# Bilevel Coreset Selection in Continual Learning: A New Formulation and Algorithm

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## Abstract

Coreset is a small set that provides a data summary for a large dataset, such that training solely on the small set achieves competitive performance compared with a large dataset. In rehearsal-based continual learning, the coreset is typically used in the memory replay buffer to stand for representative samples in previous tasks, and the coreset selection procedure is typically formulated as a bilevel problem. However, the typical bilevel formulation for coreset selection explicitly performs optimization over discrete decision variables with greedy search, which is computationally expensive. Several works consider other formulations to address this issue, but they ignore the nested nature of bilevel optimization problems and may not solve the bilevel coreset selection problem accurately. To address these issues, we propose a new bilevel formulation, where the inner problem tries to find a model which minimizes the expected training error sampled from a given probability distribution, and the outer problem aims to learn the probability distribution with approximately K (coreset size) nonzero entries such that learned model in the inner problem minimizes the training error over the whole data. To ensure the learned probability has approximately K nonzero entries, we introduce a novel regularizer based on the smoothed top-K loss in the upper problem. We design a new optimization algorithm that provably converges to the  $\epsilon$ -stationary point with  $O(1/\epsilon^4)$  computational complexity. We conduct extensive experiments in various settings in continual learning, including balanced data, imbalanced data, and label noise, to show that our proposed formulation and new algorithm significantly outperform competitive baselines. From bilevel optimization point of view, our algorithm significantly improves the vanilla greedy coreset selection method in terms of running time on continual learning benchmark datasets. The code is available at https://github.com/MingruiLiu-ML-Lab/ Bilevel-Coreset-Selection-via-Regularization.

## 1 Introduction

Deep Neural Networks (DNNs) have achieved tremendous successes in various domains, including computer vision [41, 30], natural language processing [72, 15], generative modeling [26] and

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Figure 1: Illustration of our algorithm. There are two neural network models, one is  $M_{tr}$  for model training, and the other is  $M_{cs}$  for coreset selection. A coreset is selected from the current data stream  $B_t$  by conducting six steps. (1) Feed a stream mini-batch  $B_t$  and sampled buffer data to  $M_{tr}$ . (2) Copy model parameters from  $M_{tr}$  to  $M_{cs}$ :  $\theta_{cs} \leftarrow \theta_{tr}$ . (3) Feed a mini-batch  $B_t$  into model  $M_{cs}$ . (4) Conduct bilevel optimization to update the model parameter  $\theta_{cs}$  in  $M_{cs}$  and output a probability distribution w. (5) Sample a coreset from  $B_t$  based on the distribution of w and add the sampled data into buffer. (6) Calculate stochastic gradient based on  $B_t$  and sampled data in the buffer in Step 1, and update  $\theta_{tr}$  based on gradient information. Repeat the above steps for each stream mini-batch.

games [68]. However, in continual learning, where DNNs are trained on a sequence of tasks with possibly non-i.i.d. data, the performance will be degraded on the previously trained tasks. This is referred to as *catastrophic forgetting* [53, 52, 60]. To alleviate catastrophic forgetting, one of the effective ways is *rehearsal-based continual learning*, where a small replay buffer is maintained and revisited during the continuous learning process. There is a line of works studying how to efficiently maintain the replay buffer using the coreset selection approach [6, 78, 83], in which a small set of data is selected as representative samples to be used in continual learning.

The coreset selection in continual learning is formulated as a cardinality-constrained bilevel optimization problem which is solved by incremental subset selection [6]. This greedy approach is computationally expensive and hence is not scalable when the coreset size is large. To address this issue, Zhou et al. [83] propose a relaxation of the bilevel formulation in [6], which drops the nested nature of bilevel formulation and actually becomes two sequential optimization problems. Tiwari et al.proposed a gradient approximation method in [71], which selects a coreset that approximates the gradient of model parameters over the entirety of the data seen so far. Yoon et al. [78] proposes an online coreset selection method by maximizing several similarity metrics based on data pairs within each minibatch, and sample pairs between each minibatch and coreset. These approaches do not directly address the algorithmic challenges caused by the nested nature of the bilevel optimization problem, and may not solve the original bilevel coreset selection problem efficiently.

The key challenges in the bilevel coreset selection problems are two folds. First, the bilevel formulation in [6] needs to directly perform optimization over cardinality constraint, which is a nonconvex set and greedy approaches are expensive when the coreset size is large. Second, the bilevel formulation in [6] has a nested structure: one problem is embedded within another, and the outer and inner functions both have dependencies over the same set of decision variables. It remains unclear how to design efficient algorithms to solve constrained bilevel optimization algorithms for the coreset selection problem with provable theoretical guarantees.

Our proposed solution addresses these challenges with a novel bilevel formulation and provably efficient optimization algorithms. The proposed new bilevel formulation is referred to as *Bilevel Coreset Selection via Regularization* (BCSR). The main differences between our approach and the standard bilevel approach in [6] are: (i) unlike the standard bilevel formulation which requires performing optimization based on a cardinality constraint, we propose to solve a bilevel optimization on a probability simplex over training examples; (ii) to make sure the probability distribution lies in a low dimensional manifold, we propose to add a smoothed top-K loss as a regularizer to the upper-level problem; (iii) due to our new formulation, we are able to design a simple and effective first-order method to solve this new bilevel problem with provable non-asymptotic convergence guarantees. The first-order method is easy to implement and much faster than the greedy approach as in [6]. Our main contribution is listed as follows.

Algorithm 1 PyTorch-style pseudocode for BCSR

```
1 # tasks: the task sequences; T: the number of tasks
2 # L(): loss function; x: image batch, y: label batch
3 # model, model_proxy: for training and coreset selection
4 # update_w: a function updating outer variable w
5 M = [[] * T]
                 # memory buffer
6 for ind, task in tasks:
      for (x, y) in dataloader:
          model_proxy.load_state_dict(model.parameters())
8
9
          (x_m, y_m) = next_batch(M)
          out1 = model(x)
10
          out2 = model(x_m)
          loss = L (out1, y) + L (out2, y_m)
          loss.backward()
          (x_core, y_core) = find_coreset(x, y, K, model_proxy)
14
          M[ind].append((x_core, y_core))
15
          update(model.params)
16
17 def find_coreset(x, y, K, model_proxy):
18
      coreset_w = 1.0/y.size()
      for j in range(outer_loops):
19
          for i in range(inner_loops):
20
               lower_loss = L (coreset_w * model (x, y) )
21
              lower_loss.backward()
23
              update(model_proxy.params)
          coreset_w = update_w(coreset_w)
24
      return torch.multinomial(coreset_w , K)
25
```

- We propose a new bilevel formulation, namely BCSR, for the coreset selection in rehearsalbased continual learning. Instead of directly learning the binary masks for each sample, the new formulation tries to learn a probability distribution in a low-dimensional manifold by adding a smoothed top-K loss as a regularizer in the upper problem. This formulation is designed to satisfy two important features in continual learning with DNNs: (i) keeping the nested structure in the coreset selection; (ii) being amenable to first-order algorithms, which makes it easy to implement in modern deep learning frameworks such as PyTorch and TensorFlow. Based on the new formulation, we propose an efficient first-order algorithm for solving it. The main workflow of our algorithm is illustrated in Figure 1, and the corresponding Pytorch-style pseudocode is presented in Algorithm 1.
- We have conducted extensive experiments among various scenarios to verify the effectiveness of our proposed algorithm, including balanced, imbalanced, and label-noise data. Our algorithm outperforms all baselines for all settings in terms of average accuracy, and it is much better than all other coreset selection algorithms. For example, on imbalanced data of Multiple Datasets, BCSR is better than the best coreset selection algorithm by 4.65% in average accuracy. From bilevel optimization point of view, our algorithm significantly improves the vanilla greedy coreset selection method [6] in terms of running time on continual learning benchmark datasets.
- Under the standard smoothness assumptions of the loss function, we show that our algorithm requires at most  $O(1/\epsilon^4)$  complexity for finding an  $\epsilon$ -stationary point in the constrained case<sup>2</sup>. Notably, the  $O(1/\epsilon^4)$  complexity consists of  $O(1/\epsilon^2)$  backpropagations and  $O(1/\epsilon^4)$  samplings from Gaussian distribution, where the latter cost is computationally cheap.

# 2 Related Work

**Continual Learning** There are different classes of continual learning methods, including regularization-based approaches [39, 81, 10, 1, 59, 64, 17], dynamic architecture methods [61,

<sup>&</sup>lt;sup>2</sup>In the constrained setting, the definition of  $\epsilon$ -stationary point is defined with gradient mapping, i.e., w is a  $\epsilon$ -stationary point of the function  $\phi$  if  $\frac{1}{\beta} || w - \mathcal{P}_{\Delta}(w - \beta \nabla \phi(w)) || \le \epsilon$ , where  $\beta$  is the stepsize,  $\mathcal{P}$  is the projection operator,  $\Delta$  is the probability simplex. This matches the best iteration complexity as in the single level optimization problem [24].

79, 62, 51, 76, 44, 77], and rehearsal-based methods [48, 57, 11, 58, 31, 3, 18, 28, 80, 6, 83, 78, 84]. In the rehearsal-based continual learning, the memory is either reproduced experience replay [48] or generative replay [67]. Our work focuses on the aspect of the coreset selection on the replay memory and can be flexibly integrated into rehearsal-based methods in continual learning.

**Coreset Selection** The coreset selection methods were used frequently in supervised and unsupervised learning, such as k-means [19], Gaussian mixture model [49], logistic regression [33] and bayesian inference [9]. They were also used frequently in the active learning literature [74, 63]. The coreset selection in continual learning is related to the sample selection [34, 2, 3]. Nguyen et al. [55] introduce variational continual learning which is combined with coreset summarization [5]. Borsos et al. [6] proposed the first bilevel formulation for the coreset selection in continual learning, which is later improved by [83, 78]. Compared with these works, our work focuses on improved bilevel coreset selection: we provide a better bilevel formulation than [6] and design a provably efficient optimization algorithm.

**Bilevel optimization** Bilevel optimization is used to model nested structure in the decision-making process [73]. Recently, gradient-based bilevel optimization methods have broad applications in machine learning, including meta-learning [20], hyperparameter optimization [56, 22], neural architecture search [46], and reinforcement learning [40, 32]. These methods can be generally categorized into implicit differentiation [16, 56, 45, 4] and iterative differentiation [50, 21, 20, 65, 27] based approaches. Recently, various stochastic bilevel algorithms have been also proposed and analyzed by [12, 37, 25, 32, 29, 4, 14]. A comprehensive introduction can be found in the survey [47]. In this work, we propose a novel stochastic bilevel optimizer with very flexible parameter selection, which shows great promise in the coreset selection for continual learning.

# 3 New Bilevel Formulation for Coreset Selection in Continual Learning

In this section, we first introduce our new bilevel formulation, namely Bilevel Coreset Selection via Regularization (BCSR). The key idea of this approach is to learn a probability distribution over the whole dataset such that the best model parameter obtained by minimizing the loss on the sampled dataset (i.e., the minimizer for the lower-level problem) is also the best for the whole dataset (i.e., the minimizer for the upper-level problem), and then a coreset can be sampled based on the learned probability distribution. In addition, the learned probability distribution is expected to lie in a low dimensional manifold (i.e., with K nonzero entries where K is the coreset size). To achieve this, we added a smooth top-K loss as a regularizer to promote the probability distribution to have K nonzero entries. Specifically, the objective function of BCSR is:

$$\min_{\substack{0 \le w_{(i)} \le 1 \\ ||w||_1 = 1}} \left[ \phi(w) = \sum_{i=1}^n \ell_i(\theta^*(w)) - \lambda \sum_{i=1}^K \mathbb{E}_z(w + \delta z)_{[i]} \right]$$

$$s.t., \theta^*(w) = \arg\min_{\theta} \left[ L(\theta, w) = \sum_{i=1}^n w_{(i)}\ell_i(\theta) \right]$$
(1)

where *n* is the sample size,  $\theta$  is the model parameter, *w* is the sample weights,  $\ell_i(\theta)$  denote the loss function calculated based on *i*-th sample with model parameter  $\theta$ ,  $w_{(i)}$  is the *i*-th coordinate of *w*,  $w_{[i]}$ is the *i*-th largest component of *w*,  $\lambda > 0$  is the regularization parameter,  $w + \delta z$  denote to adding  $\delta z$ on each coordinate of *w* where  $z \sim \mathcal{N}(0, 1)$ . Note that  $R(w, \delta) := -\lambda \sum_{i=1}^{K} \mathbb{E}_z(w + \delta z)_{[i]}$  denote the smoothed top-*K* regularization. We add this regularization to make sure the summation of the top-*K* entries of the learned probability vector is large, such that we can confidently choose a coreset with size *K*. The goal of employing Gaussian noise to the regularizer is for the ease of algorithm design: this Gaussian smoothing technique can make the regularizer to be smooth such that it is easier to design efficient first-order bilevel optimization solvers. Otherwise, the upper-level problem would become nonconvex and nonsmooth, and it would be difficult for algorithm design under this case.

