Dataset condensation with latent quantile matching

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Abstract

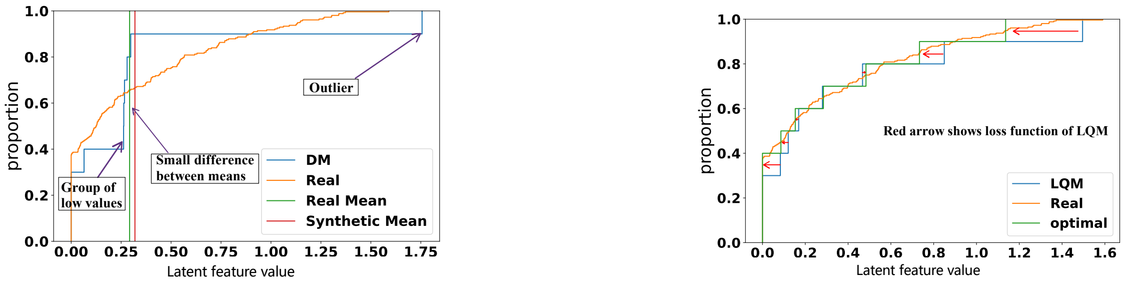
Dataset condensation (DC) methods aim to learn a smaller, synthesized dataset with informative data records to accelerate the training of machine learning models. Current distribution matching (DM) based DC methods learn a synthesized dataset by matching the mean of the latent embeddings between the synthetic and the real dataset. However, two distributions with the same mean can still be vastly different. In this work, we demonstrate the shortcomings of using Maximum Mean Discrepancy to match latent distributions, i.e., the weak matching power and lack of outlier regularization. To alleviate these shortcomings, we propose our new method: Latent Quantile Matching (LQM), which matches the quantiles of the latent embeddings to minimize the goodness of fit test statistic between two distributions. Empirical experiments on both image and graph-structured datasets show that LQM matches or outperforms previous state of the art in distribution matching based DC. Moreover, we show that LQM improves the performance in continual graph learning (CGL) setting, where memory efficiency and privacy can be important. Our work sheds light on the application of DM based DC for CGL.

1. INTRODUCTION

As the world becomes more connected, the available data increases exponentially. In order to learn knowledge that is generalizable to all the available data, large and complex deep models are proposed. The immense computational cost of training these models hinders their development, which is undesirable. Next, real-world datasets may contain sensitive data. These data can't be made public due to the privacy concerns. This hinders the research transparency and reproducibility. Dataset condensation (DC) can solve these issues by reducing the size of the training set. Instead of a large training set with potential redundant data records, DC methods aim to generate a small, synthetic dataset that is highly informative, which is also shown to be more privacy-preserving [13]. The deep learning models trained on the synthetic dataset should have similar evaluation performance compared to the models trained on the original, large training set. DC is applied to many problems, such as continual learning (CL) [28] [41], federated learning [15] and neural architecture search [37]. DC improves the state-of-the-art (SOTA) performance of CL with graph-structured data significantly [28]. However, the studies on applying DC to continual graph learning (CGL) problems are still scarce [28]. Our work focuses on improving DC and its application on CGL, we hope that our work sheds light on this under-explored field. We use the terms real dataset and original dataset interchangeably to refer to the dataset to condense.

Based on Sachdeva and McAuley [33], the SOTA dataset condensation methods are categorized into four categories: 1) Meta-Model Matching, 2) Gradient Matching, 3) Trajectory Matching, 4) Distribution Matching. The former three categories involve expensive bi-level optimization to achieve the goal of DC. I.e., they train a model for each optimization step of the synthetic dataset. Our work focuses on the last category, the distribution matching (DM) based DC methods. These methods do not have the costly bi-level optimization. Instead of comparing the distance between the learned parameters, or the gradients of the trained models, DM based DC methods initialize different models for each optimization steps, extract latent embeddings of both real and the synthetic dataset, and matches their distribution.

SOTA DM based DC methods use the Maximum Mean Discrepancy (MMD) to measure the distance between synthetic and real latent embeddings [38, 44, 46]. We note that comparing the mean of the latent embeddings is equivalent to comparing the sum of the mean of each individual latent feature distribution in the latent embedding. In the remainder of this work, we focus on the comparison between individual latent feature distributions. MMD only matches the mean of these distributions (i.e., first-order moment). As it does not provide any guarantee about other aspects of the matched distributions, they can still differ in statistics such as the variance, skewness, and kurtosis. This issue was identified



(a) Synthetic latent feature generated using MMD as distance function. The mean of the distribution matches. However, the synthetic distribution contains an outlier and there are no values in between 0.5 and 1.5. MMD fails to approximate the distribution.

(b) Synthetic latent feature generated using LQM as distance function. LQM minimizes the distance between synthetic data records and the optimal k-point approximations of the real distribution. LQM approximates the distribution better.

Figure 1. The empirical cumulative distribution function (ECDF) of a latent feature of class 0 in CIFAR-10 after 1900 epochs of training.

by Zhao et al. [46]. However, the author still used MMD as the distance function despite this shortcoming. As an empirical evidence, an example where the MMD fails to match the latent distribution is shown in Fig. 1a. In the synthetic dataset generated by MMD, there is one sample with very high value, while other samples have relatively low values. This matches the mean correctly, but it does not reflect the real distribution. The synthetic feature with the highest value is also larger than the maximum value in the real dataset, this may harm the learning process of the model.

Based on this observation, we believe that replacing MMD with a more suitable metric that reflects the distance between the distributions better, can improve the performance of DM based DC methods. We are inspired by goodness of fit tests in the field of statistics, which quantifies a distance between two empirical cumulative distribution functions (ECDF). Specifically, we propose a novel DM based DC method: Latent Quantile Matching (LQM) based on the two-sample Cramér-von Mises (CvM) test [2]. It estimates the squared difference between the two ECDFs. It is empirically shown to be more powerful [36] than the widely used Kolmogorov-Smirnov test [30], and there is a simple way to minimize the CvM test statistics for any number of data records k based on the optimal k-point discrete approximation studied in Kennan [21].

