# Department of AI, University of Seoul Machine Learning and Artificial Intelligence Lab

< 2022/05/02 >

**Dataset Condensation with Gradient Matching** 

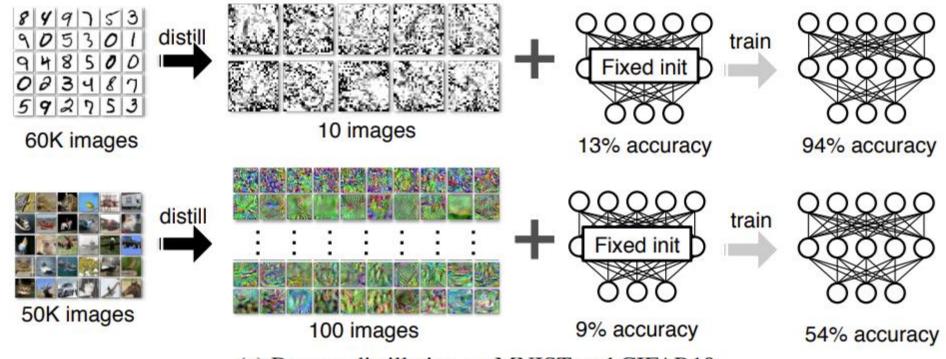
Lab seminar IN-DEPTH

YongTaek Lim

# **Dataset Distillation**

### **Dataset Distillation**

#### Concept



(a) Dataset distillation on MNIST and CIFAR10

 Goal: Compress the knowledge of an entire dataset into a few synthetic training images while achieving close to original performance with only a few gradient descent steps.

# **Dataset Distillation**

#### **Method**

#### **Algorithm 1** Dataset Distillation

```
Input: p(\theta_0): distribution of initial weights; M: the number of distilled data
Input: \alpha: step size; n: batch size; T: the number of optimization iterations; \tilde{\eta}_0: initial value for \tilde{\eta}
 1: Initialize \tilde{\mathbf{x}} = {\{\tilde{x}_i\}_{i=1}^{M} \text{ randomly, } \tilde{\eta} \leftarrow \tilde{\eta}_0}
 2: for each training step t = 1 to T do
            Get a minibatch of real training data \mathbf{x}_t = \{x_{t,j}\}_{j=1}^n
 3:
             Sample a batch of initial weights \theta_0^{(j)} \sim p(\theta_0)
 4:
            for each sampled \theta_0^{(j)} do
 5:
                  Compute updated parameter with GD: \theta_1^{(j)} = \theta_0^{(j)} - \tilde{\eta} \nabla_{\theta_0^{(j)}} \ell(\tilde{\mathbf{x}}, \theta_0^{(j)})
 6:
                   Evaluate the objective function on real training data: \mathcal{L}^{(j)} = \ell(\mathbf{x}_t, \theta_1^{(j)})
 7:
 8:
             end for
             Update \tilde{\mathbf{x}} \leftarrow \tilde{\mathbf{x}} - \alpha \nabla_{\tilde{\mathbf{x}}} \sum_{i} \mathcal{L}^{(j)}, and \tilde{\eta} \leftarrow \tilde{\eta} - \alpha \nabla_{\tilde{\eta}} \sum_{i} \mathcal{L}^{(j)}
 9:
10: end for
Output: distilled data \tilde{\mathbf{x}} and optimized learning rate \tilde{\eta}
```

Source:

# Motivation

## **Motivation**

#### Why Dataset Condenstation?

- storing datasets and training models on them become more expensive.
  - classical data selection methods have two shortcomings.
    - they rely on heuristics which does not guarantee optimal solution for the downstream tasks.
    - presence of representative sample maybe not guaranteed.
- Applications
  - Continual Learning
    - goal: To preserve the performance on the old tasks while learning the new ones.
    - herding(<u>Castro et al.,2018</u>): Produces a sorted list of samples of one class based on the distance to the mean sample of that class.
    - replace herding to Dataset Condensation
  - Neural Architecture Search(NAS)
    - Goal: To automate the design of DNN.
    - Training model with whole dataset requires expensive time.
    - Achieving the highest testing performance and performance correlation(Mentioned Later).

