On Large-Batch Training for Deep Learning: Generalization Gap and Sharp Minima

Nitish Shirish Keskar[1] Dheevatsa Mudigere[2] Jorge Nocedal[1]
Mikhail Smelyanskiy[2] Ping Tak Peter Tang[2]

[1]Northwestern University

[2]Intel Corporation

ICLR, 2017
Presenter: Tianlu Wang

Outline

1. Introduction
   - Batch Size of Stochastic Gradient Methods
2. Drawbacks of Large-Batch Methods
   - Main Observation
   - Numerical Results
   - Parametric Plots
   - Sharpness of Minima
3. Success of Small-Batch Methods
   - Deterioration along Increasing of Batch-Size
   - Warm-started Large Batch experiments
4. Summary

Outline

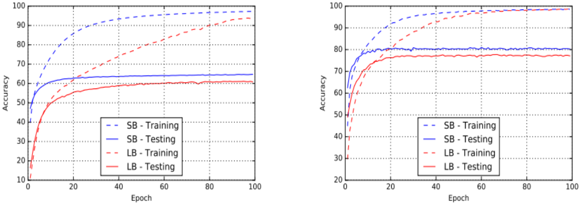
1. Introduction
   - Batch Size of Stochastic Gradient Methods
2. Drawbacks of Large-Batch Methods
   - Main Observation
   - Numerical Results
   - Parametric Plots
   - Sharpness of Minima
3. Success of Small-Batch Methods
   - Deterioration along Increasing of Batch-Size
   - Warm-started Large Batch experiments
4. Summary

Batch Size of Stochastic Gradient Methods

- Non-convex optimization in deep learning:
  $\min_{x \in \mathbb{R}^n} f(x) := \frac{1}{M} \sum_{i=1}^{M} f_i(x)$
- Stochastic Gradient Methods and its variants:
  $|B_k| \in \{32, 64, \ldots, 512\}$
- Increase batch size to improve parallelism leads to a loss in generalization performance

Batch Size of Stochastic Gradient Methods

- Non-convex optimization in deep learning:
  $\min_{x\in\mathbb{R}^n} f(x) := \frac{1}{M}\sum_{i=1}^{M} f_i(x)$
- Stochastic Gradient Methods and its variants:
  $|B_k| \in \{32, 64, \ldots, 512\}$
- Increase batch size to improve parallelism leads to a loss in generalization performance



(a) Network F_2

(b) Network C_1

Figure 2: Training and testing accuracy for SB and LB methods as a function of epochs.

Outline

1 Introduction
- Batch Size of Stochastic Gradient Methods

2 Drawbacks of Large-Batch Methods
- Main Observation
- Numerical Results
- Parametric Plots
- Sharpness of Minima

3 Success of Small-Batch Methods
- Deterioration along Increasing of Batch-Size
- Warm-started Large Batch experiments

4 Summary

Main Observations

- Large-batch methods tend to converge to sharp minimizers of the training function and tend to generalize less well.
  Small-batch methods converge to flat minimizers and are able to escape basins of attraction of sharp minimizers.

Main Observations

- Large-batch methods tend to converge to sharp minimizers of the training function and tend to generalize less well.
  Small-batch methods converge to flat minimizers and are able to escape basins of attraction of sharp minimizers.
- Sharp Minimizer $\hat{x}$: function increases rapidly in a small neighborhood of $\hat{x}$
  Flat Minimizer $\bar{x}$: function varies slowly in a large neighborhood of $\bar{x}$

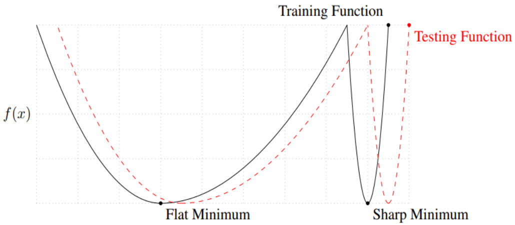


Figure 1: A Conceptual Sketch of Flat and Sharp Minima. The Y-axis indicates value of the loss function and the X-axis the variables (parameters)

Outline

1 Introduction
- Batch Size of Stochastic Gradient Methods

2 Drawbacks of Large-Batch Methods
- Main Observation
- Numerical Results
- Parametric Plots
- Sharpness of Minima

3 Success of Small-Batch Methods
- Deterioration along Increasing of Batch-Size
- Warm-started Large Batch experiments

4 Summary

Numerical Results

- 6 multi-class classification networks, mean cross entropy, ADAM optimizer, LB: 10% of training data, SB: 256 data points

Numerical Results

- 6 multi-class classification networks, mean cross entropy, ADAM optimizer, LB: 10% of training data, SB: 256 data points

Table 1: Network Configurations

Name	Network Type	Architecture	Data set
F_1	Fully Connected	Section B.1	MNIST (LeCun et al., 1998a)
F_2	Fully Connected	Section B.2	TIMIT (Garofolo et al., 1993)
C_1	(Shallow) Convolutional	Section B.3	CIFAR-10 (Krizhevsky & Hinton, 2009)
C_2	(Deep) Convolutional	Section B.4	CIFAR-10
C_3	(Shallow) Convolutional	Section B.3	CIFAR-100 (Krizhevsky & Hinton, 2009)
C_4	(Deep) Convolutional	Section B.4	CIFAR-100