The objective of LQM is to minimize the difference between synthetic data records and optimal quantiles k in the latent space, which corresponds to the optimal k-point discrete approximation of the original latent distribution. This objective is similar to the Quantile Regression (QR) problem in the field of statistics [23]. However, the objective of QR is to express the quantiles of the distribution of the response variables as functions of the observable input variable. Our approach does not explicitly learn a model which predicts the values at a certain quantile. Instead, LQM tries to learn a small synthetic dataset that matches the different quantiles of the real dataset in the different latent spaces extracted by the feature extractors. Our approach tries to minimize the difference between synthetic latent features and the quantiles of the real latent features. In Fig. 1b, we show that the objective function is defined by the horizontal difference between the blue ECDF and the optimal green ECDF. As a result, the synthetic dataset produced by LQM discourages any outliers and approximates the real distribution better. Our contributions are as follows.

- We demonstrate the shortcomings of Maximum Mean Discrepancy as a metric to measure the distance between two empirical distributions. We reveal that two distribution with the same mean may not be similar.
- We propose a novel distribution matching based dataset condensation method: Latent Quantile Matching. We learn a small set of synthetic samples which match the different quantiles of the original dataset in the latent space. The quantiles are chosen based on the optimal k-point discrete approximation of the original latent distribution [21].
- We extensively evaluate LQM on image and graph datasets. Compared to previous studies, our experiments show the efficacy of our method with different data structure. Next, the experimental results show that the model trained on dataset learned by LQM outperform the models trained on dataset learned by MMD on most datasets. I.e., the performance gap between the model trained on the smaller synthetic dataset and the full, original dataset is reduced.
- We evaluate LQM in continual graph learning (CGL) setting with CaT-CGL [28]. We show that LQM outperforms SOTA CGL method. The performance improvement is larger when the synthetic dataset is small.

2. RELATED WORKS

Dataset Condensation. Dataset condensation (DC) aims to condense large training datasets into small synthetic datasets, while preserving the same evaluation performance when the model is trained only on the synthetic datasets. Wang et al. [39] proposed a way to maximize the performance of model trained using the synthetic dataset by using meta-learning.

Subsequent studies introduced different techniques such as soft-label [6], gradient-matching [45], data-augmentation [43], trajectory matching [9] and data-parameterization [22]. Despite their good performance, most of the methods rely on bi-level optimization involving second-order derivatives, which is computationally expensive.

On the contrary, Distribution Matching (DM) [44] proposes to condense the large training dataset into a synthetic dataset by matching the latent distribution between the two datasets using different, randomly initialized feature extractors. The distance between the latent distributions is measured by the Maximum Mean Discrepancy (MMD). DM does not require bi-level optimizations and is less computationally expensive compared to other approaches. Subsequent studies outperform DM by introducing techniques such as partition and expansion augmentation [46], trained feature extractors [46] and attention matching [34]. Despite the improvement in performance, all the above-mentioned methods use MMD to measure the distance between the two distributions. This makes them vulnerable to the shortcoming shown in Fig. 1a. In this work, we replace MMD with a distance function inspired by the goodness of fit tests in the field of statistics. Our distance function only reaches zero if the synthetic latent distribution is close to the specified quantiles of the original latent distribution for all classes.

Recently, Liu et al. [27] also studied the shortcomings of MMD, and replaces it with more powerful metrics. Our work is concurrent with theirs. Their work is based on optimal transport theory and uses Wasserstein Barycenter [1] as the matching metric. The computation of Wasserstein Barycenter is computationally expensive [8], and they used an approximation algorithm proposed by Cuturi and Doucet [12] to reduce it. In contrary, our work is not computationally expensive as it is based on statistical goodness of fit tests and uses the mean squared errors to the target quantiles as the metric. The computation of quantiles of an empirical distribution is not computationally expensive. By sorting the empirically drawn samples, we can retrieve all the quantiles of an ECDF. As an example, the time complexity of quicksort is $O(nlog(n))$ [19].

Goodness of Fit Tests. In statistics, a goodness of fit test measures how well a set of observed values fits a given statistical model. A subset of the tests quantifies the distance between two ECDFs. The Kolmogorov–Smirnov (KS) test [30] measures the maximum difference between the two ECDFs. The Cramér–von Mises (CvM) test [2] estimates the squared differences between the two ECDFs. The Anderson-Darling (AD) test [35] extends the CvM test by assigning more weights to the tails of the distributions. Previous studies show that the CvM and AD test are more powerful than the KS test [32]. Compared to MMD, these goodness of fit tests can match distributions beyond the first-moment. Our work uses optimal quantiles that minimize the CvM test statistic (CvM stat), proved by Kennan [21] and reported in Barbiero and Hitaj [4], as the regression target for the synthetic dataset. This ensures the similarity of the synthetic and the real latent distributions.

Continual (Graph) Learning. Continual Learning (CL) is a research field that benefits from DC. CL aims to build deep models that can acquire knowledge across different tasks without retraining from scratch. Amongst different CL methods, replay based methods obtain exceptional performances [31] [42] [3] [40]. They store a fraction of the data from the past tasks as memory buffer and replay them during the training of the new tasks. However, they require additional storage space and may raise privacy concerns. The advancements in dataset condensation show a promising direction to solve these problems. By condensing the dataset, the storage overhead can be reduced. Next, the privacy issue is alleviated, as the synthetic dataset is an obscured version of the real dataset, which is shown to be safe against membership-inference privacy attacks [13]. To the best of our knowledge, CaT-CGL [28] is the only work that studies DC in Continual Graph Learning (CGL). We incorporate our method into CaT-CGL and outperforms their method.

3. PRELIMINARIES

Dataset Condensation. Given a large training set $\mathcal{T} = (x_1, y_1), ..., (x_{|\mathcal{T}|}, y_{|\mathcal{T}|})$ containing $|\mathcal{T}|$ data records and their labels, DC aims to synthesize a smaller set $\mathcal{S} = (s_1, y_1^s), ..., (s_{|\mathcal{T}|}, y_{|\mathcal{T}|}^s)$, $|\mathcal{S}| \ll |\mathcal{T}|$, such that the deep models trained on $\mathcal{S}$ maintain similar evaluation performance as models trained on $\mathcal{T}$. Let x be a sample from the real data distribution P_D with label y, $\phi_{\theta^\mathcal{T}}$ and $\phi_{\theta^\mathcal{S}}$ be two variants of the same model ϕ with parameters θ trained on dataset $\mathcal{T}$ and $\mathcal{S}$, respectively, and $\mathcal{L}$ denotes the loss function (e.g., cross-entropy loss). The objective of DC is to find the ideal dataset $\mathcal{S}^*$ defined by the following equation.

