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Incremental Without Replacement Sampling in Nonconvex Optimization

Edouard Pauwels*

Abstract

Minibatch decomposition methods for empirical risk minimization are commonly analysed in a stochastic approximation setting, also known as sampling with replacement. On the other hands modern implementations of such techniques are incremental, they rely on sampling without replacement. We reduce this gap between theory and common usage by analysing a versatile incremental gradient scheme. We consider constant, decreasing or adaptive step sizes. In the smooth setting we obtain explicit rates and in the nonsmooth setting we prove that the sequence is attracted by solutions of optimality conditions of the problem.

Keywords. Without Replacement Sampling, Incremental Methods, Nonconvex Optimization, First order Methods, Stochastic Gradient, Adaptive Methods, Backpropagation, Deep Learning

1 Introduction

1.1 Context and motivation

Training of modern learning architectures is mostly achieved by empirical risk minimization, relying on minibatch decomposition first order methods [17, 28]. The goal is to solve optimization problems of the form

$$F^* = \inf_{x \in \mathbb{R}^p} F(x) = \frac{1}{n} \sum_{i=1}^n f_i(x) \quad (1)$$

where $f_i: \mathbb{R}^p \rightarrow \mathbb{R}$ are Lipschitz functions and the infimum is finite. In this context minibatching takes advantage of redundancy in large sums and perform steps which only rely on partial sums [16]. The most widely studied variant is the Stochastic Gradient algorithm, each step consists in sampling with replacement in $\{1, \dots, n\}$, and moving in the direction of the gradient of F corrupted by centered noise inherent to subsampling. This allows to study such algorithms in the broader context of stochastic approximation, initiated by Robins and Monro [39] with many subsequent work [30, 6, 26, 15, 34, 20, 14].

On the other hand most widely used implementations of such learning strategies for deep network [1, 37] rely on sampling without replacement, an epoch being the result of a single path during which first order information for each f_i is computed exactly once. Although very close to stochastic approximation, this strategy does not satisfy the “gradient plus centered noise” hypothesis. Hence all existing theoretical guaranties relying on stochastic approximation arguments do not hold true for many practical implementation of learning algorithm. The purpose of this work is to reduce this gap and analyse “without replacement minibatch strategies” for problem (1), also known as incremental methods [10].

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Algorithm 1: Without replacement descent algorithm

Program data: For $i = 1 \dots, n$, f_i and the corresponding search direction oracle d_i .

Input: $x_0 \in \mathbb{R}^p$.

1: Decreasing steps:	1: Adaptive steps:
2: $(\alpha_{K,i})_{K \in \mathbb{N}, i \in \{1, \dots, n\}}$.	2: $v_0 = \delta^2 > 0, \beta > 0$.
3: for $K \in \mathbb{N}$ do	3: for $K \in \mathbb{N}$ do
4: Set: $z_{K,0} = x_K$	4: Set: $z_{K,0} = x_K, v_{K,0} = v_K$
5: for $i = 1, \dots, n$ do	5: for $i = 1, \dots, n$ do
6: $\hat{z}_{K,i-1} \in \text{conv}((z_{K,j})_{j=0}^{i-1})$.	6: $\hat{z}_{K,i-1} \in \text{conv}((z_{K,j})_{j=0}^{i-1})$.
7: $z_{K,i} = z_{K,i-1} - \alpha_{K,i} d_i(\hat{z}_{K,i-1})$	7: $v_{K,i} = v_{K,i-1} + \beta \ d_i(\hat{z}_{K,i-1})\ ^2$
8: end for	8: $\alpha_{K,i} = 1/\sqrt{v_{K,i}}$
9: Set: $x_{K+1} = z_{K,n}$	9: $z_{K,i} = z_{K,i-1} - \alpha_{K,i} d_i(\hat{z}_{K,i-1})$
10: end for	10: end for
	11: Set: $x_{K+1} = z_{K,n}, v_{K+1} = v_{K,n}$.
	12: end for

1.2 Problem setting

We consider problem (1) and assume that for each f_i we have access to an oracle which provides a search direction $d_i: \mathbb{R}^p \mapsto \mathbb{R}^p, i = 1, \dots, n$. We consider two settings

Smooth setting: f_i are C^1 with Lipschitz gradient, in which case we set $d_i = \nabla f_i, i = 1, \dots, n$.

Nonsmooth setting: f_i are path differentiable. Such functions constitute a subclass of Lipschitz functions which enjoy some of the nice properties of nonsmooth convex functions [14] in particular, an operational chain rule [20]. In this case, d_i is a selection in a conservative field for f_i . Examples of such object include convex subgradients if f_i is convex, the Clarke subgradient, which is an extension to the nonconvex setting, as well as the output of automatic differentiation applied to a nonsmooth program, see [14] for more details. In both settings we impose the following standing assumption.

Assumption 1 For $i = 1, \dots, n$, $f_i: \mathbb{R}^p \rightarrow \mathbb{R}$ is an M_i Lipschitz functions and $d_i: \mathbb{R}^p \mapsto \mathbb{R}^p$ is such that for all $x \in \mathbb{R}^p, \|d_i(x)\| \leq M_i$. We let $M = \sqrt{\frac{1}{n} \sum_{i=1}^n M_i^2}$. Note that in this case F is M -Lipschitz.

We consider a class of descent methods described by Algorithm 1. Notice that there is no randomness specified in the algorithm, all our results are worst case and hold deterministically. Algorithm 1 allows to model:

Gradient descent: Set $\hat{z}_{K,i-1} = z_{K,0} = x_K$, for all $K \in \mathbb{N}$ and $i = 1 \dots, n$.

Incremental algorithms: Set $\hat{z}_{K,i-1} = z_{K,i-1}$, for all $K \in \mathbb{N}$ and $i = 1 \dots, n$.

