Contents

1 On large-batch training for deep learning: Generalization gap and sharp minima

1.1 Existing problems

1. large batch methods over-fit the model.
2. large batch methods are attracted to saddle points.
3. large batch methods tend to zoom-in on the minimizer closest to the initial point.
4. small batch and large batch methods converge to qualitatively different minimizers with different properties.

1.2 Conclusions/Founding in this paper

- The generalization gap is not due to over-fitting or over-training.
- Due to the ***inherent noise*** in the gradient estimation:
  - large-batch methods tend to converge to sharp minimizers of the training and testing functions.
    * the sharp minimizers are characterized by ***a significant number of large positive eigenvalues*** in $\bigtriangledown^2 f(x)$.
    * flat minimizers tend to generalize well.
  - small-batch methods consistently converge to flat minimizers.
    * flat minimizers characterized by ***having numerous small eigenvalues of*** $\bigtriangledown^2 f(x)$.
- The loss function landscape of deep neural networks is such that large-batch methods are attracted to the region with sharp minimizers and are unable to escape basins of attraction of these minimizers.
- **using a large-batch method that is warm-start with a small-batch method**.

1.3 Some background information

- What is a flat minimizer and a sharp minimizer?
  - **flat minimizer** $\mathbf{x}^*$: the function varies slowly in a relatively large neighborhood of $\mathbf{x}^*$.
  - **sharp minimizer** $\mathbf{x}^*$: the function increases rapidly in a small neighborhood of $\mathbf{x}^*$.
- Many theoretial properties of SGD in small batch regime are known:
  1. converge to minimizers of strongly-convex functions and to stationary points for non-convex functions[1].
  2. saddle-point avoidance[2].
  3. robustness to input data[3].
- The loss function of deep learning models is fraught with many local minimizers, and many of these minimizers correspond to a similar loss function value.
  - both flat and sharp minimizer have very similar loss function values.

1.4 Experimental Study

1.4.1 How to measure the sharpness of a minimizer

- the sharpness of a minimizer can be characterized by the magnitude of the eigenvalues of $\bigtriangledown^2 f(x)$
  - however, the computation cost is prohibitive.
- a computationally feasible metric: exploring a small neighborhood of a solution and computing the largest value that the function f can attain in that neighborhood.

space $\mathbb{R}^n$ as well as in random manifolds. For that purpose, we introduce an $n \times p$ matrix A, whose columns are randomly generated. Here p determines the dimension of the manifold, which in our experiments is chosen as $p = 100$.

Specifically, let $\mathcal{C}_\epsilon$ denote a box around the solution over which the maximization of f is performed, and let $A \in \mathbb{R}^{n \times p}$ be the matrix defined above. In order to ensure invariance of sharpness to problem dimension and sparsity, we define the constraint set $\mathcal{C}_\epsilon$ as:

$$\mathcal{C}_\epsilon = \{z \in \mathbb{R}^p : -\epsilon(|(A^+x)_i| + 1) \leq z_i \leq \epsilon(|(A^+x)_i| + 1) \quad \forall i \in \{1, 2, \cdots, p\}\}, \tag{3}$$

where A^+ denotes the pseudo-inverse of A. Thus ϵ controls the size of the box. We can now define our measure of sharpness (or sensitivity).

Metric 2.1. *Given $x \in \mathbb{R}^n$, $\epsilon > 0$ and $A \in \mathbb{R}^{n \times p}$, we define the $(\mathcal{C}_\epsilon, A)$-sharpness of f at x as:*

$$\boxed{\phi_{x,f}(\epsilon, A) := \frac{(\max_{y \in \mathcal{C}_\epsilon} f(x + Ay)) - f(x)}{1 + f(x)} \times 100.} \tag{4}$$

  - pseudo-inverse

1.4.2 Comparison of the sharpness of the minimizers

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

- experiment 1:

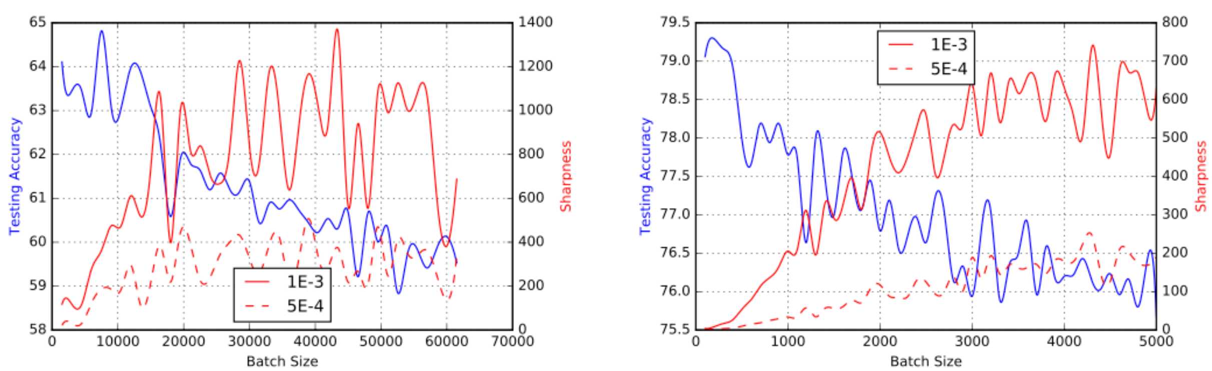
Table 3: Sharpness of Minima in Full Space; ϵ is defined in (3).

