Provable Stochastic Optimization for Global Contrastive Learning: Small Batch Does Not Harm Performance

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Self-Supervised Learning

- Learning representations on large amount of unlabeled data (e.g., image, text)
  - **Contrastive learning** – SimCLR (Google), CLIP (OpenAI)
- Challenges of contrastive learning, such as
  - **Large batch size** – high computation resource demand
- In this work, we explain **why** SimCLR is sensitive to batch size and **how** to tackle this challenge by proposing a new framework

SimCLR: Mini-batch Contrastive Objective

- SimCLR defines contrastive objective for each augmented pair $(\mathcal{A}(\mathbf{x}_i), \mathcal{A}'(\mathbf{x}_i))$ for an image $\mathrm{x_i}$ in **mini-batch level** B :

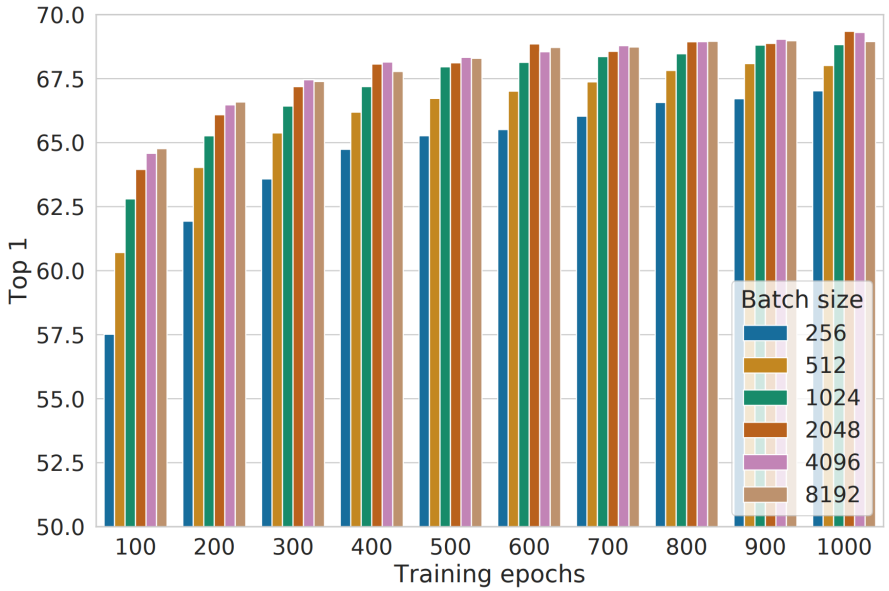
Positive Pair

$$L_{\mathcal{B}}(\mathbf{w}; \mathbf{x}_i, \mathcal{A}, \mathcal{A}') = -\ln \frac{\exp(E(\mathcal{A}(\mathbf{x}_i))^\top E(\mathcal{A}'(\mathbf{x}_i))/\tau)}{g(\mathbf{w}; \mathbf{x}_i, \mathcal{A}, \mathcal{B})},$$

$$g(\mathbf{w}; \mathbf{x}_i, \mathcal{A}, \mathcal{B}_i) = \sum_{\mathbf{z}_j \in \mathcal{B}_i} (\exp(E(\mathcal{A}(\mathbf{x}_i))^\top E(\mathbf{z}_j)/\tau)$$

Mini-batch

Negative Pairs



Why Large batch sizes work better?

Global Contrastive Objective

- To explain of issues of InfoNCE loss, we use **Global Contrastive Objective** for each augmented pair $(\mathcal{A}(\mathbf{x}_i), \mathcal{A}'(\mathbf{x}_i))$ of an image $\mathrm{x_i}$ in all data S:

Mini-batch Contrastive Objective

$$L_{\mathcal{B}}(\mathbf{w}; \mathbf{x}_i, \mathcal{A}, \mathcal{A}') = -\ln \frac{\exp(E(\mathcal{A}(\mathbf{x}_i))^\top E(\mathcal{A}'(\mathbf{x}_i))/\tau)}{g(\mathbf{w}; \mathbf{x}_i, \mathcal{A}, \mathcal{B})},$$

$$g(\mathbf{w}; \mathbf{x}_i, \mathcal{A}, \mathcal{B}_i) = \sum_{\mathbf{z}_j \in \mathcal{B}_i} (\exp(E(\mathcal{A}(\mathbf{x}_i))^\top E(\mathbf{z}_j)/\tau)$$

Negative Pairs (**mini-batch**)

Global Contrastive Objective

$$L(\mathbf{w}; \mathbf{x}_i, \mathcal{A}, \mathcal{A}') = -\ln \frac{\exp(E(\mathcal{A}(\mathbf{x}_i))^\top E(\mathcal{A}'(\mathbf{x}_i))/\tau)}{\varepsilon' + g(\mathbf{w}; \mathbf{x}_i, \mathcal{A}, \mathcal{S}_i)},$$

$$g(\mathbf{w}; \mathbf{x}_i, \mathcal{A}, \mathcal{S}_i) = \sum_{\mathbf{z} \in \mathcal{S}_i} (\exp(E(\mathcal{A}(\mathbf{x}_i))^\top E(\mathbf{z})/\tau),$$

Negative Pairs (**All data**)

Analysis of Optimization Error for SimCLR

Theorem 1. Assume $\mathbf{F}$ is smooth, $\mathbf{g}$ is smooth and Lipchitiz continuous, SimCLR ensures that $\mathbb{E}\left[\|\nabla F(\mathbf{w}_{t'})\|^2\right] \leq O\left(\frac{1}{\eta T} + \eta + \frac{1}{B}\right)$ for a random $t' \in \{1, \ldots, T\}$.