#### **Dataset Condensation**

• Method aims to find the optimum set of synthetic images  $S^*$  such that model  $\phi_{\theta^S}$  trained on them minimizes the training loss over the original data.

$$\bullet \quad \mathcal{S}^* = \mathop{\arg\min}_{\mathcal{S}} \mathcal{L}^{\mathcal{T}}(\boldsymbol{\theta}^{\mathcal{S}}(\mathcal{S})) \qquad \text{subject to} \qquad \boldsymbol{\theta}^{\mathcal{S}}(\mathcal{S}) = \mathop{\arg\min}_{\boldsymbol{\theta}} \mathcal{L}^{\mathcal{S}}(\boldsymbol{\theta}).$$

where

$$\bullet \quad \boldsymbol{\theta}^{\mathcal{T}} = \operatorname*{arg\,min}_{\boldsymbol{\theta}} \mathcal{L}^{\mathcal{T}}(\boldsymbol{\theta})$$

$$\bullet \ \theta^{\mathcal{S}} = \arg\min_{\boldsymbol{\theta}} \mathcal{L}^{\mathcal{S}}(\boldsymbol{\theta})$$

- But, optimizing this equation requires a computationally expensive procedure.
- So alternative formulation for dataset condensation proposed.

#### **Dataset Condensation with parameter matching**

- Motivation :
  - Pure dataset condensation requires computationally expensive procedure.
  - So, it does not scale to large and accurate inner-loop optimizers with many steps.
- Goal : To learn S such that the model  $\phi_{\theta^S}$  trained on them achieves not only comparable generalization performance to  $\phi_{\theta^T}$  but also converges to a similar solution in the parameter space so  $\theta^S \approx \theta^T$ .
- $\min_{\mathcal{S}} D(\boldsymbol{\theta}^{\mathcal{S}}, \boldsymbol{\theta}^{\mathcal{T}})$  subject to  $\boldsymbol{\theta}^{\mathcal{S}}(\mathcal{S}) = \arg\min_{\boldsymbol{\theta}} \mathcal{L}^{\mathcal{S}}(\boldsymbol{\theta})$  (4)
  - where  $D(\cdot,\cdot)$  is a distance function.
- But, optimization in eq. (4) aims to obtain an optimum set of S only for  $\phi_{\theta^T}$

with initialization  $\theta_0$ 

SK Song Kyungwoo 11 hours ago

Dataset Distillation에서, Dataset Consendation으로 넘어가는 motivation 부분이 잘 와닿지 않는것 같습니다. 즉, 식 (3)이 기존의 방법들이고, 식(4)번이 본 논문의 방법론으로 보이는데요. 식(3)번의 어떤 부분이 문제라서 식 (4)로 넘어가야만 하는지 (즉 이 연구를 왜 해야하는지) 궁금합니다. 본문에서는 계산상의 어려움을 많이 이유로 들고 있는데, 이유가 단순히 그것뿐인가요?

#### Dataset Condensation with parameter matching

- So, modify eq.(4) as follows
  - $\min_{\mathcal{S}} E_{\boldsymbol{\theta}_0 \sim P_{\boldsymbol{\theta}_0}} [D(\boldsymbol{\theta}^{\mathcal{S}}(\boldsymbol{\theta}_0), \boldsymbol{\theta}^{\mathcal{T}}(\boldsymbol{\theta}_0))] \quad \text{subject to} \quad \boldsymbol{\theta}^{\mathcal{S}}(\mathcal{S}) = \arg\min_{\boldsymbol{\theta}} \mathcal{L}^{\mathcal{S}}(\boldsymbol{\theta}(\boldsymbol{\theta}_0))$  (5)
  - but inner loop optimization  $\theta^S(S) = argmin_\theta L^S(\theta)$  can be computationally expensive.
- So modify eq.(5) by adopting the back-optimization approach
  - $oldsymbol{ heta}^{\mathcal{S}}(\mathcal{S}) = exttt{opt-alg}_{oldsymbol{ heta}}(\mathcal{L}^{\mathcal{S}}(oldsymbol{ heta}), arsigma)$
  - whre opt-alg is a specific optimization procedure with a fixed number of steps.