	$\epsilon = 10^{-3}$		$\epsilon = 5 \cdot 10^{-4}$	
	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

Table 4: Sharpness of Minima in Random Subspaces of Dimension 100

	$\epsilon = 10^{-3}$		$\epsilon = 5 \cdot 10^{-4}$	
	SB	LB	SB	LB
F_1	0.11 ± 0.00	9.22 ± 0.56	0.05 ± 0.00	9.17 ± 0.14
F_2	0.29 ± 0.02	23.63 ± 0.54	0.05 ± 0.00	6.28 ± 0.19
C_1	2.18 ± 0.23	137.25 ± 21.60	0.71 ± 0.15	29.50 ± 7.48
C_2	0.95 ± 0.34	25.09 ± 2.61	0.31 ± 0.08	5.82 ± 0.52
C_3	17.02 ± 2.20	236.03 ± 31.26	4.03 ± 1.45	86.96 ± 27.39
C_4	6.05 ± 1.13	72.99 ± 10.96	1.89 ± 0.33	19.85 ± 4.12

- experiment 2:



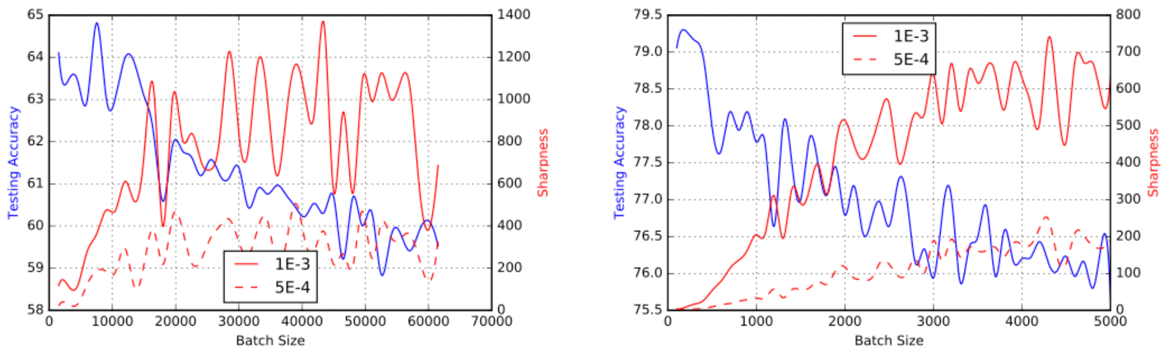
(a) F_2 (b) C_1

Figure 4: Testing Accuracy and Sharpness v/s Batch Size. The X-axis corresponds to the batch size used for training the network for 100 epochs, left Y-axis corresponds to the testing accuracy at the final iterate and right Y-axis corresponds to the sharpness of that iterate. We report sharpness for two values of ϵ: 10^{-3} and $5 \cdot 10^{-4}$.

- sharp minimizers identified in the experiments **do not resemble a cone**
  - sampling the loss function in the neighborhood
  - the loss function rises steeply only along a small dimensional subspace.

1.4.3 minimizers and the starting point

- experimental method:
  1. train the network using Adam with a batch size of 256 (small batch size), then we get 100 solutions.
  2. use these 100 solutions as start points and train the network use a larget batch size.
- founding
  1. when warm-stared with only a few initial epochs, the larget batch method does not yield a generalization improvement.
  2. after a certain number of epochs of warm-starting, the accuracy improves and sharpness of the large-batch iterations drop.



(a) F_2 (b) C_1

Figure 4: Testing Accuracy and Sharpness v/s Batch Size. The X-axis corresponds to the batch size used for training the network for 100 epochs, left Y-axis corresponds to the testing accuracy at the final iterate and right Y-axis corresponds to the sharpness of that iterate. We report sharpness for two values of ϵ: 10^{-3} and $5 \cdot 10^{-4}$.

the small batch method has ended its exploration phase and discovered a flat minimizer, the large batch method is then able to converge toward it, leading to a good testing accuracy.

1.5 References

1. Bottou L, Curtis F E, Nocedal J. Optimization methods for large-scale machine learning[J]. arXiv preprint arXiv:1606.04838, 2016.
2. Lee J D, Simchowitz M, Jordan M I, et al. Gradient descent converges to minimizers[J]. arXiv preprint arXiv:1602.04915, 2016.
3. Hardt M, Recht B, Singer Y. Train faster, generalize better: Stability of stochastic gradient descent[J]. arXiv preprint arXiv:1509.01240, 2015.