**Discussion and Comparison with Prior Works** In this part, we illustrate how this new formulation addresses the drawbacks of the previous approaches. The work of [6] does not use any regularizer and regards the weight of each sample as a binary mask. This formulation needs to solve a combinatorial

#### Algorithm 2 Bilevel Coreset Selection via Regularization (BCSR)

Input: Dataset  $\mathcal{D}$ Initialize: model parameter  $\theta_0$ , memory  $\mathcal{M} = \{\}$ 1: for batch  $\mathcal{B}_t \sim \mathcal{D}$  do 2: Compute coreset  $\mathcal{S}_t = \text{Find-coreset}(\theta_{t-1}, \mathcal{B}_t)$ 3:  $\mathcal{M} = \mathcal{M} \cup \mathcal{S}_t$ 4: end for

## Algorithm 3 Find-coreset( $\theta$ , $\mathcal{B}$ )

**Input**: the current model parameter  $\theta$ , the current batch  $\mathcal{B}$ , the iteration parameters J, N, Q**Initialize**: coreset size  $K, n = |\mathcal{B}|$ , and  $v_0$ 

1:  $w_0 = \left[\frac{1}{n}, \ldots, \frac{1}{n}\right]$  (uniform probability initialization) 2:  $\theta_1^0 = \theta$ 2.  $\theta_1 = 0$ 3. for j = 0, 2, ..., J - 1 do 4. Set initialization  $\theta_j^0 = \theta_{j-1}^N$  if j > 0 and  $\theta_1^0$  otherwise 5. for k = 1, ..., N do 6. update  $\theta_j^k$  according to eq. (2). 7: end for Set initialization  $v_j^0 = v_{j-1}^Q$  if j > 0 and  $v_0$  otherwise 8: Compute estimate  $v_i^Q$  by solving QP in (4) by GD with stepsize  $\eta$  and initial  $v_i^0 = v_{i-1}^Q$ . 9: Compute hypergradient estimate in (3) 10: Update  $w_{i+1}$  and project it onto simplex by (5) 11: 12: end for 13:  $\mathcal{S} \leftarrow$  a set of K data points sampled from  $\mathcal{B}$  according to the probability distribution  $w_J$ 14: Return S

optimization problem and their approach of incremental subset selection is computationally expensive. The work of [83] relaxes the bilevel formulation in [6] to minimize the expected loss function over the Bernoulli distribution s, i.e.,  $\min_{s \in C} \Phi(s)$ , and develops a policy gradient solver to optimize the Bernoulli variable. Their gradient  $\nabla_s \Phi(s) = \mathbb{E}_{p(m|s)} L(\theta^*(m)) \nabla_s \ln p(m|s)$  does not include the implicit gradient of  $L(\theta^*(m))$  in terms of s. However,  $\theta^*(m)$  actually depends on the mask m, and m depends on the Bernoulli variable s. In contrast, our bilevel optimization computes the hypergradients for the coreset weights w ( $0 \le w \le 1$  and  $||w||_1 = 1$ ), which considers the dependence between  $\theta(w)$  and  $w^3$ . In addition, Zhou et al. [83] assume that the inner loop can obtain the exact minimizer  $\theta^*(m)$ , which may not hold in practice. In contrast, we carefully analyze the gap between the estimated  $\theta^*(w)$  and itself by our algorithm and analysis.

# 4 Algorithm Design

Equipped with the new formulation, the entire algorithm is presented in Algorithm 2, which calls Algorithm 3 as a subroutine. Each time the algorithm encounters a minibatch  $\mathcal{B}$ , a coreset is selected within this minibatch by invoking Algorithm 3. Algorithm 3 is a first-order algorithm for solving the bilevel formulation (1). In Algorithm 3, the model parameter  $\theta$  and the weight distribution w are updated alternatively. We first perform N steps of gradient descent steps to find a sufficiently good  $\theta$ for the lower-level problem (lines 5-7) by the update rule:

$$\theta_j^k = \theta_j^{k-1} - \alpha \nabla_\theta L(\theta_j^{k-1}, w_j), \tag{2}$$

where  $\theta_j^k$  denotes the model parameters at the *j*-th outer loop and the *k*-th inner loop. To update the outer variable *w*, BCSR approximates the true gradient  $\nabla \phi(w)$  of the outer function w.r.t *w*, which is called hypergradient [56]. BCSR constructs a hypergradient estimator:

$$\varphi_j = \frac{1}{|\mathcal{B}|} \sum_{\widetilde{z} \in \mathcal{B}} \nabla_w R(w, \delta; \widetilde{z}) - \nabla_w \nabla_\theta L(\theta_j^N, w_j) \Big[ (\nabla_\theta^2 L(\theta_j^N, w_j))^{-1} (\sum_{i=1}^n \nabla_\theta \ell_i(\theta_j^N)) \Big], \quad (3)$$

<sup>&</sup>lt;sup>3</sup>The coreset weight w in our formulation is equivalent to sample mask s in [83]

Table 1: Experiment results on Split CIFAR-100

	Bala	anced	Imba	lanced	Labe	l Noise
Methods	$A_T$	$FGT_T$	$A_T$	$FGT_T$	$A_T$	$FGT_T$
K-means Features	57.82±0.69	0.070±0.003	45.44±0.76	0.037±0.002	57.38±1.26	0.098±0.003
K-means Embedding	59.77±0.24	0.061±0.001	43.91±0.15	0.044±0.001	57.92±1.25	0.091±0.016
Uniform	58.99±0.54	$0.074 \pm 0.004$	44.73±0.11	0.033±0.007	58.76±1.07	0.087±0.006
iCaRL	60.74±0.09	0.044±0.026	44.25±2.04	0.042±0.019	59.70±0.70	0.071±0.010
Grad Matching	59.17±0.38	0.067±0.003	45.44±0.64	0.038±0.001	59.58±0.28	0.073±0.008
SPR	59.56±0.73	0.143±0.064	44.45±0.55	0.086±0.023	58.74±0.63	0.073±0.010
MetaSP	60.14±0.25	0.056±0.230	43.74±0.36	0.079±0.014	57.43±0.54	0.086±0.007
Greedy Coreset	59.39±0.16	0.066±0.017	43.80±0.01	0.039±0.007	58.22±0.16	0.066±0.001
GCR	58.73±0.43	0.073±0.013	44.48±0.05	0.035±0.005	58.72±0.63	0.081±0.005
PBCS	55.64±2.26	0.062±0.001	39.87±1.12	0.076±0.011	56.93±0.14	0.100±0.003
OCS	52.57±0.37	$0.088 \pm 0.001$	46.54±0.34	0.022±0.003	51.77±0.81	0.103±0.007
BCSR	61.60±0.14	0.051±0.015	47.30±0.57	0.022±0.005	60.70±0.08	0.059±0.013

where  $R(w, \delta; \tilde{z}) := -\lambda \sum_{i=1}^{K} (w + \delta \tilde{z})_{[i]}$  and  $\tilde{z} \sim \mathcal{N}(0, 1)$ . Solving the Hessian-inverse-vector product in eq. (3) is computationally intractable. We denote  $v^* := (\nabla^2_{\theta} L(\theta^N_j, w_j))^{-1} (\sum_{i=1}^n \nabla_{\theta} \ell_i(\theta^N_j))$  in eq. (3), where  $v^*$  can be approximated by solving the following quadratic programming problem efficiently by Q steps of gradient descent (line 9):

$$\min_{v} \frac{1}{2} v^T \nabla^2_{\theta} L(\theta^N_j, w_j) v - v^T \sum_{i=1}^n \nabla_{\theta} \ell_i(\theta^N_j).$$
(4)

Next, the hypergradient estimate (line 10) is computed based on the output of approximated quadratic programming. Note both model parameters and sample weights need to use warm start initialization (line 4 and line 8). Then the weight is updated and projected onto simplex (line 11):

$$\hat{w}_{j+1} = w_j - \beta \varphi_j, \quad w_{j+1} = \mathcal{P}_{\Delta^n}(\hat{w}_{j+1}), \tag{5}$$

where  $\Delta^n := \{w \in \mathbb{R}^n : 0 \le w_{(i)} \le 1, ||w||_1 = 1\}$ . In terms of other experimental hyperparameters, we allow very flexible choices of hyperparameters (e.g., N, Q) as shown in our theory to achieve polynomial time complexity for finding a  $\epsilon$ -stationary point.

The selected coresets for each task are stored in a memory buffer with a fixed size m. There is a separated memory slot for each task with size [m/i] when the task i comes. After each task i, the memory slots before i will randomly remove some samples to adjust all the memory slots to [m/i]. That means the memory size for each task decreases as the task ID increase to maintain the total buffer size m unchanged. The same memory strategy is also used in the greedy coreset approach [6].

# 5 Experiments

We conduct extensive experiments under various settings, including balanced data, imbalanced data, and label-noise data. The empirical results demonstrate the effectiveness of our method in rehearsal-based continual learning.

#### 5.1 Experimental Setup

**Datasets** We use commonly-used datasets in the field of continual learning, including Split CIFAR-100, Permuted MNIST, Multiple Datasets, Tiny-ImageNet, and Split Food-101. We follow the experimental settings as that in prior work [78] and [83]. Each dataset is processed with three approaches: balanced, imbalanced, and label-noise. Please refer to Appendix L for more details about data processing and settings.

**Baselines** We compare our algorithm BCSR with other continual learning methods based on coreset strategy, including *k*-means features [55], *k*-means embedding [63], Uniform Sampling, iCaRL [57], Grad Matching [9], Greedy Coreset [6], PBCS [83], GCR [71], and OCS [78]. We also compare with non-coreset reply method, SPR [38], MetaSP [70]. All algorithms are built upon episodic memory, which stores coreset selected from stream data. Then a model, such as ResNet-18 [30], is trained over the data from the current stream and the episodic memory.

**Metrics** Average accuracy and forgetting measure [10] are two primary evaluation metrics that are used in continual learning literature. AVG ACC  $(A_T)$  is the average accuracy tested on all tasks after finishing the task  $T: A_T = \frac{1}{T} \sum_{i=1}^{T} a_{T,i}$ , where  $a_{T,i}$  is the test accuracy of task *i* after training

		1		1		
	Bala	anced	Imba	lanced	Label Noise	
Methods	$A_T$	$FGT_T$	$A_T$	$FGT_T$	$A_T$	$FGT_T$
K-means Features	54.63±0.88	0.138±0.007	33.63±2.66	0.136±0.063	45.46±3.50	0.120±0.049
K-means Embedding	56.83±1.65	0.106±0.019	35.93±1.60	0.106±0.031	46.32±3.19	0.084±0.030
Uniform	55.93±0.03	0.101±0.032	35.48±2.96	0.104±0.025	48.68±0.44	0.079±0.002
iCaRL	56.19±0.32	0.130±0.012	42.18±1.59	0.057±0.022	49.22±0.54	0.067±0.010
Grad Matching	53.41±0.46	0.119±0.020	38.16±3.90	0.082±0.003	46.96±1.05	0.091±0.029
SPR	56.20±1.91	0.124±0.036	40.79±1.73	0.143±0.051	49.77±1.58	0.062±0.024
MetaSP	57.14±1.10	0.113±0.042	41.32±1.50	0.103±0.053	47.14±1.66	0.081±0.027
Greedy Coreset	53.56±0.06	0.099±0.005	22.57±1.10	0.265±0.022	41.32±1.51	0.137±0.009
GCR	54.35±0.31	0.125±0.014	35.13±2.79	0.105±0.043	47.58±1.30	0.078±0.016
PBCS	52.93±0.28	0.152±0.016	37.25±2.93	0.115±0.033	47.51±1.56	0.101±0.021
OCS	55.65±2.26	$0.062 \pm 0.001$	40.48±1.39	0.051±0.003	45.03±4.16	0.049±0.012
BCSR	59.89±0.95	$0.096 \pm 0.005$	45.13±0.54	0.046±0.008	49.97±1.14	0.064±0.031