$$\mathcal{S}^* = \underset{S}{argmin}\, \mathbb{E}_{x \sim P_D} ||\mathcal{L}(\phi_{\theta^\mathcal{T}}(x), y) - \mathcal{L}(\phi_{\theta^\mathcal{S}}(x), y)|| \quad (1)$$

Distribution Matching. Distribution Matching (DM) [44] proposed to tackle the DC problem by matching the distributions of the latent embeddings $\phi_\theta(x_i)$ and $\phi_\theta(s_j)$ for $\mathcal{T}$ and $\mathcal{S}$, respectively. The objective of distribution matching based DC methods is to find the ideal dataset $\mathcal{S}^*$ such that:

$$\mathcal{S}^* = \underset{S}{argmin}\, \mathcal{D}(\phi_\theta(\mathcal{T}), \phi_\theta(\mathcal{S})) \quad (2)$$

Where $\mathcal{D}$ denotes a distance function which takes as input the latent embeddings extracted by randomly initialized networks with parameter $\theta \sim P_{\theta_0}$. Compared to the general objective of DC, described in Eq. (1), DM's objective function does not require the model to be trained. Instead, DM attempts to learn the synthetic dataset with the same distribution as the real dataset with randomly initialized networks.

This surrogate objective makes the computational cost of DM based DC methods lower than the approaches that require bi-level optimization. When the distance function $\mathcal{D}$ is MMD, the objective is defined as:

$$\mathcal{S}^* = \underset{S}{arg\,min}\, \mathbb{E}_{\theta \sim P_{\theta_0}} || \frac{1}{|\mathcal{T}|} \sum_{i=1}^{|\mathcal{T}|} \phi_\theta(x_i) - \sum_{j=1}^{|\mathcal{S}|} \phi_\theta(s_j) || \quad (3)$$

Continual (Graph) Learning. The two most used settings in CL are Task-incremental (Task-IL) and Class-incremental (Class-IL). We focus on the more difficult Class-IL setting [47]. We assume a sequence of B tasks: $\{D^1, D^2, D^3, ...D^B\}$. $D^b = \{(x_i^b, y_i^b)\}_{i=1}^{n_b}$ denotes the b-th incremental training task with n_b data instances. Each task D contains data instances from one or more classes $c \in C$. We denote function Cls as a function that maps the task to the classes of the data instances it contains. The classes in each task D do not overlap with any other tasks defined in the sequence. Thus:

$$Cls(D^a) \cap Cls(D^b) = \emptyset, \forall a, b \in \{1, ..., B\}, a \neq b \quad (4)$$

During the b-th incremental training process, the model only has access to the data instances from the current task D^b. Rehearsal based methods can still access their memory buffer. After each incremental training process, the model is evaluated over all seen classes $C_{seen}^b = Cls(D^1) \cup ... \cup Cls(D^b)$. Class-IL aims to find the model $f(x) : X \mapsto C$ that minimizes the loss over all the tasks in the sequence.

4. METHODOLOGY

The base of our method lies on the two shortcomings that we observed with dataset condensation methods that use Maximum Mean Discrepancy (MMD) to measure the distance between the synthetic and the real latent embeddings. In this section, we explain the two shortcomings in detail, show that they can harm the distribution matching objective, and propose our new method: Latent Quantile Matching that alleviates the shortcomings.

4.1. Shortcomings of MMD

Inadequate distribution matching power. As the name Maximum Mean Discrepancy suggests, MMD only matches the mean of the empirical distributions (i.e., first-order moment). A previous study [16] has shown that, in the universal reproducing kernel Hilbert space (RKHS), asymptotically, MMD is 0 if and only if $P_X = P_Y$. Characterizing the function space explored by neural networks is a difficult and ongoing field of study. Recent works show that the function space of fully connected layers can be defined as trainable ladders of Hilbert spaces [10], or as reproducing kernel Banach space [5]. However, there are no studies that characterizes function spaces explored by the convolutional layers or graph neural networks yet. Our empirical observation in Fig. 1a suggests that in DC, there are cases where the mean of the latent feature distribution matches, but still differs in other statistics. This suggests that the feature extractors does not map the input to the universal RKHS. Therefore, a metric with stronger distribution matching power may be beneficial to the dataset condensation process.

No penalization for outliers/extreme values. The synthetic dataset is initialized by randomly choosing existing data records in the original dataset. Thus, it is probable that the initial synthetic dataset contains data records that yield extreme values in the latent space. During the distribution matching process, they may become more extreme, as the objective of MMD only matches the mean of the compared distributions. An example is shown in Fig. 1a. In the synthetic dataset, the largest value for the shown latent feature is larger than the corresponding largest value in the original dataset. They provide little information and waste valuable memory space that is limited for the synthetic dataset.

4.2. Proposed Method

To address the abovementioned shortcomings, we propose our new method: Latent Quantile Matching (LQM) which learns a synthetic dataset that minimizes the mean squared error between the latent features in the synthetic dataset and the target quantiles of the latent feature distributions in the real dataset. The objective of LQM is to find the optimal synthetic dataset S^* as defined in Eq. (2), where D denotes the sum of CvM test statistic (CvM stat) of the latent feature distributions. However, computing the CvM stat for each feature distribution for each epoch is time-consuming. Next, if we use it as the loss function, it will never reach zero. A zero CvM stat denotes that the ECDF of the synthetic latent distribution is the same as the ECDF of the real latent distribution, this is only possible if the number of data in the synthetic dataset is equal or larger than the number of data in the real dataset. Thus, a zero CvM stat is impossible and not desired in the scenario of DM based DC.

