Revisiting and Advancing Fast Adversarial Training Through The Lens of Bi-Level Optimization

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Abstract

Adversarial training (AT) is a widely recognized defense mechanism to gain the robustness of deep neural networks against adversarial attacks. It is built on min-max optimization (MMO), where the minimizer (i.e., defender) seeks a robust model to minimize the worst-case training loss in the presence of adversarial examples crafted by the maximizer (i.e., attacker). However, the conventional MMO method makes AT hard to scale. Thus, FAST-AT [40] and other recent algorithms attempt to simplify MMO by replacing its maximization step with the single gradient sign-based attack generation step. Although easy to implement, FAST-AT lacks theoretical guarantees, and its empirical performance is unsatisfactory due to the issue of robust catastrophic overfitting when training with strong adversaries. In this paper, we advance FAST-AT from the fresh perspective of bi-level optimization (BLO). We first show that the commonly-used FAST-AT is equivalent to using a stochastic gradient algorithm to solve a linearized BLO problem involving a sign operation. However, the discrete nature of the sign operation makes it difficult to understand the algorithm performance. Inspired by BLO, we design and analyze a new set of robust training algorithms termed Fast Bi-level AT (FAST-BAT), which effectively defends sign-based projected gradient descent (PGD) attacks without using any gradient sign method or explicit robust regularization. In practice, we show that our method yields substantial robustness improvements over multiple baselines across multiple models and datasets.

1 Introduction

Given the fact that machine learning (ML) models can be easily fooled by tiny adversarial perturbations (also known as adversarial attacks) on the input [15, 5, 28], training robust deep neural networks is now a major focus in research. Nearly all existing effective defense mechanisms [26, 46, 35, 40, 45, 3] are built on the adversarial training (AT) recipe, introduced by [36] and later formalized in [26] using min-max optimization (MMO), where a minimizer (i.e. defender) seeks to update model parameters against a maximizer (i.e. attacker) that aims to increase the training loss by perturbing the training data.

Despite the effectiveness of the AT-type defenses in various application domains, the min-max nature makes them difficult to scale, because of the multiple maximization steps required by the iterative attack generator at each training step. The resulting prohibitive computation cost makes AT not suitable in practical settings. For example, [41] used 128 GPUs to run AT on ImageNet. Thereby, how to speed up AT without losing accuracy and robustness is now a grand challenge for adversarial defense [40].

Recently, [40, 35, 45, 2] attempted to develop computationally-efficient alternatives of AT, that is, the ‘fast’ versions of AT. To the best of our knowledge, FAST-AT [40] and FAST-AT with gradient alignment (GA) regularization, termed FAST-AT-GA [2], are the two state-of-the-art (SOTA) ‘fast’ versions of AT, since they
Table 1: Performance overview of proposed Fast-BAT vs. the baselines Fast-AT [40] and Fast-AT-GA [2] on CIFAR-10, CIFAR-100 and Tiny-ImageNet with PreActResNet-18. All methods are robustly trained under two perturbation budgets $\epsilon = 8/255$ and 16/255 over 20 epochs. We use the early-stopping policy [33] to report the model with best robustness for each method. The evaluation metrics include robust accuracy (RA) against PGD-50-10 attacks (50-step PGD attack with 10 restarts) [26] at $\epsilon = 8/255$ and 16/255 (the test-time $\epsilon$ is the same as the train-time), RA against AutoAttack (AA) [7] at $\epsilon = 8/255$ and 16/255, and computation time (per epoch). The result $a \pm b$ represents mean $a$ and standard deviation $b$ over 10 random trials. All experiments are run on a single GeForce RTX 3090 GPU.

| Method      | SA (%) $\pm$ (e = 8/255) | RA-PGD (%) $\pm$ (e = 8/255) | RA-AA (%) $\pm$ (e = 8/255) | SA (%) $\pm$ (e = 16/255) | RA-PGD (%) $\pm$ (e = 16/255) | RA-AA (%) $\pm$ (e = 16/255) | Time (s/epoch) |
|-------------|-----------------------------|-------------------------------|-------------------------------|-----------------------------|-------------------------------|-------------------------------|----------------|
| Fast-AT     | 82.39 $\pm$ 0.14            | 45.49 $\pm$ 0.21              | 41.87 $\pm$ 0.15              | 44.15 $\pm$ 0.27           | 21.83 $\pm$ 0.32             | 12.49 $\pm$ 0.33             | 23.1           |
| Fast-AT-GA  | 79.71 $\pm$ 0.24            | 47.27 $\pm$ 0.22              | 43.24 $\pm$ 0.07              | 58.29 $\pm$ 0.32           | 26.01 $\pm$ 0.16             | 17.97 $\pm$ 0.33             | 75.3           |
| Fast-BAT    | 79.97 $\pm$ 0.12            | 48.83 $\pm$ 0.17              | 45.19 $\pm$ 0.12              | 68.16 $\pm$ 0.25           | 27.09 $\pm$ 0.16             | 18.79 $\pm$ 0.24             | 61.4           |

| Method      | RA-PGD (%) $\pm$ (e = 8/255) | RA-AA (%) $\pm$ (e = 8/255) | RA-PGD (%) $\pm$ (e = 16/255) | RA-AA (%) $\pm$ (e = 16/255) | Time (s/epoch) |
|-------------|-------------------------------|-------------------------------|-------------------------------|-------------------------------|----------------|
| Fast-AT     | 52.62 $\pm$ 0.18              | 24.66 $\pm$ 0.21              | 21.72 $\pm$ 0.17              | 21.32 $\pm$ 0.27             | 8.62 $\pm$ 0.13             | 6.22 $\pm$ 0.61             | 23.8           |
| Fast-AT-GA  | 50.06 $\pm$ 0.27              | 24.97 $\pm$ 0.23              | 21.82 $\pm$ 0.21              | 32.51 $\pm$ 0.27             | 12.27 $\pm$ 0.36             | 9.43 $\pm$ 0.19             | 77.1           |
| Fast-BAT    | 50.19 $\pm$ 0.21              | 26.49 $\pm$ 0.20              | 23.97 $\pm$ 0.15              | 39.29 $\pm$ 0.53             | 13.97 $\pm$ 0.17             | 11.32 $\pm$ 0.22             | 61.6           |

| Method      | RA-PGD (%) $\pm$ (e = 8/255) | RA-AA (%) $\pm$ (e = 8/255) | RA-PGD (%) $\pm$ (e = 16/255) | RA-AA (%) $\pm$ (e = 16/255) | Time (s/epoch) |
|-------------|-------------------------------|-------------------------------|-------------------------------|-------------------------------|----------------|
| Fast-AT     | 41.37 $\pm$ 0.08              | 17.05 $\pm$ 0.25              | 12.31 $\pm$ 0.73              | 31.38 $\pm$ 0.19             | 5.42 $\pm$ 0.17             | 3.13 $\pm$ 0.24             | 284.6          |
| Fast-AT-GA  | 45.52 $\pm$ 0.24              | 20.39 $\pm$ 0.19              | 16.25 $\pm$ 0.17              | 29.17 $\pm$ 0.33             | 6.79 $\pm$ 0.27             | 4.27 $\pm$ 0.15             | 592.7          |
| Fast-BAT    | 45.50 $\pm$ 0.22              | 21.97 $\pm$ 0.21              | 17.64 $\pm$ 0.15              | 33.78 $\pm$ 0.23             | 8.83 $\pm$ 0.22             | 5.52 $\pm$ 0.14             | 572.4          |

Achieve a significant reduction in computational complexity and preserve accuracy and robustness to some extent. To be specific, Fast-AT [40] replaces an iterative attack generator in AT with a heuristic single-step attack generation method. Yet, Fast-AT suffers from two main issues: (i) lack of stability, i.e., it has a large variance in performance [25], and (ii) catastrophic overfitting, i.e., when training with strong adversaries, the robustness of the resulting model can drop significantly. To alleviate these problems, Andriushchenko and Flammarion [2] proposed Fast-AT-GA by penalizing Fast-AT using an explicit GA regularization. However, we will show that Fast-AT-GA encounters another problem: (iii) it improves robust accuracy (RA) at the cost of a sharp drop in standard accuracy (SA), leading to a poor accuracy-robustness tradeoff for large attack budget (e.g., $\epsilon = 16/255$ in Table I). Moreover, (iv) there has been no theoretical guarantee for the optimization algorithms used in Fast-AT and Fast-AT-GA. Given the limitations (i)-(iv), we ask:

**How to design a ‘fast’ AT with improved stability, mitigated catastrophic overfitting, enhanced RA-SA tradeoff, and some theoretical guarantees?**

To address the above question, we formulate the AT problem as a unified bi-level optimization (BLO) problem [10]. In the new formulation, the attack generation is cast as a constrained lower-level optimization problem, while the defense serves as the upper-level optimization problem. To the best of our knowledge, this is the first work that makes a rigorous connection between adversarial defense and BLO. Technically, we show that Fast-AT can be interpreted as BLO with linearized lower-level problems. Delving into the linearization of BLO, we propose a novel, theoretically-grounded ‘fast’ AT framework, termed fast bi-level AT (Fast-BAT). Practically, Table I highlights some achieved improvements over Fast-AT and Fast-AT-GA: When a stronger train-time attack (i.e., $\epsilon = 16/255$) is adopted, Fast-AT suffers from a large degradation of RA and SA, together with higher variances than proposed Fast-BAT. Although Fast-AT-GA outperforms Fast-AT, it still incurs a significant SA loss at $\epsilon = 16/255$. In contrast, Fast-BAT produces a more graceful SA-Ra tradeoff: As Fast-BAT achieves the best RA in all experimental settings, its SA still remains at a high level, e.g. a significant improvement on SA by 9.9%, 6.7%, and 4.6% at $\epsilon = 16/255$ for CIFAR-10, CIFAR-100, and Tiny-ImageNet.