# changdae oh

스텝 수가 1이면 SAM, meta learning등에서 사용되는 taylor first order approximation랑 동일하다고 봐도 될까요?

#### **Dataset Condensation with gradient matching**

- Motivation
  - Dataset condensation with parameter matching has two issues.
    - $D(\theta^T, \theta^S)$  can be too big in the parameter space.  $\rightarrow$  hard to optimize
    - opt-alg may not be sufficient to take enough steps for reaching the optimal solution.
- Goal: make  $\theta^S$  to be close to not only the final  $\theta^T$  but also to follow a similar path to  $\theta^T$  throughout the optimization steps.
- eq. (5) decomposed as follows

$$\min_{\mathcal{S}} \mathcal{E}_{\boldsymbol{\theta}_0 \sim P_{\boldsymbol{\theta}_0}} [\sum_{t=0}^{T-1} D(\boldsymbol{\theta}_t^{\mathcal{S}}, \boldsymbol{\theta}_t^{\mathcal{T}})] \quad \text{subject to}$$

$$\boldsymbol{\theta}_{t+1}^{\mathcal{S}}(\mathcal{S}) = \text{opt-alg}_{\boldsymbol{\theta}}(\mathcal{L}^{\mathcal{S}}(\boldsymbol{\theta}_t^{\mathcal{S}}), \varsigma^{\mathcal{S}}) \quad \text{and} \quad \boldsymbol{\theta}_{t+1}^{\mathcal{T}} = \text{opt-alg}_{\boldsymbol{\theta}}(\mathcal{L}^{\mathcal{T}}(\boldsymbol{\theta}_t^{\mathcal{T}}), \varsigma^{\mathcal{T}})$$

$$(7)$$

each iteration t. In our preliminary experiments, we observe that  $\theta_{t+1}^{\mathcal{S}}$ , which is parameterized with  $\mathcal{S}$ , can successfully track  $\theta_{t+1}^{\mathcal{T}}$  by updating  $\mathcal{S}$  and minimizing  $D(\theta_t^{\mathcal{S}}, \theta_t^{\mathcal{T}})$  close to zero.



제가 영어를 잘 해석하지 못한건지.. 여기서 Preliminary experiment가 어 떤 것을 말하는 것일까요? 해당 진술 이 확인되는 과정을 알고 싶은데 찾 을 수가 없어서 여쭤봅니다.

#### **Dataset Condensation with gradient matching**

• parameters  $\theta^T$ ,  $\theta^S$  updated as follows.

$$\theta_{t+1}^{\mathcal{S}} \leftarrow \theta_{t}^{\mathcal{S}} - \eta_{\theta} \nabla_{\theta} \mathcal{L}^{\mathcal{S}}(\theta_{t}^{\mathcal{S}})$$
 and  $\theta_{t+1}^{\mathcal{T}} \leftarrow \theta_{t}^{\mathcal{T}} - \eta_{\theta} \nabla_{\theta} \mathcal{L}^{\mathcal{T}}(\theta_{t}^{\mathcal{T}}),$ 

- Based on authors observation that  $D(\theta_t^S, \theta_t^T) \approx 0$ , formulation in eq. (7) simplified by replacing  $\theta_t^T$  with  $\theta_t^S$  and use  $\theta$  to denote  $\theta^S$  so,
- $\min_{\mathcal{S}} \mathrm{E}_{\boldsymbol{\theta}_0 \sim P_{\boldsymbol{\theta}_0}} [\sum_{t=0}^{T-1} D(\nabla_{\boldsymbol{\theta}} \mathcal{L}^{\mathcal{S}}(\boldsymbol{\theta}_t), \nabla_{\boldsymbol{\theta}} \mathcal{L}^{\mathcal{T}}(\boldsymbol{\theta}_t))].$
- joint optimization data and label is challenging, thus in this paper model learn to synthesize images for fixex labels.