To establish an achievable objective, we utilize the optimal k-point discrete approximation of any distribution, as proposed in Kennan [21]. We define the set of optimal quantiles Q that minimizes the CvM stats for a synthetic dataset with k data records:

$$Q = \{\frac{2*1-1}{2k}, \frac{2*2-1}{2k}, ..., \frac{2k-1}{2k}\} \quad (5)$$

The ECDF constructed using values from these quantiles has the smallest CvM stat to the original distribution. The proof of this property can be found in Barbiero and Hitaj [4]. Using this property, and the fact that we have a predefined memory budget for the synthetic dataset, we can compute the quantiles that corresponds to the optimal points that minimizes the CvM stats for each latent feature distribution. This

Algorithm 1: Distribution Matching + Latent Quantile Matching

```
Input  : Training set $\mathcal{T}$
Params : Randomly initialized set of synthetic samples $\mathcal{S}$ for $\mathcal{C}$ classes, $|\mathcal{S}_c| = \beta_c$ for $c \in \mathcal{C}$, model $\phi_\theta$ parameterized
         with $\theta$, probability distribution over parameters $P_\theta$, train iterations $K$, learning rate $\eta$, quantile function
         $\mathcal{F}_q(Q, E) : \mathbb{R}^{D \times F} \mapsto \mathbb{R}^{|Q| \times F}$, $Q$ is the set of quantiles, $E$ is the batch of embeddings with $D$ data records
         and $F$ features, sort function $\mathcal{F}_s(E) : \mathbb{R}^{D \times F} \mapsto \mathbb{R}^{D \times F}$ sorts feature vectors $F$ in the ascending order.
for $k = 0$ to $K - 1$ do
    Sample $\theta$ from $P_\theta$
    for $c \in \mathcal{C}$ do
        Sample mini-batch $B_c^{\mathcal{T}} \sim \mathcal{T}$ and synthetic image $\mathcal{S}_c \subset \mathcal{S}$ for class $c$, $|S_c| = \beta_c$
        Compute the embeddings $\mathcal{E}_c^{\mathcal{T}} = \phi_\theta(x), x \in B_c^{\mathcal{T}}$ and $\mathcal{E}_c^{\mathcal{S}} = \phi_\theta(s), s \in \mathcal{S}_c$
        Compute the optimal quantiles $Q = \{\frac{2*1-1}{2\beta_c}, \frac{2*2-1}{2\beta_c}, ..., \frac{2*\beta_c-1}{2\beta_c}\}$, $|Q| = \beta_c$
        Compute $\mathcal{L} = \frac{1}{\beta_c}||\mathcal{F}_q(Q, \mathcal{E}_c^{\mathcal{T}}) - \mathcal{F}_s(\mathcal{E}_c^{\mathcal{S}})||^2$
        Update $S \leftarrow S - \eta\Delta_S\mathcal{L}$
Output : Condensed synthetic set $\mathcal{S}$
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provides us with a realistic objective that can be reached for the condensation process: When the loss reaches zero, the synthetic latent distribution represents the most optimal approximation, measured by the CvM stat, of the real latent distribution when we only have k data records. This objective is formally defined as:

$$S^* = \underset{S}{argmin} \frac{1}{|C|} \sum_{c \in C} ||\mathcal{F}_q(Q, \phi_\theta(\mathcal{T}_c)) - \mathcal{F}_s(\phi_\theta(\mathcal{S}_c))||^2 \quad (6)$$

Where $c \in C$, denotes the classes in the datasets. Q denotes the optimal quantiles computed using Eq. (5). $\mathcal{F}_q(Q, E) : \mathbb{R}^{D \times F} \mapsto \mathbb{R}^{|Q| \times F}$ denotes a quantile computation function with a set of quantiles and a series of embeddings as inputs, and outputs the quantiles for each latent feature. $\mathcal{F}_s(E) : \mathbb{R}^{D \times F} \mapsto \mathbb{R}^{D \times F}$ denotes a sort function that sorts each latent feature in the input embeddings in ascending order. LQM minimizes the distance between the latent feature in the synthetic dataset and the optimal quantiles that minimizes the CvM stat by sorting the synthetic latent feature and aligning them with the corresponding values of the optimal quantiles of the original latent feature distribution.

As our method only replaces the distance computation in the distribution matching process, it can be implemented on top of any existing DM based DC methods that compares the distance between two distributions. In Algorithm 1, the procedure of the proposed method, build on top of the basic distribution matching based DC algorithm is shown.

Limitation. As the initial data records are selected randomly, when the memory budget becomes larger, the initial synthetic latent distribution will already be similar to the original latent distribution. This diminishes the advantage of LQM as the difference in high-order moments between the synthetic and real latent distributions is smaller. Therefore, the impact of the first shortcoming of MMD is smaller. Next, when the budget is large, the impact of few outliers being selected in the initialization process and kept in the synthetic dataset is less severe. There are many other data records with latent features within the normal range, which will provide the model with enough information. Thus, when the synthetic dataset is large, the improvement of LQM compared to MMD may be less noticeable.

5. EXPERIMENTS

To validate the performance of LQM empirically. We implemented LQM on top of the SOTA DM based DC methods: 'Improved Distribution Matching' (IDM) [46] and 'Condense and Train' (CaT) [28] for image and graph-structured data, respectively. For DC with graph-structured data, we use the framework implemented by CaT-CGL [28] to evaluate our method in both the normal dataset condensation setting and in the continual graph learning (CGL) setting. CaT-CGL framework is implemented for CGL, However, the normal DC setting can be imitated by considering the full dataset as one task. We validate that LQM's performance in CGL by implementing it in Cat-CGL, and compare it with CaT: a CGL method that utilizes DM based DC with MMD as distance function [28]. Additionally, we include two baselines for the CGL experiments: 1) Finetuning, 2) Joint. They refer to training a model in CGL setting without any CGL method, and training a model using the full dataset, respectively.