Random permutations: Although not explicitly stated in the algorithm, all our proof argument hold independantly of the order of query of the indices $i = 1, \dots, n$ for each epoch. Hence our results actually hold deterministically for “random shuffling” or, “without replacement sampling” strategies.

Mini-batching: Set $\hat{z}_{K,i-1} = \hat{z}_{K,i-2} = z_{K,i-2}$, which results in computation of gradients of f_i and f_{i-1} at the same point $z_{K,i-2}$.

Asynchronous computation in a parameter server setting: Consider that $(z_{K,i})_{K \in \mathbb{N}, i=1 \dots n}$ is stored on a server, accessed by workers which compute $d_i(z_{K,i-1})$. Due to communication and computation delays, d_i may be evaluated using an outdated estimate of z , called \hat{z} . In Algorithm 1, asynchronicity and delays between workers may be arbitrary within each epoch. However, we enforce that the whole system waits for all workers to communicate results before starting a new epoch, a form of partial synchronization.

1.3 Contributions

We propose a detailed convergence analysis of Algorithm 1 in a nonconvex setting. Our analysis is worst case and our results hold deterministically. When each f_i is smooth with Lipschitz gradient, we

obtain an $O(1/\sqrt{K})$ convergence rate in terms of gradient norm squared, for both step size regimes, adaptive steps allowing to improve dependency in problem constants. For general nonsmooth objectives, convergence rate do not exist for the simplest subgradient oracle, see for example [43] with an attempt for more complex oracles. We prove that the sequence $(x_K)_{K \in \mathbb{N}}$ is attracted by subsets of \mathbb{R}^p which are solutions to optimality condition related to problem (1), for both step size strategies.

1.4 Relation to existing literature

Incremental gradient was introduced by Bertsekas in the late 90's [8], extended with a gradient plus error analysis [9] and nonsmooth version [35]. An overview is given in [10], see also [11]. Most convergence analyses are qualitative and limited to convex objectives, only few rates are available, to our knowledge, our convergence rates are new. The prescribed step size strategy in Algorithm 1 is directly inspired from these works. We analyse the incremental method as a perturbed gradient method, a view which was exploited in [9, 31] and in distributed settings, see for example [32, 33, 27, 38].

The adaptive step size is taken from adagrad algorithm introduced in [22]. Analysis of such algorithms in a nonconvex setting has attracted a lot of attention, see for example [29, 42, 3, 21] in the stochastic and smooth setting. To our knowledge the combination of adaptive step sizes with incremental methods has not been considered. We use the ‘‘scalar step variant’’ of adagrad, called adagrad-norm in [42] or global step size in [29], in contrast with the originally proposed coordinatewise step sizes analysed in [21].

Out nonsmooth convergence analysis relies on the ODE method, see [30] with many subsequent developments [6, 26, 7, 15, 3]. In particular we build upon a nonsmooth ODE formulation, differential inclusions [19, 2]. This was used in [20] to analyse the stochastic subgradient algorithm in nonconvex settings using the subgradient projection formula [12]. In the nonsmooth world the backpropagation algorithm [41] used in deep learning suffers from inconsistent behaviors and may not provide subgradient of any kind [24, 25]. We use the recently introduced tool of conservative fields and path differentiable function [14] capturing the full complexity of backpropagation oracles. Our proof essentially relies on the notion of Asymptotic Pseudo Trajectory (APT) for differential inclusions [5, 7].

1.5 Preliminary results

It is important to emphasize that in Algorithm 1, the adaptive step strategy is a special case of the prescribed step strategy. Hence our analysis will start by general considerations for the prescribed step strategy followed by specific considerations to the adaptive steps. We start with a simple claim whose proof is given in appendix A and asserts provides a bound on the length of the steps taken by the algorithm.

Claim 1 *For all $K \in \mathbb{N}$ and all $i = 1, \dots, n$, we have*

$$\max \{ \|z_{K,i} - x_K\|^2, \|x_{K+1} - x_K\|^2, \|\hat{z}_{K,i-1} - x_K\|^2 \} \leq n \sum_{i=1}^n \alpha_{K,i}^2 \|d(\hat{z}_{K,i-1})\|^2, \quad (2)$$

Throughout this paper, we will work under decreasing step size condition which meaning is described in the following assumption. We remark that both step size strategies provided in Algorithm 1 comply with this constraint.

Assumption 2 *The sequence $(\alpha_{K,i})_{K \in \mathbb{N}, i \in \{1, \dots, n\}}$ is non increasing with respect to the lexicographic order. That is for all $K \in \mathbb{N}$, $i = 2, \dots, n$, $\alpha_{K,i-1} \geq \alpha_{K,i} \geq \alpha_{K+1,i}$.*

2 Quantitative analysis in the smooth setting

In this section we consider that each f_i has Lipschitz gradient, in which case, d_i is set to be ∇f_i . Note that in this setting, $\nabla F = \frac{1}{n} \sum_{i=1}^n \nabla f_i$ and F also has L -Lipschitz gradient.

Assumption 3 In addition to Assumption 1, for $i = 1, \dots, n$, f_i is continuously differentiable with L_i Lipschitz gradient and we set $d_i = \nabla f_i$. We set $L = \frac{1}{n} \sum_{i=1}^n L_i$. Note that in this case F has L -Lipschitz gradient as shown in Claim 6.

The technical bulk of our analysis is given by the following claim whose proof is provided in appendix A. Note that this result holds deterministically and independantly of the considered step size strategy.

Claim 2 Under Assumptions 1, 2, 3, for all $K \in \mathbb{N}$, setting $\alpha_K = \alpha_{K-1,n}$ and $\alpha_0 = 1/\delta$, we have

$$\begin{aligned} & F(x_{K+1}) \tag{3} \\ & \leq F(x_K) - \frac{n\alpha_K}{2} \|\nabla F(x_K)\|^2 + \left(\frac{L^2 n^2}{\delta} + \frac{Ln}{2} \right) \sum_{j=1}^n \alpha_{K,j}^2 \|d_j(\hat{z}_{K,j-1})\|^2 + \frac{M^2}{\delta} \sum_{i=1}^n \left(1 - \frac{\alpha_{K,i}^2}{\alpha_K^2} \right). \end{aligned}$$

2.1 Corollaries for specific instances

The following hold under Assumptions 1, 2, 3 for Algorithm 1.

