	87.91±0.45
Our H-OT	ResNet12	65.63±0.32	82.87 ±0.43	73.71±0.26	87.46±0.35	76.28±0.40	89.87±0.36
Free-Lunch° [14]	WRN28+RTloss	68.57 ± 0.55	82.88± 0.42	75.10 ± 0.32⋆	88.42± 0.40 ⋆	79.56±0.87	90.67±0.35
Our H-OT	WRN28+RTloss	**69.04 ± 0.29**	**84.36 ± 0.41**	**75.91±0.35**	**89.33±0.48**	**81.23±0.35**	**91.45±0.38**

the previous work [33], we split the dataset into 64 base classes, 16 validation classes, and 20 novel classes. The **tieredImageNet** is a larger subset of ILSVRC-12 dataset [37]. It contains 608 classes sampled from a hierarchical category structure, where each class belongs to one of 34 higher-level categories from the high-level nodes in the ImageNet. The average number of images in each class is 1281. We adopt 351, 97, and 160 classes for training, validation, and test, respectively. The **CUB** is a fine-grained few-shot classification benchmark, which contains 200 different classes of birds with a total of 11,788 images, and we resize them as $84 \times 84 \times 3$. We follow previous works [3] and split the dataset into 100 base classes, 50 validation classes, and 50 novel classes. The **CIFAR-FS** dataset is a recently proposed few-shot image classification benchmark, consisting of all 100 classes from CIFAR-100 [38]. The classes are randomly split into 64, 16, and 20 for meta-training, meta-validation, and meta-testing, respectively. Each class contains 600 images of size $32 \times 32 \times 3$.

Implementation Details Since Free-Lunch is the SOTA distribution calibration method, we mainly compare with Free-Lunch. For miniImageNet and CUB, we directly use pre-extracted features from Free-Lunch's code [14], which are produced by WideResNet trained from scratch on the base classes by following Mangla et al. [39] to optimize a classification loss and a self-supervised rotation loss jointly, denoted as WRN28+RTLoss. Free-lunch did not share the features on tieredImageNet and CIFAR-FS, thus we have taken the pre-trained WRN28+RTloss backbone of Mangla et al. [39] to extract the features, where we use this same backbone to implement Free-lunch with its official code and we have explored and selected an appropriate w for Free-lunch. To confirm the validity of our proposed method on the commonly-used backbone, we also take the ResNet12 as the example, which is trained from scratch by minimizing a standard classification loss (without the rotation loss). To make sure the log transform in TLPT is valid to its inputs, we need to guarantee the non-negativity of features. Therefore, we extract the features of given samples from the penultimate layer (with a ReLU activation function) of the feature extractor. To demonstrate the effectiveness of our method, we consider the simple Logistic Regression (LR) classifier for θ and ϕ in Algorithm 1, where the LR implementation of scikit-learn [40] with the default settings is adopted. We use the same hyper-parameter value for all datasets except for λ. Specifically, the number of generated features is 750, the ϵ in Sinkhorn algorithm is 0.01, the α in (10) is 0.21; and λ is 0.5, 1, 1 and 0.8 for miniImageNet, tieredImageNet, CUB, and CIFAR-FS, respectively, selected by a grid search using the validation set. The maximum iteration number in Sinkhorn algorithm is set as 200. The reported results are the averaged classification accuracy over 10,000 tasks.

5.2 Evaluation with the Standard Setting

We now conduct experiments on the most common setting in few-shot classification, 1-shot and 5-shot classification, where the results of different models on miniImageNet, tieredImagenet, CUB and CIFAR-FS are shown in Tables 1 and 2. To validate the effectiveness of our proposed model, we compare it with three main groups of the few-shot learning method, including optimization-based, metric-based, and distribution calibration-based. There are several observations. First, we can find

Table 2: 5way1shot and 5way5shot classification accuracy (%) on CIFAR-FS with 95% confidence intervals. ∗ means the results cited from [44] and ÷ denotes our implementation of Free-Lunch with their official code.

Methods	Backbone	CIFAR-FS	
		5way1shot	5way5shot
MAML∗ [6]	32-32-32-32	58.9 ± 1.9	71.5 ± 1.0
ProtoNet∗ [9]	64-64-64-64	55.5 ± 0.7	72.0 ± 0.6
RelaNet∗ [45]	64-96-128-256	55.0 ± 1.0	69.3 ± 0.8
R2D2∗ [46]	96-192-384-512	65.3 ± 0.2	79.4 ± 0.1
Shot-Free∗ [47]	ResNet12	69.2 ± n/a	84.7 ± n/a
MetaOpt∗ [48]	ResNet12	72.6 ± 0.7	84.3 ± 0.5
RFS∗ [44]	ResNet12	73.9 ± 0.8	86.9 ± 0.5
Free-Lunch÷ [14]	ResNet12	73.8 ± 0.4	86.0 ± 0.4
Our H-OT	ResNet12	74.5 ± 0.4	87.1 ± 0.3
Free-Lunch [14]	WRN28+RTloss	74.9 ± 0.4	86.2 ± 0.5
Our H-OT	WRN28+RTloss	**75.4 ± 0.3**	**87.5 ± 0.3**