Datasets. For the evaluation with image data, we used datasets of various complexity and sizes. CIFAR-10, CIFAR-100 [24] and TinyImageNet [25]. The task is to classify each image to the correct category. For graph-structured data, we used datasets from different domains. CoraFull [7], Arxiv [20], Reddit [18] and Product [20] graph datasets were used in our experiments. The tasks of these datasets are to classify each node into their corresponding category.

The details of the used datasets are reported in Sec. 5 and

Sec. 5. The budget per task row in Sec. 5 refers to the total number of nodes that we store in the synthetic dataset for each task in the CGL experiment. The budget is chosen such that each task is condensed to 1% of the original size.

DATASET	CIFAR10	CIFAR100	TINYIMAGENET
IMAGES	60,000	60,000	100,000
IMAGE SIZE	32x32x3	32x32x3	64x64x3
CLASSES	10	100	200

Table 1. Statistics of the experimented image datasets.

Dataset	CoraFull	Arxiv	Reddit	Products
Nodes	19,793	169,343	227,853	2,449,028
Edges	130,622	1,166,243	114,615,892	61,859,036
Features	8,710	128	602	100
Classes	70	40	40	46
Tasks	35	20	20	23
Budget/task	4	29	40	219

Table 2. Statistics of the experimented graph datasets.

Experimental settings. For both experiments, we evaluate the classification performance of deep learning models that are trained on the synthetic dataset learned by LQM. All experiments are run on a Tesla V100-SXM3-32GB GPU.

For image datasets, we learn 1/10/50 synthetic images per class. The training set is used to generate the synthetic dataset. The default hyperparameters of Zhao et al. [46] are used for all of our experiments. The performance is measured by the mean accuracy and standard deviation of 5 runs, where the models are randomly initialized and trained on the condensed synthetic dataset and evaluated on the test set of the real dataset.

For graph datasets, we learn a synthetic dataset that is 1% of the size of the original dataset. The number of nodes for each class is proportional to its ratio in the original dataset. In addition, a continual graph learning setting is used to show that LQM improves the performance in a more complex learning settings. Our work focus on the class-incremental CGL, where the model does not know from which task a sample belongs to. This is more difficult and realistic than the task-incremental setting, where the task identifier is available to the model at any time. To transform the dataset into the class-incremental setting, we first divided each dataset into train, validation, and test sets using a 6:2:2 ratio. Next, each set is divided into tasks. Each task only contains data of two unique, non-overlapping classes. The objective is to condense each task into a small synthetic dataset that is 1% of the original size. We use the default hyperparameters of Liu et al. [28] for all of our experiments. Performance is measured by the mean and standard deviation of average accuracy (AA) and backward transfer (BWT) of 5 runs. In each run, a model sequentially learns different tasks on the condensed dataset.

The average accuracy is defined as the average of accuracies $A_{k,i}$ for each previously learned task i. It measures the average performance of the model across all learned tasks.

$$AA_k = \frac{1}{k}\sum_{i=1}^{k} A_{k,i} \tag{7}$$

The backward transfer [29] indicates how the training of current tasks affects past tasks. A large number implies a greater impact, and the sign of the number denotes whether the impact is positive or negative. BWT is defined as:

$$BWT_k = \frac{1}{k-1}\sum_{i=1}^{k-1}(A_{k,i} - A_{i,i}) \tag{8}$$

6. RESULTS

6.1. Image datasets

We compare the performance of IDM+LQM against the SOTA dataset condensation (DC) methods in Tab. 3 and the CvM test statistic (CvM stat) between the synthetic and the real dataset for IDM and IDM+LQM in Fig. 2. We show the images in the synthetic dataset learned by IDM+LQM in the appendices. In Tab. 3, we include the performance of bi-level optimization based DC methods [11, 14, 17, 26, 38, 43, 45] to show that distribution matching (DM) based DC methods can match their performance. However, the focus of our work is on the comparison between our method 'IDM+LQM' and other DM based DC methods [34, 46]. IDM+LQM outperforms both the reported and our replicated results of IDM on CIFAR-10 and CIFAR-100 for all synthetic dataset size. On TinyImageNet, IDM+LQM match the replicated performance on 1 and 10 image per class, and underperforms in the 50 image per class setting.

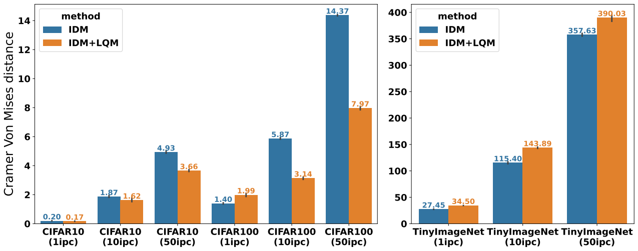

Figure 2. Comparison of average Cramér-von Mises stats between the synthetic dataset and the real dataset for each latent feature distribution. Lower number denotes higher probabilities that the compared samples (synthetic and real dataset in latent space) are drawn from the same distribution. The latent features are extracted by a pretrained model on the synthetic dataset.

Comparing the results from Tab. 3 and Fig. 2, we see that IDM+LQM outperforms IDM when the CvM stat between

Category	Methods	CIFAR-10			CIFAR-100			TinyImageNet		
Img / Cls		1	10	50	1	10	50	1	10	50
Ratio(%)		0.02	0.2	1	0.2	2	10	0.2	2	10
Bi-level Optimization	DC	28.3±0.5	44.9±0.5	53.9±0.5	12.8±0.3	25.2±0.3	-	-	-	-
	DSA	28.8±0.7	52.1±0.5	60.6±0.5	13.9±0.3	32.3±0.3	42.8±0.4	-	-	-
	CAFE	30.3±1.1	46.3±1.6	55.5±0.6	12.9±0.3	27.8±0.3	37.9±0.3	-	-	-
	CAFE+DSA	31.6±0.8	50.9±0.5	62.3±0.4	14.0±0.3	31.5±0.2	42.9±0.2	-	-	-
	DSAC	34.0±0.7	54.5±0.5	64.2±0.4	14.6±0.3	33.5±0.3	39.3±0.4	-	-	-
	FTD	46.8±0.3	66.6±0.3	73.8±0.2	25.2±0.2	43.4±0.3	50.7±0.3	10.4±0.3	24.5±0.2	-
	TESLA	48.5±0.8	66.4±0.8	72.6±0.7	24.8±0.4	41.7±0.3	47.9±0.3	-	-	-
	DATM	46.9±0.5	66.8±0.2	76.1±0.3	27.9±0.2	47.2±0.4	55.0±0.2	17.1±0.3	31.1±0.3	39.7±0.3
Distribution matching	DM	26.0±0.8	48.9±0.6	63.0±0.4	11.4±0.3	29.7±0.3	43.6±0.4	3.9±0.2	12.9±0.4	24.1±0.3
	DataDAM	32.0±1.2	54.2±0.8	67.0±0.4	14.5±0.5	34.8±0.5	49.4±0.3	8.3±0.4	18.7±0.3	**28.7±0.3**
	IDM	45.6±0.7	58.6±0.1	67.5±0.1	20.1±0.3	45.1±0.1	50.0±0.2	10.1±0.2	**21.9±0.2**	27.7±0.3