Corollary 1 If the step size is constant, $\alpha_{K,i} = \alpha/n$ for all $K \in \mathbb{N}$, $i = 1 \dots, n$, we have

$$\min_{K=0, \dots, N} \|\nabla F(x_K)\|^2 \leq \frac{2(F(x_0) - F^*)}{(N+1)\alpha} + 2 \left(\alpha L^2 M^2 + \frac{LM^2}{2} \right) \alpha$$

Corollary 2 If the step size is decreasing $\alpha_{K,i} = 1/(n\sqrt{K+1})$, for all $K \in \mathbb{N}$, $i = 1 \dots, n$, then

$$\min_{K=0, \dots, N} \|\nabla F(x_K)\|^2 \leq \frac{1}{\sqrt{N+1}-1} \left(F(x_0) - F^* + \left(L^2 M^2 + \frac{LM^2}{2} \right) (1 + \log(N+1)) \right)$$

Corollary 3 If we consider the adaptive step size strategy with $\beta = \delta = n$, then

$$\min_{K=0, \dots, N} \|\nabla F(x_K)\|^2 \leq 2 \left(F(x_0) - F^* + \left(L^2 + \frac{L}{2} + M^2 \right) \log(1 + M^2(N+1)) \right) \frac{\sqrt{M^2+1}}{\sqrt{N+1}}.$$

2.2 Discussion on the obtained convergence rates

All the rates deccribed in Section 2.1 are of the order $O(1/\sqrt{K})$ where K is the number of epochs. In particular, there is no dependency in the size of the sum n or in the dimension p beyond problem constants L and M . Compared to “with replacement” stochastic variants of similar algorithms, the dependency in n may look unfavorable. Indeed, our rates are in terms of number of epochs rather than number of iterations as it is customary in stochastic settings [16, 34, 17]. This is due to the nature of our analysis, which is worst case, in contrast with average case analysis usually performed when considering “with replacement” strategies. If the situation is very adversarial, for example only f_n is nonzero, then there is only a single non zero update per epoch which suggests that the convergence should indeed be measured in term of number of epochs. On the other hand, if the index i is chosen uniformly at random at each step within the first epoch, although in the worst case, no improvement is made for the first steps, there is improvement on average. In the noiseless setting, the gradient algorithm achieves $O(1/K)$ rate and the drop in order of convergence speed is due to the perturbation of the exact gradient algorithm. Although our perturbation are worst case deterministic, we still pay a similar drop in convergence speed which is natural.

Dependency in problem constants L and M are worse than deterministic gradient descent algorithm. The prescribed step size strategy comes with a very bad dependency in M and L . If these constants were known, we could use them to devise better strategies. For example optimizing over α in Corollary 1, one ends up with a rate of the form $O\left(M\sqrt{L}\sqrt{F}/\sqrt{N+1}\right)$ which is homogeneuous. However these constants are not known. It is important to notice that the adaptive step size strategy leads to a better dependency in L and M , closer to homogeneity and comparable to dependencies obtained for “with replacement” variants of the same algorithm. In particular the adaptative step size strategy improves the dependancy in problem constants.

2.3 Proofs for the obtained rates

Proof of Corollary 1: Fix $K \in \mathbb{N}$, fix $\alpha_{K,i} = \alpha_K$ for all $i = 1, \dots, n$, we have $1 - \frac{\alpha_{K,i}^2}{\alpha_K^2} = 0$. Combining with Claim 2, we have

$$\frac{n\alpha_K}{2} \|\nabla F(x_K)\|^2 \leq F(x_K) - F(x_{K+1}) + \left(\frac{L^2 M^2 n}{\delta} + \frac{LM^2}{2} \right) n^2 \alpha_K^2.$$

Summing for $K = 0, \dots, N$ and dividing by $\sum_{K=0}^N n\alpha_K$, we obtain

$$\min_{K=0, \dots, N} \|\nabla F(x_K)\|^2 \leq \frac{2}{\sum_{K=0}^N n\alpha_K} \left(F(x_0) - F^* + \left(\frac{L^2 M^2 n}{\delta} + \frac{LM^2}{2} \right) \sum_{K=0}^N n^2 \alpha_K^2 \right) \quad (4)$$

Choosing constant step α/n with $\delta = n/\alpha$ for $\alpha > 0$, we obtain

$$\min_{K=0, \dots, N} \|\nabla F(x_K)\|^2 \leq \frac{2(F(x_0) - F^*)}{(N+1)\alpha} + 2 \left(\alpha L^2 M^2 + \frac{LM^2}{2} \right) \alpha$$

□

Proof of Corollary 2: In this setting (4) is still valid. Choosing $\alpha_K = \frac{1}{n\sqrt{K+1}}$, with $\delta = n$, we have

$$\begin{aligned} \sum_{K=0}^N \alpha_K &\geq \int_{t=0}^{t=N+1} \frac{1}{n\sqrt{t+1}} dt \geq \frac{2}{n} (\sqrt{N+1} - 1) \\ \sum_{K=0}^N \alpha_K^2 &\leq \frac{1}{n^2} \left(1 + \sum_{K=1}^N \frac{1}{K+1} \right) \leq \frac{1}{n^2} \left(1 + \int_{t=0}^{t=N} \frac{dt}{t+1} \right) = \frac{1}{n^2} (1 + \log(N+1)) \end{aligned}$$

and we obtain in (4)

$$\min_{K=0, \dots, N} \|\nabla F(x_K)\|^2 \leq \frac{1}{\sqrt{N+1} - 1} \left(F(x_0) - F^* + \left(L^2 M^2 + \frac{LM^2}{2} \right) (1 + \log(N+1)) \right)$$

□

Proof of Corollary 3: We write for all $K \in \mathbb{N}$ and all $i = 1, \dots, n$, $\alpha_K = \frac{1}{\sqrt{v_K}}$. Let us start with the following.