이거 맞아요?

total set이랑 small set에 대해 각각 따로 가정했던 theta를 별 차이 안날 테니까 그냥 공통 shared 파라미터 로 하겠다는건데, 업데이트 별로 안 된 학습 초기에는 많이 다를거같은데 그냥 첨부터 하나로 보고 이렇게 formulate해도 될지



저도 이 부분이 동일하게 궁금합니다. 이와 관련된 실험이 본문 또는 appendix에 있나요?

#### Dataset Condensation with gradient matching

# Algorithm

#### Algorithm 1: Dataset condensation with gradient matching

**Input:** Training set  $\mathcal{T}$ 

**Required**: Randomly initialized set of synthetic samples S for C classes, probability distribution over randomly initialized weights  $P_{\theta_0}$ , deep neural network  $\phi_{\theta}$ , number of outer-loop steps K, number of inner-loop steps T, number of steps for updating weights  $\varsigma_{\theta}$  and synthetic samples  $\varsigma_{S}$  in each inner-loop step respectively, learning rates for updating weights  $\eta_{\theta}$  and synthetic samples  $\eta_{S}$ .

#### Output: S

# changdae oh

각 synthetic sample들은 learnable 한 다차원 텐서일텐데 shape은 꼭 원 래 original image랑 같아야 할 필요 는 없는거같은데 맞죠??

#### 임용택

5 hours ago 하나의 실험에서 사용된 (NAS) MNIST, SVHN, USPS 가 각각 28\*28, 32\*32, 16\*16의 크기를 가지는 것으로 보아 다 르게 해도 상관 없을 것 같습니다

#### 변호윤 a day ago

클래스별로 샘플들을 평균을 내거나 간단한 알고리즘으로 군집화 하는 등 의 전처리를 통해서 더 빠른 수렴을 기대할 수 있을까요? 좀 더 학습 데이터셋을 활용하여 synthetic dataset을 구축할 수도 있 었을 텐데, Synthetic sample은 랜덤해야만 하 는가 궁금합니다.

Source:

#### **Dataset Condensation with gradient matching**

# Algorithm

#### Algorithm 1: Dataset condensation with gradient matching

**Input:** Training set  $\mathcal{T}$ 

**Required**: Randomly initialized set of synthetic samples S for C classes, probability distribution over randomly initialized weights  $P_{\theta_0}$ , deep neural network  $\phi_{\theta}$ , number of outer-loop steps K, number of inner-loop steps T, number of steps for updating weights  $S_{\theta}$  and synthetic samples  $S_{\theta}$  in each inner-loop step respectively, learning rates for updating weights  $S_{\theta}$  and synthetic samples  $S_{\theta}$ .

#### Output: S

# SK Song Kyungwoo

Class 마다 비교하고 있는데요. 혹시 Class 마다 하지 않을 때는 어떠한지 성능 실험이 있을까요? + Unlabeled data 에 대해서는 그럼 현재의 Dataset condensation 모델 적용이 가능한가요? 실제로 우리가다루는 large-scale data는 대부분이 class가 없는것일텐데요

#### 임용택 12 hours ago

OpenReview에서 저자들이 말하길 Our method could be used in selfsupervised learning problems such as estimating rotation of an image (Gidaris et al 2018 ICLR) without any major modification. 라고 하네요. 사용 될 수도 있다고는 하는데 본 논문에 정 리된 부분은 없네요

# changdae oh

loss function에 따라서도 결과 꽤 다 를수도 있을거같은데 여기선 cross entropy만 실험한거같은데 다른것들 에 대해서는 어떨지 개인적으로 궁금 하네요

# 임용택 12 hours ago openreview에 같은 질문이 있었네요. 저자들은 "다른 loss에서 특별히 안 좋 은 결과를 낼 이유가 없어보인다" 정도 로만 답했습니다!



이부분 B^S\_C ~ S에 대해 제가 이해한 바가 맞는지 확인하고싶은데, 우리가 S의 사이즈 N를 미리 설정하고 (예를들어 5천장) 이후 N \* C \* H \* W의 전체 S를 한번에 parameterize하고 이후 loop 돌때는 이 N \* C \* H \* W의 텐서에서 일부를 BS \* C \* H \* W만큼 샘플링해서 모델에 집어넣는거 맞죠?? 그럼 얘는 랜덤하게 샘플링하면 안되고 순서대로 집어넣겠군요?! 얘네 전부가 학습대상이니까.