	IDM (replicated)	**45.3±0.5**	57.1±0.4	67.2±0.2	26.5±0.3	44.8±0.3	50.5±0.2	**10.3±0.4**	21.5±0.5	25.2±0.6
Full dataset	Full dataset	84.8±0.1			56.2±0.3			37.6±0.4		
Ours	IDM+LQM	**45.9±0.6**	**60.9±0.3**	**70.2±0.1**	**27.2±0.4**	**47.7±0.3**	**52.4±0.4**	**10.4±0.3**	20.8±0.4	24.3±0.3

Table 3. Comparison of test accuracy of randomly initialized model trained on condensed dataset. We evaluate our method on three different datasets with different numbers of synthetic images per class. Img/Cls: number of images per class. Ratio(%): the ratio of condensed images to the whole training set. Full Dataset: the accuracy of the model trained on the whole training set. The bold results are the best performance of the distribution matching-based dataset condensation methods within the margin of error, excluding 'Full Dataset' baseline. The best results of bi-level optimization based approaches are underlined. IDM+LQM uses the default parameter provided by IDM [46].

the synthetic and real dataset in the latent space is lowered noticeably, i.e., with 10 and 50 image per class. This supports our hypothesis that using a distribution matching metric beyond the first moment yields better DC performance.

Next, we note that all our experiments are performed using the default hyperparameters provided by IDM, except the training epoch of the network on the synthetic dataset during the evaluation. We increased it from 1000 to 2000 to ensure the model learns the synthetic dataset produced by LQM optimally. As LQM changes the loss function of the method, the hyperparameters used by IDM with MMD may not be optimal to IDM with LQM anymore. Combined with the limitation we discussed in Sec. 4, our LQM underperforms on the TinyImageNet dataset. Due to the time constraint, we were unable to optimize the hyperparameters. However, we believe that the performance of IDM+LQM in CIFAR-10 and CIFAR-100 is already sufficient to demonstrate the efficacy of our new method.

6.2. Graph datasets

To show that the efficacy of our method on complex learning settings, we compare the performance of CaT+LQM with other CGL baselines in Tab. 4. We experiment in two different settings, as indicated in the brackets on the category column. They are explained in Sec. 5. Our experiments use the default hyperparameters provided by CaT. Thus, the performance of CaT+LQM may benefit from further hyperparameter optimization. However, CaT+LQM already consistently matches or outperforms the replicated result of CaT that uses MMD. In the one task setting, CaT+LQM consistently outperform CaT. This validates that our method generalizes to graph-structured data. In the CGL setting, CaT+LQM has a higher average accuracy with similar or less negative impacts on past tasks in CGL setting, which is denoted by the higher backward transfer metric.

We observe that the improvement of AA is larger when the synthetic dataset is small, corresponding to the limitation we discussed in Sec. 4. On CoraFull and Arxiv, we have 4 and 29 nodes for the synthetic dataset per task, respectively. Compared to the replicated results, LQM improves AA by 2% and 1.4%, respectively. For larger datasets: Reddit and Product, where we have 40 and 318 nodes for the synthetic dataset per task, respectively, the improvement of LQM is less noticeable. LQM is 0.1% worse and 0.7% better in AA compared to the replicated results of CaT.

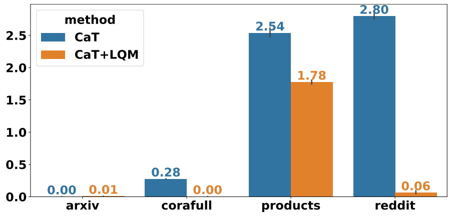

Figure 3. The average percentage of extreme latent values for each class. A value of one denotes that one percent of the latent features in each class in the synthetic dataset exceed the maximum or dropped below the minimum of the corresponding class latent distribution in the real dataset. The latent features are extracted by a pretrained model on the synthetic dataset.

The influence of the shortcomings of MMD is especially intriguing in the context of CGL experiments, where tasks are learned sequentially. When the first few tasks contain

Category	Methods	CoraFull		Arxiv		Reddit		Product	
		AA(%)↑	BWT(%)↑	AA(%)↑	BWT(%)↑	AA(%)↑	BWT(%)↑	AA(%)↑	BWT(%)↑
Dataset Condensation (One task)	CaT (replicated)	54.6±1.0	-	64.8±1.3	-	92.7±0.3	-	84.3±0.0	-
Ours (One task)	CaT+LQM	**57.5±0.2**	-	**67.6±0.4**	-	**92.8±0.1**	-	**84.4±0.1**	-
Lower Bound (CGL)	Finetuning	2.2±0.0	-96.6±0.1	5.0±0.0	-96.7±0.1	5.0±0.0	-99.6±0.0	4.3±0.0	-97.2±0.1
Dataset condensation (CGL)	CaT	64.5±1.4	**-3.3±2.6**	66.0±1.1	-13.1±1.0	**97.6**±0.1	**-0.2±0.2**	**71.0±0.2**	**-4.8±0.4**
	CaT (replicated)	66.1±0.6	-8.4±0.7	66.6±0.6	-12.4±0.5	97.2±0.0	-0.5±0.1	70.3±0.1	-5.0±0.1
Full dataset (CGL)	Joint	85.3±0.1	-2.7±0.0	63.5±0.3	-15.7±0.0	98.2±0.0	-0.5±0.0	72.2±0.4	-5.3±0.5
Ours (CGL)	CaT+LQM	**68.1±0.2**	-8.7±0.3	**68.0±0.3**	**-10.7±0.2**	97.1±0.0	-0.5±0.0	**71.0±0.2**	-4.9±0.2

Table 4. Comparison of AA and BWT of dataset condensation based CGL methods in Class-IL setting without inter-task edges. The bold results are the best performance excluding Joint baseline. ↑ denotes the greater value represents greater performance. Two different settings are expressed in the category column. CGL setting splits dataset into tasks with two classes per task, one task setting considers whole dataset as one task, which imitates the usual dataset condensation setting. In one task setting, BWT is not available as the model only learns one task, thus there is no transfer of knowledge between the tasks.