Table 2: Experiment results on Multiple Datasets

Table 3: Experiment results on Tiny-ImageNet

	Bala	inced	Imba	lanced	Label	Noise
Methods	AVG ACC	FGT	AVG ACC	FGT	AVG ACC	FGT
K-means Features	41.20±0.75	0.131±0.004	36.27±0.30	0.079±0.014	36.68±1.35	0.095±0.004
K-means Embedding	41.48±1.21	0.129±0.007	36.29±0.23	0.085±0.003	36.01±1.51	0.083±0.005
Uniform	42.11±0.52	0.129±0.002	37.07±0.53	0.083±0.009	37.14±1.05	0.099±0.003
iCaRL	43.84±0.09	0.114±0.004	37.65±0.84	0.058±0.003	38.52±0.25	0.063±0.006
Grad Matching	43.45±0.32	0.105±0.007	37.58±0.39	$0.066 \pm 0.004$	38.84±0.42	$0.064 \pm 0.006$
SPR	42.79±0.50	0.102±0.009	36.55±0.74	0.070±0.026	39.89±0.53	0.065±0.021
MetaSP	43.33±0.32	0.127±0.002	36.75±0.57	$0.086 \pm 0.006$	37.18±0.76	$0.068 \pm 0.007$
Greedy Coreset	41.02±0.33	0.119±0.017	33.43±0.86	0.103±0.002	36.37±0.16	0.079±0.006
GCR	41.45±0.35	0.125±0.008	36.08±0.62	0.072±0.017	37.46±0.40	0.115±0.011
PBCS	36.99±0.15	0.177±0.002	35.88±0.16	0.071±0.080	37.02±0.16	0.133±0.029
OCS	41.29±0.09	0.112±0.001	35.09±0.60	0.036±0.011	35.36±0.94	0.061±0.005
BCSR	44.13±0.33	$0.106 \pm 0.001$	38.59±0.11	$0.070 \pm 0.004$	40.72±0.56	$0.055 \pm 0.006$

the task T.  $FGT_T$  evaluates the performance drop on the past tasks after training on the task T:  $FGT_T = \frac{1}{T} \sum_{j=1}^{T} [\max_{j \in 1, \dots, T-1} (a_{j,i} - a_{T,i})].$ 

**Implementation Details** Following the implementation of the coreset-based algorithm [6], we use two models for the purposes of model training and coreset selection respectively, where the first model is denoted as  $M_{tr}$  for model training, and the second model (also known as a proxy model) is denoted as  $M_{cs}$  for coreset selection. In the section of the model training, we adopt a single-head MLP with two hidden layers for Permuted MNIST, and a ResNet-18 for Split CIFAR-100 and other datasets. In the section of the coreset selection,  $M_{cs}$  adopts the same architecture as  $M_{tr}$ . This is the key difference between our work and the Greedy Coreset [6]: they use Neural Tangent Kernels (NTK) [35] while we use a specific deep neural network. Note that NTK performs learning based on fixed features, which is shown to be limited [66]. In contrast, our algorithm allows hierarchical feature learning during the training process. In addition, our algorithm does not rely on discrete decision variables as in [6]: we use first-order methods with gradient and Hessian-inverse-vector product information with convergence guarantee and hence is more efficient in practice. For non-coreset reply methods SPR and MetaSP, we set the size of the method buffer as that in coreset-based methods. Especially for SPR, there are two memory buffers: the delayed buffer D temporarily stocks the incoming data stream, and the purified buffer P maintains the cleansed data. To satisfy the

Table 4: Experiment results on Food-101

	Bala	anced	Imba	lanced	Label	Noise
Methods	AVG ACC	FGT	AVG ACC	FGT	AVG ACC	FGT
K-means Features	46.35±1.41	$0.057 \pm 0.004$	33.35±0.93	$0.064 \pm 0.008$	34.88±0.64	0.127±0.011
K-means Embedding	49.47±0.46	$0.040 \pm 0.004$	34.07±0.89	0.057±0.014	35.54±0.57	0.141±0.008
Uniform	46.50±0.13	0.048±0.001	34.61±0.16	0.060±0.007	36.69±1.13	0.123±0.007
iCaRL	48.12±0.78	0.035±0.001	36.83±1.06	$0.032 \pm 0.001$	39.22±0.30	0.084±0.010
Grad Matching	49.13±0.44	$0.026 \pm 0.002$	36.51±0.04	0.043±0.003	38.86±0.31	0.086±0.019
SPR	48.34±0.54	0.042±0.003	37.41±0.68	0.037±0.006	38.63±0.34	0.069±0.016
MetaSP	48.84±0.38	0.053±0.006	38.41±0.78	0.053±0.011	38.78±0.41	0.063±0.013
Greedy Coreset	49.19±0.91	$0.030 \pm 0.008$	38.78±0.01	0.038±0.001	38.61±0.18	0.096±0.004
GCR	47.03±1.17	$0.048 \pm 0.004$	36.99±0.30	0.042±0.005	35.78±1.08	0.126±0.013
PBCS	47.98±0.42	0.098±0.006	38.00±0.16	0.046±0.001	37.77±0.40	0.123±0.013
OCS	46.80±1.05	0.103±0.013	34.44±0.29	0.067±0.001	35.50±0.04	0.135±0.004
BCSR	51.30±0.62	$0.039 \pm 0.008$	39.05±0.99	0.044±0.001	39.63±0.22	0.060±0.071



Figure 2: The average accuracy during the continual learning. After each task, the training model is tested on all encountered tasks. Due to the nature of forgetting, the average test performance of all the methods tends to decrease.

Table 5: Random initialization with (W) and without (WO) bilevel optimizers (BO)

	Split CI	FAR-100	Permute	d MNIST	Multiple	e Datasets
BO	$A_T$	$FGT_T$	$A_T$	$FGT_T$	$A_T$	$FGT_T$
WO	58.37±0.37	0.073±0.004	53.34±0.74	0.074±0.009	55.50±0.80	0.128±0.027
W	61.60±0.14	0.051±0.015	56.23±0.29	$0.058 \pm 0.002$	59.89±0.95	0.096±0.005

requirement of coreset experiments, we keep the size of P and D buffers the same. The detailed hyperparameter settings can be found in Appendix C.

## 5.2 Results

We report the results of average accuracy (AVG ACC) and forgetting (FGT) for all the algorithms on the balanced, imbalanced, and label-noise benchmarks, and the results are presented in Table 1, Table 2, Table 3, Table 4, and Table 9 (Appendix E) respectively. We have the following observations. (i) In the balanced setting, our method outperforms other baselines significantly in terms of AVG ACC. For example, compared with the best coreset selection methods, our BCSR shows 2.21%, 4.24%, 2.68%, 2.11%, and 1.7% improvements in AVG ACC on five benchmarks, respectively. (ii) In the imbalanced and label-noise setting, our method also demonstrates relatively higher performance. For example, on imbalanced data of Multiple Datasets, BCSR is better than the best coreset selection algorithm by 4.65% in average accuracy. An interesting observation is that Greedy Coreset [6] does not perform very well, especially in imbalanced and label-noise settings. The reason is that the inner optimization in Greedy Coreset is conducted by an NTK, where only a fixed feature is used but not the learned feature. (iii) From bilevel optimization point of view, our algorithm significantly reduces the running time of the vanilla greedy coreset selection method [6] by at least 58% on continual learning benchmark datasets. For detailed comparison, please check Table 8 in Appendix D. (iv) In addition, the test AVG ACC (Figure 2 and Figure 4 in Appendix F) of the BCSR during the training process shows that our algorithm alleviates catastrophic forgetting and it is comparable to other best baselines. For example, BCSR enjoys the lowest forgetting for almost all datasets under the label-noise setting (except for Multiple Datasets in Table 2). For most experiments on other settings, BCSR achieves a forgetting performance that is comparable to the best methods with at most 1% gap.

#### 5.3 Ablation Studies

We conduct ablation studies to inspect the effectiveness of individual components in our proposed approach, including the effect of the bilevel optimizer, the smoothed top-K regularizer, and the coreset size K (Appendix J) respectively.

**Random initialization with and without bilevel optimizers.** Our new bilevel optimization algorithm (Algorithm 3) is of vital importance for finding a good distribution w for selecting the coreset. To demonstrate this, we design comparative experiments: one experiment initializes w randomly without updating it, and the other one adopts the same initialization strategy but updates w by the proposed bilevel optimizer. Then we sample coresets based on w from two methods respectively. As you can see, the random initialization method is equivalent to Uniform Sampling. We report the experimental results of average accuracy and forgetting on three balanced datasets in Table 5. It can be observed that the sampling strategy based on bilevel optimization significantly outperforms random sampling. In particular, the strategy with bilevel optimization shows 3.23%, 2.89%, and 4.39% AVG ACC improvement on three benchmarks. Meanwhile, it also obtains 2.20%, 1.60%, and 3.20% FGT reduction on three benchmarks.

Split CIFAR-100 Permuted MNIST Multiple Datasets λ  $A_T$  $FGT_T$  $A_T$  $FGT_T$  $A_T$  $FGT_T$ 0.00 60.43±0.15 0.064±0.005 54.20±1.53 0.116±0.030 55.71±0.32 0.055±0.003 60.56±2.05 0.074±0.016 55.09±2.94  $0.097 \pm 0.020$ 55.39±0.95 0.065±0.012 0.01 0.10 61.04±0.53 0.063±0.007 57.20±0.58  $0.064 \pm 0.010$  $55.69 \pm 0.40$ 0.057±0.002 1.0059.43±1.20  $0.072 \pm 0.008$ 55.43±1.53 0 108+0 019 58.18±0.77 0.046±0.006 5.00 58 80+1 58  $0.084 \pm 0.017$ 53 13+2 74 0 120+0 021 56.67±0.78 0.051+0.007  $0.060 \pm 0.010$ 10.00 0.075±0.012 0.118±0.029 55.57±1.05 59.53±0.42 53.54±2.02

Table 6: The impact of different values of  $\lambda$ 



Figure 3: The upper loss of bilevel optimization. Each distinct spike means the arrival of a new task.

To verify the effectiveness of our bilevel optimizer, we compare the loss curve with Greedy Coreset that uses NTK. The result is presented in Figure 3. There are a number of stream mini-batches in each task. The bilevel optimizer trains over each mini-batch, where the upper loss is plotted in the figure. In the experiment, we plot the loss value for every 5 mini-batches. Within each task, the loss from BCSR gradually decreases with slight fluctuations, and it increases only when encountering a new task. In contrast, the loss value of the Greedy Coreset approach always stays large. It indicates that our bilevel optimizer is more effective than the Greedy Coreset approach.

Effectiveness of the regularizer. In our algorithm, the bilevel formulation has a smooth top-K loss as a regularizer in the objective function to promote the probability distribution to have K nonzero entries. The goal is to make sure that the summation of top-K entries of the learned probability vector is large, which increases confidence in the coreset selection. The hyperparameter  $\lambda$  is used to balance the cross-entropy loss and the regularization term. We explore the effects on the performance with different  $\lambda$ , and list the results in Table 6.

This ablation experiment is performed on our framework BCSR, and average accuracy and forgetting on three balanced benchmarks are reported. When  $\lambda = 0.10$ , BCSR can reach the best performance (The highest AVG ACC and lowest FGT) on Split CIFAR-100 and Permuted MNIST. While on Multiple Datasets, BCSR performs the best when  $\lambda = 1.0$ . This dataset contains more categories, and hence it is more challenging to select the appropriate representative samples. In this case, larger  $\lambda$  would emphasize more on maximizing the top-K probability and help select better representative samples. In addition, we observe that  $\lambda$  set as a too large or too small value will damage the performance, which is in line with the observations in standard regularized empirical risk minimization problems such as overfitting and underfitting. Please refer to Appendix H for further analysis.

# 6 Theoretical Analysis

In this section, we provide a theoretical analysis for our proposed method. In particular, we establish convergence rate for our algorithm BCSR.

**Theorem 1.** Suppose standard assumptions hold in bilevel optimization (see Assumptions 1, 2 and 3 in Appendix M). Choose parameters  $\lambda$ ,  $\alpha$ ,  $\eta$  and N such that  $(1 + \lambda)(1 - \alpha\mu)^N(1 + \frac{8rL^2}{\eta\mu}) \leq 1 - \eta\mu$ , where  $r = \frac{C_Q^2}{(\frac{\rho M}{\mu} + L)^2}$  and  $C_Q = \frac{Q\rho M\eta}{\mu} + \eta^2 Q^2 \rho M + \eta QL$ . Furthermore, choose the stepsize  $\beta$  such that  $6\omega\beta^2 L^2 < \frac{1}{9}\eta\mu$  and  $\beta \leq \frac{1}{4L_{\phi}}$ , where the constant  $\omega$  is given by Equation (16) in Appendix A.