**Contributions.** We summarize our contributions below.

(i) (Formulation-wise) We propose a unified BLO-based formulation for the robust training problem. Within this formulation, we show the conventional Fast-AT method is solving a low-level linearized BLO problem, rather than the vanilla min-max problem. This key observation not only provides a new interpretation of Fast-AT, but most importantly, also explains why Fast-AT is difficult to possess strong theoretical guarantees.
We propose the new FAST-BAT algorithm based on our new understanding of FAST-AT. The key enabling technique is to introduce a new smooth lower-level objective of BLO for robust training. In contrast to MMO, BLO adopts a different optimization routine that requires implicit gradient (IG) computation. We derive the closed-form of IG for FAST-BAT.

We made a comprehensive experimental study to demonstrate the effectiveness of FAST-BAT over SOTA baselines across datasets and model types. Besides its merit in robustness enhancement, we also show its improved stability, lifted accuracy-robustness trade-off, and mitigated catastrophic overfitting.

2 Related work

Adversarial attack. Adversarial attacks are techniques to generate malicious perturbations that are imperceptible to humans but can mislead the ML models [15, 5, 9, 42, 4]. The adversarial attack has become a major approach to evaluate the robustness of deep neural networks and thus, help build safe artificial intelligence in many high-stakes applications such as autonomous driving [12, 24] and surveillance [37, 43].

Adversarial defense and robust training at scale. Our work falls into the category of robust training, which was mostly built on MMO. For example, [26] established the framework of AT for the first time, always recognized as one of the most powerful defenses [3]. Extended from AT, TRADES [46] sought the optimal balance between robustness and generalization ability. Further, AT-type defense has been generalized to the semi-/self-supervised settings [6, 2] and integrated Eq. [1] with certified defense techniques such as randomized smoothing [34].

Despite the effectiveness of AT and its variants, how to speed up AT without losing performance remains an open question. Some recent works attempted to impose algorithmic simplifications to AT, leading to fast but approximate AT algorithms, such as ‘free’ AT [35], you only propagate once (YOPO) [45], FAST-AT [40], and FAST-AT regularized by gradient alignment (termed FAST-AT-GA) [2]. In particular, FAST-AT and FAST-AT-GA are the baselines most relevant to ours due to their low computational complexity. However, their defense performance is still unsatisfactory. For example, FAST-AT has poor training stability [25] and suffers catastrophic overfitting when facing strong attacks [2]. In contrast, FAST-AT-GA yields improved robustness but has a poor accuracy-robustness tradeoff (see Table 1).

Bi-level optimization (BLO). BLO is a unified hierarchical learning framework, where the objective and variables of the upper-level problem depend on the lower-level problems. The BLO problem in its most generic form is very challenging, and thus, the design of algorithms and theory for BLO focuses on special cases [38, 32, 16, 14, 22, 21, 19]. In practice, BLO has been successfully applied to meta-learning [30], data poisoning attack design [20], and reinforcement learning [8]. However, as will be evident later, the existing BLO approach is not directly applied to adversarial defense due to the presence of the constrained non-convex lower-level problem (for attack generation). To the best of our knowledge, our work makes a rigorous connection between adversarial defense and BLO for the first time.

3 A Bi-Level Optimization View on FAST-AT

Preliminaries on AT and FAST-AT. Let us consider the following standard min-max formulation for the robust adversarial training problem [26]

\[
\begin{align*}
\minimize_{\theta} \quad & \mathbb{E}_{(x, y) \in \mathcal{D}} \left[ \maximize_{\delta \in \mathcal{C}} \ell_{\text{tr}}(\theta, x + \delta, y) \right], \\
\end{align*}
\]
where $\theta \in \mathbb{R}^n$ denotes model parameters; $D$ is the training set consisting (a finite number) of labeled data pairs with feature $x$ and label $y$; $\delta \in \mathbb{R}^d$ represents adversarial perturbations subject to the perturbation constraint $C$, e.g., $C = \{ \delta \mid \| \delta \|_\infty \leq \epsilon, \delta \in [0, 1] \}$ for $\epsilon$-tolerance $\ell_\infty$-norm constrained attack (normalized to $[0, 1]$); $\ell_{tr}(\cdot)$ is the training loss; $(x + \delta)$ represents an adversarial example.

The standard solver for problem $[1]$ is known as AT $[26]$. However, it has to call an iterative optimization method (e.g., $K$-step PGD attack) to solve the inner maximization problem of $[1]$, which is computationally expensive. To improve its scalability, the FAST-AT algorithm $[40]$ was proposed to take a single-step PGD attack for inner maximization. The algorithm backbone of FAST-AT is summarized below.

**FAST-AT algorithm** Let $\theta_t$ be parameters at iteration $t$. The $(t + 1)$th iteration becomes $[40]$:

- **Inner maximization by 1-step PGD**:
  \[
  \delta \leftarrow \mathcal{P}_C (\delta_0 + \alpha \cdot \text{sign} (\nabla_{\delta t} \ell_{tr}(\theta_t, x + \delta_0, y))) ,
  \]
  where $\mathcal{P}_C(a)$ denotes the projection operation that projects the point $a$ onto $C$, i.e., $\mathcal{P}_C(z) = \arg \min_{\delta \in C} \| \delta - z \|_2^2$. $\delta_0$ is a random uniform initialization within $[0, 1]$, $\alpha > 0$ is a proper learning rate (e.g., 1.25$\epsilon$), and $\text{sign}(\cdot)$ is the element-wise sign operation.

- **Outer minimization for model training**: This can be conducted by any standard optimizer, e.g.,
  \[
  \theta_{t+1} \leftarrow \theta_t - \beta \nabla_{\theta} \ell_{tr}(\theta_t, x + \delta, y)
  \]
  where $\beta > 0$ is a proper learning rate (e.g., cyclic learning rate), and $\delta$ is provided from the inner maximization step.

A few remarks about FAST-AT are given below.

1. Roughly speaking, FAST-AT is a simplification of AT using 1-step PGD for inner maximization. However, it is not entirely clear which problem FAST-AT is actually solving. If we take a closer look at the algorithm, we will see that the inner update only changes to the initial $\delta_0$, not the most recent $\delta$. Clearly, this scheme is fundamentally different from the classical gradient descent-ascent algorithm for min-max optimization $[32]$, which alternatively updates the inner and outer variables. Therefore, it remains elusive if FAST-AT is solving the original problem $[7]$.

2. Andriushchenko and Flammarion $[2]$ demonstrated that FAST-AT could lead to catastrophic overfitting when using strong adversaries for training. However, there was no grounded theory to justify the pros and cons of FAST-AT. We will show that BLO provides a promising solution.

**BLO: Towards a unified formulation of robust training.** BLO (bi-level optimization) is an optimization problem that involves two levels of optimization tasks, where the lower-level task is nested inside the upper-level task. More precisely, it has the following generic form:

\[
\begin{aligned}
\min_{u \in \mathcal{U}} & \quad f(u, v^*(u)) \\
\text{s.t.} & \quad v^*(u) = \arg \min_{v \in \mathcal{V}} \quad g(v, u)
\end{aligned}
\]  

(2)

where $\mathcal{U}$ and $\mathcal{V}$ are the feasible sets for the variables $u$ and $v$, respectively; $f(\cdot)$ and $g(\cdot)$ are the upper- and the lower-level objective functions, respectively. Intuitively, the BLO $[2]$ can be used to formulate the adversarial training problem as the latter also involves two problems, one nested in the other. Importantly, it is more powerful than the min-max formulation $[1]$ as it allows the two problems to have different objective functions. This flexibility provided by BLO is the key to the generality of our proposed framework.

To make the above intuition precise, we use the upper-level problem to model the training loss minimization,
while the lower-level problem to model the attack generation process, and consider the following BLO problem:

$$\min_{\theta} \mathbb{E}_{(x,y) \in D}[\ell_{\text{tr}}(\theta, x + \delta^*(\theta; x, y); y)]$$

subject to $$\delta^*(\theta; x, y) = \arg \min_{\delta \in C} \ell_{\text{atk}}(\theta, \delta; x, y),$$

(3)

where the training loss function $$\ell_{\text{tr}}(\cdot)$$ has been defined in [1], and $$\ell_{\text{atk}}(\cdot)$$ denotes an attack objective. For the notation simplicity, in the subsequent discussion, we will not indicate the dependency of the functions $$\ell_{\text{tr}}, \ell_{\text{atk}},$$ and $$\delta^*$$ with respect to (w.r.t.) the data samples $$(x, y)$$. The formulation (3) has two key differences from (1):

1. When we choose $$\ell_{\text{atk}} = -\ell_{\text{tr}}$$, problem (3) becomes equivalent to the min-max formulation (1). It follows that the BLO is suitable to formulate the adversarial training problem. Moreover, we will see shortly that the flexibility provided by choosing the lower-level objective independently of the upper-level one enables us to interpret FAST-AT as solving a certain special form of the BLO problem. Note that prior to our work, it was not entirely clear what is the problem that FAST-AT is trying to solve.