that our H-OT equipped with WRN28+RTLoss and simple linear classifier outperforms all previous competing methods on 5-way-1-shot and 5-way-5-shot settings, which illustrates the superiority of the proposed framework. Second, our H-OT equipped with ResNet12 is better than other baselines except for the 5way1shot task on miniImageNet, where in this case our H-OT is still competitive with DeepEMD [30]. This observation proves the effectiveness of distribution calibration and transferring the statistics from base classes to novel classes using OT. Third, the comparison between our model and the strong baseline of distribution calibration-based methods, i.e., Free-Lunch [14], confirms the validity of incorporating the adaptive weight matrix when transferring the statistics from the base classes to the novel classes. Although both methods utilize distribution calibration to perform few-shot classification, our model can more effectively transfer the knowledge of the base classes to estimate the distribution of novel samples more accurately with the help of hierarchical OT (H-OT). Fourth, in terms of 5-way 1-shot tasks on all datasets, the performance gain from our model over Free-Lunch on the CUB is larger than that of other datasets. However, for 5-way 5-shot tasks on all datasets, the improvement gain from our model over Free-Lunch on the CUB is not as significant as that on other datasets. The reason behind this might be that CUB is a fine-grained image classification dataset, which makes it more effective for statistics transfer compared to other datasets under the 1-shot setting. Furthermore, with the development of label examples in the novel classes (5-shot), our method can perform more effective knowledge transfer from base classes to novel samples in the coarse-grained image classification dataset. The results reveal that the granularity of the dataset is an important factor in the current few-shot classification setting. Our model avoids the costly fine-tuning for backbone and it only takes time at the testing stage. We defer the details on comparison of computational cost to Appendix A and summary of test results to Appendix B.

5.3 Evaluation with the Cross-domain Setting

To explore the cross-domain generalization ability of H-OT for the few-shot classification task, we consider a practical evaluation setting following Chen et al. [3], where there exists domain shift between base and novel classes (e.g., sampling base classes from a coarse-grained dataset and novel classes from a fine-grained dataset). We design two cross-domain scenarios: miniImageNet → CUB, CIFAR-FS → CUB, where CUB is the target domain while both miniImageNet and CIFAR-FS are the source domains. Compared with collecting images from a general class, collecting images from fine-grained classes might be more difficult, so these two scenarios are very meaningful in reality. We consider the comparison with Free-Lunch, which is closely related to ours. As shown in Fig. 1, both H-OT and Free-Lunch achieve acceptable performance in these two scenarios, proving the effectiveness of the distribution calibration framework in the cross-domain case. Besides, H-OT shows its clear advantage over Free-Lunch. It indicates that H-OT can

Figure 1: 5way1shot accuracy under the cross-domain scenarios, i.e., miniImageNet → CUB and CIFAR-FS → CUB. CUB indicates that both base and novel classes are from CUB.

Figure 2: Accuracy on miniImageNet for 5way1shot task with varying number of generated features.

Figure 3: Top-5 closest base classes for a novel sample from the "plain" class on CIFAR-FS based on our learned transport plan.

better utilize the statistics from the base classes of the source domain with the adaptive weight matrix and transfer them to the novel classes of the target domain. Moreover, H-OT under the CIFAR-FS $\rightarrow$ CUB (blue bar in the 3rd column) scenario still outperforms Free-Lunch under CUB (orange bar in the 1st column). These results show that H-OT is less affected by domain shift between the base and novel classes and possesses the desired cross-domain generalization ability.

Table 3: Ablation study with different cost functions (5way1shot).

Models	miniImageNet	CUB	CIFAR-FS	tieredImagenet
Free-lunch [14]	68.57 ± 0.55	79.56 ± 0.87	74.94 ± 0.64	75.10 ± 0.32
High-level OT+Euc	68.79 ± 0.31	80.29 ± 0.25	75.09 ± 0.33	75.31 ± 0.36
High-level OT+Euc+weighted	68.80 ± 0.32	80.33 ± 0.27	75.13 ± 0.31	75.35 ± 0.40
High-level OT+cos	68.82 ± 0.36	81.01 ± 0.41	75.12 ± 0.31	75.52 ± 0.36
High-level OT+cos+weighted	68.78 ± 0.33	81.02 ± 0.30	75.10 ± 0.34	75.55 ± 0.41
Our H-OT	$\mathbf{69.04 \pm 0.29}$	$\mathbf{81.23 \pm 0.35}$	$\mathbf{75.42 \pm 0.32}$	$\mathbf{75.91 \pm 0.35}$

Table 4: 5way1shot performance on miniImageNet with different backbones.