Then, we have the following convergence result.

$$\frac{1}{J}\sum_{j=0}^{J-1} \mathbb{E} \|G_j\|^2 \le \mathcal{O}\Big(\frac{D_{\phi}}{\beta J} + \frac{1}{|\mathcal{B}|} + \frac{D_0}{\eta \mu J}\Big).$$

where  $G_j := \frac{1}{\beta}(w_j - \mathcal{P}_{\Delta^n}(w_j - \beta \nabla \phi(w_j)))$  denote the generalized projected gradient,  $D_{\phi} := \phi(w_0) - \min_w \phi(w) > 0$ ,  $D_0 = \|\theta_0^0 - \theta_0^*\|^2 + \|v_0^0 - v_0^*\|^2$ ,  $L_{\phi}$  is the smoothness parameter of the total objective  $\phi(w)$  whose form is proved in Appendix A.

Theorem 1 provides a general convergence result for the proposed bilevel algorithm, which allows for a very flexible selection of subloop lengths N and Q as long as the inequality  $(1 + \lambda)(1 - \alpha \mu)^N(1 + \frac{8rL^2}{\eta\mu}) \leq 1 - \eta\mu$  holds given proper stepsizes  $\lambda, \eta, \alpha$ . For example, in most of our experiments, the choice of N = 1 and Q = 3 works the best. Then, in this case, we further specify the parameters in Theorem 1, and provide the following corollary.

**Corollary 1.** Under the same setting as in Theorem 1, choose N = 1, Q = 3 and set  $\lambda = \frac{\alpha \mu}{2}, \eta \leq \frac{\mu^2 \alpha}{4608L^2}$  and  $\alpha \leq \frac{1}{L}$ . Then, to make sure an  $\epsilon$ -accurate stationary point, i.e.,  $\frac{1}{J} \sum_{j=0}^{J-1} \mathbb{E} ||G_j||^2 \leq \epsilon^2$ , the number of iterations is  $\mathcal{O}(\epsilon^{-2})$ , each using  $|\mathcal{B}| = \mathcal{O}(\epsilon^{-2})$  of samples from the standard Gaussian distribution  $\mathcal{N}(0, 1)$ .

Corollary 1 shows that the proposed bilevel algorithm converges to an  $\epsilon$ -accurate stationary point using only  $\mathcal{O}(\epsilon^{-2})$  iterations and  $\mathcal{O}(\epsilon^{-2})$  samples drawn from  $\mathcal{N}(0, 1)$  per iteration. Note the the large batch size  $|\mathcal{B}| = \mathcal{O}(\epsilon^{-2})$  is necessary here to guarantee a convergence rate of  $\mathcal{O}(1/T)$ , which matches the results in solving single-level constrained nonconvex problems [24]. In addition, it is computationally tractable because sampling from a known Gaussian distribution is easy and cheap.

#### 7 Conclusion

In this paper, we advance the state-of-the-art bilevel coreset selection in continual learning. We first introduce a new bilevel formulation with smoothed top-K regularization and then design an efficient bilevel optimizer as a solver. We conduct extensive experiments in continual learning benchmark datasets to demonstrate the effectiveness of our proposed approach. We also show that the bilevel optimizer can efficiently find  $\epsilon$ -stationary point with  $O(1/\epsilon^4)$  computational complexity, which matches the best complexity of projected SGD for a single-level problem.

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#### References

- Rahaf Aljundi, Francesca Babiloni, Mohamed Elhoseiny, Marcus Rohrbach, and Tinne Tuytelaars. Memory aware synapses: Learning what (not) to forget. In *Proceedings of the European Conference on Computer Vision (ECCV)*, pages 139–154, 2018.
- [2] Rahaf Aljundi, Eugene Belilovsky, Tinne Tuytelaars, Laurent Charlin, Massimo Caccia, Min Lin, and Lucas Page-Caccia. Online continual learning with maximal interfered retrieval. In Advances in Neural Information Processing Systems 32, pages 11849–11860. 2019.
- [3] Rahaf Aljundi, Min Lin, Baptiste Goujaud, and Yoshua Bengio. Gradient based sample selection for online continual learning. *Advances in neural information processing systems*, 32, 2019.
- [4] Michael Arbel and Julien Mairal. Amortized implicit differentiation for stochastic bilevel optimization. In *International Conference on Learning Representations*, 2022.

- [5] Olivier Bachem, Mario Lucic, and Andreas Krause. Coresets for nonparametric estimation-the case of dp-means. In *International Conference on Machine Learning*, pages 209–217. PMLR, 2015.
- [6] Zalán Borsos, Mojmir Mutny, and Andreas Krause. Coresets via bilevel optimization for continual learning and streaming. Advances in Neural Information Processing Systems, 33:14879– 14890, 2020.
- [7] Lukas Bossard, Matthieu Guillaumin, and Luc Van Gool. Food-101 mining discriminative components with random forests. In *European Conference on Computer Vision*, 2014.
- [8] Yaroslav Bulatov. Notmnist dataset. Google (Books/OCR), Tech. Rep.[Online]. Available: http://yaroslavvb. blogspot. it/2011/09/notmnist-dataset. html, 2, 2011.
- [9] Trevor Campbell and Tamara Broderick. Automated scalable bayesian inference via hilbert coresets. *The Journal of Machine Learning Research*, 20(1):551–588, 2019.
- [10] Arslan Chaudhry, Puneet K Dokania, Thalaiyasingam Ajanthan, and Philip HS Torr. Riemannian walk for incremental learning: Understanding forgetting and intransigence. In *Proceedings of* the European Conference on Computer Vision (ECCV), pages 532–547, 2018.
- [11] Arslan Chaudhry, Marc'Aurelio Ranzato, Marcus Rohrbach, and Mohamed Elhoseiny. Efficient lifelong learning with a-gem. *arXiv preprint arXiv:1812.00420*, 2018.
- [12] Tianyi Chen, Yuejiao Sun, and Wotao Yin. A single-timescale stochastic bilevel optimization method. arXiv preprint arXiv:2102.04671, 2021.
- [13] Yin Cui, Menglin Jia, Tsung-Yi Lin, Yang Song, and Serge Belongie. Class-balanced loss based on effective number of samples. In *Proceedings of the IEEE/CVF conference on computer* vision and pattern recognition, pages 9268–9277, 2019.
- [14] Mathieu Dagréou, Pierre Ablin, Samuel Vaiter, and Thomas Moreau. A framework for bilevel optimization that enables stochastic and global variance reduction algorithms. arXiv preprint arXiv:2201.13409, 2022.
- [15] Jacob Devlin, Ming-Wei Chang, Kenton Lee, and Kristina Toutanova. Bert: Pre-training of deep bidirectional transformers for language understanding. arXiv preprint arXiv:1810.04805, 2018.
- [16] Justin Domke. Generic methods for optimization-based modeling. In *Artificial Intelligence and Statistics (AISTATS)*, pages 318–326, 2012.
- [17] Sayna Ebrahimi, Mohamed Elhoseiny, Trevor Darrell, and Marcus Rohrbach. Uncertaintyguided continual learning with bayesian neural networks. arXiv preprint arXiv:1906.02425, 2019.
- [18] Mehrdad Farajtabar, Navid Azizan, Alex Mott, and Ang Li. Orthogonal gradient descent for continual learning. arXiv preprint arXiv:1910.07104, 2019.
- [19] Dan Feldman and Michael Langberg. A unified framework for approximating and clustering data. In *Proceedings of the forty-third annual ACM symposium on Theory of computing*, pages 569–578, 2011.
- [20] Chelsea Finn, Pieter Abbeel, and Sergey Levine. Model-agnostic meta-learning for fast adaptation of deep networks. In *Proceedings of the 34th International Conference on Machine Learning-Volume 70*, pages 1126–1135. JMLR. org, 2017.
- [21] Luca Franceschi, Michele Donini, Paolo Frasconi, and Massimiliano Pontil. Forward and reverse gradient-based hyperparameter optimization. In *International Conference on Machine Learning (ICML)*, pages 1165–1173, 2017.
- [22] Luca Franceschi, Paolo Frasconi, Saverio Salzo, Riccardo Grazzi, and Massimiliano Pontil. Bilevel programming for hyperparameter optimization and meta-learning. In *International Conference on Machine Learning*, pages 1568–1577. PMLR, 2018.

- [23] Camille Garcin, Maximilien Servajean, Alexis Joly, and Joseph Salmon. Stochastic smoothing of the top-k calibrated hinge loss for deep imbalanced classification. *arXiv preprint arXiv:2202.02193*, 2022.
- [24] Saeed Ghadimi, Guanghui Lan, and Hongchao Zhang. Mini-batch stochastic approximation methods for nonconvex stochastic composite optimization. *Mathematical Programming*, 155(1):267–305, 2016.
- [25] Saeed Ghadimi and Mengdi Wang. Approximation methods for bilevel programming. *arXiv* preprint arXiv:1802.02246, 2018.
- [26] Ian Goodfellow, Jean Pouget-Abadie, Mehdi Mirza, Bing Xu, David Warde-Farley, Sherjil Ozair, Aaron Courville, and Yoshua Bengio. Generative adversarial nets. In Advances in neural information processing systems, pages 2672–2680, 2014.
- [27] Riccardo Grazzi, Luca Franceschi, Massimiliano Pontil, and Saverio Salzo. On the iteration complexity of hypergradient computation. In *Proc. International Conference on Machine Learning (ICML)*, 2020.
- [28] Yunhui Guo, Mingrui Liu, Tianbao Yang, and Tajana Rosing. Improved schemes for episodic memory-based lifelong learning. Advances in Neural Information Processing Systems, 33, 2020.
- [29] Zhishuai Guo and Tianbao Yang. Randomized stochastic variance-reduced methods for stochastic bilevel optimization. arXiv preprint arXiv:2105.02266, 2021.
- [30] 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.
- [31] Xu He and Herbert Jaeger. Overcoming catastrophic interference using conceptor-aided backpropagation. 2018.
- [32] Mingyi Hong, Hoi-To Wai, Zhaoran Wang, and Zhuoran Yang. A two-timescale framework for bilevel optimization: Complexity analysis and application to actor-critic. *arXiv preprint arXiv:2007.05170*, 2020.
- [33] Jonathan Huggins, Trevor Campbell, and Tamara Broderick. Coresets for scalable bayesian logistic regression. *Advances in Neural Information Processing Systems*, 29, 2016.
- [34] David Isele and Akansel Cosgun. Selective experience replay for lifelong learning. In Proceedings of the AAAI Conference on Artificial Intelligence, volume 32, 2018.
- [35] Arthur Jacot, Franck Gabriel, and Clément Hongler. Neural tangent kernel: Convergence and generalization in neural networks. *Advances in neural information processing systems*, 31, 2018.
- [36] Kaiyi Ji, Mingrui Liu, Yingbin Liang, and Lei Ying. Will bilevel optimizers benefit from loops. arXiv preprint arXiv:2205.14224, 2022.
- [37] Kaiyi Ji, Junjie Yang, and Yingbin Liang. Bilevel optimization: Convergence analysis and enhanced design. In *International Conference on Machine Learning (ICML)*, pages 4882–4892. PMLR, 2021.
- [38] Chris Dongjoo Kim, Jinseo Jeong, Sangwoo Moon, and Gunhee Kim. Continual learning on noisy data streams via self-purified replay. In *Proceedings of the IEEE/CVF international conference on computer vision*, pages 537–547, 2021.
- [39] James Kirkpatrick, Razvan Pascanu, Neil Rabinowitz, Joel Veness, Guillaume Desjardins, Andrei A Rusu, Kieran Milan, John Quan, Tiago Ramalho, Agnieszka Grabska-Barwinska, et al. Overcoming catastrophic forgetting in neural networks. *Proceedings of the national academy of sciences*, 114(13):3521–3526, 2017.
- [40] Vijay Konda and John Tsitsiklis. Actor-critic algorithms. Advances in neural information processing systems, 12, 1999.