2. BLO calls a different optimization routine from those to solve the original min-max problem (1). As will be evident later, even if we set $$\ell_{\text{atk}} = -\ell_{\text{tr}}$$ in (3), the BLO-enabled solver does not simplify to FAST-AT (see more details in Appendix B). This is because for a given data sample $$(x, y)$$, the gradient for the upper-level problem of (3) yields:

$$\frac{d\ell_{\text{tr}}(\theta, \delta^*(\theta))}{d\theta} = \nabla_{\theta} \ell_{\text{tr}}(\theta, \delta^*(\theta)) + \frac{d\delta^*(\theta)^T}{d\theta} \nabla_{\delta} \ell_{\text{tr}}(\theta, \delta^*(\theta)),$$

(4)

where the superscript $$^T$$ denotes the transpose operation, and $$\nabla_{\delta} \ell_{\text{tr}}(\theta, \delta^*(\theta))$$ denotes the partial derivative w.r.t. the first input argument $$\theta$$; and $$\frac{d\delta^*(\theta)^T}{d\theta} \in \mathbb{R}^{n \times d}$$, if exists, is referred to as implicit gradient (IG) because it is defined through an implicitly constrained optimization problem $$\min_{\delta \in C} \ell_{\text{atk}}$$. The dependence on IG is a ‘fingerprint’ of BLO [1] in contrast to AT or FAST-AT.

**BLO-enabled interpretation of FAST-AT.** Next, we demonstrate how FAST-AT relates to BLO. FAST-AT can be interpreted as an approximated stochastic gradient algorithm for solving the following lower-level linearized BLO. That is to say, FAST-AT is not solving the original min-max problem [1], but its linearized version below:

$$\begin{align*}
\text{minimize} & \quad \mathbb{E}_{(x,y) \in D}[\ell_{\text{tr}}(\theta, \delta^*(\theta))] \\
\text{subject to} & \quad \delta^*(\theta) = \arg \min_{\delta \in C} [(\delta - z)^T \text{sign}(\nabla_{\delta = z} \ell_{\text{atk}}(\theta, \delta))] + (\lambda/2)\|\delta - z\|_2^2,
\end{align*}$$

(5)

where $$z = \delta_0$$ and $$\lambda = 1/\alpha$$. Our justification for the above interpretation is elaborated on below.

1. The simplified lower-level problem of (5) leads to the closed-form solution:

$$\delta^*(\theta) = \arg \min_{\delta \in C} (\lambda/2)\|\delta - z + (1/\lambda)\text{sign}(\nabla_{\delta = z} \ell_{\text{atk}}(\theta, \delta))\|_2^2$$

$$\begin{align*}
= & \mathcal{P}_C (z - (1/\lambda)\text{sign}(\nabla_{\delta = z} \ell_{\text{atk}}(\theta, \delta))),
\end{align*}$$

(6)

which is exactly given by the 1-step PGD attack with initialization $$z$$ and learning rate $$(1/\lambda)$$. In the linearization used in (5), a quadratic regularization term (with regularization parameter $$\lambda$$) is introduced to ensure the strong convexity of the lower-level objective within the constraint set $$\delta \in C$$ so as to achieve the unique minimizer (6). Note that imposing such a strongly convex regularizer is also commonly used to stabilize the convergence of MMO (min-max optimization) and BLO [29, 19]. If we set $$z = \delta_0$$ and $$\lambda = 1/\alpha$$, (6) precisely depicts the inner maximization step used in FAST-AT.

2. By substituting (6) into the upper-level problem of (5), we can then use (4) to compute the stochastic gradients of the upper-level problem. If the stochastic gradient can be precisely computed, then we can update the model
parameters $\theta$ using SGD based on [4]. That is, $\theta \leftarrow \theta - \beta \frac{d\ell(\theta, \delta^*(\theta))}{d\theta}$ (with learning rate $\beta$). However, generally speaking, the IG function $\frac{d\delta^*(\theta)^T}{d\theta}$ involved in [4] may not be differentiable, and even it is, the computation may not be easy. For our case, $\delta^*(\theta)$ expressed in (6) involves both a projection and a sign operation, which can be particularly difficult to compute. To proceed, let us make the following approximations. We assume that the chain rule of the derivative of $\delta^*(\theta)$ holds w.r.t. $\theta$, implying the differentiability of the projection operation and the sign operation. Then, based on the closed-form of $\delta^*(\theta)$ in (6), IG is approximately equal to $\frac{d\delta^*(\theta)^T}{d\theta} \approx -\delta$, where we use two facts: (1) The linearization point $z$ is independent of $\theta$, i.e. $z = \delta_0$; And (2) $\frac{d\text{sign}(\cdot)}{d\theta} = 0$ holds almost everywhere. Clearly, the use of the gradient sign method simplifies the IG computation. Further, the upper-level gradient is approximated by $\frac{d\ell(\theta, \delta^*(\theta))}{d\theta} \approx \nabla_{\theta} \ell(\theta, \delta^*(\theta)) = \delta$, and the upper-level optimization of problem [5] becomes $\theta \leftarrow \theta - \beta_0 \delta(\theta)$, which is the same as the outer minimization step in FAST-AT. In a nutshell, the BLO solver of problem [5], which calls the IG computation based on [6], eventually reduces to the FAST-AT algorithm.

The aforementioned analysis shows that FAST-AT can be viewed as using an approximated stochastic gradient algorithm to solve the linearized BLO [5], with the linearization point $z$ and the regularization parameter $\lambda$ set as $z = \delta_0$ and $\lambda = 1/\alpha$. However, since a series of approximations have been used when arriving at the approximated gradient $h(\theta)$ used by FAST-AT, it is no longer clear if the resulting algorithm can still sufficiently reduce the objective function of the upper-level problem. Additionally, based on the fact that the lower-level problem of [5] involves the discrete sign operator, it is unlikely (if not impossible) that any approximated stochastic gradient-based algorithms developed for it can possess any strong theoretical guarantees.

4 FAST-BAT: Advancing FAST-AT by BLO

**FAST-BAT and rationale.** The key take-away from [5] is that the conventional FAST-AT adopts the sign of input gradient to linearize the lower-level attack objective. However, a more natural choice is to use the first-order Taylor expansion for linearization. By doing so, problem [5] can be modified to the following form:

$$\begin{align*}
\text{minimize} & \quad \mathbb{E}_{(x,y) \in D}[\ell_{tr}(\theta, \delta^*(\theta))] \\
\text{subject to} & \quad \delta^*(\theta) = \arg\min_{\delta \in \mathcal{C}} [(\delta - z)^T (\nabla_{\delta=\delta_{\text{atk}}} \ell(\theta, \delta)) + (\lambda/2) \|\delta - z\|^2_2],
\end{align*}$$

(7)

Similar to [6], problem (7) can be solved as:

$$\delta^*(\theta) = \mathcal{P}_C (z - (1/\lambda) \nabla_{\delta=\delta_{\text{atk}}} \ell(\theta, \delta)) .$$

(8)

In contrast to [6], the IG associated with (7) cannot be approximated by zeros since the gradient sign operation is not present in (8). To compute IG, the auto-differentiation (the chain rule) can be applied to the closed-form of $\delta^*(\theta)$. However, this will not give us an accurate and generalizable IG solution since the projection operation $\mathcal{P}_C$ is not smooth everywhere and thus, the use of chain rule does not yield a rigorous derivation. In the following subsection, we address the IG challenge in a theoretically-grounded manner.

**IG theory for FAST-BAT.** The problem of FAST-BAT (7) falls into a class of very challenging BLO problems, which requires constrained lower-level optimization. The unconstrained case is easier to handle since one can apply the implicit function theory to the stationary condition of the lower-level problem to obtain IG [19]. Yet, in our case with constrained problems, a stationary point could violate the constraints, and thus, the stationary condition becomes non-applicable. Fortunately, in problem (7), we are dealing with a special class of lower-level constraints – linear constraints. Let us rewrite the constraints below:

$$\|\delta\|_\infty \leq \epsilon, \delta \in [-x, 1 - x] \iff B\delta \leq b,$$

(9)
With (11), we can simplify closed-form of IG as below:

\[ \alpha \]

where \( B \) is approximated as:

\[ H \]

This is computationally intensive. Recall from (7) that the Hessian matrix \( \nabla \delta \ell(\theta, \delta^*) \) is given by the second-order partial derivatives evaluated at \((\theta, \delta^*)\), and \( B_0 \) denotes the sub-matrix of \( B \) that only corresponds to the active constraints at \( \delta^* \), i.e., those in \( B \delta^* \leq b \) satisfied with equality.

It is clear from (10) that the computation of IG requires the second-order derivatives as well as matrix inversion. This is computationally intensive. Recall from (7) that the Hessian matrix \( \nabla \delta \ell(\theta, \delta^*) \) is approximated as: \[ \nabla \delta \ell(\theta, \delta^*) = \nabla \delta \ell_{\text{atk}} + \lambda I \] This inspires us to impose the Hessian-free approximation, i.e., \( \nabla \delta \ell_{\text{atk}} = 0 \). The rationale behind the Hessian-free assumption is that ReLU-based neural networks commonly lead to a piece-wise linear decision boundary w.r.t. the inputs [27, 1], and thus, its second-order derivative (Hessian) \( \nabla \delta \ell_{\text{atk}} \) is close to zero. In Sec. 5.2 and Appendix B, we will empirically show that the Hessian-free assumption is reasonable for both ReLU and non-ReLU neural networks. Thus, the Hessian matrix is approximated as:

\[ \nabla \delta \ell(\theta, \delta^*) = \nabla \delta \ell_{\text{atk}} + \lambda I = 0 + \lambda I. \] (11)

With (11), we can simplify closed-form of IG as below:

**Corollary 1** With the Hessian-free assumption, namely \( \nabla \delta \ell_{\text{atk}} = 0 \), the IG (implicit gradient) of (7) is

\[ \frac{d\delta^*(\theta)^\top}{d\theta} = -(1/\lambda)\nabla \delta \ell_{\text{atk}}(\theta, \delta^*)H_C, \] (12)

where \( H_C := [1_{p_1 < \delta_i^* < q_1} \cdots 1_{p_n < \delta_i^* < q_n}] \in \mathbb{R}^{d \times d} \) and the function \( 1_{\{p_i < \delta_i^* < q_i\}} \in \{0, 1\} \) denotes the indicator over the constraint of \( \{\delta_i | p_i < \delta_i^* < q_i\} \), which returns 1 if the constraint is satisfied. \( \delta_i^* \) denotes the \( i \)th entry of \( \delta^*(\theta) \), \( p_i = \max(-\epsilon, -x_i) \) and \( q_i = \min(\epsilon, 1 - x_i) \) characterize the boundary of the linear constraint (7) for the variable \( \delta_i \), and \( e_i \in \mathbb{R}^d \) denotes the basis vector with the \( i \)th entry being 1 and others being 0.