- **Remarks:**
  - SimCLR suffers a large optimization error depending on the batch size in the order of $\boldsymbol{O(1/\sqrt{B})}$ for the gradient norm term,
  - This also explains why SimCLR achieves good performance using large batch size B

SogCLR

- The key idea is to maintain a moving average on $g(\mathbf{w}; \mathbf{x}_i, \mathcal{A}, S_i)$ for each original image $\mathbf{x_i}$

$$\min_{\mathbf{w}} F(\mathbf{w}) = \mathbb{E}_{\mathbf{x}_i \sim \mathcal{D}, \mathcal{A}, \mathcal{A}' \sim \mathcal{P}}[\tau L(\mathbf{w}; \mathbf{x}_i, \mathcal{A}, \mathcal{A}')]$$

Mini-batch Gradient

(1) $\tau \nabla L(\mathbf{w}; \mathbf{x}_i, \mathcal{A}, \mathcal{A}') = -\nabla(E(\mathcal{A}(\mathbf{x}_i))^\top E(\mathcal{A}'(\mathbf{x}_i)))$

$$+ \frac{\tau}{\varepsilon' + g(\mathbf{w}; \mathbf{x}_i, \mathcal{A}, \mathcal{S}_i)} \nabla g(\mathbf{w}; \mathbf{x}_i, \mathcal{A}, \mathcal{S}_i).$$

Non-linear function of g(•) !

Mini-batch Gradient

(2) $\mathbf{u}_{i,t} = (1-\gamma)\mathbf{u}_{i,t-1}$

$$+ \gamma \frac{1}{2|\mathcal{B}_i|}(g(\mathbf{w}_t; \mathbf{x}_i, \mathcal{A}, \mathcal{B}_i) + g(\mathbf{w}_t; \mathbf{x}_i, \mathcal{A}', \mathcal{B}_i))$$

maintain a scalar $\mathbf{u_i}$ for each image to track g(•) by using a mini-batch $\mathbf{B_i}$

Using mini-batch doesn't work !

Analysis of Optimization Error for SogCLR

Theorem 2&3 Assume $\mathbb{E}_{\mathcal{A},\mathcal{A}',\mathbf{z}} \left| E\left(\mathcal{A}\left(\mathbf{x}_i\right)\right)^\top E(\mathbf{z}) - E\left(\mathcal{A}'\left(\mathbf{x}_i\right)\right)^\top E(\mathbf{z}) \right|^2 \leq \epsilon^2$, after T iterations, SogCLR ensures $\mathrm{E}[\|\nabla F_{v1}(\mathbf{w}_{t'})\|^2] \leq O(\frac{1}{\sqrt{BT}} + \frac{\sqrt{n}}{B\sqrt{T}} + \epsilon^2)$ and $\mathrm{E}[\|\nabla F_{v2}(\mathbf{w}_{t'})\|^2] \leq O(\frac{1}{\sqrt{BT}} + \frac{\sqrt{n}}{B\sqrt{T}})$ for a random $t' \in \{1, \ldots, T\}$.

- **Remarks:**
  - V1: When ϵ is small enough, the optimization error of SogCLRv1 is negligible
  - V2: SogCLRv2 can converges to a stationary solution, i.e., zero optimization error

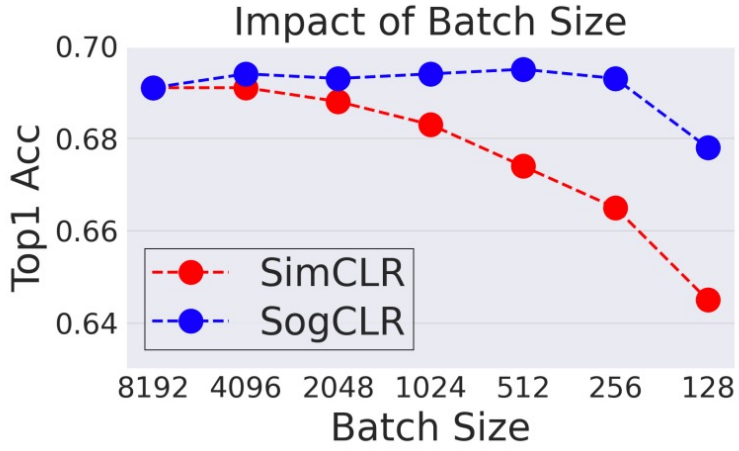
Experiments

- Experiments of image pretraining task on ImageNet-1K

Table 3. Linear evaluation (top-1 accuracy) under different batch sizes and training epoch on ResNet-50 and ImageNet-1K.