Numerical Results

- 6 multi-class classification networks, mean cross entropy, ADAM optimizer, LB: 10% of training data, SB: 256 data points

Table 1: Network Configurations

Name	Network Type	Architecture	Data set
F_1	Fully Connected	Section B.1	MNIST (LeCun et al., 1998a)
F_2	Fully Connected	Section B.2	TIMIT (Garofolo et al., 1993)
C_1	(Shallow) Convolutional	Section B.3	CIFAR-10 (Krizhevsky & Hinton, 2009)
C_2	(Deep) Convolutional	Section B.4	CIFAR-10
C_3	(Shallow) Convolutional	Section B.3	CIFAR-100 (Krizhevsky & Hinton, 2009)
C_4	(Deep) Convolutional	Section B.4	CIFAR-100

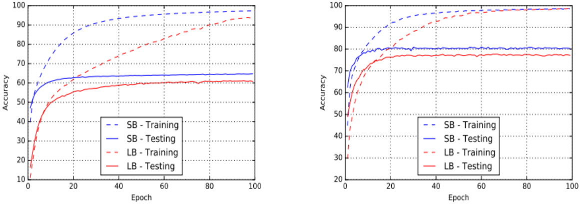
	Training Accuracy		Testing Accuracy	
Name	SB	LB	SB	LB
F_1	$99.66\% \pm 0.05\%$	$99.92\% \pm 0.01\%$	$98.03\% \pm 0.07\%$	$97.81\% \pm 0.07\%$
F_2	$99.99\% \pm 0.03\%$	$98.35\% \pm 2.08\%$	$64.02\% \pm 0.2\%$	$59.45\% \pm 1.05\%$
C_1	$99.89\% \pm 0.02\%$	$99.66\% \pm 0.2\%$	$80.04\% \pm 0.12\%$	$77.26\% \pm 0.42\%$
C_2	$99.99\% \pm 0.04\%$	$99.99\% \pm 0.01\%$	$89.24\% \pm 0.12\%$	$87.26\% \pm 0.07\%$
C_3	$99.56\% \pm 0.44\%$	$99.88\% \pm 0.30\%$	$49.58\% \pm 0.39\%$	$46.45\% \pm 0.43\%$
C_4	$99.10\% \pm 1.23\%$	$99.57\% \pm 1.84\%$	$63.08\% \pm 0.5\%$	$57.81\% \pm 0.17\%$

Question

- Generalization gap is not due to *over-fitting* or *over-training* ???

Question

- Generalization gap is not due to *over-fitting* or *over-training* ???



(a) Network F_2 (b) Network C_1

Figure 2: Training and testing accuracy for SB and LB methods as a function of epochs.

Outline

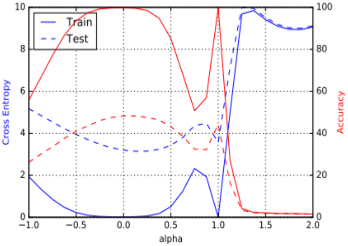
1. Introduction
    - Batch Size of Stochastic Gradient Methods
2. Drawbacks of Large-Batch Methods
    - Main Observation
    - Numerical Results
    - Parametric Plots
    - Sharpness of Minima
3. Success of Small-Batch Methods
    - Deterioration along Increasing of Batch-Size
    - Warm-started Large Batch experiments
4. Summary

Parametric Plots

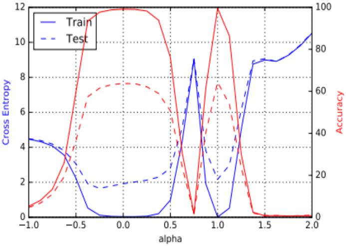
- x_s^* and x_l^*:solutions obtained by SB and LB
- plot $f(\alpha x_l^* + (1-\alpha)x_s^*)$:

Parametric Plots

- x_s^* and x_l^*:solutions obtained by SB and LB
- plot $f(\alpha x_l^* + (1-\alpha)x_s^*)$:



(e) C_3



(f) C_4

Outline

1 Introduction
- Batch Size of Stochastic Gradient Methods

2 Drawbacks of Large-Batch Methods
- Main Observation
- Numerical Results
- Parametric Plots
- Sharpness of Minima

3 Success of Small-Batch Methods
- Deterioration along Increasing of Batch-Size
- Warm-started Large Batch experiments

4 Summary

Sharpness of Minima

- Motivation: Measure the sensitivity of training function at the given local minimizer, so we want to explore **a small neighborhood** of a minimizer and compute **the largest value** that f can attain in this neighborhood.