**FAST-BAT algorithm and implementation.** Similar to FAST-AT or AT, the FAST-BAT algorithm also follows the principle of alternating optimization. Specifically, it consists of the IG-based upper-level gradient descent [4], interlaced with the lower-level optimal attack [3]. We summarize the FAST-BAT algorithm below.

**Lower-level solution:** Obtain \( \delta^*(\theta) \) from (8):

\[ \delta^*(\theta) = P_C(z - (1/\lambda)\nabla \delta = \delta_{\text{atk}}(\theta, \delta)) \cdot \]

**Upper-level model training:** Integrating the IG (12) into (4), call SGD to update the model parameters as:

\[ \theta_{t+1} = \theta_t - \alpha_1 \nabla \theta \ell_{\text{tr}}(\theta_t, \delta^*) - \alpha_2 (-1/\lambda)\nabla \delta \ell_{\text{atk}}(\theta_t, \delta^*)H_C \nabla \delta \ell_{\text{tr}}(\theta_t, \delta^*), \] (13)

where \( \alpha_1, \alpha_2 > 0 \) are learning rates associated with the model gradient and the IG-augmented descent direction.
It is clear from (13) that to train a robust model, FAST-BAT can be decomposed into the regular FAST-AT update (i.e., the term multiplied by \( \alpha_1 \)) and the additional update that involves IG, (i.e., the term multiplied by \( \alpha_2 \)). To implement FAST-BAT, we highlight some key hyper-parameter setups that are different from FAST-AT \([40]\) and FAST-AT-GA \([2]\).

**Remark on implementation details** In what follows, we discuss the practical setups of hyperparameters used in Fast-BAT; see more details and empirical justifications in Appendix \([C]\). In Sec. 5.1, we will show that a proper \( \alpha_2 \) helps mitigate catastrophic overfitting. In practice, we set \( \alpha_2/\lambda = 0.1\alpha_1 \) (see Table \([A2]\) for empirical justifications). To specify the linearization point \( z \) in (7), we investigate two types of linearization schemes: (1) the random constant linearization (uniformly random linearization and random corner linearization) and (2) the 1-step perturbation warm-up-based linearization (1-step sign-based PGD and 1-step PGD w/o sign). We consider these linearization schemes since they have computational complexities up to the one-step attack generation. Empirically, we find that FAST-BAT using “1-step PGD w/o sign” leads to the best defensive performance; see justification in Table \([A4]\). We follow this experiment setup in the sequel.

**Remark on convergence analysis** We prove the convergence of FAST-BAT in Appendix \([E]\). It is worth mentioning that the main analysis difficulty lies in the last term of the model updating rule (13), which involves two coupled derivatives built upon the same mini-batch.

5 Experiments

5.1 Experiment Setup

**Datasets and model architectures.** We will evaluate the effectiveness of our proposal under CIFAR-10 \([23]\), CIFAR-100 \([23]\), Tiny-ImageNet \([11]\), and ImageNet \([11]\). Unless specified otherwise, we will train DNN models PreActResNet (PARN)-18 \([18]\) for all datasets except ImageNet, and ResNet (RN)-50 \([17]\) for ImageNet. As a part of the ablation study, we also train larger models PARN-50 and WideResNet (WRN)-16-8 \([44]\) on CIFAR-10. Some preliminary ImageNet results are reported in Appendix \([D]\).

**Baselines.** We consider three baseline methods: FAST-AT \([40]\), FAST-AT-GA \([2]\), and PGD-2-AT \([26]\), i.e., the 2-step PGD attack-based AT. The primal criterion of baseline selection is computational complexity. The training time of all methods including ours falls between the time of FAST-AT and FAST-AT-GA.

**Training details.** We choose the training perturbation strength \( \epsilon \in \{8, 16\}/255 \) for CIFAR-10, CIFAR-100, and Tiny-ImageNet; and \( \epsilon = 2/255 \) for ImageNet following \([40]\) \([2]\). Throughout the experiments, we utilize an SGD optimizer with a momentum of 0.9 and weight decay of \( 5 \times 10^{-4} \). For CIFAR-10, CIFAR-100 and Tiny-ImageNet, we train each model for 20 epochs in total, where we use the cyclic scheduler to adjust the learning rate. The learning rate linearly ascends from 0 to 0.2 within the first 10 epochs and then reduces to 0 within the last 10 epochs. Our batch size is set to 128 for all settings. In the implementation of FAST-BAT, we follow the dataset-agnostic hyperparameter scheme for \( \lambda \), such that \( \lambda = 255/5000 \) for \( \epsilon = 8/255 \) and \( \lambda = 255/2500 \) for \( \epsilon = 16/255 \) for CIFAR-10, CIFAR-100 and Tiny-ImageNet. For ImageNet, we strictly follow the setup given by \([40]\) and we choose the train-time attack budget as \( \epsilon = 2/255 \). For each method, we use the early stopping method to pick the model with the best robust accuracy, following \([33]\). All the experiments are conducted on a single GeForce RTX 3090 GPU. All the baselines are trained with the recommended configurations in their official GitHub repos. We refer readers to Appendix \([C]\) for more details on the training setup.
Table 2: SA, RA-PGD, and RA-AA of different robust training methods in the setup (CIFAR-10, PARN-18 training with $\epsilon = 8/255$) and (CIFAR-10, PARN-18 training with $\epsilon = 16/255$), respectively. All the results are averaged over 10 independent trials with different random seeds.

| Method       | SA (%) | RA-PGD (%) | RA-AA (%) |
|--------------|--------|------------|-----------|
|              | $\epsilon = 8$ | $\epsilon = 16$ | $\epsilon = 8$ | $\epsilon = 16$ |
| FAST-AT      | 82.39 ± 0.44 | 45.49 ± 0.41 | 9.56 ± 0.26 | 41.87 ± 0.15 | 7.91 ± 0.06 |
| FAST-AT-GA   | 79.71 ± 0.44 | 47.27 ± 0.42 | 11.75 ± 0.32 | 43.24 ± 0.27 | 9.48 ± 0.15 |
| PGD-2-AT     | 87.91 ± 0.41 | 44.62 ± 0.39 | 9.39 ± 0.32 | 41.73 ± 0.20 | 7.54 ± 0.25 |
| FAST-BAT     | 79.97 ± 0.12 | 48.83 ± 0.17 | 14.00 ± 0.21 | 45.19 ± 0.12 | 41.51 ± 0.20 |
|              | $\epsilon = 16$ | $\epsilon = 255$ | $\epsilon = 16$ | $\epsilon = 255$ |
| FAST-AT      | 44.15 ± 7.27 | 37.17 ± 0.74 | 21.83 ± 1.32 | 31.66 ± 0.27 | 12.49 ± 0.33 |
| FAST-AT-GA   | 58.29 ± 1.32 | 43.86 ± 0.67 | 26.01 ± 0.16 | 38.69 ± 0.56 | 17.97 ± 0.33 |
| PGD-2-AT     | 68.04 ± 0.30 | 48.79 ± 0.31 | 24.30 ± 0.46 | 41.59 ± 0.22 | 15.40 ± 0.29 |
| FAST-BAT     | 68.16 ± 0.25 | 49.05 ± 0.12 | 27.69 ± 0.10 | 43.64 ± 0.20 | 18.79 ± 0.24 |

Table 3: Performance of different robust training methods under different model types. All the models are both trained and evaluated with the same perturbation strength $\epsilon$.

| Model       | Method       | SA (%) | RA-PGD (%) | SA (%) | RA-PGD (%) |
|-------------|--------------|--------|------------|--------|------------|
|             | $\epsilon = 8/255$ | $\epsilon = 16/255$ | $\epsilon = 8/255$ | $\epsilon = 16/255$ |
| PARN-50     | FAST-AT      | 73.15 ± 0.10 | 41.03 ± 2.09 | 43.86 ± 4.31 | 22.08 ± 0.27 |
|             | FAST-AT-GA   | 77.40 ± 0.81 | 46.16 ± 0.98 | 42.28 ± 0.69 | 22.87 ± 1.25 |
|             | PGD-2-AT     | 83.53 ± 0.17 | 46.17 ± 0.59 | 68.88 ± 0.39 | 22.57 ± 0.41 |
|             | FAST-BAT     | 78.91 ± 0.68 | 49.18 ± 0.35 | 69.01 ± 0.19 | 24.55 ± 0.06 |
| WRN-16-8    | FAST-AT      | 84.39 ± 0.46 | 45.80 ± 0.57 | 49.39 ± 2.17 | 21.99 ± 0.41 |
|             | FAST-AT-GA   | 81.51 ± 0.38 | 48.29 ± 0.20 | 45.95 ± 1.63 | 23.10 ± 0.90 |
|             | PGD-2-AT     | 85.52 ± 0.14 | 45.47 ± 0.14 | 72.11 ± 0.33 | 23.61 ± 0.16 |
|             | FAST-BAT     | 81.66 ± 0.54 | 49.93 ± 0.36 | 68.12 ± 0.47 | 25.63 ± 0.44 |

Evaluation details. For adversarial evaluation, we report robust test accuracy (RA) of a learned model against PGD attacks (RA-PGD). Unless otherwise specified, we set the test-time perturbation strength ($\epsilon$) the same as the train-time value, and take 50-step PGD with 10 restarts all the datasets. Since AutoAttack [9] is known as the strongest robust benchmark evaluation metric (given as an ensemble attack), we also measure robust accuracy against AutoAttack, termed RA-AA. Further, we measure the standard accuracy (SA) against natural examples. Results are averaged over 10 independent trials. We would like to highlight that all the methods share the same batch size, epoch number, and training hardware. Thus, the time consumption per epoch reported in Table and Table5 will serve as a fair indicator of the algorithm complexity of different methods.