Method	BatchSize\Epoch	100	200	400	800
SimCLR	128	62.6	64.0	64.1	64.5
SogCLR	128	**64.9**	**66.2**	**67.4**	**67.9**
SimCLR	256	62.8	64.3	65.7	66.5
SogCLR	256	**65.2**	**67.1**	**68.7**	**69.4**
SimCLR	512	63.8	65.6	66.7	67.4
SogCLR	512	**65.0**	**67.2**	**68.8**	**69.6**

Linear evaluation with small batch sizes for different epochs.



Linear evaluation by varying batch sizes from 128 to 8192 on ImageNet-1K.

Experiments

- Comparison of different InfoNCE-based contrastive learning methods

Method	Batch Size	Memory Bank	Momentum Encoder	Other Tricks	Convergence	Top1 Acc.
SimCLR (Chen et al., 2020a)	Large-batch	No	No	Strong Aug.	No	66.5
NNCLR (Dwibedi et al., 2021)	Large-batch	No	No	Nearest Neighbors	No	68.7
SiMo (Zhu et al., 2020a)	Small-batch	No	Yes	Margin Trick	No	72.1
MoCov2 (Chen et al., 2020c)	Small-batch	Yes	Yes	Strong Aug.	No	71.1
InfoMin (Tian et al., 2020)	Small-batch	Yes	Yes	InfoMin Aug.	No	73.0
SogCLR (Ours)	Small-batch	No	No	GC Optimization	Yes	72.5

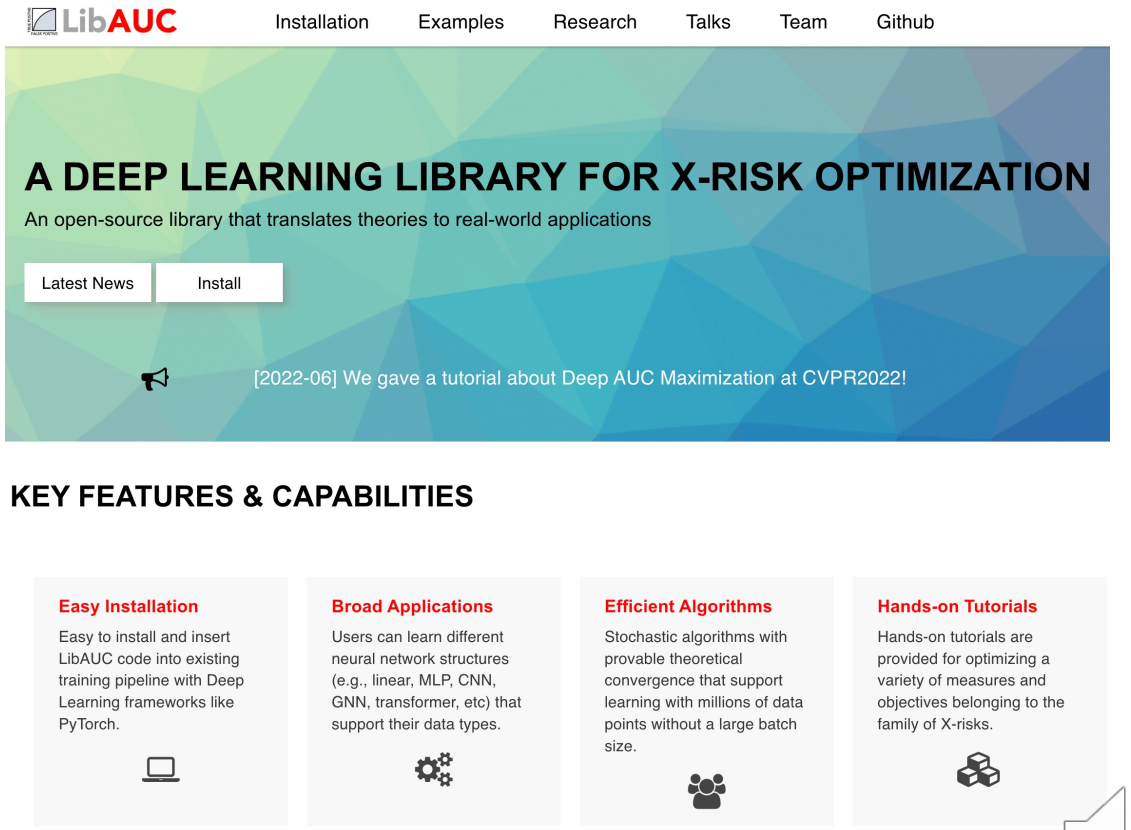
Notes: Linear evaluation accuracy by using 800 epochs, a batch size of 256, and ResNet-50 on ImageNet-1K. Momentum Bank/Encoder is introduced by MoCov1 (He et al. 2019).

Implementations

- Code is integrated with LibAUC: https://github.com/Optimization-AI/SogCLR

LibAUC

https://libauc.org



Thank You!