Backbone	Free-Lunch	Ours
Conv4	54.62 ± 0.64	$\mathbf{55.23 \pm 0.59}$
Conv6	57.14 ± 0.45	$\mathbf{58.01 \pm 0.42}$
ResNet10	64.41 ± 0.33	$\mathbf{65.22 \pm 0.37}$
Resnet18	61.50 ± 0.47	$\mathbf{62.61 \pm 0.41}$
WRN28+RTloss	68.57 ± 0.55	$\mathbf{69.04 \pm 0.29}$

5.4 Ablation Study and Qualitative Analysis

Impact of adaptive cost from low-level OT Recall that we formulate our general goal as a high-level OT problem and we propose a low-level OT for computing the cost function for the high-level one in an adaptive way. The low-level OT captures the distance between a base class and a novel class. Here we consider two commonly-used cost functions to replace the adaptive cost, including Euclidean distance and cosine similarity between the feature space of the novel classes and the mean of the features from the base classes, denoted as High-level OT+Euc and High-level OT+cos. Besides, to exclude the possibility that the gain of our H-OT comes only from the effect of introducing weighted mean in the low-level OT, we also consider use the weighted mean with (7) to implement High-level OT, denoted as High-level OT+Euc+weighted and High-level OT+cos+weighted. As summarized in Table 6, our proposed H-OT achieves better performance than these degraded variants, which confirms the validity of adaptive cost from low-level OT in few-shot classification. And introducing the weighted mean into the cost function of high-level OT does not improve the performance. It indicates that the performance gain comes mainly from the low-level OT rather than the effect of weighted mean. The reason behind this might be that our proposed low-level OT considers all samples within a base class when deciding the cost between novel samples and this base class, instead of using the mean of the features from the base class. Besides, even with the given cost functions, our proposed method still outperforms the competing baseline (i.e., Free-Lunch), indicating the usefulness of the transport plan (i.e., adaptive matrix) learned from high-level OT.

Different backbones Since our framework is agnostic with the choice of backbones, following Yang et al. [14], we further employ other commonly used backbones, such as networks with four or six convolutional layers (Conv4 or Conv6), Resnet10 and Resnet18, which are trained from scratch following [3]. Table 4 illustrates the classification performance (5-way-1-shot) comparison between our H-OT and strong baseline (Free-Lunch) on miniImageNet with different backbones. We find that H-OT always outperforms its baseline given the same backbone. This result reveals the superiority of learning an adaptive weight matrix to select statistics of base classes on different backbones. As H-OT is agnostic to the feature extractor and does not require costly fine-tuning, it can also conveniently work with more advanced feature extractors to get better performance.

Number of generated features Fig. 2 shows the variation of the classification performance of distribution calibration models with the increasing number of generated features, where we consider our H-OT (red) and Free-Lunch (green) in a 5-way-1-shot classification setting for miniImageNet. We can see that increasing the number of generated samples results in consistent improvement in both cases. However, given the same number of generated samples, H-OT outperforms its baseline, which only selects the $top - k$ base classes for each novel sample using Euclidean distance [14]. Interestingly, our model achieves around 68.5 accuracy with only 50 generated samples, while Free-Lunch takes 750 generated samples to achieve a similar result. Hence, the adaptive weight matrix learned by H-OT can contribute to the distribution calibration strategy for sampling more representative features.

Learned transport plan To explore whether the learned transport plan can capture the correlations between the base classes and one given sample from the novel class ("plain"), we show a list of base classes with decreasing ranks in Fig. 3. The top-5 base classes are highly related to the given novel sample about their semantic meanings. It is reasonable since the images from wild animal-related classes are usually taken on the plain, such as "elephant" and "bear". It indicates that the transport plan can be successfully optimized by our H-OT and provides an elegant way to measure the closeness between base classes and novel samples. Different from Free-Lunch that only selects top-k base classes (k=2), our model takes full advantage of all base classes for learning adaptive weight for each base class. Additional quantitative results and qualitative are deferred to the Appendix B.

6 Conclusion

This paper introduces a novel hierarchical OT to improve the existing distribution calibration-based algorithm for few-shot learning. We first develop a low-level OT problem to learn the cost between novel samples and a base class, which takes into account different weights of the samples in the base class. Moreover, we further design a high-level OT for measuring the distance between novel samples and all base classes, which uses the cost learned from the low-level one to define the cost function rather than manually chosen cost functions. The proposed H-OT can capture the correlations between the novel samples and base classes with a two-level hierarchy. When transferring the statistics from base classes to novel samples, we view the learned optimal transport plan between them as the adaptive weight matrix, providing an effective way to weigh each base class for a novel sample. Extensive experiments have been conducted, showing that our proposed framework achieves competing performance on commonly few-shot learning problems and cross-domain scenarios.

7 Negative Societal Impacts

We develop a simple and effective distribution calibration approach to the few-shot learning, which has the potential to encourage researchers to derive new and better methods for few-shot learning or meta-learning. Our work may indirectly lead to a negative outcome if there is a sufficiently malicious or ill-informed choice of a few-shot classification task.

Acknowledgements. This work is partially supported by a grant from the Shenzhen Science and Technology Program (JCYJ20210324120011032) and Shenzhen Institute of Artificial Intelligence and Robotics for Society.

References

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

[2] Karen Simonyan and Andrew Zisserman. Very deep convolutional networks for large-scale image recognition. In Yoshua Bengio and Yann LeCun, editors, *3rd International Conference on Learning Representations, ICLR 2015, San Diego, CA, USA, May 7-9, 2015, Conference Track Proceedings*, 2015. URL http://arxiv.org/abs/1409.1556.

[3] Wei-Yu Chen, Yen-Cheng Liu, Zsolt Kira, Yu-Chiang Frank Wang, and Jia-Bin Huang. A closer look at few-shot classification. In *International Conference on Learning Representations*, 2019.