5.2 Results

Overall performance of FAST-BAT. In Table and Table we compare the overall performance of our proposed FAST-BAT with baselines.

1. We find that FAST-BAT consistently outperforms the other baselines across the datasets and attack types. In Table, FAST-BAT improves the RA-PGD performance consistently by over 1.5% and RA-AA by around 1% across all the datasets on both attack strengths. For stronger attacks with a larger perturbation budget the advantage of FAST-BAT is even clearer, e.g. a gain of over 2% in Tiny-ImageNet with $\epsilon = 16/255$. On ImageNet, FAST-BAT outperforms FAST-AT by 1.23% with $\epsilon = 2/255$.

2. FAST-BAT leads to a much better SA-RA trade-off compared with the baselines. For example, in Table the improvement in RA is not at cost of a huge drop in SA. Instead, when models are trained with $\epsilon = 16/255$, FAST-BAT even enjoys a significant boost over FAST-AT-GA in SA by 9.9%, 6.7%, and 4.6% for CIFAR-10,
CIFAR-100, and Tiny-ImageNet respectively.

**Performance under different model architectures.** Besides PARN-18 reported above, Table 3 presents results on both deeper (PARN-50) and wider (WRN-18-6) models. As we can see, FAST-BAT consistently yields RA improvement over other methods. We also note that PGD-2-AT could be a competitive baseline in terms of SA. In contrast to FAST-AT and FAST-AT-GA, FAST-BAT is the only approach that yields an evident RA improvement over PGD-2-AT.

![Figure 1: RA-PGD of different robust training methods for CIFAR-10 with the same training and evaluation attack strengths.](image)

**Mitigation of robust catastrophic overfitting.** As shown in [2], FAST-AT suffers robust catastrophic overfitting when the train-time and test-time attack strength $\epsilon$ grows. Following [2], Figure 1 presents two RA-PGD trajectories, i.e., training without early stopping and training with early stopping, versus the train/test-time $\epsilon$. As we can see, FAST-AT encounters a sharp RA drop when $\epsilon > 8$ when early stopping is not used, consistent with [2]. With early stopping, the overfitting of RA can be alleviated to some extent for FAST-AT, but its performance still remains the worst. Moreover, different from [2], we find that PGD-2-AT yields resilient performance against catastrophic overfitting. Our implementation gives a more positive baseline for PGD-2-AT, since the implementation in [2] did not use random initialization to generate train-time attacks. Furthermore, Figure 1 shows that FAST-BAT mitigates the issue of catastrophic overfitting and yields improved RA over other methods. We highlight that such an achievement is free of any robustness stability regularization, like gradient alignment used in FAST-AT-GA.

**Gradient alignment for ‘free’.** As shown by [2], catastrophic overfitting occurs with the local non-linearity of deep networks, which can be measured by the gradient alignment (GA) score:

$$E_{(x,y) \sim D, \eta \sim \mathcal{U}([-\epsilon, \epsilon]^d)} \left[ \cos(\nabla_x \ell_{tr}(x, y; \theta), \nabla_x \ell_{tr}(x + \eta, y; \theta)) \right],$$

where $\mathcal{U}$ denotes the randomly uniform distribution.

GA is a key performance indicator to measure the appearance of robustness catastrophic overfitting, as catastrophic overfitting is always accompanied by a sharp GA drop in the training trajectory of the robustly trained network. Figure 2 shows the training curve of GA score over different training methods on CIFAR-10.
Table 4: RA of robust PARN-18 trained by different methods against adaptive attacks (RA-PGD) and transfer attacks (RA-Transfer Attack). Regarding transfer attacks, naturally trained PARN-18, PARN-50, and WRN-16-8 serve as surrogate models for PGD-20 attack with $\epsilon = 8/255$.

| Method          | RA-PGD(%)       | RA-Transfer Attack(%) |
|-----------------|-----------------|-----------------------|
|                 | PARN-18 | PARN-50 | WRN-16-8 | PARN-18 | PARN-50 | WRN-16-8 |
| FAST-AT         | 45.44±0.06      | 76.35±0.12            | 76.94±0.14            | 77.23±0.21 |
| PGD-2-AT        | 44.71±0.04      | 77.56±0.14            | 78.64±0.12            | 78.84±0.17 |
| FAST-AT-GA      | 47.31±0.05      | 77.34±0.13            | 78.34±0.13            | 78.53±0.12 |
| FAST-BAT(Ours)  | 48.67±0.05      | 78.03±0.15            | 79.93±0.12            | 79.21±0.15 |

Table 5: Performance of Hessian-free and Hessian-aware FAST-BAT on CIFAR-10. We train and evaluate with the same attack budgets $\epsilon = 8/255$ and $\epsilon = 16/255$ to show the influence brought by Hessian matrix.

| Method         | RA-PGD(%)       | RA-Transfer Attack(%) |
|----------------|-----------------|-----------------------|
| Hessian-free   |                 |                       |
| (\epsilon = 8/255) | 79.97±0.12      | 48.83±0.17            | 68.16±0.25            | 27.69±0.16 |
| Hessian-aware  |                 |                       |
| (\epsilon = 16/255) | 79.62±0.17      | 49.13±0.14            | 67.82±0.23            | 27.82±0.19 |

Table 5: Performance of Hessian-free and Hessian-aware FAST-BAT on CIFAR-10. We train and evaluate with the same attack budgets $\epsilon = 8/255$ and $\epsilon = 16/255$ to show the influence brought by Hessian matrix.

model. In our paper, we calculate the GA for each method on the test set at the end of each epoch throughout the training process. Figure 1 suggested that FAST-BAT can mitigate overfitting without explicit GA regularization, and Figure 2 presents the GA score versus the training epoch number. As can be seen, FAST-BAT automatically enforces GA and remains very close to FAST-AT-GA, which maximizes GA with an explicit regularization. Therefore, a high GA score may just be a necessary but not a sufficient condition for avoiding catastrophic overfitting. As additional evidence, Fig. A[1] shows that similar to FAST-AT-GA, FAST-BAT has a flatter loss landscape than FAST-AT as well. Therefore, a direct penalization on the input gradient norm may not achieve the state-of-the-art model robustness.

**Sanity check for obfuscated gradients** As pointed out by [3], model robustness could be overestimated due to obfuscated gradients. The model with obfuscated gradients could have ‘obfuscated’ stronger resilience to white-box (adaptive) attacks than black-box (transfer) attacks. To justify the validity of FAST-BAT, Table 4 summarizes the comparison between our proposal and the other baselines when facing adaptive and transfer attacks. Firstly, for all the methods, RA increases if the transfer attack is applied, implying that the transfer attack is weaker than the adaptive attack. This is desired in the absence of obfuscated gradients. Moreover, FAST-BAT consistently outperforms the other baselines against both adaptive and transfer attacks. The absence of obfuscated gradients can also be justified by the flatness of the adversarial loss landscape in Figure A[1].

**The validity of the Hessian-free assumption on ReLU-based neural networks.** In Corollary 1 the Hessian-free assumption, $i.e. \nabla_{\delta \delta} \ell_{\text{atk}} = 0$, was made to simplify the computation of implicit gradient. To justify this assumption we conduct experiments to compare the Hessian-free FAST-BAT with the Hessian-aware version. In Hessian-aware FAST-BAT, the implicit gradient is calculated based on (23). In Table 5 the results do not indicate much difference when Hessian is used. However, the extra computations required to evaluate the Hessian heavily slows down FAST-BAT as around 30% more time is needed. Therefore, the Hessian-free assumption is reasonable and also necessary in terms of the efficiency of the algorithm. We also justify this assumption on some non-ReLU neural networks and for more results please refer to Appendix D.

6 Conclusion

In this paper, we introduce a novel bi-level optimization-based fast adversarial training framework, termed FAST-BAT. The rationale behind designing FAST-BAT lies in two aspects. First, from the perspective of implicit gradients, we show that the existing FAST-AT framework is equivalent to the lower-level linearized BLO along
the sign direction of the input gradient. Second, we show that FAST-BAT is able to achieve improved stability of performance, mitigated catastrophic overfitting, and enhanced accuracy-robustness trade-off. To the best of our knowledge, we for the first time establish the theory and the algorithmic foundation of BLO for adversarial training. Extensive experiments are provided to demonstrate the superiority of our method to state-of-the-art accelerated AT baselines.
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A Proof of Proposition 1 and Corollary 1

Proof: Upon defining \( g(\theta, \delta) = (\delta - z)\nabla_{\delta=x}\ell_{\text{atk}}(\theta, \delta) + (\lambda/2)\|\delta - z\|_2^2 \), we repeat (7) as

\[
\begin{align*}
\text{minimize} & \quad \mathbb{E}_{(x,y) \in D}[\ell_{\text{tr}}(\theta, \delta^*(\theta))] \\
\text{subject to} & \quad \delta^*(\theta) = \arg\min_{B \delta \leq b} g(\theta, \delta),
\end{align*}
\]

where we have used the expression of linear constraints in (9).