추가로 그럼 이 방법론을 적용했을때 최종적으로 학습되는 파라미터는 (사용되는 backbone 모델의 파라미 터 총 개수 + (N \* C \* H \* W)갰네요?

Source:

#### **Dataset Condensation with gradient matching**

Gradient matching loss

$$d(\mathbf{A}, \mathbf{B}) = \sum_{i=1}^{\text{out}} \left( 1 - \frac{\mathbf{A_{i \cdot} \cdot B_{i \cdot}}}{\|\mathbf{A_{i \cdot}}\| \|\mathbf{B_{i \cdot}}\|} \right)$$



식 10에서 두 gradient의 방향만 고려 하는데 각 gradient의 크기는 고려할 필요가 없을까요??

#### Show less

changdae oh

저도 비슷한 맥락에서 cosine distance 말고 다른 distance로 했을때는 어떨지 궁금하네요



12 hours ago

1. gradient크기가 필요한 지 여부에 대 해서는 좀 더 찾아보고 답변 준비하겠 습니다.

임용택 12 hours ago

2.유클리디안, 코사인 에 대해서 추가적 으로 실험한 결과가 오픈리뷰에 있습니 다. 코사인과 여기서 제안한 방법의 차 이가 무엇인지는 잘 모르겠으나.. 정리 해가도록 하겠습니다

	MLP	ConvNet	LeNet	AlexNet	VGG	ResNet
Euclidean	69.3±0.9	92.7±0.3	65.0±5.1	66.2±5.6	57.1±7.0	68.0±5.2
Cosine	45.2±3.6	69.2±2.7	61.1±8.2	58.3±4.1	55.0±5.0	68.8±7.8
Ours	70.5±1.2	91.7±0.5	85.0±1.7	82.7±2.9	81.7±2.6	89.4±0.9

#### **Dataset Condensation**

- Datasets
  - MNIST
  - SVHN
  - FashionMNIST
  - CIFAR10
- Deep Network Architectures
  - MLP
  - ConvNet
  - LeNet
  - AlexNet
  - VGG
  - ResNet

#### **Dataset Condensation**

# Comparison to coreset methods

	Img/Cls	Ratio %	Random	Coreset Herding	Selection K-Center	Forgetting	Ours	Whole Dataset
MNIST	1 10 50	0.017 0.17 0.83	64.9±3.5 95.1±0.9 97.9±0.2	89.2±1.6 93.7±0.3 94.9±0.2	89.3±1.5 84.4±1.7 97.4±0.3	35.5±5.6 68.1±3.3 88.2±1.2	$91.7 \pm 0.5$ $97.4 \pm 0.2$ $98.8 \pm 0.2$	99.6±0.0
FashionMNIST	1 10 50	0.017 0.17 0.83	51.4±3.8 73.8±0.7 82.5±0.7	67.0±1.9 71.1±0.7 71.9±0.8	66.9±1.8 54.7±1.5 68.3±0.8	42.0±5.5 53.9±2.0 55.0±1.1	70.5±0.6 82.3±0.4 83.6±0.4	93.5±0.1
SVHN	1 10 50	0.014 0.14 0.7	14.6±1.6 35.1±4.1 70.9±0.9	20.9±1.3 50.5±3.3 72.6±0.8	21.0±1.5 14.0±1.3 20.1±1.4	12.1±1.7 16.8±1.2 27.2±1.5	31.2±1.4 76.1±0.6 82.3±0.3	95.4±0.1
CIFAR10	1 10 50	0.02 0.2 1	14.4±2.0 26.0±1.2 43.4±1.0	21.5±1.2 31.6±0.7 40.4±0.6	21.5±1.3 14.7±0.9 27.0±1.4	13.5±1.2 23.3±1.0 23.3±1.1	28.3±0.5 44.9±0.5 53.9±0.5	84.8±0.1