[4] Sinno Jialin Pan and Qiang Yang. A survey on transfer learning. *IEEE Transactions on knowledge and data engineering*, 22(10):1345–1359, 2009.

[5] Yaroslav Ganin and Victor Lempitsky. Unsupervised domain adaptation by backpropagation. In *International conference on machine learning*, pages 1180–1189. PMLR, 2015.

[6] Chelsea Finn, Pieter Abbeel, and Sergey Levine. Model-agnostic meta-learning for fast adaptation of deep networks. In *International Conference on Machine Learning*, pages 1126–1135. PMLR, 2017.

[7] Sachin Ravi and Hugo Larochelle. Optimization as a model for few-shot learning. In *5th International Conference on Learning Representations, ICLR 2017, Toulon, France, April 24-26, 2017, Conference Track Proceedings*, 2017.

[8] Oriol Vinyals, Charles Blundell, Tim Lillicrap, Koray Kavukcuoglu, and Daan Wierstra. Matching networks for one shot learning. In *Advances in Neural Information Processing Systems 29: Annual Conference on Neural Information Processing Systems 2016, December 5-10, 2016, Barcelona, Spain*, pages 3630–3638, 2016.

[9] Jake Snell, Kevin Swersky, and Richard S. Zemel. Prototypical networks for few-shot learning. In *Advances in Neural Information Processing Systems*, pages 4077–4087, 2017.

[10] Bharath Hariharan and Ross B. Girshick. Low-shot visual recognition by shrinking and hallucinating features. In *IEEE International Conference on Computer Vision, ICCV 2017, Venice, Italy, October 22-29, 2017*, pages 3037–3046. IEEE Computer Society, 2017.

[11] Yu-Xiong Wang, Ross B. Girshick, Martial Hebert, and Bharath Hariharan. Low-shot learning from imaginary data. In *2018 IEEE Conference on Computer Vision and Pattern Recognition, CVPR 2018, Salt Lake City, UT, USA, June 18-22, 2018*, pages 7278–7286. Computer Vision Foundation / IEEE Computer Society, 2018.

[12] Spyros Gidaris and Nikos Komodakis. Dynamic few-shot visual learning without forgetting. In *2018 IEEE Conference on Computer Vision and Pattern Recognition, CVPR 2018, Salt Lake City, UT, USA, June 18-22, 2018*, pages 4367–4375. Computer Vision Foundation / IEEE Computer Society, 2018.

[13] Hang Qi, Matthew Brown, and David G. Lowe. Low-shot learning with imprinted weights. In *2018 IEEE Conference on Computer Vision and Pattern Recognition, CVPR 2018, Salt Lake City, UT, USA, June 18-22, 2018*, pages 5822–5830. Computer Vision Foundation / IEEE Computer Society, 2018.

[14] Shuo Yang, Lu Liu, and Min Xu. Free lunch for few-shot learning: Distribution calibration. In *International Conference on Learning Representations*, 2021.

[15] Viet Huynh, Dinh Q Phung, and He Zhao. Optimal transport for deep generative models: State of the art and research challenges. In *IJCAI*, pages 4450–4457, 2021.

[16] He Zhao, Dinh Phung, Viet Huynh, Trung Le, and Wray Buntine. Neural topic model via optimal transport. In *International Conference on Learning Representations*, 2021.

[17] Dongsheng Wang, Dandan Guo, He Zhao, Huangjie Zheng, Korawat Tanwisuth, Bo Chen, and Mingyuan Zhou. Representing mixtures of word embeddings with mixtures of topic embeddings. In *International Conference on Learning Representations*, 2022.

[18] Anh Tuan Bui, Trung Le, Quan Hung Tran, He Zhao, and Dinh Phung. A unified Wasserstein distributional robustness framework for adversarial training. In *International Conference on Learning Representations*, 2022.

[19] Dandan Guo, Zhuo Li, Meixi Zheng, He Zhao, Mingyuan Zhou, and Hongyuan Zha. Learning to re-weight examples with optimal transport for imbalanced classification. *arXiv preprint arXiv:2208.02951*, 2022.

[20] Gabriel Peyré and Marco Cuturi. Computational optimal transport. *Found. Trends Mach. Learn.*, 11(5-6):355–607, 2019.

[21] Marco Cuturi. Sinkhorn distances: Lightspeed computation of optimal transport. *Advances in neural information processing systems*, 26:2292–2300, 2013.

[22] John W Tukey et al. *Exploratory data analysis*, volume 2. Reading, Mass., 1977.

[23] Ian Goodfellow, Jean Pouget-Abadie, Mehdi Mirza, Bing Xu, David Warde-Farley, Sherjil Ozair, Aaron Courville, and Yoshua Bengio. Generative adversarial nets. volume 27, 2014.

[24] David E Rumelhart, Geoffrey E Hinton, and Ronald J Williams. Learning representations by back-propagating errors. *nature*, 323(6088):533–536, 1986.

[25] Ruixiang Zhang, Tong Che, Zoubin Ghahramani, Yoshua Bengio, and Yangqiu Song. Metagan: An adversarial approach to few-shot learning. *NeurIPS*, 2:8, 2018.