Claim 3 For all $K \in \mathbb{N}$ and all $i = 1, \dots, n$

$$1 - \frac{\alpha_{K,i}^2}{\alpha_K^2} \leq \beta \sum_{j=1}^n \frac{\|d_j(\hat{z}_{K,j-1})\|^2}{v_{K,j}} \quad (5)$$

Proof of claim 3: Fix $K \in \mathbb{N}$ and i in $1, \dots, n$, we have

$$v_K \leq v_{K,i} = v_K + \beta \sum_{j=1}^i \|d_j(\hat{z}_{K,j-1})\|^2.$$

From this we deduce, using the fact that $v_{K,j}$ is non decreasing in j ,

$$1 - \frac{\alpha_{K,i}^2}{\alpha_K^2} = \frac{v_{K,i} - v_K}{v_{K,i}} = \frac{\beta \sum_{j=1}^i \|d_j(\hat{z}_{K,j-1})\|^2}{v_{K,i}} \leq \beta \sum_{j=1}^i \frac{\|d_j(\hat{z}_{K,j-1})\|^2}{v_{K,j}} \leq \beta \sum_{j=1}^n \frac{\|d_j(\hat{z}_{K,j-1})\|^2}{v_{K,j}},$$

□

Combining Claim 2 and Claim 3, we have for all $K \in \mathbb{N}$,

$$\frac{n\alpha_K}{2} \|\nabla F(x_K)\|^2 \leq F(x_K) - F(x_{K+1}) + \left(\frac{L^2 n^2}{\delta} + \frac{Ln}{2} + \frac{M^2 n \beta}{\delta} \right) \sum_{j=1}^n \alpha_{K,j}^2 \|d_j(\hat{z}_{K,j-1})\|^2. \quad (6)$$

We remark that for all $K \in \mathbb{N}$, $\alpha_K \geq \frac{1}{\sqrt{Kn\beta M^2 + \delta^2}}$. Summing (6) for $K = 0, \dots, N$, we obtain

$$\frac{n(N+1)}{2\sqrt{Nn\beta M^2 + \delta^2}} \min_{K=0, \dots, N} \|\nabla F(x_K)\|^2 \leq F(x_0) - F^* + \left(\frac{L^2 n^2}{\delta} + \frac{Ln}{2} + \frac{M^2 n \beta}{\delta} \right) \sum_{K=0}^N \sum_{j=1}^n \alpha_{K,j}^2 \|d_j(\hat{z}_{K,j-1})\|^2 \quad (7)$$

Now, we use the lexicographic order on pairs of integers, $(a, b) \leq (c, d)$ if $a < c$ or $a = c$ and $b \leq d$. From Lemma 3, we have

$$\begin{aligned} \sum_{K=0}^N \sum_{i=1}^n \alpha_{K,i}^2 \|d_i(\hat{z}_{K,i-1})\|^2 &= \sum_{(K,i) \leq (N,n)} \frac{\|d_i(\hat{z}_{K,i-1})\|^2}{\delta^2 + \beta \sum_{(k,j) \leq (K,i)} \|d_j(\hat{z}_{k,j-1})\|^2} \\ &\leq \frac{1}{\beta} \log \left(1 + \frac{\beta \sum_{(K,i) \leq (N,n)} \|d_i(\hat{z}_{K,i-1})\|^2}{\delta^2} \right) \leq \frac{1}{\beta} \log \left(1 + \frac{\beta n M^2 (N+1)}{\delta^2} \right), \end{aligned} \quad (8)$$

where the last identity follows by applying Lemma 3 in appendix C, noticing that we sum over $(N+1)n$ instances and that $\sum_{i=1}^n \|d_i\|^2 \leq nM^2$. Combining (7) and (8) and choosing $\beta = \delta = n$, we obtain

$$\min_{K=0, \dots, N} \|\nabla F(x_K)\|^2 \leq 2 \left(F(x_0) - F^* + \left(L^2 + \frac{L}{2} + M^2 \right) \log(1 + M^2(N+1)) \right) \frac{\sqrt{M^2 + 1}}{\sqrt{N+1}}. \quad \square$$

3 Qualitative analysis for nonsmooth objectives

In this section we consider nonsmooth objectives such as typical losses arising when training deep networks. Our analysis will be performed under the following standing assumption.

Assumption 4 *In addition to Assumption 2, we set for each $K \in \mathbb{N}$, $\alpha_K = \alpha_{K-1, n}$, and assume that*

$$\sum_{K=0}^{\infty} \alpha_K = +\infty, \quad \text{and} \quad \alpha_K \xrightarrow{K \rightarrow \infty} 0, \quad \text{and} \quad \frac{\alpha_K}{\alpha_{K+1}} \xrightarrow{K \rightarrow \infty} 1. \quad (9)$$

We follow the ODE approach, our arguments closely follow those developed in [7]. We start by defining a continuous time piecewise affine interpolant of the sequence.