- [41] Alex Krizhevsky, Ilya Sutskever, and Geoffrey E Hinton. Imagenet classification with deep convolutional neural networks. In Advances in neural information processing systems, pages 1097–1105, 2012.
- [42] Ya Le and Xuan Yang. Tiny imagenet visual recognition challenge. CS 231N, 7(7):3, 2015.
- [43] Yann LeCun, Léon Bottou, Yoshua Bengio, and Patrick Haffner. Gradient-based learning applied to document recognition. *Proceedings of the IEEE*, 86(11):2278–2324, 1998.
- [44] Xilai Li, Yingbo Zhou, Tianfu Wu, Richard Socher, and Caiming Xiong. Learn to grow: A continual structure learning framework for overcoming catastrophic forgetting. In *International Conference on Machine Learning*, pages 3925–3934. PMLR, 2019.
- [45] Renjie Liao, Yuwen Xiong, Ethan Fetaya, Lisa Zhang, KiJung Yoon, Xaq Pitkow, Raquel Urtasun, and Richard Zemel. Reviving and improving recurrent back-propagation. In Proc. International Conference on Machine Learning (ICML), 2018.
- [46] Hanxiao Liu, Karen Simonyan, and Yiming Yang. Darts: Differentiable architecture search. *ICLR*, 2019.
- [47] Risheng Liu, Jiaxin Gao, Jin Zhang, Deyu Meng, and Zhouchen Lin. Investigating bi-level optimization for learning and vision from a unified perspective: A survey and beyond. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 2021.
- [48] David Lopez-Paz et al. Gradient episodic memory for continual learning. In *Advances in Neural Information Processing Systems*, pages 6467–6476, 2017.
- [49] Mario Lucic, Matthew Faulkner, Andreas Krause, and Dan Feldman. Training gaussian mixture models at scale via coresets. *The Journal of Machine Learning Research*, 18(1):5885–5909, 2017.
- [50] Dougal Maclaurin, David Duvenaud, and Ryan Adams. Gradient-based hyperparameter optimization through reversible learning. In *International Conference on Machine Learning (ICML)*, pages 2113–2122, 2015.
- [51] Arun Mallya and Svetlana Lazebnik. Packnet: Adding multiple tasks to a single network by iterative pruning. In *Proceedings of the IEEE conference on Computer Vision and Pattern Recognition*, pages 7765–7773, 2018.
- [52] James L McClelland, Bruce L McNaughton, and Randall C O'Reilly. Why there are complementary learning systems in the hippocampus and neocortex: insights from the successes and failures of connectionist models of learning and memory. *Psychological review*, 102(3):419, 1995.
- [53] Michael McCloskey and Neal J Cohen. Catastrophic interference in connectionist networks: The sequential learning problem. In *Psychology of learning and motivation*, volume 24, pages 109–165. Elsevier, 1989.
- [54] Yuval Netzer, Tao Wang, Adam Coates, Alessandro Bissacco, Bo Wu, and Andrew Y Ng. Reading digits in natural images with unsupervised feature learning. 2011.
- [55] Cuong V Nguyen, Yingzhen Li, Thang D Bui, and Richard E Turner. Variational continual learning. *arXiv preprint arXiv:1710.10628*, 2017.
- [56] Fabian Pedregosa. Hyperparameter optimization with approximate gradient. In *International conference on machine learning*, pages 737–746. PMLR, 2016.
- [57] Sylvestre-Alvise Rebuffi, Alexander Kolesnikov, Georg Sperl, and Christoph H Lampert. icarl: Incremental classifier and representation learning. In *Proceedings of the IEEE conference on Computer Vision and Pattern Recognition*, pages 2001–2010, 2017.
- [58] Matthew Riemer, Ignacio Cases, Robert Ajemian, Miao Liu, Irina Rish, Yuhai Tu, and Gerald Tesauro. Learning to learn without forgetting by maximizing transfer and minimizing interference. arXiv preprint arXiv:1810.11910, 2018.

- [59] Hippolyt Ritter, Aleksandar Botev, and David Barber. Online structured laplace approximations for overcoming catastrophic forgetting. In *Advances in Neural Information Processing Systems*, pages 3738–3748, 2018.
- [60] Anthony Robins. Catastrophic forgetting, rehearsal and pseudorehearsal. *Connection Science*, 7(2):123–146, 1995.
- [61] Andrei A Rusu, Neil C Rabinowitz, Guillaume Desjardins, Hubert Soyer, James Kirkpatrick, Koray Kavukcuoglu, Razvan Pascanu, and Raia Hadsell. Progressive neural networks. arXiv preprint arXiv:1606.04671, 2016.
- [62] Jonathan Schwarz, Wojciech Czarnecki, Jelena Luketina, Agnieszka Grabska-Barwinska, Yee Whye Teh, Razvan Pascanu, and Raia Hadsell. Progress & compress: A scalable framework for continual learning. In *International Conference on Machine Learning*, pages 4528–4537. PMLR, 2018.
- [63] Ozan Sener and Silvio Savarese. Active learning for convolutional neural networks: A core-set approach. *arXiv preprint arXiv:1708.00489*, 2017.
- [64] Joan Serra, Didac Suris, Marius Miron, and Alexandros Karatzoglou. Overcoming catastrophic forgetting with hard attention to the task. In *International Conference on Machine Learning*, pages 4548–4557. PMLR, 2018.
- [65] Amirreza Shaban, Ching-An Cheng, Nathan Hatch, and Byron Boots. Truncated backpropagation for bilevel optimization. In *International Conference on Artificial Intelligence and Statistics (AISTATS)*, pages 1723–1732, 2019.
- [66] Zhenmei Shi, Junyi Wei, and Yingyu Liang. A theoretical analysis on feature learning in neural networks: Emergence from inputs and advantage over fixed features. *arXiv preprint arXiv:2206.01717*, 2022.
- [67] Hanul Shin, Jung Kwon Lee, Jaehong Kim, and Jiwon Kim. Continual learning with deep generative replay. *Advances in neural information processing systems*, 30, 2017.
- [68] David Silver, Aja Huang, Chris J Maddison, Arthur Guez, Laurent Sifre, George Van Den Driessche, Julian Schrittwieser, Ioannis Antonoglou, Veda Panneershelvam, Marc Lanctot, et al. Mastering the game of go with deep neural networks and tree search. *nature*, 529(7587):484, 2016.
- [69] Johannes Stallkamp, Marc Schlipsing, Jan Salmen, and Christian Igel. The german traffic sign recognition benchmark: a multi-class classification competition. In *The 2011 international joint conference on neural networks*, pages 1453–1460. IEEE, 2011.
- [70] Qing Sun, Fan Lyu, Fanhua Shang, Wei Feng, and Liang Wan. Exploring example influence in continual learning. Advances in Neural Information Processing Systems, 35:27075–27086, 2022.
- [71] Rishabh Tiwari, Krishnateja Killamsetty, Rishabh Iyer, and Pradeep Shenoy. Gcr: Gradient coreset based replay buffer selection for continual learning. In *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pages 99–108, 2022.
- [72] Ashish Vaswani, Noam Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N Gomez, Łukasz Kaiser, and Illia Polosukhin. Attention is all you need. Advances in neural information processing systems, 30, 2017.
- [73] Luis N Vicente and Paul H Calamai. Bilevel and multilevel programming: A bibliography review. *Journal of Global optimization*, 5(3):291–306, 1994.
- [74] Kai Wei, Rishabh Iyer, and Jeff Bilmes. Submodularity in data subset selection and active learning. In *International conference on machine learning*, pages 1954–1963. PMLR, 2015.
- [75] Han Xiao, Kashif Rasul, and Roland Vollgraf. Fashion-mnist: a novel image dataset for benchmarking machine learning algorithms. *arXiv preprint arXiv:1708.07747*, 2017.

- [76] Ju Xu and Zhanxing Zhu. Reinforced continual learning. Advances in Neural Information Processing Systems, 31, 2018.
- [77] Jaehong Yoon, Saehoon Kim, Eunho Yang, and Sung Ju Hwang. Scalable and order-robust continual learning with additive parameter decomposition. *International Conference on Learning Representations*, 2020.
- [78] Jaehong Yoon, Divyam Madaan, Eunho Yang, and Sung Ju Hwang. Online coreset selection for rehearsal-based continual learning. *arXiv preprint arXiv:2106.01085*, 2021.
- [79] Jaehong Yoon, Eunho Yang, Jeongtae Lee, and Sung Ju Hwang. Lifelong learning with dynamically expandable networks. arXiv preprint arXiv:1708.01547, 2017.
- [80] Tianhe Yu, Saurabh Kumar, Abhishek Gupta, Sergey Levine, Karol Hausman, and Chelsea Finn. Gradient surgery for multi-task learning. *Advances in Neural Information Processing Systems*, 33:5824–5836, 2020.
- [81] Friedemann Zenke, Ben Poole, and Surya Ganguli. Continual learning through synaptic intelligence. In *Proceedings of the 34th International Conference on Machine Learning-Volume* 70, pages 3987–3995. JMLR. org, 2017.
- [82] Guodong Zhang, James Martens, and Roger B Grosse. Fast convergence of natural gradient descent for over-parameterized neural networks. *Advances in Neural Information Processing Systems (NeurIPS)*, 32, 2019.
- [83] Xiao Zhou, Renjie Pi, Weizhong Zhang, Yong Lin, Zonghao Chen, and Tong Zhang. Probabilistic bilevel coreset selection. In Kamalika Chaudhuri, Stefanie Jegelka, Le Song, Csaba Szepesvari, Gang Niu, and Sivan Sabato, editors, *Proceedings of the 39th International Conference on Machine Learning*, volume 162 of *Proceedings of Machine Learning Research*, pages 27287–27302. PMLR, 17–23 Jul 2022.
- [84] Xiangyu Zhu, Jie Hao, Yunhui Guo, and Mingrui Liu. Auc maximization in imbalanced lifelong learning. In Uncertainty in Artificial Intelligence, pages 2574–2585. PMLR, 2023.

# A Proof of Theorem 1

Let  $\Delta^{(n)} := \{w : 0 \le w_{(i)} \le 1, ||w||_1 = 1\}$  denote the constraint set of the upper-level problem. We first provide some important inequalities.

Recall that  $v_j^q$  be the  $q^{th}$  GD iterate in solving the linear system  $\nabla_{\theta}^2 L(\theta_j^N, w_j)v = \sum_{i=1}^n \nabla \ell_i(\theta_j^N)$  at iteration j via the following process:

$$v_{j}^{q+1} = (I - \eta \nabla_{\theta}^{2} L(\theta_{j}^{N}, w_{j})) v_{j}^{q} + \eta \sum_{i=1}^{n} \nabla \ell_{i}(\theta_{j}^{N}).$$
(6)

which, by telescoping Equation (6) over q from 0 to Q - 1, yields

$$v_j^Q = (I - \eta \nabla_\theta^2 L(\theta_j^N, w_j))^Q v_k^0 + \eta \sum_{q=0}^{Q-1} (I - \eta \nabla_\theta^2 L(\theta_j^N, w_j))^q \sum_{i=1}^n \nabla \ell_i(\theta_j^N).$$
(7)

Let  $v_j^*$  be the solution of the linear system  $\nabla_{\theta}^2 L(\theta_j^*, w_j)v = \sum_{i=1}^n \nabla \ell_i(\theta_j^*)$ , and then we have

$$v_{j}^{*} = (I - \eta \nabla_{\theta}^{2} L(\theta_{j}^{*}, w_{j}))^{Q} v_{j}^{*} + \eta \sum_{q=0}^{Q-1} (I - \eta \nabla_{\theta}^{2} L(\theta_{j}^{*}, w_{j}))^{q} \sum_{i=1}^{n} \nabla \ell_{i}(\theta_{j}^{*}).$$
(8)