[26] Hang Gao, Zheng Shou, Alireza Zareian, Hanwang Zhang, and Shih-Fu Chang. Low-shot learning via covariance-preserving adversarial augmentation networks. In *Advances in Neural Information Processing Systems 31: Annual Conference on Neural Information Processing Systems 2018, NeurIPS 2018, December 3-8, 2018, Montréal, Canada*, pages 983–993, 2018.

[27] Eli Schwartz, Leonid Karlinsky, Joseph Shtok, Sivan Harary, Mattias Marder, Abhishek Kumar, Rogério Schmidt Feris, Raja Giryes, and Alexander M. Bronstein. Delta-encoder: an effective sample synthesis method for few-shot object recognition. In *Advances in Neural Information Processing Systems 31: Annual Conference on Neural Information Processing Systems 2018, NeurIPS 2018, December 3-8, 2018, Montréal, Canada*, pages 2850–2860, 2018.

[28] Yongqin Xian, Tobias Lorenz, Bernt Schiele, and Zeynep Akata. Feature generating networks for zero-shot learning. In *Proceedings of the IEEE conference on computer vision and pattern recognition*, pages 5542–5551, 2018.

[29] Jian Zhang, Chenglong Zhao, Bingbing Ni, Minghao Xu, and Xiaokang Yang. Variational few-shot learning. In *2019 IEEE/CVF International Conference on Computer Vision, ICCV 2019, Seoul, Korea (South), October 27 - November 2, 2019*, pages 1685–1694. IEEE, 2019.

[30] Chi Zhang, Yujun Cai, Guosheng Lin, and Chunhua Shen. Deepemd: Few-shot image classification with differentiable earth mover's distance and structured classifiers. In *Proceedings of the IEEE/CVF conference on computer vision and pattern recognition*, pages 12203–12213, 2020.

[31] Dan dan Guo, Long Tian, Minghe Zhang, Mingyuan Zhou, and Hongyuan Zha. Learning prototype-oriented set representations for meta-learning. In *International Conference on Learning Representations*, 2022.

[32] Mikhail Yurochkin, Sebastian Claici, Edward Chien, Farzaneh Mirzazadeh, and Justin M. Solomon. Hierarchical optimal transport for document representation. In Hanna M. Wallach, Hugo Larochelle, Alina Beygelzimer, Florence d'Alché-Buc, Emily B. Fox, and Roman Garnett, editors, *Advances in Neural Information Processing Systems 32: Annual Conference on Neural Information Processing Systems 2019, NeurIPS 2019, December 8-14, 2019, Vancouver, BC, Canada*, pages 1599–1609, 2019.

[33] Sachin Ravi and Hugo Larochelle. Optimization as a model for few-shot learning. 2016.

[34] Mengye Ren, Eleni Triantafillou, Sachin Ravi, Jake Snell, Kevin Swersky, Joshua B. Tenenbaum, Hugo Larochelle, and Richard S. Zemel. Meta-learning for semi-supervised few-shot classification. In *6th International Conference on Learning Representations, ICLR 2018, Vancouver, BC, Canada, April 30 - May 3, 2018, Conference Track Proceedings*. OpenReview.net, 2018. URL https://openreview.net/forum?id=HJcSzz-CZ.

[35] Peter Welinder, Steve Branson, Takeshi Mita, Catherine Wah, Florian Schroff, Serge Belongie, and Pietro Perona. Caltech-ucsd birds 200. 2010.

[36] Luca Bertinetto, Joao F Henriques, Philip HS Torr, and Andrea Vedaldi. Meta-learning with differentiable closed-form solvers. *arXiv preprint arXiv:1805.08136*, 2018.

[37] Olga Russakovsky, Jia Deng, Hao Su, Jonathan Krause, Sanjeev Satheesh, Sean Ma, Zhiheng Huang, Andrej Karpathy, Aditya Khosla, Michael S. Bernstein, Alexander C. Berg, and Li Fei-Fei. Imagenet large scale visual recognition challenge. *Int. J. Comput. Vis.*, 115(3):211–252, 2015.

[38] Alex Krizhevsky, Vinod Nair, and Geoffrey Hinton. Cifar-10 (canadian institute for advanced research). *URL http://www. cs. toronto. edu/kriz/cifar. html*, 5:4, 2010.

[39] Puneet Mangla, Nupur Kumari, Abhishek Sinha, Mayank Singh, Balaji Krishnamurthy, and Vineeth N Balasubramanian. Charting the right manifold: Manifold mixup for few-shot learning. In *Proceedings of the IEEE/CVF Winter Conference on Applications of Computer Vision*, pages 2218–2227, 2020.

[40] Fabian Pedregosa, Gaël Varoquaux, Alexandre Gramfort, Vincent Michel, Bertrand Thirion, Olivier Grisel, Mathieu Blondel, Peter Prettenhofer, Ron Weiss, Vincent Dubourg, et al. Scikit-learn: Machine learning in python. *the Journal of machine Learning research*, 12:2825–2830, 2011.