Our goal is to derive the IG \( \frac{d \delta^*(\theta)^T}{d \theta} \) shown in (4). To this end, we first build implicit functions by leveraging KKT conditions of the lower-level problem of (14). We say \( \delta^*(\theta) \) and \( \lambda^*(\theta) \) (Lagrangian multipliers) satisfy the KKT conditions:

\[
\begin{align*}
\text{Stationarity:} & \quad \nabla g(\theta, \delta^*(\theta)) + B^\top \lambda^*(\theta) = 0, \\
\text{Complementary slackness:} & \quad \lambda^*(\theta) \cdot (B\delta^*(\theta) - b) = 0, \\
\text{Dual feasibility:} & \quad \lambda^*(\theta) \geq 0
\end{align*}
\]

where \( \cdot \) denotes the elementwise product.

Active constraints \& definition of \( B_0 \): Let \( B_0 \) denote the sub-matrix of \( B \) and \( b_0 \) the sub-vector of \( b \), which consists of only the active constraints at \( \delta^*(\theta) \), i.e., those satisfied with the equality \( B_0\delta^*(\theta) = b_0 \) (corresponding to nonzero dual variables). The determination of active constraints is done given \( \theta \) at each iteration.

With the aid of \( (B_0, b_0) \), KKT (15) becomes

\[
\nabla g(\theta, \delta^*(\theta)) + B_0^\top \lambda^*(\theta) = 0, \quad \text{and} \quad B_0\delta^*(\theta) - b_0 = 0,
\]

where the nonzero \( \lambda^*(\theta) \) only corresponds to the active constraints. We take derivatives w.r.t. \( \theta \) of (16), and thus obtain the following

\[
\begin{align*}
\frac{d \nabla g(\theta, \delta^*(\theta))^T}{d \theta} + \nabla \lambda^*(\theta)^T B_0 &= 0 \\
\implies \nabla g(\theta, \delta^*(\theta)) + \frac{d \delta^*(\theta)^T}{d \theta} \nabla g(\theta, \delta^*(\theta)) + \nabla \lambda^*(\theta)^T B_0 &= 0, \\
\text{and} \quad \frac{d \delta^*(\theta)^T}{d \theta} B_0^\top &= 0,
\end{align*}
\]

where \( \nabla_{\theta \delta} \in \mathbb{R}^{[\theta] \times [\delta]} \) denotes second-order partial derivatives (recall that \( |\theta| = n \) and \( |\delta| = d \)). According to (17), we have

\[
\frac{d \delta^*(\theta)^T}{d \theta} = -[\nabla g(\theta, \delta^*(\theta)) + \nabla \lambda^*(\theta)^T B_0] \nabla g(\theta, \delta^*(\theta))^{-1}.
\]

Substituting the above into (18), we obtain

\[
\nabla g(\theta, \delta^*(\theta)) \nabla g(\theta, \delta^*(\theta))^{-1} B_0^\top + \nabla \lambda^*(\theta)^T B_0 \nabla g(\theta, \delta^*(\theta))^{-1} B_0^\top = 0,
\]

which yields:

\[
\nabla \lambda^*(\theta)^T = -\nabla g(\theta, \delta^*(\theta)) \nabla g(\theta, \delta^*(\theta))^{-1} B_0^\top [B_0 \nabla g(\theta, \delta^*(\theta))^{-1} B_0^\top]^{-1},
\]

and thus,

\[
\nabla \lambda^*(\theta)^T B_0 = -\nabla g(\theta, \delta^*(\theta)) \nabla g(\theta, \delta^*(\theta))^{-1} B_0^\top [B_0 \nabla g(\theta, \delta^*(\theta))^{-1} B_0^\top]^{-1} B_0.
\]
Substituting (22) into (19), we obtain the IG

$$\frac{d\delta^*(\theta)^T}{d\theta} = -\nabla_{\theta^*g}(\theta, \delta^*(\theta))\nabla_{\delta g}(\theta, \delta^*(\theta))^{-1} - \nabla_{\theta^*}(\theta)^T B_0 \nabla_{\delta g}(\theta, \delta^*(\theta))^{-1}$$

$$= -\nabla_{\theta^*g}(\theta, \delta^*(\theta))\nabla_{\delta g}(\theta, \delta^*(\theta))^{-1} + \nabla_{\theta^*g}(\theta, \delta^*(\theta))\nabla_{\delta g}(\theta, \delta^*(\theta))^{-1} B_0^T [B_0 \nabla_{\delta g}(\theta, \delta^*(\theta))^{-1} B_0^T]^{-1} B_0 \nabla_{\delta g}(\theta, \delta^*(\theta))^{-1}.$$

(23)

The above completes the proof of Proposition 1. □

To further compute (23), the Hessian matrix $\nabla_{\delta^*\ell_{atk}}$ is needed. Recall from the definition of the lower-level objective that the Hessian matrix is given by

$$\nabla_{\delta^*\ell}(\theta, \delta^*(\theta)) = \nabla_{\delta^*\ell_{atk}} + \lambda I = 0 + \lambda I.$$  

(24)

Here we used the assumption that $\nabla_{\delta^*\ell_{atk}} = 0$. The rationale behind that is neural networks commonly leads to a piece-wise linear decision boundary w.r.t. the inputs (27), and thus, its second-order derivative (Hessian) $\nabla_{\delta^*\ell_{atk}}$ is close to zero.

Based on the simplification (24), we have

$$\frac{d\delta^*(\theta)^T}{d\theta} = - (1/\lambda) \nabla_{\theta^*g}(\theta, \delta^*(\theta)) \left( I - B_0^T [B_0 B_0^T]^{-1} B_0 \right)$$

$$- (1/\lambda) \nabla_{\theta^*\ell_{atk}}(\theta, \delta^*(\theta)) H_C,$$

(25)

where we have used the fact that $\nabla_{\theta^*g} = \nabla_{\theta^*\ell_{atk}}$.

What is $H_C$ in (25)? Since $B = \begin{bmatrix} I \\ -I \end{bmatrix}$, we can obtain that $B_0 B_0^T = I$ and $B_0^T B_0$ is a sparse diagonal matrix with diagonal entries being 0 or 1. Thus, $H_C$ can be first simplified to

$$H_C = I - B_0^T B_0.$$  

(26)

Clearly, $H_C$ is also a diagonal matrix with either 0 or 1 diagonal entries. The 1-valued diagonal entry of $H_C$ corresponds to the inactive constraints in $B \delta^*(\theta) < b$, i.e., those satisfied with strict inequalities in $\{\|\delta\|_\infty \leq \epsilon, 0 \leq \delta \leq 1\}$. This can be expressed as

$$H_C = \left[1_{p_1 \leq \delta^*_1 \leq q_1}, 1_{p_2 \leq \delta^*_2 \leq q_2}, \ldots, 1_{p_d \leq \delta^*_d \leq q_d}, e_d\right]$$

(27)

where $1_{p_i \leq \delta^*_i \leq q_i} \in \{0, 1\}$ denotes the indicator function over the constraint $\{p_i \leq \delta^*_i \leq q_i\}$ and returns 1 if the constraint is satisfied, $\delta^*_i$ denotes the $i$th entry of $\delta^*(\theta)$, $p_i = \max\{-\epsilon, -x_i\}$ and $q_i = \min\{\epsilon, 1 - x_i\}$, and $e_i \in \mathbb{R}^d$ denotes the basis vector with the $i$th entry being 1 and others being 0s.

Based on the definition of $g$, (23) and (27), we can eventually achieve the desired IG formula (12). The proof of Corollary 1 is now complete. □
B Discussion on case $\ell_{atk} = -\ell_{tr}$

We provide an in-depth explanation on the fact that even if we set $\ell_{atk} = -\ell_{tr}$, the optimization routine given by (4) to solve problem (3) does not reduce to the ordinary IG-absent gradient descent to solve problem (1) because of the presence of lower-level constraints.

- In the absence of the constraint $\delta \in \mathcal{C}$, if we set $\ell_{atk} = -\ell_{tr}$, then solving problem (3) via IG-involved descent method (4) will reduce to the ordinary IG-absent method that solves problem (1). This is a known BLO result (e.g., [14]) and can be readily proven using the stationary condition. To be specific, based on the stationary condition of unconstrained lower-level optimization, we have $\nabla_\delta \ell_{atk}(\theta, \delta^*) = 0$. Since $\ell_{atk} = -\ell_{tr}$, we have $\nabla_\delta \ell_{tr}(\theta, \delta^*) = 0$. As a result, the second term in (4) becomes 0 and solving problem (3) becomes identical to solving the min-max problem (1).

- In the presence of the constraint $\delta \in \mathcal{C}$, the stationary condition cannot be applied since the stationary point may not be a feasible point in the constraint. In other words, $\nabla_\delta \ell_{atk}(\theta, \delta^*) = 0$ does not hold in the case of $\ell_{atk} = -\ell_{tr}$. As a matter of fact, one has to resort to KKT conditions instead of the stationary condition for a constrained lower-level problem. Similar to our proof in Proposition 1, the implicit gradient (and thus the second term of (4)) cannot be omitted in general. This makes the optimization routine to solve problem (3) different from solving problem (1).

C Detailed Experiment settings

C.1 Training Set-up

For CIFAR-10, we summarize the training setup for each method. 1) FAST-AT: We use FGSM with an attack step size of $1.25\epsilon$ to generate perturbations; 2) PGD-2-AT: 2-step PGD attacks $\delta$ with an attack step size of $0.5\epsilon$ is implemented; 3) FAST-AT-GA: The gradient alignment regularization parameter is set to the recommended value for each $\epsilon$; 4) FAST-BAT: We select $\lambda$ from $255/5000$ to $255/2000$ for different $\epsilon$. At the same time, we adjust $\alpha_2$ accordingly, so that the coefficient of the second term in (13), namely $\alpha_2/\lambda$ always equals to $0.1\alpha_1$.