outliers, the model trained on these tasks will overfit to the outliers, which negatively impacts the generalization towards future tasks. In the non-continual learning experiments, all the data are available at the start, the model must generalize to all the samples at once. Thus, the effect of the outlier in the synthetic dataset is smaller. Our method penalizes the outliers explicitly, which results in better performance in the CGL setting. In Fig. 3, we show the average number of latent features of each class in the synthetic datasets that is higher than the maximum or lower than the minimum of the corresponding latent feature in the real dataset of the same class. We observe that CaT+LQM has low(er) number of extreme values in the latent feature. However, this does not fully explain why Arxiv performs much better than Reddit. We observe that CoraFull and Arxiv both have a low number of edges per node. As the graph convolutional layer aggregates neighboring features, the extreme values will be smoothed out. When there are many neighbors, the majority of the neighbor features will not be extreme values. On CoraFull and Arxiv, the smoothing effect is not strong, thus, LQM outperforms the MMD counterpart.

7. CONCLUSION

We propose a novel distribution matching (DM) based dataset condensation (DC) method: Latent Quantile Matching (LQM). It alleviates two shortcomings of the widely used Maximum Mean Discrepancy (MMD) based loss function, i.e., inadequate distribution matching power and lack of penalization for outliers/extreme values. Our method chooses specific values which the synthetic dataset should be aligned to based on the optimal k-point approximation that minimizes the Cramér-von Mises (CvM) test statistics between the two distributions, as studied in Kennan [21] and reported in Barbiero and Hitaj [4]. This alleviates the first shortcoming, as the goodness of fit tests matches the distributions on higher-order moments, while MMD only matches the mean, or the first-order moment. It also alleviates the second shortcoming, the extreme values will be penalized more as they are located further from the values at the optimal quantiles.

As the core of our method is the adapted computation of the distance between two distributions, we can easily implement it on top of other DM based DC methods that use MMD [28, 34, 44, 46]. Extensive empirical experiments on both image and graph datasets show that LQM outperforms or matches the performance of the counterpart that uses MMD. Moreover, the improvement of LQM is more noticeable with constraint memory budgets in the continual graph learning (CGL) setting. The severity of the two shortcomings increases as the memory budget decreases, since the outlier will have a higher influence within the limited synthetic dataset. This effect is more noticeable in CGL as the model can only learn a subset of the dataset for each task, therefore, the model is more likely to overfit to the outliers in the synthetic dataset. Thus, the improved result of LQM in CGL at low memory budget shows that LQM effectively alleviates the two shortcomings. As the objective of DC is to create small synthetic datasets, the advantage of LQM compared to MMD is going to be more prominent in future research. This property makes LQM a future direction on follow-up research regarding the DM distance functions in DM based DC methods.

Some future works include: 1) Evaluate the performance of LQM with other DM based DC methods. 2) Incorporate a heuristic based initialization procedure for the synthetic dataset to improve the performance. 3) Study the possibility of using other statistical metrics for DM based DC.

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References

[1] Martial Agueh and Guillaume Carlier. Barycenters in the wasserstein space. *SIAM Journal on Mathematical Analysis*, 43(2):904–924, 2011. 3

[2] Theodore W Anderson. On the distribution of the two-sample cramer-von mises criterion. *The Annals of Mathematical Statistics*, pages 1148–1159, 1962. 2, 3

[3] Benedikt Bagus and Alexander Gepperth. An investigation of replay-based approaches for continual learning. In *2021 International Joint Conference on Neural Networks (IJCNN)*, pages 1–9. IEEE, 2021. 3

[4] Alessandro Barbiero and Asmerilda Hitaj. Discrete approximations of continuous probability distributions obtained by minimizing cramér-von mises-type distances. *Statistical Papers*, 64(5):1669–1697, 2023. 3, 4, 8

[5] Francesca Bartolucci, Ernesto De Vito, Lorenzo Rosasco, and Stefano Vigogna. Understanding neural networks with reproducing kernel banach spaces. *Applied and Computational Harmonic Analysis*, 62:194–236, 2023. 4

[6] Ondrej Bohdal, Yongxin Yang, and Timothy Hospedales. Flexible dataset distillation: Learn labels instead of images. *arXiv preprint arXiv:2006.08572*, 2020. 3

[7] Aleksandar Bojchevski and Stephan Günnemann. Deep gaussian embedding of graphs: Unsupervised inductive learning via ranking. *arXiv preprint arXiv:1707.03815*, 2017. 5

[8] Steffen Borgwardt and Stephan Patterson. On the computational complexity of finding a sparse wasserstein barycenter. *Journal of Combinatorial Optimization*, 41(3):736–761, 2021. 3

[9] George Cazenavette, Tongzhou Wang, Antonio Torralba, Alexei A Efros, and Jun-Yan Zhu. Dataset distillation by matching training trajectories. In *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pages 4750–4759, 2022. 3

[10] Zhengdao Chen. Multi-layer neural networks as trainable ladders of hilbert spaces. In *International Conference on Machine Learning*, pages 4294–4329. PMLR, 2023. 4

[11] Justin Cui, Ruochen Wang, Si Si, and Cho-Jui Hsieh. Scaling up dataset distillation to imagenet-1k with constant memory. In *International Conference on Machine Learning*, pages 6565–6590. PMLR, 2023. 6

[12] Marco Cuturi and Arnaud Doucet. Fast computation of wasserstein barycenters. In *International conference on machine learning*, pages 685–693. PMLR, 2014. 3

[13] Tian Dong, Bo Zhao, and Lingjuan Lyu. Privacy for free: How does dataset condensation help privacy? In *International Conference on Machine Learning*, pages 5378–5396. PMLR, 2022. 1, 3

[14] Jiawei Du, Yidi Jiang, Vincent YF Tan, Joey Tianyi Zhou, and Haizhou Li. Minimizing the accumulated trajectory error to improve dataset distillation. In *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pages 3749–3758, 2023. 6

[15] Jack Goetz and Ambuj Tewari. Federated learning via synthetic data. *arXiv preprint arXiv:2008.04489*, 2020. 1