Definition 1 *For all $K \in \mathbb{N}$, we let $\tau_K = \sum_{k=0}^K \sum_{i=1}^n \alpha_{k,i}$. We fix the sequence given by Algorithm (1) and consider the associated Lipschitz interpolant such that $\mathbf{w}: \mathbb{R}^+ \mapsto \mathbb{R}^p$, such that $\mathbf{w}(\tau_K) = x_K$ for all $K \in \mathbb{N}$ and the interpolation is affine on (τ_K, τ_{K+1}) for all $K \in \mathbb{N}$.*

3.1 Differential inclusion setting

The main argument in this Section is connecting the continuous time interpolant in Definition 1 and continuous dynamics. The continuous time counterpart of Algorithm 1, is $\dot{\mathbf{x}} = \frac{-1}{n} \sum_{i=1}^n d_i(\mathbf{x})$, which right hand side is not continuous, classical Cauch-Lipschitz type theorems for existence of solutions cannot be applied. We need to resort to a continuous extension of the right hand side, which becomes set valued, providing a weaker notion of solution. We use the recently introduced notion of conservativity [14] which captures the complexity of automatic differentiation oracles in nonsmooth settings. Recall that the set valued map D is conservative for the locally Lipschitz function f , if it has a closed graph and for any locally Lipschitz curve $\mathbf{x}: [0, 1] \mapsto \mathbb{R}^p$ and almost all $t \in [0, 1]$

$$\frac{d}{dt} f(\mathbf{x}(t)) = \langle v, \dot{\mathbf{x}}(t) \rangle, \quad \forall v \in D(\mathbf{x}(t)). \quad (10)$$

This is the counterpart to $\frac{d}{dt} f(\mathbf{x}(t)) = \langle \nabla f(\mathbf{x}(t)), \dot{\mathbf{x}}(t) \rangle$ for C^1 function f and C^1 curve \mathbf{x} . This property is known as the chain rule of subdifferential inclusions, see for example [20]. The main specificity is that the property holds for almost all t due to the fact that we have nondifferentiable objects, and for all possible choices in D which is set valued, again due to nondifferentiability.

Assumption 5 For $i = 1, \dots, n$, we let D_i be a conservative field for f_i with $\max_{v \in D_i(x)} \|v\| \leq M$ for all $x \in \mathbb{R}^p$ and $d_i: \mathbb{R}^p \mapsto \mathbb{R}^p$ is measurable such that for all $x \in \mathbb{R}^p$, $d_i(x) \in D_i(x)$. We set $D = \text{conv}(\frac{1}{n} \sum_{i=1}^n D_i)$, note that D is conservative for F , it has convex compact values and a closed graph. We set crit_F to be the set of $x \in \mathbb{R}^p$ such that $0 \in D(x)$.

Main examples in deep learning: If each f_i , $i = 1, \dots, n$ is the loss associated to a sample point and a neural network architecture, assuming that f_i is defined using a compositional formula involving piecewise polynomials, logarithms and exponentials (which covers most of deep network architectures), then the Clarke subgradient [19] is a conservative field for f_i . Recall that the Clarke subgradient extends the notion of convex subgradient to nonconvex locally Lipschitz functions. This was proved in [20] using the projection formula in [14], see also [18, 14]. In deep learning context, backpropagation may fail to provide Clarke subgradients in nonsmooth contexts [24, 25]. Nonetheless, it was shown in [14] that backpropagation computes a conservative field. Hence our analysis applies to training of deep networks using a backpropagation oracle such as the ones implemented in [1, 37].

Definition 2 A solution to the differential inclusion

$$\dot{\mathbf{x}} \in -D(\mathbf{x})$$

with initial point $x \in \mathbb{R}^p$ is a locally Lipschitz mapping $\mathbf{x}: \mathbb{R} \mapsto \mathbb{R}^p$ such that $\mathbf{x}(0) = x$ and for almost all $t \in \mathbb{R}$, $\dot{\mathbf{x}}(t) \in -D(\mathbf{x}(t))$. We denote by S_x the set of such solutions.

Standard results in this field [2, Chapter 2, Theorem 3] ensure that, since D has closed graph and compact convex values, for any $x \in \mathbb{R}^p$ the set S_x is nonempty, note that it could be non unique.

3.2 Main result

The following notion was introduced in [7], see also [5]. It captures the fact that a continuous trajectory is a solution to the differential inclusion in Definition 2 asymptotically.

Definition 3 (Asymptotic pseudo trajectory) A continuous function $\mathbf{z}: \mathbb{R}_+ \mapsto \mathbb{R}^p$ is an asymptotic pseudotrajectory (APT), if for all $T > 0$,

$$\lim_{t \rightarrow \infty} \inf_{\mathbf{x} \in S_{\mathbf{z}(t)}} \sup_{0 \leq s \leq T} \|\mathbf{z}(t+s) - \mathbf{x}(s)\| = 0.$$

Claim 4 Under Assumptions 1, 2, 4 and 5, assume that $(x_K)_{K \in \mathbb{N}}$ produced by Algorithm 1 with prescribed step size is bounded. Then the interpolant \mathbf{w} given in Definition 1 is an asymptotic pseudo trajectory as described in Definition 3.

The proof follows by combining Lemma 1 and Theorem 1. In order to deduce convergence of Algorithm 1 from the Asymptotic pseudo trajectory property, we need the following Morse-Sard assumption. We stress that for deep network involving piecewise polynomials, logarithms and exponentials, this assumption is satisfied for both the Clarke subgradient and the backpropagation oracle [12, 20, 14].

Assumption 6 The function F and D are such that $F(\text{crit}_F)$, does not contain any open interval, where crit_F is given in Assumption 5 and contains all $x \in \mathbb{R}^p$, with $0 \in D(x)$.

Corollary 4 Under Assumptions 1, 2, 4 and 5, assume that $(x_K)_{K \in \mathbb{N}}$ produced by Algorithm 1 with prescribed step size is bounded and that Assumption 6 holds. Then $F(x_K)$ converges to a critical value of F as $K \rightarrow \infty$ and all accumulation points of the sequence are critical points for D .