Combining Equation (6) and Equation (7), noting that  $v_j^0 = v_{j-1}^Q$  and using Assumption 2 that  $\|v_j^*\| \leq \|(\nabla_{\theta}^2 L(\theta_j^*, w_j))^{-1}\|\|\sum_{i=1}^n \nabla \ell_i(\theta_j^*)\| \leq \frac{M}{\mu}$ , the difference between  $v_j^Q$  and  $v_j^*$  can be bounded as

$$\|v_{j}^{Q} - v_{j}^{*}\| \leq \|(I - \eta \nabla_{\theta}^{2} L(\theta_{j}^{N}, w_{j}))^{Q} - (I - \eta \nabla_{\theta}^{2} L(\theta_{j}^{*}, w_{j}))^{Q}\|\frac{M}{\mu} + (1 - \eta \mu)^{Q}\|v_{j-1}^{Q} - v_{j}^{*}\| + \eta M \|\sum_{q=0}^{Q-1} (I - \eta \nabla_{\theta}^{2} L(\theta_{j}^{N}, w_{j}))^{q} - \sum_{q=0}^{Q-1} (I - \eta \nabla_{\theta}^{2} L(\theta_{j}^{*}, w_{j}))^{q} \| + (1 - (1 - \eta \mu)^{Q})\frac{L}{\mu}\|\theta_{j}^{*} - \theta_{j}^{N}\|.$$

$$(9)$$

We next bound  $\Delta_q := \|(I - \eta \nabla^2_{\theta} L(\theta^N_j, w_j))^q - (I - \eta \nabla^2_{\theta} L(\theta^*_j, w_j))^q\|$  in Equation (9) as:

$$\Delta_q \stackrel{(i)}{\leq} (1 - \eta \mu) \Delta_{q-1} + (1 - \eta \mu)^{q-1} \eta \rho \|\theta_j^N - \theta_j^*\|.$$
(10)

which, by telescoping Equation (10) and in conjunction with Equation (9), yields

$$\begin{aligned} |v_{j}^{Q} - v_{j}^{*}|| &\leq Q(1 - \eta\mu)^{Q-1}\eta\rho\frac{M}{\mu} \|\theta_{j}^{N} - \theta_{j}^{*}\| + (1 - \eta\mu)^{Q} \|v_{j-1}^{Q} - v_{j}^{*}\| \\ &+ \eta M \sum_{q=0}^{Q-1} q(1 - \eta\mu)^{q-1}\eta\rho \|\theta_{j}^{N} - \theta_{j}^{*}\| + (1 - (1 - \eta\mu)^{Q})\frac{L}{\mu} \|\theta_{j}^{*} - \theta_{j}^{N}\| \quad (11) \\ &\leq \frac{Q(1 - \eta\mu)^{Q-1}\rho M\eta}{\mu} \|\theta_{j}^{N} - \theta_{j}^{*}\| + (1 - \eta\mu)^{Q} \|v_{j-1}^{Q} - v_{j-1}^{*}\| \\ &+ (1 - \eta\mu)^{Q} \|v_{j-1}^{*} - v_{j}^{*}\| + \frac{1 - (1 - \eta\mu)^{Q}(1 + \eta Q\mu)}{\mu^{2}} \rho M \|\theta_{j}^{N} - \theta_{j}^{*}\| \\ &+ (1 - (1 - \eta\mu)^{Q})\frac{L}{\mu} \|\theta_{j}^{*} - \theta_{j}^{N}\| \end{aligned}$$

which, combined with  $||v_j^* - v_{j-1}^*|| \le \left(\frac{L}{\mu} + \frac{M\rho}{\mu^2}\right)\left(\frac{L}{\mu} + 1\right)||w_j - w_{j-1}||$  and using the fact that  $(1-x)^Q \ge 1 - xQ$  for  $0 \le x \le 1$ , yields

$$\mathbb{E} \|v_{j}^{Q} - v_{j}^{*}\|^{2} \leq (1 - \eta\mu) \mathbb{E} \|v_{j-1}^{Q} - v_{j-1}^{*}\|^{2} + \frac{4}{\eta\mu} C_{Q}^{2} \|\theta_{j}^{*} - \theta_{j}^{N}\|^{2} + \frac{4}{\eta\mu} \Big(\frac{L}{\mu} + \frac{M\rho}{\mu^{2}}\Big)^{2} \Big(\frac{L}{\mu} + 1\Big) \|w_{j} - w_{j-1}\|^{2}$$
(12)

where the constant  $C_Q := \frac{Q\rho M\eta}{\mu} + \eta^2 Q^2 \rho M + \eta Q L.$ 

The next step is to characterize the error induced by the lower-level updates on  $\theta$ .

Note that  $\theta_j^* = \arg \min_{\theta} L(\theta, w_j)$ . Using Assumptions 1 and 2, we have

$$\|\theta_j^N - \theta_j^*\|^2 \le (1 - \alpha \mu)^N \|\theta_j^0 - \theta_j^*\|^2,$$
(13)

which, in conjunction with  $\theta_j^0 = \theta_{j-1}^N$  and Lemma 2.2 in [25], yields

$$\mathbb{E} \|\theta_{j}^{N} - \theta_{j}^{*}\|^{2} \leq (1 - \alpha \mu)^{N} (1 + \lambda) \mathbb{E} \|\theta_{j-1}^{N} - \theta_{j-1}^{*}\|^{2} + (1 - \alpha \mu)^{N} (1 + \frac{1}{\lambda}) \frac{L^{2}}{\mu^{2}} \mathbb{E} \|w_{j} - w_{j-1}\|^{2}.$$
(14)

Recall the definition that  $r = \frac{C_Q^2}{(\frac{\rho M}{\mu} + L)^2}$ . Then, combining Equation (12) and Equation (14) yields we can obtain

$$\left(1 + \frac{\rho^2 M^2}{L^2 \mu^2}\right) \mathbb{E} \|\theta_j^N - \theta_j^*\|^2 + \mathbb{E} \|v_j^Q - v_j^*\|^2$$

$$\leq (1 + \lambda)(1 - \alpha \mu)^N \left(1 + \frac{\rho^2 M^2}{L^2 \mu^2}\right) \left(1 + \frac{8rL^2}{\eta \mu}\right) \mathbb{E} \|\theta_{j-1}^N - \theta_{j-1}^*\|^2$$

$$+ (1 - \eta \mu) \mathbb{E} \|v_{j-1}^Q - v_{j-1}^*\|^2 + \omega \mathbb{E} \|w_j - w_{j-1}\|^2,$$
(15)

where the constant  $\omega$  is given by

$$\omega := \left(1 + \frac{1}{\lambda}\right) (1 - \alpha \mu)^N \left(1 + \frac{\rho^2 M^2}{L^2 \mu^2}\right) \frac{L^2}{\mu^2} + \frac{8}{\eta \mu} \frac{L^4}{\mu^2} \left(1 + \frac{\rho^2 M^2}{L^2 \mu^2}\right) \left(\frac{4}{\mu^2} + r(1 - \alpha \mu)^N \left(1 + \frac{1}{\lambda}\right)\right).$$
(16)

Recall that we choose  $(1 + \lambda)(1 - \alpha \mu)^N (1 + \frac{8rL^2}{\eta \mu}) \le 1 - \eta \mu$ . Then, we obtain from Equation (15) that

$$\left(1 + \frac{\rho^2 M^2}{L^2 \mu^2}\right) \mathbb{E} \|\theta_j^N - \theta_j^*\|^2 + \mathbb{E} \|v_j^Q - v_j^*\|^2$$

$$\leq (1 - \eta \mu) \left(1 + \frac{\rho^2 M^2}{L^2 \mu^2}\right) \mathbb{E} \|\theta_{j-1}^N - \theta_{j-1}^*\|^2$$

$$+ (1 - \eta \mu) \mathbb{E} \|v_{j-1}^Q - v_{j-1}^*\|^2 + \omega \mathbb{E} \|w_j - w_{j-1}\|^2.$$

$$(17)$$

Let  $\delta_j := \left(1 + \frac{\rho^2 M^2}{L^2 \mu^2}\right) \mathbb{E} \|\theta_j^N - \theta_j^*\|^2 + \mathbb{E} \|v_j^Q - v_j^*\|^2$ . Then, incorporating the update that  $w_j = \mathcal{P}_{\Delta^n}(w_{j-1} - \beta \varphi_{j-1})$  into Equation (17) yields

$$\delta_{j} \leq (1 - \eta \mu) \delta_{j-1} + 2\omega \beta^{2} \mathbb{E} \left\| \underbrace{\frac{1}{\beta} (w_{j-1} - \mathcal{P}_{\Delta^{n}} (w_{j-1} - \beta \nabla \phi(w_{j-1})))}_{G_{j-1}} \right\|^{2} + 2\omega \beta^{2} \|\varphi_{j-1} - \nabla \phi(w_{j-1})\|^{2}.$$
(18)

We next bound the last term in the above Equation (18). Based on the definition of the hypergradient estimate  $\varphi_j = \nabla_w R(w, \delta; \mathcal{B}) - \nabla_w \nabla_\theta L(\theta_j^N, w_j) v_j^Q$ , we have

$$\mathbb{E} \|\varphi_{j} - \nabla\phi(w_{j})\|^{2} \\
\leq 3\mathbb{E} \|\nabla R(w_{j}, \delta; \mathcal{B}) - \nabla R(w_{j}, \delta)\|^{2} + \frac{3\rho^{2}M^{2}}{\mu^{2}} \mathbb{E} \|\theta_{j}^{*} - \theta_{j}^{N}\|^{2} + 3L^{2}\mathbb{E} \|v_{j}^{*} - v_{j}^{Q}\|^{2} \\
\stackrel{(i)}{=} \frac{3}{|\mathcal{B}|^{2}} \sum_{\widetilde{z} \in \mathcal{B}} \|\nabla R(w_{j}, \delta; \widetilde{z}) - \nabla R(w, \delta)\|^{2} + 3L^{2} \Big(1 + \frac{\rho^{2}M^{2}}{\mu^{2}L^{2}}\Big) \mathbb{E} \|\theta_{j}^{*} - \theta_{j}^{N}\|^{2} + 3L^{2} \mathbb{E} \|v_{j}^{*} - v_{j}^{Q}\|^{2} \\
\leq \frac{6K}{|\mathcal{B}|} + 3L^{2} \Big(1 + \frac{\rho^{2}M^{2}}{\mu^{2}L^{2}}\Big) \mathbb{E} \|\theta_{j}^{*} - \theta_{j}^{N}\|^{2} + 3L^{2} \mathbb{E} \|v_{j}^{*} - v_{j}^{Q}\|^{2} = \frac{6K}{|\mathcal{B}|} + 3L^{2}\delta_{j},$$
(19)

where (i) follows because  $\nabla R(w_j, \delta; \tilde{z})$  is an unbiased estimate of  $\nabla R(w, \delta)$  and (ii) follows from Proposition 1. Substituting Equation (19) into Equation (18) yields

$$\delta_j \le (1 - \eta\mu + 6\omega\beta^2 L^2)\delta_{j-1} + \frac{12\omega K\beta^2}{|\mathcal{B}|} + 2\omega\beta^2 \mathbb{E} \|G_{j-1}\|^2.$$
(20)

Let  $\tau := 1 - \eta \mu + 6\omega \beta^2 L^2$ . Then, telescoping Equation (20) yields

$$\delta_{j} \leq \tau^{j} \delta_{0} + \frac{12\omega K\beta^{2}}{(1-\tau)|\mathcal{B}|} + 2\omega\beta^{2} \sum_{t=0}^{j-1} \tau^{t} \mathbb{E} \|G_{j-1-t}\|^{2}.$$
(21)

Based on Equation (21), we are ready to provide the final convergence result. First, based on the Lipschitz continuity in Assumption 1, Assumption 2 and Assumption 3, we have

 $\|\nabla \phi(w_1) - \nabla \phi(w_2)\| \le L_{\phi} \|w_1 - w_2\|,$ 

where the constant  $L_{\phi} = \frac{\sqrt{Kn}}{\delta} + \frac{L^2 + \rho M^2}{\mu} + \frac{2\rho LM + L^3}{\mu^2} + \frac{\rho L^2 M}{\mu^3}$  is the smoothness parameter. Then, this inequality further implies

$$\phi(w_{j+1}) \leq \phi(w_j) + \langle \nabla \phi(w_j), w_{j+1} - w_j \rangle + \frac{L_{\phi}}{2} \|w_{j+1} - w_j\|^2 \\
\leq \phi(w_j) + \frac{1}{\beta} \langle \beta \varphi_j, \mathcal{P}_{\Delta^n}(w_j - \beta \varphi_j) - w_j \rangle + \langle \nabla \phi(w_j) - \varphi_j, \mathcal{P}_{\Delta^n}(w_j - \beta \varphi_j) - w_j \rangle \\
+ \frac{L_{\phi}}{2} \|w_{j+1} - w_j\|^2.$$
(22)

To analyze the second term at the right hand side of the above Equation (22), we note that

 $-\langle \beta \varphi_j, \mathcal{P}_{\Delta^n}(w_j - \beta \varphi_j) - w_j \rangle$ 

 $= \langle w_j - \beta \varphi_j - \mathcal{P}_{\Delta^n}(w_j - \beta \varphi_j), \mathcal{P}_{\Delta^n}(w_j - \beta \varphi_j) - w_j \rangle + \|\mathcal{P}_{\Delta^n}(w_j - \beta \varphi_j) - w_j\|^2,$ which, in conjunction with the property of projection on convex set that  $\langle x - \mathcal{P}_{\Delta^n}(x), y - \mathcal{P}_{\Delta^n}(x) \rangle \leq 0$ for any  $y \in \mathcal{S}$  and the fact that  $w_j = \mathcal{P}_{\Delta^n}(w_{j-1} - \beta \varphi_{j-1}) \in \mathcal{S}$ , yields

$$-\langle \beta \varphi_j, \mathcal{P}_{\Delta^n}(w_j - \beta \varphi_j) - w_j \rangle \ge \|\mathcal{P}_{\Delta^n}(w_j - \beta \varphi_j) - w_j\|^2 \ge 0.$$
(23)