[16] Arthur Gretton, Karsten M Borgwardt, Malte J Rasch, Bernhard Schölkopf, and Alexander Smola. A kernel two-sample test. *The Journal of Machine Learning Research*, 13(1):723–773, 2012. 4

[17] Ziyao Guo, Kai Wang, George Cazenavette, Hui Li, Kaipeng Zhang, and Yang You. Towards lossless dataset distillation via difficulty-aligned trajectory matching. *arXiv preprint arXiv:2310.05773*, 2023. 6

[18] Will Hamilton, Zhitao Ying, and Jure Leskovec. Inductive representation learning on large graphs. *Advances in neural information processing systems*, 30, 2017. 5

[19] Charles AR Hoare. Quicksort. *The computer journal*, 5(1): 10–16, 1962. 3

[20] Weihua Hu, Matthias Fey, Marinka Zitnik, Yuxiao Dong, Hongyu Ren, Bowen Liu, Michele Catasta, and Jure Leskovec. Open graph benchmark: Datasets for machine learning on graphs. *Advances in neural information processing systems*, 33:22118–22133, 2020. 5

[21] John Kennan. A note on discrete approximations of continuous distributions. *University of*, 2006. 2, 3, 4, 8

[22] Jang-Hyun Kim, Jinuk Kim, Seong Joon Oh, Sangdoo Yun, Hwanjun Song, Joonhyun Jeong, Jung-Woo Ha, and Hyun Oh Song. Dataset condensation via efficient synthetic-data parameterization. In *International Conference on Machine Learning*, pages 11102–11118. PMLR, 2022. 3

[23] Roger Koenker and Kevin F Hallock. Quantile regression. *Journal of economic perspectives*, 15(4):143–156, 2001. 2

[24] Alex Krizhevsky, Geoffrey Hinton, et al. Learning multiple layers of features from tiny images. 2009. 5

[25] Ya Le and Xuan Yang. Tiny imagenet visual recognition challenge. *CS 231N*, 7(7):3, 2015. 5

[26] Saehyung Lee, Sanghyuk Chun, Sangwon Jung, Sangdoo Yun, and Sungroh Yoon. Dataset condensation with contrastive signals. In *International Conference on Machine Learning*, pages 12352–12364. PMLR, 2022. 6

[27] Haoyang Liu, Tiancheng Xing, Luwei Li, Vibhu Dalal, Jingrui He, and Haohan Wang. Dataset distillation via the wasserstein metric. *arXiv preprint arXiv:2311.18531*, 2023. 3

[28] Yilun Liu, Ruihong Qiu, and Zi Huang. Cat: Balanced continual graph learning with graph condensation. *arXiv preprint arXiv:2309.09455*, 2023. 1, 2, 3, 5, 6, 8

[29] David Lopez-Paz and Marc'Aurelio Ranzato. Gradient episodic memory for continual learning. *Advances in neural information processing systems*, 30, 2017. 6

[30] Frank J Massey Jr. The kolmogorov-smirnov test for goodness of fit. *Journal of the American statistical Association*, 46(253): 68–78, 1951. 2, 3

[31] Ameya Prabhu, Philip HS Torr, and Puneet K Dokania. Gdumb: A simple approach that questions our progress in continual learning. In *Computer Vision–ECCV 2020: 16th European Conference, Glasgow, UK, August 23–28, 2020, Proceedings, Part II 16*, pages 524–540. Springer, 2020. 3

[32] Nornadiah Mohd Razali, Yap Bee Wah, et al. Power comparisons of shapiro-wilk, kolmogorov-smirnov, lilliefors and anderson-darling tests. *Journal of statistical modeling and analytics*, 2(1):21–33, 2011. 3

[33] Noveen Sachdeva and Julian McAuley. Data distillation: A survey. *arXiv preprint arXiv:2301.04272*, 2023. 1

[34] Ahmad Sajedi, Samir Khaki, Ehsan Amjadian, Lucy Z Liu, Yuri A Lawryshyn, and Konstantinos N Plataniotis. Datadam: Efficient dataset distillation with attention matching. In *Proceedings of the IEEE/CVF International Conference on Computer Vision*, pages 17097–17107, 2023. 3, 6, 8

[35] Fritz W Scholz and Michael A Stephens. K-sample anderson–darling tests. *Journal of the American Statistical Association*, 82(399):918–924, 1987. 3

[36] Michael A Stephens. Edf statistics for goodness of fit and some comparisons. *Journal of the American statistical Association*, 69(347):730–737, 1974. 2

[37] Felipe Petroski Such, Aditya Rawal, Joel Lehman, Kenneth Stanley, and Jeffrey Clune. Generative teaching networks: Accelerating neural architecture search by learning to generate synthetic training data. In *International Conference on Machine Learning*, pages 9206–9216. PMLR, 2020. 1

[38] Kai Wang, Bo Zhao, Xiangyu Peng, Zheng Zhu, Shuo Yang, Shuo Wang, Guan Huang, Hakan Bilen, Xinchao Wang, and Yang You. Cafe: Learning to condense dataset by aligning features. In *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pages 12196–12205, 2022. 1, 6

[39] Tongzhou Wang, Jun-Yan Zhu, Antonio Torralba, and Alexei A Efros. Dataset distillation. *arXiv preprint arXiv:1811.10959*, 2018. 2

[40] Wei Wei, Tom De Schepper, and Kevin Mets. Benchmarking sensitivity of continual graph learning for skeleton-based action recognition. *arXiv preprint arXiv:2401.18054*, 2024. 3

[41] Enneng Yang, Li Shen, Zhenyi Wang, Tongliang Liu, and Guibing Guo. An efficient dataset condensation plugin and its application to continual learning. In *Thirty-seventh Conference on Neural Information Processing Systems*, 2023. 1

[42] Xikun Zhang, Dongjin Song, and Dacheng Tao. Cglb: Benchmark tasks for continual graph learning. *Advances in Neural Information Processing Systems*, 35:13006–13021, 2022. 3

[43] Bo Zhao and Hakan Bilen. Dataset condensation with differentiable siamese augmentation. In *International Conference on Machine Learning*, pages 12674–12685. PMLR, 2021. 3, 6

[44] Bo Zhao and Hakan Bilen. Dataset condensation with distribution matching. In *Proceedings of the IEEE/CVF Winter Conference on Applications of Computer Vision*, pages 6514–6523, 2023. 1, 3, 8

[45] Bo Zhao, Konda Reddy Mopuri, and Hakan Bilen. Dataset condensation with gradient matching. *arXiv preprint arXiv:2006.05929*, 2020. 3, 6

[46] Ganlong Zhao, Guanbin Li, Yipeng Qin, and Yizhou Yu. Improved distribution matching for dataset condensation. In *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pages 7856–7865, 2023. 1, 2, 3, 5, 6, 7, 8

[47] Da-Wei Zhou, Qi-Wei Wang, Zhi-Hong Qi, Han-Jia Ye, De-Chuan Zhan, and Ziwei Liu. Deep class-incremental learning: A survey. *arXiv preprint arXiv:2302.03648*, 2023. 4