Proof : Let $\mathbf{x}: \mathbb{R}^p \mapsto \mathbb{R}$ be a solution to the differential inclusion described in Definition 2. Then using conservativity in (10), for almost all $t \in \mathbb{R}_+$, we have

$$\frac{d}{dt} F(\mathbf{x}(t)) = - \min_{v \in D(\mathbf{x}(t))} \|v\|^2$$

Hence F is a Lyapunov function for the system: it decreases along trajectory, strictly outside crit_F . Using Claim 4, \mathbf{w} is an APT. Combining Assumption 6 with Proposition 3.27 and Theorem 4.3 in [7], all limit points of \mathbf{w} are contained in crit_F and F is constant on this set, that is $F(\mathbf{w}(t))$ converges as $t \rightarrow \infty$. \square

Corollary 5 Under Assumptions 1 and 5, assume that $(x_K)_{K \in \mathbb{N}}$ produced by Algorithm 1 with adaptive step size is bounded and that Assumption 6 holds. Then $F(x_K)$ converges to a critical value of F as $K \rightarrow \infty$ and all accumulation points of the sequence are critical points for D .

Proof : If v_K converges, this means that all d_i go to 0, and all partial increments also vanish asymptotically due to Claim 1. Hence accumulation points form a compact connected subset of crit_F , see [13, Lemma 3.5, (iii)] for details. By continuity of F , the $F(\text{crit}_F)$ is a connected subset of \mathbb{R} , that is an interval. By Morse-Sart assumption 6 it is a singleton which proves the claim. Assume otherwise that v_K diverges to $+\infty$ as $K \rightarrow \infty$, in this case, the step size goes to 0. We have

$$v_K \leq v_{K+1} \leq v_K + nM$$

which shows that $v_{K+1}/v_K \rightarrow 1$ as $K \rightarrow \infty$, and $\sum_{K \in \mathbb{N}} \alpha_K = +\infty$ so that Corollary 5 applies. \square

3.3 Proof of the main result

We extend and adapt the arguments of [7].

Definition 4 (Local extension) For any $\delta > 0$, and any $x \in \mathbb{R}^p$, we let D^δ be the following local extension of D

$$D^\delta(x) = \left\{ y \in \mathbb{R}^p, y \in \frac{1}{n} \sum_{i=1}^n \lambda_i D_i(x_i), \|x - x_i\| \leq \delta, |\lambda_i - 1| \leq \delta, i = 1, \dots, n \right\}.$$

Note that $\lim_{\delta \rightarrow 0} D^\delta(x) = \frac{1}{n} \sum_{i=1}^n D_i(x)$ by graph closedness of each D_i in Assumption 5.

Definition 5 (Perturbed differential inclusion) A locally Lipschitz path $\mathbf{x}: \mathbb{R}_+ \mapsto \mathbb{R}^p$ satisfies the perturbed differential inclusion if there exists a function $\delta: \mathbb{R}_+ \mapsto \mathbb{R}_+$ with $\lim_{t \rightarrow \infty} \delta(t) = 0$, such that for almost all $t \geq 0$

$$\dot{\mathbf{x}}(t) \in -D^{\delta(t)}(\mathbf{x}(t))$$

Lemma 1 The interpolated trajectory \mathbf{w} given in Definition 1 satisfies the perturbed differential inclusion in Definition 5.

Proof : The interpolated trajectory is piecewise affine so it is locally Lipschitz and differentiable almost everywhere. For each $K \in \mathbb{N}$ and $i = 1, \dots, n$, we have using Claim 1

$$\|x_K - \hat{z}_{K,i-1}\| \leq n\alpha_K M. \quad (11)$$

Furthermore, for all $t \in (\tau_K, \tau_{K+1})$,

$$\dot{\mathbf{w}}(t) = - \sum_{i=1}^n \alpha_{K,i} d_i(\hat{z}_{K,i-1}) / (\tau_{K+1} - \tau_K) = - \frac{1}{n} \sum_{i=1}^n \lambda_i d_i(\hat{z}_{K,i-1}), \quad (12)$$

where for all $i = 1, \dots, n$, using $\alpha_{K,i} \leq \alpha_K$ and $\tau_{K+1} - \tau_K = \sum_{i=1}^n \alpha_{K,i} \geq n\alpha_{K+1}$,

$$\lambda_i = \frac{n\alpha_{K,i}}{\tau_{K+1} - \tau_K} \leq n \frac{\alpha_K}{n\alpha_{K+1}} = \frac{\alpha_K}{\alpha_{K+1}}. \quad (13)$$

Hence combining (11) and (12), we may consider $\delta(t) = \max \left\{ n\alpha_K M, \left| 1 - \frac{\alpha_K}{\alpha_{K+1}} \right| \right\}$ for all $t \in (\tau_K, \tau_{K+1})$ which satisfies the desired hypothesis. \square

The following result is the main technical part of this section. The proof follows that of [7, Theorem 4.2] and is provided in Appendix B.

Theorem 1 Let \mathbf{z} be a perturbed differential inclusion trajectory as given in Definition 5. Then \mathbf{z} is an asymptotic pseudotrajectory as described in Definition 3.

Broader impact

This work is theoretical and the authors believe that this section does not apply to it.

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This is the appendix for “Incremental Without Replacement Sampling in Nonconvex Optimization”. We begin with the proof of the first claim of the paper.

Proof of Claim 1: We have for all $K \in \mathbb{N}$ and $i = 1 \dots n$, using the recursion in Algorithm 1,

$$z_{K,i} - x_K = \sum_{j=1}^i \alpha_{K,j} d(\hat{z}_{K,j-1}).$$

Using Lemma 2, we obtain

$$\|z_{K,i} - x_K\|^2 \leq i \sum_{j=1}^i \alpha_{K,i}^2 \|d(\hat{z}_{K,i-1})\|^2 \leq n \sum_{i=1}^n \alpha_{K,i}^2 \|d(\hat{z}_{K,i-1})\|^2.$$

Taking $i = n$, we obtain the second inequality. The result follows for $\hat{z}_{K,i-1}$ because it is in $\text{conv}(z_{K,j})_{j=0}^{i-1}$ and

$$\|\hat{z}_{K,i-1} - x_K\|^2 \leq \max_{z \in \text{conv}(z_{K,j})_{j=0}^{i-1}} \|z - x_K\|^2 = \max_{j=0, \dots, i} \|z_{K,j} - x_K\|^2 \leq n \sum_{i=1}^n \alpha_{K,i}^2 \|d(\hat{z}_{K,i-1})\|^2,$$

where the equality in the middle follows because maximum of convex function over polyhedra is achieved at vertices. \square

A Proofs for the smooth setting

For all $K \in \mathbb{N}$, we let $\alpha_K = \alpha_{K-1,n}$, with $\alpha_0 = 1/\delta$.