Then, substituting Equation (23) into Equation (22) yields

$$\phi(w_{j+1}) \leq \phi(w_j) + \langle \nabla \phi(w_j) - \varphi_j, \mathcal{P}_{\Delta^n}(w_j - \beta \varphi_j) - w_j \rangle + \frac{L_{\phi}}{2} \|w_{j+1} - w_j\|^2 \\
\leq \phi(w_j) - \frac{\beta}{2} \|\widehat{G}_j\|^2 + \frac{\beta}{2} \|\varphi_j - \nabla \phi(w_j)\|^2 + \frac{L_{\phi}\beta^2}{2} \|\widehat{G}_j\|^2 \\
\leq \phi(w_j) - \left(\frac{\beta}{4} - \frac{L_{\phi}\beta^2}{4}\right) \|G_j\|^2 + \left(\beta - \frac{L_{\phi}\beta^2}{2}\right) \|\varphi_j - \nabla \phi(w_j)\|^2,$$
(24)

where we use the notation that  $\hat{G}_j = \frac{1}{\beta} (w_j - \mathcal{P}_{\Delta^n} (w_j - \beta \varphi_j))$ , and the non-expansive property of projection. Then, taking the expectation and incorporating Equation (19) into Equation (24), we have

$$\mathbb{E}\phi(w_{j+1}) \leq \mathbb{E}\phi(w_j) - \left(\frac{\beta}{4} - \frac{L_{\phi}\beta^2}{4}\right) \mathbb{E}\|G_j\|^2 + \left(\beta - \frac{L_{\phi}\beta^2}{2}\right) \mathbb{E}\|\varphi_j - \nabla\phi(w_j)\|^2$$
$$\leq \mathbb{E}\phi(w_j) - \left(\frac{\beta}{4} - \frac{L_{\phi}\beta^2}{4}\right) \mathbb{E}\|G_j\|^2 + \left(\beta - \frac{L_{\phi}\beta^2}{2}\right) \left(\frac{6K}{|\mathcal{B}|} + 3L^2\delta_j\right). \tag{25}$$

Then, substituting Equation (21) into the above Equation (25) yields

$$\begin{split} \mathbb{E}\phi(w_{j+1}) &\leq \mathbb{E}\phi(w_{j}) - \left(\frac{\beta}{4} - \frac{L_{\phi}\beta^{2}}{4}\right) \mathbb{E}\|G_{j}\|^{2} + \left(\beta - \frac{L_{\phi}\beta^{2}}{2}\right) \frac{6K}{|\mathcal{B}|} \\ &+ 3L^{2} \left(\beta - \frac{L_{\phi}\beta^{2}}{2}\right) \left(\tau^{j}\delta_{0} + \frac{12\omega K\beta^{2}}{(1-\tau)|\mathcal{B}|} + 2\omega\beta^{2} \sum_{t=0}^{j-1} \tau^{t} \mathbb{E}\|G_{j-1-t}\|^{2}\right) \\ &\leq \mathbb{E}\phi(w_{j}) - \left(\frac{\beta}{4} - \frac{L_{\phi}\beta^{2}}{4}\right) \mathbb{E}\|G_{j}\|^{2} + \left(1 + \frac{6\omega\beta^{2}L^{2}}{1-\tau}\right) \left(\beta - \frac{L_{\phi}\beta^{2}}{2}\right) \frac{6K}{|\mathcal{B}|} \\ &+ 3L^{2} \left(\beta - \frac{L_{\phi}\beta^{2}}{2}\right) \tau^{j}\delta_{0} + 6\omega\beta^{2}L^{2} \left(\beta - \frac{L_{\phi}\beta^{2}}{2}\right) \sum_{t=0}^{j-1} \tau^{t} \mathbb{E}\|G_{j-1-t}\|^{2}, \end{split}$$

which, by taking the telescoping over j from 0 to J - 1, yields

$$\begin{split} \frac{1}{J} \sum_{j=0}^{J-1} & \left(\frac{1}{4} - \frac{L_{\phi}\beta}{4}\right) \mathbb{E} \|G_{j}\|^{2} \\ & \leq \frac{\phi(w_{0}) - \min_{w} \phi(w)}{\beta J} + \left(1 + \frac{6\omega\beta^{2}L^{2}}{1 - \tau}\right) \left(1 - \frac{L_{\phi}\beta}{2}\right) \frac{6K}{|\mathcal{B}|} \\ & + \frac{3L^{2} \left(1 - \frac{L_{\phi}\beta}{2}\right) \delta_{0}}{(1 - \tau)J} + 6\omega\beta^{2}L^{2} \left(1 - \frac{L_{\phi}\beta}{2}\right) \frac{1}{J} \sum_{j=0}^{J-1} \sum_{t=0}^{j-1} \tau^{t} \mathbb{E} \|G_{j-1-t}\|^{2} \\ & \leq \frac{\phi(w_{0}) - \min_{w} \phi(w)}{\beta J} + \left(1 + \frac{6\omega\beta^{2}L^{2}}{1 - \tau}\right) \left(1 - \frac{L_{\phi}\beta}{2}\right) \frac{6K}{|\mathcal{B}|} \\ & + \frac{3L^{2} \left(1 - \frac{L_{\phi}\beta}{2}\right) \delta_{0}}{(1 - \tau)J} + 6\omega\beta^{2}L^{2} \left(1 - \frac{L_{\phi}\beta}{2}\right) \frac{1}{(1 - \tau)J} \sum_{j=0}^{J-1} \mathbb{E} \|G_{j}\|^{2}. \end{split}$$

Rearranging the above inequality, we have

$$\frac{1}{J} \sum_{j=0}^{J-1} \left( \frac{1}{4} - \frac{L_{\phi}\beta}{4} - \frac{6\omega\beta^2 L^2}{1-\tau} \left( 1 - \frac{L_{\phi}\beta}{2} \right) \right) \mathbb{E} \|G_j\|^2 \\
\leq \frac{\phi(w_0) - \min_w \phi(w)}{\beta J} + \left( 1 + \frac{6\omega\beta^2 L^2}{1-\tau} \right) \left( 1 - \frac{L_{\phi}\beta}{2} \right) \frac{6K}{|\mathcal{B}|} + \frac{3L^2 \left( 1 - \frac{L_{\phi}\beta}{2} \right) \delta_0}{(1-\tau)J}.$$
(26)

Recalling the definition that  $\tau = 1 - \eta \mu + 6\omega \beta^2 L^2$ , and noting that we choose the stepsize  $\beta$  such that  $6\omega \beta^2 L^2 < \frac{1}{9}\eta \mu$  and  $\beta \le \frac{1}{4L_{\phi}}$ , we can simplify Equation (26) as

$$\frac{1}{16J} \sum_{j=0}^{J-1} \mathbb{E} \|G_j\|^2 \le \frac{\phi(w_0) - \min_w \phi(w)}{\beta J} + \frac{27K}{4|\mathcal{B}|} + \frac{27L^2 \delta_0}{8\eta \mu J}$$

From the gradient descent based updates, we have  $\delta_0 = \left(1 + \frac{\rho^2 M^2}{L^2 \mu^2}\right) \mathbb{E} \|\theta_0^N - \theta_0^*\|^2 + \mathbb{E} \|v_0^Q - v_0^*\|^2 \le \left(1 + \frac{\rho^2 M^2}{L^2 \mu^2}\right) \|\theta_0^0 - \theta_0^*\|^2 + \|v_0^0 - v_0^*\|^2 < +\infty.$  Then, the proof is complete.

# **B** Proof of Corollary 1

Based on the definition of  $C_Q = \frac{Q\rho M\eta}{\mu} + \eta^2 Q^2 \rho M + \eta QL$  and noting that  $\eta \leq \frac{1}{L} \leq \frac{1}{\mu}$  and Q = 3, we have  $C_Q \leq 12\eta(\frac{\rho M}{\mu} + L)$ , which, combined with the definition that  $r = \frac{C_Q^2}{(\frac{\rho M}{\mu} + L)^2}$ , yields  $r \leq 144\eta^2$ . Then, based on the choice of N = 1 and  $\lambda = \frac{\alpha\mu}{2}$ , we have

$$(1+\lambda)(1-\alpha\mu)^N \left(1+\frac{8rL^2}{\eta\mu}\right) \le \left(1-\frac{\alpha\mu}{2}\right) \left(1+\frac{1152\eta L^2}{\mu}\right) \le 1-\frac{\alpha\mu}{2} + \frac{1152\eta L^2}{\mu}$$

which, in conjunction with  $\eta \leq \frac{\mu^2}{4608L^2} \alpha$  and  $\alpha \leq \frac{1}{L}$ , yields

$$(1+\lambda)(1-\alpha\mu)^N \left(1+\frac{8rL^2}{\eta\mu}\right) \le 1-\frac{1}{4}\alpha\mu \le 1-\eta\mu.$$
 (27)

This implies that the inequality  $(1 + \lambda)(1 - \alpha \mu)^N(1 + \frac{8rL^2}{\eta\mu}) \leq 1 - \eta\mu$  required by Theorem 1 is satisfied. Then, treating  $\mu, \eta, L, \rho, M, \alpha, \beta, K$ ,  $\|\theta_0^0 - \theta_0^*\|^2$  and  $\|v_0^0 - v_0^*\|^2$  as constants independent of the total number J of iterations, we have

$$\frac{1}{J} \sum_{j=0}^{J-1} \mathbb{E} \|G_j\|^2 \le \mathcal{O}\left(\frac{1}{J} + \frac{1}{|\mathcal{B}|}\right).$$
(28)

Then, to ensure an  $\epsilon$ -accurate stationary point, the number of iterations is  $\epsilon^{-2}$  with a batch size  $|\mathcal{B}| = \mathcal{O}(\epsilon^{-2})$ .

# **C** Experiment Hyperparameters

The experimental hyperparameters are list in Table 7, including the memory size:  $|\mathcal{M}|$ , coreset size:  $|\mathcal{S}|$ , stream batch size:  $|\mathcal{B}_t|$ , learning rate for  $M_{tr}$ :  $lr_t$ , learning rate for  $M_{cs}$ :  $lr_p$ , learning rate for sample weights:  $lr_w$ , regularization efficient:  $\lambda$ , epochs for training model: E, outer loops in bilevel optimization: J, inner loops in bilevel optimization: N, loops for estimating the Hessian-inverse-vector product: Q, a factor of Gaussian noise:  $\delta$ .

Hyperparameters	Permuted MNIST	Split CIFAR-100	Split Tiny-Imagenet	Multiple Datasets	Split Food-101
$ \mathcal{M} $	200	100	200	83	100
$ \mathcal{S} $	10	10	20	10	10
$ \mathcal{B}_t $	50	50	100	50	50
$lr_t$	0.005	0.15	0.20	0.1	0.15
$lr_p$	5.0	5.0	10	5.0	10
$lr_w$	5.0	5.0	10	5.0	10
$\lambda$	0.1	0.1	0.1	0.1	0.1
E	1	1	1	1	1
J	5	10	5	5	5
N	1	1	1	1	1
Q	3	3	3	3	3
$\delta$	1e-3	1e - 3	1e-3	1e-3	1e-3

Table 7: Hyperparameters settings in experiments.

#### **D** Running Time Comparison

We evaluate the running time (wall-clock time) of baseline methods on Split Tiny-ImageNet and Split Food-101 in Table 8. All the training sections keep the same among these algorithms. Since there is no advanced coreset selection procedures in K-means Features, K-means Embedding, Uniform sampling, iCaRL, and Grad Matching, their running costs are pretty low but with worse performance (i.e., accuracy and forgetting) compared with our approach BCSR. PBCS and GCR, SPR and MetaSP don't involve bilevel formulations, they cannot guarantee accurate coreset sampling though with lower time cost against BCSR. Compared with OCS, BCSR takes 23% and 35% running time reduction on Tiny-ImageNet and Split Food-101, respectively. Because similarity computing based on data pairs is computationally expensive for OCS. Greedy Coreset takes much more time than BCSR due to the usage of NTK.

	U				
	Time (hours)				
Methods	Tiny-ImageNet	Split Food-101			
K-means Features	0.15	0.02			
K-means Embedding	0.41	0.04			
Uniform	0.13	0.03			
iCaRL	0.41	0.04			
Grad Matching	0.57	0.06			
SPR	0.77	0.11			
MetaSP	0.86	0.13			
PBCS	1.13	0.15			
GCR	0.91	0.13			
Greedy Coreset	6.26	0.83			
OCS	3.45	0.40			
BCSR	2.65	0.26			

Table 8: Running time.