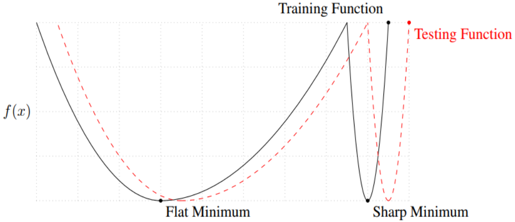


Figure 1: A Conceptual Sketch of Flat and Sharp Minima. The Y-axis indicates value of the loss function and the X-axis the variables (parameters)

Sharpness of Minima

- Small neighborhood:
  p: dimension of manifold
  A: $n \times p$ matrix,columns are randomly generated
  A^+: pesudo-inverse of A

$$C_\varepsilon = \{z \in \mathbb{R}^n : -\varepsilon(|x_i| + 1) \le z_i \le \varepsilon(|x_i| + 1)\} \\ \forall i \in \{1, 2, \dots, n\}$$

$$C_\varepsilon = \{z \in \mathbb{R}^p : -\varepsilon(|(A^+x)_i| + 1) \le z_i \le \varepsilon(|(A^+x)_i| + 1)\} \\ \forall i \in \{1, 2, \dots, p\}$$

- **Metric 2.1.** Given $x \in \mathbb{R}^n$, $\varepsilon > 0$ and $A \in \mathbb{R}^{n*p}$, the sharpness of f at x:

$$\phi_{x,f}(\varepsilon, A) := \frac{(\max_{y \in C_\varepsilon} f(x + Ay)) - f(x)}{1 + f(x)} \times 100 \quad (1)$$

- A can be the identity matrix I_n

Sharpness of Minima

- Sharpness of Minima in Full Space(A is the identity matrix):

	$\epsilon = 10^{-3}$		$\epsilon = 5 \cdot 10^{-4}$	
	SB	LB	SB	LB
F_1	1.23 ± 0.83	205.14 ± 69.52	0.61 ± 0.27	42.90 ± 17.14
F_2	1.39 ± 0.02	310.64 ± 38.46	0.90 ± 0.05	93.15 ± 6.81
C_1	28.58 ± 3.13	707.23 ± 43.04	7.08 ± 0.88	227.31 ± 23.23
C_2	8.68 ± 1.32	925.32 ± 38.29	2.07 ± 0.86	175.31 ± 18.28
C_3	29.85 ± 5.98	258.75 ± 8.96	8.56 ± 0.99	105.11 ± 13.22
C_4	12.83 ± 3.84	421.84 ± 36.97	4.07 ± 0.87	109.35 ± 16.57

Outline

1 Introduction
- Batch Size of Stochastic Gradient Methods

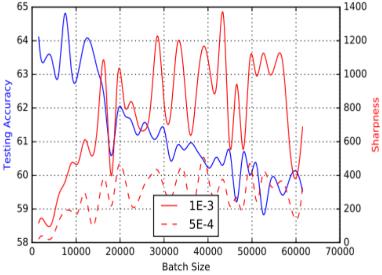
2 Drawbacks of Large-Batch Methods
- Main Observation
- Numerical Results
- Parametric Plots
- Sharpness of Minima

3 Success of Small-Batch Methods
- Deterioration along Increasing of Batch-Size
- Warm-started Large Batch experiments

4 Summary

Deterioration along Increasing of Batch-Size

- Note batch-size≈ 15000 for F_2 and batch-size≈ 500 for C_1



(a) F_2 (b) C_1

- There exists a threshold after which there is a deterioration in the quality of the model.

Outline

1 Introduction
- Batch Size of Stochastic Gradient Methods

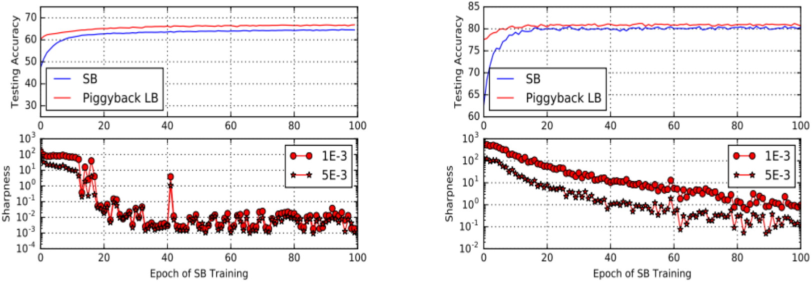
2 Drawbacks of Large-Batch Methods
- Main Observation
- Numerical Results
- Parametric Plots
- Sharpness of Minima

3 Success of Small-Batch Methods
- Deterioration along Increasing of Batch-Size
- Warm-started Large Batch experiments

4 Summary

Warm-started Large Batch experiments

- Train network for 100 epochs with batch-size=256 and use these 100 epochs as starting points.



(a) F_2 (b) C_1

- The SB method needs some epochs to explore and discover a flat minimizer.

Summary

- Numerical experiments that support the view that convergence to sharp minimizers gives rise to the poor generalization of large-batch methods for deep learning.
- SB methods have an exploration phase followed by convergence to a flat minimizer.
- Attempts to remedy the problem:
  - Data augmentation
  - Conservative training
  - Adversarial training
  - Robust optimization