[41] Yaoyao Liu, Bernt Schiele, and Qianru Sun. An ensemble of epoch-wise empirical bayes for few-shot learning. In Andrea Vedaldi, Horst Bischof, Thomas Brox, and Jan-Michael Frahm, editors, *Computer Vision - ECCV 2020 - 16th European Conference, Glasgow, UK, August 23-28, 2020, Proceedings, Part XVI*, volume 12361 of *Lecture Notes in Computer Science*, pages 404–421. Springer, 2020.

[42] Andrei A. Rusu, Dushyant Rao, Jakub Sygnowski, Oriol Vinyals, Razvan Pascanu, Simon Osindero, and Raia Hadsell. Meta-learning with latent embedding optimization. In *7th International Conference on Learning Representations, ICLR 2019, New Orleans, LA, USA, May 6-9, 2019*. OpenReview.net, 2019.

[43] Bin Liu, Yue Cao, Yutong Lin, Qi Li, Zheng Zhang, Mingsheng Long, and Han Hu. Negative margin matters: Understanding margin in few-shot classification. In Andrea Vedaldi, Horst Bischof, Thomas Brox, and Jan-Michael Frahm, editors, *Computer Vision - ECCV 2020 - 16th European Conference, Glasgow, UK, August 23-28, 2020, Proceedings, Part IV*, volume 12349 of *Lecture Notes in Computer Science*, pages 438–455. Springer, 2020.

[44] Yonglong Tian, Yue Wang, Dilip Krishnan, Joshua B Tenenbaum, and Phillip Isola. Rethinking few-shot image classification: a good embedding is all you need? In *Computer Vision–ECCV 2020: 16th European Conference, Glasgow, UK, August 23–28, 2020, Proceedings, Part XIV 16*, pages 266–282. Springer, 2020.

[45] Flood Sung, Yongxin Yang, Li Zhang, Tao Xiang, Philip HS Torr, and Timothy M Hospedales. Learning to compare: Relation network for few-shot learning. In *Proceedings of the IEEE conference on computer vision and pattern recognition*, pages 1199–1208, 2018.

[46] Luca Bertinetto, Joao F Henriques, Philip HS Torr, and Andrea Vedaldi. Meta-learning with differentiable closed-form solvers. *arXiv preprint arXiv:1805.08136*, 2018.

[47] Avinash Ravichandran, Rahul Bhotika, and Stefano Soatto. Few-shot learning with embedded class models and shot-free meta training. In *Proceedings of the IEEE/CVF International Conference on Computer Vision*, pages 331–339, 2019.

[48] Kwonjoon Lee, Subhransu Maji, Avinash Ravichandran, and Stefano Soatto. Meta-learning with differentiable convex optimization. In *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pages 10657–10665, 2019.

[49] Lénaïc Chizat, Pierre Roussillon, Flavien Léger, François-Xavier Vialard, and Gabriel Peyré. Faster wasserstein distance estimation with the sinkhorn divergence. In *Advances in Neural Information Processing Systems 33: Annual Conference on Neural Information Processing Systems 2020, NeurIPS 2020, December 6-12, 2020, virtual*, 2020.

[50] Jason Altschuler, Jonathan Weed, and Philippe Rigollet. Near-linear time approximation algorithms for optimal transport via sinkhorn iteration. In *Advances in Neural Information Processing Systems 30: Annual Conference on Neural Information Processing Systems 2017, December 4-9, 2017, Long Beach, CA, USA*, pages 1964–1974, 2017.

[51] Pavel E. Dvurechensky, Alexander V. Gasnikov, and Alexey Kroshnin. Computational optimal transport: Complexity by accelerated gradient descent is better than by sinkhorn's algorithm. In Jennifer G. Dy and Andreas Krause, editors, *Proceedings of the 35th International Conference on Machine Learning, ICML 2018, Stockholmsmässan, Stockholm, Sweden, July 10-15, 2018*, volume 80 of *Proceedings of Machine Learning Research*, pages 1366–1375. PMLR, 2018.

[52] Laurens Van der Maaten and Geoffrey Hinton. Visualizing data using t-sne. *Journal of machine learning research*, 9(11), 2008.

A   Computational Complexity

To approximate the general optimal transport (OT) distance between two discrete distributions of size n, the time complexity bound scales as $n^2 \log(n)/\varepsilon^2$ to reach ε-accuracy with Sinkhorn's algorithm, as demonstrated by Chizat et al. [49], Altschuler et al. [50], and Dvurechensky et al. [51]. In this paper, we set the maximum iteration number as Itermax $= 200$ in Sinkhorn algorithm for all experiments, which is typically enough for Sinkhorn algorithm to converge. We compare the computational cost of these two algorithms at the testing stage, on a Pentium PC with 3.7-GHz CPU and 64 GB RAM. Notably, similar to Free-Lunch, our proposed model is built on top of an arbitrary pretrained feature extractor and can avoid costly fine-tuning. Thus, we compare the computational complexity of two algorithms at the testing stage in Table 5. Although our model has a higher computational cost (our limitation) than Free-Lunch for introducing the hierarchical OT, it produces better performance with an acceptable cost. Below, we develop a deeper analysis.