	Ima/Cle		Core-set Selection Random Herding K-Center Forgetting				LD <sup>†</sup>	Ours	Whole Dataset
	mig/Cis	Katio //	Random	Herding	K-Center	Forgetting	LD	Ours	Whole Dataset
CIFAR100	1	0.2	4.2±0.3	8.4±0.3	8.3±0.3	3.5±0.3	11.5±0.4	12.8±0.3	56.2±0.3
	10	2	$14.6 \pm 0.5$	$17.3 \pm 0.3$	$7.1 \pm 0.3$	$9.8 \pm 0.2$	-	$25.2 \pm 0.3$	30.2±0.3



좀 더 크고 class가 다양한 데이터에 대한 결과가 궁금했는데 supplementary에 cifar100에 대한 결과가 나와있네요.. 성능은 ciar10 과 비슷한 이유로 안 좋은 듯 합니다.

#### Show less



a day ago 인정. 저해상도 이미지들만 있어서 아 쉽긴했네요



학습 자체가 invariant feature를 잘 뽑아내지 못해서이지 않을까요?

논문의 알고리즘에서 Domain 종류 에 대한 for loop를 추가해서 IDGM Term을 쓰면 어떨지 궁금하네요.

#### **Dataset Condensation**

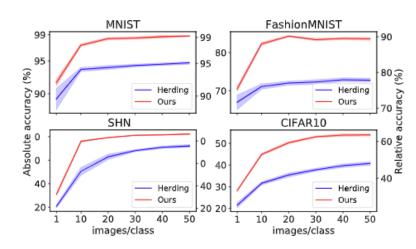
Comparison with Dataset Distillation(Wang et al., 2018)

Dataset	Img/Cls	DD	Ours	Whole Dataset
MNIST	1 10	79.5±8.1	85.0±1.6 93.9±0.6	
CIFAR10	1 10	36.8±1.2	24.2±0.9 39.1±1.2	83.1±0.2

higher accuracy and lower standard deviation.

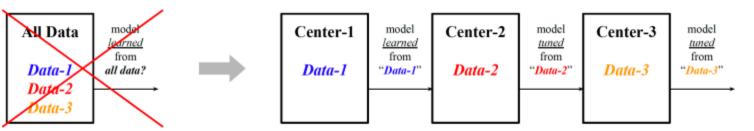
Increasing the number of condensed images improves the acc in all

benchmarks.

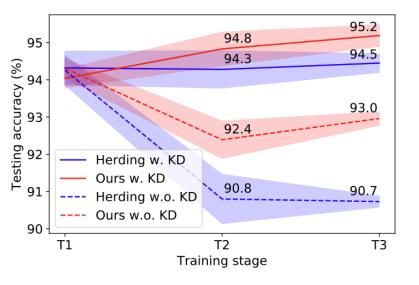


#### **Application**

# Continual Learning



#### Result



stage1: SVHN

stage2: MNIST

stage3: USPS

#### **Application**

- Neural Architecture Search(NAS)
  - varying W, N, A, P, D over an uniform grid
  - train model for 100 epochs.
  - use small proxy datasets with
    - Random Sampling
    - Herding
    - Dataset Condensation
  - searching space of 720 convnets

W: #filter

N: normalization layer

A: activation layer

P: pooling layer

D: #duplicate blocks

	Random	Herding	Ours	Early-stopping	Whole Dataset
Performance (%) Correlation Time cost (min) Storage (imgs)	76.2 -0.21 <b>18.8</b>	76.2 -0.20 <b>18.8</b> 10 <sup>2</sup>	84.5 0.79 18.8 10 <sup>2</sup>	<b>84.5</b> 0.42 <b>18.8</b> 10 <sup>4</sup>	$85.9$ $1.00$ $8604.3$ $5 \times 10^4$