For ImageNet, we set $\epsilon$ to $2/255$, and we strictly follow the training setting adopted by [40]. In FAST-BAT, we fix $\lambda$ at $255/3000$ and adopt the same $\alpha_2$ selection strategy as CIFAR-10.

Parameter for FAST-AT-GA Regarding FAST-AT-GA with different model types, we adopt the same regularization parameter recommended in its official repo intended for PreActResNet-18 (namely 0.2 for $\epsilon = 8/255$ and 2.0 for $\epsilon = 16/255$).

C.2 The choice of initialization point $z$

To specify $z$ in (7), we investigate two classes of linearization schemes. The first class is random constant linearization, including: “uniformly random linearization”, i.e., $z = \delta_0$ similar to FAST-AT, and “random corner linearization” under the $\epsilon$-radius $\ell_\infty$-ball, i.e., $z \in \{-\epsilon, \epsilon\}^d$. The second class is 1-step perturbation warm-up-based linearization, including the other two specifications: “1-step sign-based PGD”, and “1-step PGD w/o sign”. We consider this linearization schemes as their computation complexities are less than or close to the complexity of one-step attack generation. As a result, FAST-BAT takes comparable computation cost to the

1We use random initialization to generate perturbations for PGD, while in the paper of FAST-AT-GA [2], 2-step PGD is initialized at zero point, which we believe will underestimate the effect of PGD-2-AT

2FAST-AT-GA: https://github.com/ml-epfl/understanding-fast-adv-training/blob/master/sh
baselines FAST-AT, PGD-2-AT and FAST-AT-GA. Empirically, we find that FAST-BAT using “1-step PGD w/o sign” leads to the best defensive performance; see justification in Table A4. We follow this experiment setup in the sequel.
D Additional Experimental Results

Figure A1: Visualization of adversarial loss landscapes of FAST-AT, FAST-AT-GA and FAST-BAT trained using the ResNet-18 model on the CIFAR-10 dataset. The losses are calculated w.r.t. the same image example ID #001456, and the landscape is obtained by tracking the loss changes w.r.t. input variations following [13]. That is, the loss landscape is generated by $z = \text{loss}(I + x \cdot r_1 + y \cdot r_2)$, where $I$ denotes an image, and the $x$-axis and the $y$-axis correspond to linear coefficients associated with the sign-based attack direction $r_1 = \text{sign}(\nabla I \text{loss}(I)) \cdot x$ and a random direction $r_2 \sim \text{Rademacher}(0,5)$, respectively.

Results on ImageNet We train DNN models ResNet (RN)-50 [17] for ImageNet and we choose the training perturbation strength $\epsilon = 2/255$ strictly following [40] [2]. We remark that when evaluating on ImageNet, we only compare ours with FAST-AT since as shown in Table 6 of [2], the other baseline methods did not show any improvement over Fast-AT at the attack budget $\epsilon = 2/255$. RA-PGD stands for the robustness against PGD-50-10 (50-step PGD attack with 10 restarts) with $\epsilon = 2/255$. Table A1 shows the performance comparison between FAST-AT and FAST-BAT. We can see FAST-BAT outperforms FAST-AT by 1.23% when facing attacks with $\epsilon = 2/255$.

Table A1: SA and RA on ImageNet.

| Method         | SA (%) | RA-PGD (%) |
|----------------|--------|------------|
| FAST-AT        | 60.90  | 43.43      |
| FAST-BAT       | 60.18  | 44.64      |

Sensitivity to regularization parameter $\lambda$ In Table A2, we show the sensitivity of FAST-BAT to the regularization parameter $\lambda$. All the parameters remain the same as the default setting, except that for different $\lambda$. We always adjust $\alpha_2$ so that $\alpha_2/\lambda = 0.1\alpha_1$ holds. Note $1/\lambda$ also serves as the attack step in (7). As $\lambda$ decreases, the improvement in robust accuracy is evidently strengthened, and there is an obvious trade-off between robust accuracy (SA) and standard accuracy (RA). At a certain level of $\lambda$, namely when $\lambda \leq 255/3500$, RA starts to converge and stop surging.

Table A2: Performance of FAST-BAT with different parameter $\lambda$. We train and evaluate with the same attack budget $\epsilon = 16/255$ on CIFAR-10 to show the influence of $\lambda$.

| $1/\lambda (255)$ | 500 | 1000 | 1500 | 2500 | 3500 |
|-------------------|-----|------|------|------|------|
| SA (%)            | 83.20 | 75.06 | 69.31 | 68.16 | 64.37 |
| RA-PGD (%)        | 19.02 | 21.42 | 23.34 | 27.69 | 25.32 |

Sensitivity to different $\alpha_2$ choices We consider the case of robust training with the large $\epsilon$ choice (16/255). As we can see from Table A3, if $\alpha_2$ is set too small ($\alpha_2 = 0.008\alpha_1$), then both SA and RA will drop significantly. Here $\alpha_1$ is set as the cyclic learning rate and thus not a constant parameter. However, in the $\alpha_2$ interval $[0.0125\alpha_1, 0.025\alpha_1]$, we observed a tradeoff between standard accuracy (SA) and robust accuracy (RA): That is, the improvement in RA corresponds to a loss in SA. In our experiments, we choose $\alpha_2$ when the tradeoff yields the best RA without suffering a significant drop of SA (which still outperforms the baseline approaches).

Table A3: Performance of FAST-BAT with different $\alpha_2$ choices on CIFAR-10. Models are trained and evaluated with the same attack budget ($\epsilon = 16/255$). Here $\alpha_1$ is set as the cyclic learning rate and is not a constant value. $\alpha_2$ is always set proportionate to $\alpha_1$ for simplicity.

| $\alpha_2$ (CIFAR-10, PreActResNet18, $\epsilon = 16/255$) | 0.025$\alpha_1$ | 0.0167$\alpha_1$ | 0.0125$\alpha_1$ | 0.008$\alpha_1$ |
|-------------------------------------------------------------|-----------------|-----------------|-----------------|-----------------|
| SA (%)                                                      | 75.06           | 69.31           | 68.16           | 57.92           |
| RA-PGD (%)                                                  | 21.42           | 23.34           | 27.69           | 20.53           |

Sensitivity of linearization schemes Fast-BAT needs a good linearization point $z$ in (7). In experiments, we adopt the perturbation generated by 1-step PGD without sign as our default linearization scheme. In Table A4, we show the performance of the other possible linearization options. We find that 1-step PGD without sign achieves the best robust accuracy among all the choices. This is not surprising since this linearization point choice is consistent with the first-Taylor expansion that we used along the direction of the input gradient without the sign operation involved. By contrast, FAST-BAT linearized with uniformly random noise suffers from catastrophic
overfitting and reaches a rather low standard accuracy (SA). Fast-BAT with other linearizations also yields a worse SA-RA trade-off than our proposal.

The validity of the Hessian-free assumption on non-ReLU based neural networks. The Hessian-free assumption is based on the fact that the commonly used ReLU activation function is piece-wise linear w.r.t. input. We further conduct experiments to verify the feasibility of such an assumption on models with non-ReLU activation functions. We choose two commonly used activation functions, Swish [31] and Softplus, as alternatives for the non-smooth ReLU function. We compare the results both calculating Hessian as well as the Hessian-free version to see if the Hessian-free assumption still holds for the non-ReLU neural network. The results are shown in Table A5. As we can see, the use of Hessian does not affect performance much. A similar phenomenon can be observed across different ε and different model activation functions (ReLU, Softplus, and Swish). However, the introduction of Hessian leads to an increase in time consumption by more than 30%. Therefore, we can draw the conclusion that the Hessian-free assumption is reasonable across different activation function choices.

Ablation studies. In Appendix D, we present additional empirical studies including 1) the sensitivity analysis of the linearization hyperparameter λ, 2) the choice of the linearization point, and 3) the sensitivity analysis of α2.

Table A4: Performance of Fast-BAT with different linearization schemes. Besides 1-step PGD without sign (PGD w/o Sign), we further generate linearization point with the following methods: uniformly random noise [−ε, ε]d (Uniformly Random); uniformly random corner {−ε, ε}d (Random Corner); and perturbation from 1-step PGD attack with 0.5ε as attack step (PGD).

| CIFAR-10, PreActResNet-18, ε = 16/255 | Linearization Method | PGD w/o Sign | Uniformly Random | Random Corner | PGD |
|-------------------------------------|----------------------|--------------|-----------------|---------------|-----|
| SA (%)                             | 69.31 43.42 62.19    | 75.30        | 23.34 21.25 16.5 | 19.42         |     |
| RA-PGD (%)                          |                      |              |                 |               |     |

Table A5: Performance of Fast-AT and Fast-BAT with different activation functions on CIFAR-10. ReLU, Swish and Softplus are taken into consideration. For Fast-BAT, we compare the Hessian-free and Hessian-aware version to verify the influence of Hessian matrix. The results are averaged over 3 independent trials.