A.1 Analysis for both step size strategies.

Claim 5 We have for all $K \in \mathbb{N}$,

$$\begin{aligned} & \langle \nabla F(x_K), x_{K+1} - x_K \rangle \\ & \leq -n\alpha_K \|\nabla F(x_K)\|^2 + \frac{L^2 n^2}{\delta} \sum_{j=1}^n \alpha_{K,j}^2 \|d_j(\hat{z}_{K,j-1})\|^2 + \frac{M^2}{\delta} \sum_{i=1}^n \left(\frac{\alpha_{K,i}}{\alpha_K} - 1 \right)^2 \end{aligned} \quad (14)$$

Proof of Claim 5: Fix $K \in \mathbb{N}$, we have

$$x_{K+1} - x_K = - \sum_{i=1}^n \alpha_{K,i} d_i(\hat{z}_{K,i-1}) = -\alpha_K \sum_{i=1}^n \frac{\alpha_{K,i}}{\alpha_K} d_i(\hat{z}_{K,i-1}) \quad (15)$$

Recall that $\nabla F(x_K) = \frac{1}{n} \sum_{i=1}^n d_i(x_K)$, combining with (15), we deduce the following

$$\begin{aligned} & \langle \nabla F(x_K), x_{K+1} - x_K \rangle \\ & = \frac{-\alpha_K}{n} \left\langle \sum_{i=1}^n d_i(x_K), \sum_{i=1}^n \frac{\alpha_{K,i}}{\alpha_K} d_i(\hat{z}_{K,i-1}) \right\rangle \\ & = \frac{\alpha_K}{2n} \left(\left\| \sum_{i=1}^n d_i(x_K) - \sum_{i=1}^n \frac{\alpha_{K,i}}{\alpha_K} d_i(\hat{z}_{K,i-1}) \right\|^2 - \left\| \sum_{i=1}^n d_i(x_K) \right\|^2 - \left\| \sum_{i=1}^n \frac{\alpha_{K,i}}{\alpha_K} d_i(\hat{z}_{K,i-1}) \right\|^2 \right) \\ & \leq -\frac{n\alpha_K}{2} \|\nabla F(x_K)\|^2 + \frac{\alpha_K}{2n} \left\| \sum_{i=1}^n d_i(x_K) - \sum_{i=1}^n \frac{\alpha_{K,i}}{\alpha_K} d_i(\hat{z}_{K,i-1}) \right\|^2 \\ & \leq -\frac{n\alpha_K}{2} \|\nabla F(x_K)\|^2 + \frac{\alpha_K}{n} \left(\left\| \sum_{i=1}^n d_i(x_K) - \sum_{i=1}^n d_i(\hat{z}_{K,i-1}) \right\|^2 + \left\| \sum_{i=1}^n d_i(\hat{z}_{K,i-1}) - \sum_{i=1}^n \frac{\alpha_{K,i}}{\alpha_K} d_i(\hat{z}_{K,i-1}) \right\|^2 \right), \end{aligned} \quad (16)$$

where the first equalities are properties of the scalar product, the first inequality drops a negative term and the last one uses $\|a + b\|^2 \leq 2(\|a\|^2 + \|b\|^2)$. We bound each term separately, first,

$$\begin{aligned}
\left\| \sum_{i=1}^n d_i(x_K) - \sum_{i=1}^n d_i(\hat{z}_{K,i-1}) \right\|^2 &\leq \left(\sum_{i=1}^n \|d_i(x_K) - d_i(\hat{z}_{K,i-1})\| \right)^2 \\
&\leq \left(\sum_{i=1}^n L_i \|x_K - \hat{z}_{K,i-1}\| \right)^2 \\
&\leq \max_{i=1, \dots, n} \|x_K - \hat{z}_{K,i-1}\|^2 \left(\sum_{i=1}^n L_i \right)^2 \\
&\leq L^2 n^3 \sum_{j=1}^n \alpha_{K,j}^2 \|d_j(\hat{z}_{K,j-1})\|^2. \tag{17}
\end{aligned}$$

where the first step uses the triangle inequality, the second step uses L_i Lipschicity of d_i , the third step is Hölder inequality, and the fourth step uses Claim 1. Furthermore, we have using the triangle inequality and Cauchy-Schwartz inequality,

$$\begin{aligned}
\left\| \sum_{i=1}^n d_i(\hat{z}_{K,i-1}) - \sum_{i=1}^n \frac{\alpha_{K,i}}{\alpha_K} d_i(\hat{z}_{K,i-1}) \right\|^2 &\leq \left(\sum_{i=1}^n \left(\frac{\alpha_{K,i}}{\alpha_K} - 1 \right) \|d_i(\hat{z}_{K,i-1})\| \right)^2 \\
&\leq \sum_{i=1}^n \left(\frac{\alpha_{K,i}}{\alpha_K} - 1 \right)^2 \sum_{i=1}^n \|d_i(\hat{z}_{K,i-1})\|^2 \\
&\leq \sum_{i=1}^n \left(\frac{\alpha_{K,i}}{\alpha_K} - 1 \right)^2 \sum_{i=1}^n M_i^2 = nM^2 \sum_{i=1}^n \left(\frac{\alpha_{K,i}}{\alpha_K} - 1 \right)^2 \tag{18} \\
&\tag{19}
\end{aligned}$$

Combining (16), (17) and (19), we obtain using the fact that $\alpha_K \leq \alpha_0 = 1/\delta$,

$$\langle \nabla F(x_K), x_{K+1} - x_K \rangle \leq -\frac{n\alpha_K}{2} \|\nabla F(x_K)\|^2 + \frac{L^2 n^2}{\delta} \sum_{j=1}^n \alpha_{K,j}^2 \|d_j(\hat{z}_{K,j-1})\|^2 + \frac{M^2}{\delta} \sum_{i=1}^n \left(\frac{\alpha_{K,i}}{\alpha_K} - 1 \right)^2$$

□

Claim 6 F has L Lipschitz gradient.