# **E** Experiments on Permuted-MNIST

The experiment results on Permuted-MNIST is presented in this section. BCSR outperforms other baselines significantly in AVG ACC on all the data settings, while showing relatively low forgetting.

	Bala	anced	Imbal	anced	Labe	Label Noise	
Methods	$A_T$	$FGT_T$	$A_T$	$FGT_T$	$A_T$	$FGT_T$	
K-means Features	54.30±0.93	0.064±0.012	39.46±0.11	0.023±0.003	46.71±0.64	0.094±0.011	
K-means Embedding	54.78±1.83	0.056±0.009	41.97±2.02	0.013±0.005	47.36±1.58	0.082±0.015	
Uniform	53.74±0.35	0.073±0.006	38.49±1.89	0.025±0.008	46.35±1.72	0.091±0.014	
iCaRL	52.62±0.01	0.076±0.001	48.64±0.58	0.022±0.001	48.14±0.83	0.082±0.007	
Grad Matching	54.76±1.61	0.065±0.011	33.67±1.24	0.028±0.003	48.24±0.42	0.089±0.009	
SPR	54.24±0.45	0.068±0.019	40.79±0.83	0.031±0.003	48.23±0.75	0.067±0.004	
MetaSP	54.63±0.31	0.059±0.006	41.32±0.94	0.025±0.006	48.84±0.77	0.061±0.007	
Greedy Coreset	54.10±0.81	0.051±0.007	26.68±13.39	0.033±0.014	49.45±1.73	0.078±0.009	
GCR	54.53±0.64	0.067±0.021	40.63±0.50	0.032±0.005	48.64±0.75	0.074±0.014	
PBCS	51.61±1.14	0.144±0.021	41.14±0.23	0.119±0.007	39.74±1.98	0.178±0.001	
OCS	54.37±0.34	0.026±0.001	50.19±0.47	0.020±0.005	48.08±1.44	0.046±0.003	
BCSR	56.23±0.29	$0.058 \pm 0.002$	52.52±0.43	$0.010 \pm 0.002$	50.82±3.03	0.056±0.017	

Table 9: Experiment results on Permuted MNIST

# F Evolution of Average Accuracy

We present the learning process of different methods on Multiple Datasets in Figure 4. There are five tasks, where the average accuracy is tested after training each task. BCSR shows better performance than other baselines in different settings, including Balanced, Imbalanced, and label-noise.



Figure 4: Evolution of average accuracy during the continual learning process for Multiple Datasets.

# G Possibility Distribution of Candidate Coreset

To explore the effect of top-K regularizer, we observe the possibility distribution of sample weights after each bilevel optimization, where sample weights of candidate coresets are initialized uniformly. The novel top-K regularizer makes sure that the summation of the top-K entries of the learned probability vector is large, such that we can confidently choose a coreset with size K. We show the weight distribution after optimization in Figure. 5, where you can find that top-K weights are much higher than others (with a margin 2%), which easily distinguishes the top-K core samples from candidates.





Figure 5: Possibility distribution of candidate coreset for one mini-batch stream data.

Figure 6: The hypergradients in an outer-loop.

# **H** The Effect of Top-*K* Regularizer

To further analyze the effects of top-K regularizer, we conduct the ablation study with different values of regularizer coefficient  $\lambda$  on balanced Split CIFAR-100. The performance results with different  $\lambda$  are shown in Table 10 and the corresponding average top-K summations of coreset weights are in Table 11. In our experiment, there are 50 candidate samples in each mini-batch data, and the summation of 50 coreset weights is equal to 1.00. Top-K summation of weights increases as  $\lambda$ increases, which imposes higher probabilities on top-K entries and lower probabilities on the rest candidates. The best performance is achieved when  $\lambda = 0.1$ , which means  $\lambda$  balances the trade-off between the loss function and regularizer strength: if  $\lambda$  is too large, the algorithm primarily focuses on choosing the important samples instead of updating the model parameter, and vice versa.

Table 10: Ablation study for the regularize coefficient  $\lambda$ .

Measure	λ=0.01	λ=0.05	λ=0.10	<i>λ</i> =0.50	$\lambda$ =1.00
$\begin{array}{c} A_T \\ FGT_T \end{array}$	59.37±0.35	60.23±0.43	61.60±0.14	59.42±1.45	58.89±1.64
	0.095±0.098	0.074±0.054	0.051±0.015	0.138±0.075	0.128±0.076

Table 11: Top-K summation/Total summation of coreset weights (K = 10).

Measure	$\lambda$ =0.01	$\lambda$ =0.05	λ=0.10	$\lambda$ =0.50	$\lambda$ =1.00
Top- $K$ Sum/Total Sum	0.41/1.00	0.56/1.00	0.63/1.00	0.73/1.00	0.84/1.00

# I Hypergradient Evolution

To demonstrate the efficiency of bilevel optimization, we illustrate the evolution of hypergradients for a bilevel optimization on Split CIFAR-100 in Figure. 6. We observe the average norm of hypergradient reduces from  $10^{-1}$  to less than  $10^{-2}$  in each round of coreset selection with loops equal to 10. The hypergradient curves show that our designed bilevel optimization provides both theoretical and practical convergence guarantees.

Methods	K=10 A <sub>T</sub>	K=20 A <sub>T</sub>	K=40 A <sub>T</sub>
Uniform	58.99±0.54	53.57±2.93	53.03±1.97
Greedy Coreset	59.39±0.16	56.81±3.32	56.09±0.42
PBCS	55.64±2.26	49.84±1.76	40.95±0.32
OCS	52.57±0.37	54.87±0.58	56.46±0.07
BCSR	61.60±0.14	59.06±1.15	56.58±0.21

Table 12: The effect of coreset size

# J The Effect of Coreset Size K

Coreset size K also plays an important role in the experiment. We compare our BCSR with other coreset-based algorithms on different K. Note that coreset is selected from the current stream mini-batch  $\mathcal{B}_t$ , so the coreset size K satisfies  $K \leq |\mathcal{B}_t|$ . In the main experiment results, K = 10 is fixed in all the algorithms for a fair comparison. Here, we set K = 10, 20, 40 to conduct the continual learning experiments, respectively. The result is represented in Table 12. Note that all the results presented here are based on balanced Split CIFAR-100.

We mainly compare with the other four methods, including Uniform Sampling and three coresetbased methods, Greedy Coreset, PBCS, and OCS. We can observe that the performance of almost all methods becomes worse when coreset size is large. The reason is that if coreset size is larger and closer to  $\mathcal{B}_t$ , more redundant or noisy data are selected from the current stream mini-batch, and the coreset would not be representative anymore. In contrast, the smaller coreset could reduce the probability that redundant data are selected. Compared with other methods, BCSR shows the best performance (both accuracy and forgetting) and better robustness on different K.

# **K** The Effect of Inner Loops N and Hessian-inverse-vector Product Loops Q

We conduct ablation studies to explore the sensitivity of hyperparameters (N and Q) on Split CIFAR-100. The results are presented in Tables 13 (N) and Table 14 (Q). The model performance remains relatively stable when increasing inner loops (N) while fixing Q. But too large N ( $N \ge 15$ ) leads to performance degradation due to overfitting. The Q loops show similar properties that a few Qloops (e.g., Q = 3) are enough to approximate the Hessian-inverse-vector product. Too small Q and too large Q will hurt the performance due to possible underfitting (e.g., Q = 1) and overfitting (e.g., Q = 20).

Measure	N=1	N=5	N=10	N=15	N=20
$\begin{array}{c} A_T \\ FGT_T \end{array}$	61.60±0.14	61.75±0.11	61.64±0.15	60.77±0.32	59.20±0.41
	0.051±0.015	0.047±0.013	0.063±0.017	0.074±0.021	0.079±0.035

Table 13: Ablation study for the inner loops (N) with fixed Q = 3.

Table 14: Ablation study for the loops Q with fixed N = 1.

Measure	Q=1	Q=3	Q=5	Q=10	Q=20
$\begin{array}{c} A_T \\ FGT_T \end{array}$	52.14±1.53	61.60±0.14	61.57±0.15	58.42±0.53	57.80±1.31
	0.123±0.038	0.051±0.015	0.064±0.012	0.173±0.045	0.162±0.041

# L Datasets

- Spit CIFAR-100. Balanced split CIFAR-100 is based on the original CIFAR-100 and is split into 20 tasks, each consisting of 5 disjoint classes. The imbalanced setting and label noise are also applied to this dataset to make the task more challenging. We follow [13] to transform the original dataset to imbalanced long-tailed CIFAR-100. In the label-noise setting, we randomly select 20% data in each task and randomly change their labels to an arbitrary label of 10 classes.
- **Permuted MNIST**. Balanced MNIST is a handwritten digits dataset [43] containing 20 tasks, where each task applies a fixed random permutation to the image pixels. For the imbalanced setting, we randomly select 8 classes over 10 and sample 10% of the selected classes for training. We also conduct the experiments on the label noise scenario, where symmetric label noise with 20% noise rate is imposed on the data. In particular, to make the problem setting more challenging, each task only retains 3000 training data randomly sampled from the original data.
- **Multiple Datasets**. This dataset [78] contains a couple of totally different datasets, including MNIST [43], fashion-MNIST [75], NotMNIST [8], Traffic Sign [69] and SVHN [54]. There are 5 tasks, and each task is constructed by randomly selecting 1000 training samples from a different dataset. The procedure of creating the dataset in the imbalanced and label-noise settings is the same as that in Split CIFAR-100.
- Split Tiny-ImageNet. This dataset [42] contains 100000 images of 200 classes (500 for each class) downsized to  $64 \times 64$  colored images. Each class has 500 training images, 50 validation images, and 50 test images. We construct the task sequences by splitting data into 20 tasks, where each task consists of 10 disjoint classes.
- Split Food-101. This dataset [7] is a challenging data set of 101 food categories, with 101'000 images. All the images are resized to  $64 \times 64$  pixels to be fed into models. To build continual learning tasks easily, We discard the last category and split data into 20 tasks, with 5 categories within each task. Other data settings, including imbalanced and lable-noise, are the same as Split CIFAR-100.

# **M** Assumptions and Properties

We first provide standard definitions and assumptions for the convergence rate analysis of bilevel optimization [25, 36]. For notational convenience, we define  $\ell(\theta) := \sum_{i=1}^{n} \ell_i(\theta)$ .

**Definition 1.** A mapping f is  $L_f$ -Lipschitz continuous if for  $\forall z, z'$ ,  $||f(z) - f(z')|| \le L_f ||z - z'||$ . Assumption 1. The lower-level function  $L(\theta, w)$  is  $\mu$ -strongly-convex w.r.t.  $\theta$ .

Assumption 1 is a necessary geometric assumption in analyzing the convergence rate of bilevel optimization algorithms, as also widely adopted existing theories in [25, 37, 32]. We also note that this condition is satisfied for overparameterized neural networks [82]. The following assumption imposes some Lipschitz continuity conditions on the upper- and lower-level objective functions.

**Assumption 2.** The gradients  $\nabla_{\theta} L(\theta, w)$ ,  $\nabla_{w} L(\theta, w)$  and  $\ell(\theta)$  are L-Lipschitz continuous w.r.t.  $\theta$  and w. In addition, the gradient norm  $\|\nabla \ell(\theta^*(w))\| \leq M$ .

Note that we do not impose any conditions on the regularization function  $R(w, \delta)$ . The following assumption imposes the Lipschitz continuity on the second-order derivatives of the lower-level functions.

**Assumption 3.** The second-order derivatives  $\nabla_w \nabla_\theta L(\theta, w)$  and  $\nabla^2_\theta L(w, \theta)$  are  $\rho$ -Lipschitz continuous.

Then, we use the following proposition to characterize the properties of the smoothed top-K regularizer  $R(w, \delta)$ , based on the results in [23].

**Proposition 1.** The smoothed regularizer  $R(w, \delta)$  and its sampled version  $R(w, \delta; \tilde{z})$  satisfy the following two important properties: (i) The gradient  $\nabla R(w, \delta)$  exists and is  $\frac{\sqrt{Kn}}{\delta}$ -Lipschitz continuous; (ii) The gradient norm  $||R(w, \delta; \tilde{z})||$  is bounded by  $\sqrt{K}$  for any sample  $\tilde{z}$ .

Proposition 1 shows that the regularizer  $R(w, \delta)$  is smooth and its stochastic version  $R(w, \delta; \tilde{z})$  is bounded. These two properties are important to guarantee the non-asymptotic convergence of our proposed bilevel method.