For the high-level OT, we approximate the OT distance between the discrete distribution P and distribution Q, where the former has the size of B for B base classes, and the latter has the size of $N*K$ for the N-way-K-shot task. Now the time complexity bound scales as $O(\max(B, N * K)^2 \log(\max(B, N * K)))/\varepsilon^2$ to reach ε-accuracy with Sinkhorn's algorithm. For the low-level OT, we approximate the OT distance between the distribution R_b from the bth base class with J_b samples and distribution Q, where the former has the size of J_b and the latter has the size of $N*K$ for the N-way-K-shot task. Notably, when the number of samples in the bth base class is especially much, we can use the sub-sampling to build the empirical distribution R_b and then solve the low-level OT problem for saving the computational complexity. For high-level OT, B is usually larger than $N*K$ and its time complexity is $O(B^2 \log(B)/\varepsilon^2)$. For low-level OT, the J_b is generally larger than $N*K$ and thus the time complexity of low-level OT bound scales as $O(J_b{}^2 \log(J_b)/\varepsilon^2)$. Here, the number B of base classes of miniImageNet, CIFAR-FS, CUB, and tieredImageNet is 64, 64, 100, and 351, respectively. Besides, the average number J_b of images in each base class of miniImageNet, CIFAR-FS, CUB, and tieredImageNet is 600, 600, 59, and 1281, respectively. As we can see, tieredImageNet owns the largest B and J_b, whose running time is $9.31s$ for 5way1shot and $41.12s$ for 5way5shot. Therefore, our model can produce better performance with an acceptable overhead on large-scale dataset with larger numbers of classes and images. Notably, our model avoids the costly fine-tuning for backbone and it only takes time at the testing stage.

B   Additional results

Table 5: Comparison of computational cost when testing a novel task, where s denotes seconds.

Dataset	Free-Lunch[14]		Our Hierarchical OT	
	5way1shot	5way5shot	5way1shot	5way5shot
miniImageNet	2.34s	8.41s	2.91s	10.06s
tieredImageNet	5.76s	24.61s	9.31	41.12s
CUB	2.11s	8.24s	2.60s	11.12s
CIFAR-FS	2.22s	8.52s	3.06s	9.72s

B.1   Summary of the test results

To explore how our proposed model improves its baseline (Free-Lunch), we perform the experiments on 10,000 tasks from CIFAR-FS dataset using these two distribution calibration models, where the statistics about the classification results are shown in Fig. 4. We can see that our proposed model can effectively reduce the number of tasks with classification rates of less than 60%. To be our best knowledge, those novel tasks performed poorly by few-shot learning methods usually have the relatively large domain differences with all base classes, where the importance of each base class for novel sample might be similar. Different from Free-lunch, which only selects topw base classes to estimate the distribution of novel sample and might omit some relevant information, we utilizes all base classes by introducing the adaptive weight information over all base classes for each novel sample. It indicates that our proposed H-OT can effectively enhance distribution calibration method when there is a big domain difference between base and novel classes.

Figure 4: Statistics of the number of tasks among 10,000 tasks in total by their test accuracy.

B.2 Ablation study about the number of retrieved base classes

To explore how the classification performance of distribution calibration models is influenced by the number of retrieved base classes, we compare Free-Lunch, our high-level OT+Euc, and our H-OT in a 5-way-1-shot classification setting for CUB, as summarized in Tab. 6. We consider 5 different settings to select the base classes, including top-1, top-2, top-5, top-10, and all. We find that increasing the number of retrieved base classes results in a sharp drop in performance in terms of Free-lunch, but gradually enhances the performance of our proposed methods. We attribute this to the learning of the adaptive weight for each base class in our method, which is more flexible and effective than Free-lunch.

Table 6: Ablation study with number of retrieved base class statistics (5way1shot on CUB).

Models	top-1	top-2	top-5	top-10	all
Free-lunch	78.37 ± 0.75	$\mathbf{79.56 \pm 0.87}$	78.97 ± 0.80	78.49 ± 0.91	69.14 ± 0.88
High-level OT+Euc	80.08 ± 0.24	80.11 ± 0.23	80.15 ± 0.23	80.20 ± 0.26	$\mathbf{80.29 \pm 0.25}$
Our H-OT	80.77 ± 0.33	80.79 ± 0.30	80.87 ± 0.32	81.05 ± 0.32	$\mathbf{81.23 \pm 0.35}$

B.3 Visualization of generated features

To qualitatively show the effectiveness of our proposed methods, we show the t-SNE [52] representation of generated features by Free-Lunch and our proposed method in Fig. 5 and Fig. 6 given a same 5-way-1-shot task. We find that both our proposed model and Free-Lunch can generate more representative comprehensive features for each novel data. Besides, the generated features by ours are more discriminative than those by Free-Lunch. The phenomenon proves the benefits of learning the adaptive weight over base classes for novel sample.

B.4 Learned weights on the toy dataset.