| Setting               | SA (%) (ε = 8/255) | RA-PGD (%) (ε = 8/255) | SA (%) (ε = 16/255) | RA-PGD (%) (ε = 16/255) | Time (s/epoch) |
|-----------------------|--------------------|------------------------|---------------------|-------------------------|----------------|
| Fast-AT-ReLU          | 82.39 ±0.14        | 45.49 ±0.21            | 44.15 ±7.27         | 21.83 ±1.32             | 23.1           |
| Fast-BAT-ReLU Hessian-free | 79.97 ±0.12    | 48.83 ±0.17            | 68.16 ±0.25         | 27.69 ±0.16             | 61.4           |
| Fast-BAT-ReLU Hessian-aware | 79.62 ±0.17       | 49.13 ±0.14            | 67.82 ±0.23         | 27.82 ±0.19             | 82.6           |
| Fast-AT-Softplus      | 81.29 ±0.16        | 47.26 ±0.24            | 45.39 ±3.27         | 22.40 ±0.75             | 23.3           |
| Fast-BAT-Softplus Hessian-free | 79.48 ±0.18    | 49.74 ±0.21            | 68.57 ±0.27         | 25.59 ±0.15             | 61.7           |
| Fast-BAT-Softplus Hessian-aware | 79.59 ±0.21       | 49.74 ±0.12            | 68.63 ±0.23         | 25.54 ±0.19             | 82.8           |
| Fast-AT-Swish         | 75.61 ±0.15        | 44.43 ±0.18            | 52.03 ±4.29         | 23.08 ±2.23             | 23.1           |
| Fast-BAT-Swish Hessian-free | 73.89 ±0.14    | 45.90 ±0.23            | 62.59 ±0.29         | 23.81 ±0.17             | 61.7           |
| Fast-BAT-Swish Hessian-aware | 73.93 ±0.16       | 45.97 ±0.19            | 62.49 ±0.27         | 23.99 ±0.17             | 82.6           |
E Convergence Analysis

Let us consider we have data samples \( \{x_i, y_i\}_{i=1}^{N} \), where \( N \) denotes the number of the training data. Then the goal of FAST-BAT algorithm is to solve:

\[
\min_{\theta} L_{tr}(\theta, \delta^*(\theta)) = \frac{1}{N} \sum_{i=1}^{N} \ell_{tr}(\theta; x_i + \delta^*_i(\theta), y_i)
\]

\[
\delta^*(\theta) \in \arg \min_{\delta \in C} L_{atk}(\theta, \delta^*(\theta))
\]

(28)

Let us denote the batch size as \( b \). Then the problem can be reformulated as:

\[
\min_{\theta} L_{bt}^{b_t}(\theta, \delta^*(\theta)) = \frac{1}{b_t} \sum_{i=1}^{b_t} \ell_{tr}(\theta; x_i + \delta^*_i(\theta), y_i)
\]

\[
\delta^*(\theta) \in \arg \min_{\delta \in C} L_{atk}^{b_t}(\theta, \delta^*(\theta))
\]

(29)

The way to computes the gradient (4) is equal to the case where \( b = N \).

\[
\frac{dL_{bt}^{N}(\theta, \delta^*(\theta))}{d\theta} = \nabla_\theta L_{tr}^{N}(\theta, \delta^*(\theta)) + \frac{d\delta^*(\theta)}{d\theta}^\top \nabla_\delta L_{atk}^{N}(\theta, \delta^*(\theta))
\]

(30)

If we approximate the gradient \( \nabla_\theta L_{tr}(\theta, \delta^*(\theta)) \) using a batch size of \( b \), then we have the following assumptions:

- Bias assumption:

\[
\mathbb{E}[\nabla_\theta L_{bt}^{b_t}(\theta, \delta^*(\theta))] = \nabla_\theta L_{tr}(\theta, \delta^*(\theta)) + \beta(b),
\]

(31)

where \( \beta(b) \) is the bias and the expectation is taken w.r.t. batches. Note that \( \beta(b) = 0 \) for \( b = N \).

- Variance assumption:

\[
\mathbb{E}[\|\nabla_\theta L_{bt}^{b_t}(\theta, \delta^*(\theta)) - \nabla_\theta L_{tr}(\theta, \delta^*(\theta)) - \beta(b)\|^2] = \sigma^2[1 + \|\nabla_\theta L_{tr}(\theta, \delta^*(\theta))\|^2].
\]

(32)

Note that the variance equals 0 for \( b = N \).

Now the FAST-BAT algorithm with batch size \( b \) can be stated as follows:

- Initialization: \( \theta_0 \in \mathbb{R}^n \), step size \( \{\alpha_t\}_{t=0}^{T-1} \), batch size \( \{\alpha_{bt}\}_{t=0}^{T-1} \).

- for \( t = 1 \) to \( T \):
  - Choose batch size \( b_t \) at each iteration \( t \in [T] \).
  - \( L_{tr}(\theta, \delta^*(\theta)) \approx L_{bt}^{b_t}(\theta, \delta^*(\theta)), L_{atk}(\theta, \delta^*(\theta)) \approx L_{atk}^{b_t}(\theta, \delta^*(\theta)) \)
Assuming smoothness of $L_{tv}(\theta)$ w.r.t. $\theta$, we get:

$$L_{tv}(\theta_{t+1}) \leq L_{tv}(\theta_t) + \left\langle \nabla_\theta L_{tv}(\theta_t), \theta_{t+1} - \theta_t \right\rangle + \frac{L}{2} \|\theta_{t+1} - \theta_t\|^2$$

$$= L_{tv}(\theta_t) - \alpha \left( \nabla_\theta L_{tv}(\theta_t), \nabla_\theta L_{tv}(\theta_t) \right) + \frac{\alpha^2 L}{2} \|\nabla_\theta L_{tv}(\theta_t)\|^2$$

Taking expectation w.r.t. random samples, we get:

$$E[L_{tv}(\theta_{t+1})] \leq E[L_{tv}(\theta_t)] - \alpha E[\|\nabla_\theta L_{tv}(\theta_t)\|^2] - \alpha E[\|\nabla_\theta L_{tv}(\theta_t), \beta(b_t)\|] + \alpha^2 \sigma^2 L E[1 + \|\nabla_\theta L_{tv}(\theta_t)\|^2]
+ 2\alpha^2 \sigma L E[\|\nabla_\theta L_{tv}(\theta_t)\|^2] + 2\alpha^2 \sigma^2 L E[\|\beta(b_t)\|^2]$$

$$\leq E \left[ L_{tv}(\theta_t) - \left( \frac{\alpha t}{2} - \alpha^2 \sigma^2 L \right) \|\nabla_\theta L_{tv}(\theta_t)\|^2 + \left( \frac{\alpha t}{2} + 2\alpha^2 L \right) \|\beta(b_t)\|^2 + \alpha^2 L \sigma^2 \right]$$

Using $\alpha_t \leq \frac{1}{4L(2+\sigma^2)}$, we get:

$$E[L_{tv}(\theta_{t+1})] \leq E \left[ L_{tv}(\theta_t) - \frac{\alpha t}{4} \|\nabla_\theta L_{tv}(\theta_t)\|^2 + \alpha_1 \|\beta(b_t)\|^2 + \alpha_2 L \sigma^2 \right].$$

Finally, after rearranging the terms, we get:

$$\frac{\alpha t}{4} E[\|\nabla_\theta L_{tv}(\theta_t)\|^2] \leq E[(L_{tv}(\theta_t) - L_{tv}(\theta_{t+1})) + \alpha_1 \|\beta(b_t)\|^2 + \alpha_2 L \sigma^2]$$

Summing over $t = 1$ to $T$ and multiplying by $1/T$, we get:

$$\frac{1}{T} \sum_{t=1}^T \frac{\alpha t}{4} E[\|\nabla_\theta L_{tv}(\theta_t)\|^2] \leq \frac{L_{tv}(\theta_0) - L_{tv}(\theta^*)}{T} + \frac{1}{T} \sum_{t=1}^T \alpha t \|\beta(b_t)\|^2 + \frac{1}{T} \sum_{t=1}^T \alpha^2 \sigma^2.$$

Taking $\alpha_t = \alpha$ and $b_t = b$, we get:

$$\frac{1}{T} \sum_{t=1}^T E[\|\nabla_\theta L_{tv}(\theta_t)\|^2] \leq \frac{4[L_{tv}(\theta_0) - L_{tv}(\theta^*)]}{\alpha T} + 4\|\beta(b)\|^2 + 4\alpha \sigma^2.$$
Recall if \( b = N \), we have \( \sigma^2 = 0 \) and \( \beta(b) = 0 \), we can further get:

\[
\frac{1}{T} \sum_{t=1}^{T} \| \nabla_{\theta} L_{tr}(\theta_t) \|_2^2 \leq \frac{4[L_{tr}(\theta_0) - L_{tr}(\theta^*)]}{\alpha T}.
\]

(40)

Case I: We can choose \( \alpha = \frac{1}{8L} \) and get:

\[
\frac{1}{T} \| \nabla_{\theta} L_{tr}(\theta_t) \|_2^2 = O\left(\frac{1}{T}\right).
\]

(41)

Case II: We can choose \( \alpha = \sqrt{\frac{1}{T}} \):

\[
\frac{1}{T} \sum_{t=1}^{T} \mathbb{E}[\| \nabla_{\theta} L_{tr}(\theta_t) \|_2^2] \leq \frac{4[L_{tr}(\theta_0) - L_{tr}(\theta^*)]}{\sqrt{T}} + \frac{4\sigma^2}{\alpha T} \underbrace{[\beta(b)]^2}_{O(1)}
\]

Now if \( \| \beta(b) \|_2^2 = O\left(\frac{1}{\sqrt{T}}\right) \), then

\[
\frac{1}{T} \sum_{t=1}^{T} \mathbb{E}[\| \nabla_{\theta} L_{tr}(\theta_t) \|_2^2] \leq O\left(\frac{1}{\sqrt{T}}\right),
\]

(42)

otherwise we get in the worst case:

\[
\frac{1}{T} \sum_{t=1}^{T} \mathbb{E}[\| \nabla_{\theta} L_{tr}(\theta_t) \|_2^2] \leq O\left(\frac{1}{\sqrt{T}}\right) + O(1).
\]

(43)