To intuitively reveal whether our proposed model can address the limitations of Free-Lunch and learn effective weights to measure base classes, we design a synthetic dataset with the following procedure.
1. We sample B base classes from CIFAR-FS to build the base dataset. For easy observation, we set $B = 20$ and represent $\mu_b \in \mathbb{R}^V$ as the mean of the bth base class, and obtain the mean matrix $\mathbf{U} \in \mathbb{R}^{B \times V}$.
2. For the 5way1shot task, i.e., $N = 5, K = 1$, we use the gamma distribution with shape 0.8 and scale 1 to sample N vectors and normalize each vector. Now we get a weight matrix $\mathbf{W} \in \mathbb{R}_{\geq 0}^{N \times B}$, where $\boldsymbol{w}_n \in \Delta^B$ is the probability simplex of $\mathbb{R}^B$.

Figure 5: t-SNE projection of the generated features of Free-Lunch, where different colors represent different classes, the starts are the support set features and the small diamond are the generated features from the calibrated distributions, respectively.

Figure 6: t-SNE projection of the generated features of our H-OT, where different colors represent different classes, the starts are the support set features and the small diamond are the generated features from the calibrated distributions, respectively.

3. Finally, we synthesize N novel samples by weighting the mean matrix $\mathbf{U}$ with $\mathbf{W}$, i.e., $\mathbf{X} = \mathbf{UW}, \boldsymbol{x}_n \in \mathbb{R}^V$.

Given the base classes and 5way1shot task built from the generated novel samples, we adopt Free-Lunch and our high-level OT to learn the weight matrix, respectively, where the latter specifies the cost function with Euclidean distance between the novel sample and mean μ_b for a fair comparison. As shown in Fig. 7 in our revised version, we visualize the learned weights of different methods for a selected novel sample. Clearly, Free-Lunch does a hard selection of the top-2 base classes for the novel sample based on the Euclidean distance. However, the weights of the top-2 base classes are equal and the other base classes are ignored although some of them are also closely related to this novel sample. We observe that the weights based on our high-level OT can fit the ground-truth well. It indicates that our method can learn effective transport plan to weight the base classes for the novel sample.

B.5   Learned transport plan matrix and adaptive cost based on Hierarchical OT

One of the benefits of developing the hierarchical optimal transport for the adaptive distribution calibration is the enhancement of model interpretability. To further examine whether our proposed H-OT can capture the correlations between the base classes and novel samples, in Fig. 8, we visualize the adaptive cost learned from low-level OT and the transport plan learned from the high-level OT given the adaptive cost on CIFAR-FS for 5way1shot task. It is clear that the adaptive cost function can effectively reflect the distance between base classes and novel samples. For example, the novel sample from class "baby" is closely related with the base classes, such as "house" , "couch", "castle". And the novel sample from class "plain" is closely related with "elephant", "dinosaur", "kangaroo", "bear", "lion", "tiger", "wolf" and others. Benefiting from the cost function, the transport plan learned from the high-level OT can measure the importance of each base class for each novel sample in a more adaptive way. We note that the transport probability between a base class and a novel class is usually larger if their cost is smaller (*i.e.*, more relevant). Therefore, it is reasonable to view the learned transport probability matrix as the adaptive weight matrix, which can reflect the different contributions of the base classes. These observations suggest that our proposed H-OT can produce adaptive cost function and the adaptive weight matrix, providing an elegant and principled way to transfer the statistics from base classes to the novel classes.

Figure 7: Examples of learned weights of different methods for two synthetic novel samples, respectively.

B.6 Learned transport plan based on low-level OT

Taking the 5way1shot task on CIFAR-FS as an example, we further explore the per-example weights learned by our low-level OT. Specifically, we select the bth base class and the nth novel sample, and we visualize the learned J_b-dimensional weight vector $\{M_{j,n}^b\}_{j=1}^{J_b}$ in Fig. 9, where J_b denotes the number of samples within the bth base class. As expected, $M_{j,n}^b$, which tells us the transport weight between the nth novel sample and jth sample in the bth base class, is very different among J_b examples within the same base class. That is to say, each sample within the bth base class contributes to the nth novel class differently. Different from Free-lunch that measures the distance between novel sample n and base class b by only characterizing the base class as the unweighted average over all its samples, we use the learned weight vector to adaptively compute the distance between novel sample n and base class b.

B.7 Learned transport plan on the cross-domain setting

To further explore the learned transport plan when there is a significant shift between base and novel classes, in Fig. 10, we consider in-domain setting (CUB, top) and cross-domain setting (CIFAR-FS $\rightarrow$ CUB, bottom), both of which adopt same 5way1shot novel task from CUB. Compared with the in-domain scenario, we find that the transport plan learned in the cross-domain setting has a smaller magnitude of change. The reason might be that the distance between a base class and a novel class under the cross-domain settings is generally larger than that of the in-domain setting, making the importance of each base class for the novel sample more similar and reducing the gap between weights for base classes.

Figure 8: Learned cost between the base classes and novel samples and the resultant transport probability matrix, where we randomly select a novel task (5way1shot) from CIFAR-FS. The lighter the color is, the smaller the value is.

Figure 9: Learned per-example weights within base class Laysan Albatross, where the novel sample in the left figure is from the European Goldfinch class and novel sample in the right figure is from the Chipping Sparrow class.

Figure 10: Learned transport plan for same 5way1shot task on CUB (only a novel class is presented for simplify). The base classes in top figure (in-domain) and bottom figure (cross-domain) are from CUB and CIFAR-FS, respectively.