Proof : For any x, y , we have

$$\begin{aligned}
\|\nabla F(x) - \nabla F(y)\| &= \frac{1}{n} \left\| \sum_{i=1}^n d_i(x) - d_i(y) \right\| \leq \frac{1}{n} \sum_{i=1}^n \|d_i(x) - d_i(y)\| \leq \frac{1}{n} \sum_{i=1}^n L_i \|x - y\| \\
&= L \|x - y\|
\end{aligned}$$

where we used triangle inequality and L_i Lipschicity of d_i . □

Proof of Claim 2:

Using smoothness of F in Claim 6, we have from the descent Lemma [36, Lemma 1.2.3], for all $x, y \in \mathbb{R}^p$

$$F(y) \leq F(x) + \langle \nabla F(x), y - x \rangle + \frac{L}{2} \|y - x\|^2. \tag{20}$$

Choosing $y = x_{K+1}$ and $x = x_K$ in (20), using Claim 5 and Claim 1, we obtain

$$\begin{aligned}
F(x_{K+1}) &\leq F(x_K) + \langle \nabla F(x_K), x_{K+1} - x_K \rangle + \frac{L}{2} \|x_{K+1} - x_K\|^2 \\
&\leq F(x_K) - \frac{n\alpha_K}{2} \|\nabla F(x_K)\|^2 + \left(\frac{L^2 n^2}{\delta} + \frac{Ln}{2} \right) \sum_{j=1}^n \alpha_{K,j}^2 \|d_j(\hat{z}_{K,j-1})\|^2 + \frac{M^2}{\delta} \sum_{i=1}^n \left(\frac{\alpha_{K,i}}{\alpha_K} - 1 \right)^2
\end{aligned}$$

Since $\alpha_{K,i} \leq \alpha_K$ for all $K \in \mathbb{N}$ and $i = 1 \dots, n$, we have $0 \leq \alpha_{K,i}/\alpha_K \leq 1$, and using $(t-1)^2 \leq 1-t^2$ for all $t \in [0, 1]$

$$\left(\frac{\alpha_{K,i}}{\alpha_K} - 1\right)^2 \leq 1 - \frac{\alpha_{K,i}^2}{\alpha_K^2},$$

and the result follows. \square

B Proofs for the nonsmooth setting

Proof of Theorem 1: Fix $T > 0$, we consider the sequence of functions, for each $k \in \mathbb{N}$

$$\begin{aligned} \mathbf{w}_k &: [0, T] \mapsto \mathbb{R}^p \\ t &\mapsto \mathbf{w}(\tau_k + t) \end{aligned}$$

From Assumption 5 and Definition 5, it is clear that all functions in the sequence are M Lipschitz. Since the sequence $(x_k)_{k \in \mathbb{N}}$ is bounded, $(\mathbf{w}_k)_{k \in \mathbb{N}}$ is also uniformly bounded, hence by Arzelà-Ascoli theorem [40, Chapter 10, Lemma 2], there is a subsequence converging uniformly, let $\mathbf{z}: [0, T] \mapsto \mathbb{R}^p$ be any such uniform limit. By discarding terms, we actually have $\mathbf{w}_k \rightarrow \mathbf{z}$ as $k \rightarrow \infty$, uniformly on $[0, T]$. Note that we have for all $t \in [0, 1]$, and all $\delta > 0$

$$D^\delta(\mathbf{w}_k(t)) \subset D^{\delta + \|\mathbf{w}_k - \mathbf{z}\|_\infty}(\mathbf{z}(t)). \quad (21)$$

For all $k \in \mathbb{N}$, we set $\mathbf{v}_k \in L^2([0, T], \mathbb{R}^p)$ such that $\mathbf{v}_k = \mathbf{w}'_k$ at points where \mathbf{w}_k is differentiable (almost everywhere since it is piecewise affine). We have for all $k \in \mathbb{N}$ and all $s \in [0, T]$

$$\mathbf{w}_k(s) - \mathbf{w}_k(0) = \int_{t=0}^{t=s} \mathbf{v}_k(t) dt, \quad (22)$$

and from Definition 5, we have for almost all $t \in [0, T]$,

$$\mathbf{v}_k(t) \in -D^{\delta(\tau_k+t)}(\mathbf{w}_k(t)). \quad (23)$$

Hence, the functions \mathbf{v}_k are uniformly bounded thanks to Assumption 5 and hence the sequence $(\mathbf{v}_k)_{k \in \mathbb{N}}$ is bounded in $L^2([0, T], \mathbb{R}^p)$ and by Banach-Alaoglu theorem [40, Section 15.1], it has a weak cluster point. Denote by \mathbf{v} a weak limit of $(\mathbf{v}_k)_{k \in \mathbb{N}}$ in $L^2([0, T], \mathbb{R}^p)$. Discarding terms, we may assume that $\mathbf{v}_k \rightarrow \mathbf{v}$ weakly in $L^2([0, T], \mathbb{R}^p)$ as $k \rightarrow \infty$ and hence, passing to the limit in (22), for all $s \in [0, T]$,

$$\mathbf{z}(s) - \mathbf{z}(0) = \int_{t=0}^{t=s} \mathbf{v}(t) dt. \quad (24)$$

By Mazur's Lemma (see for example [23]), there exists a sequence $(N_k)_{k \in \mathbb{N}}$, with $N_k \geq k$ and a sequence $\tilde{\mathbf{v}}_k \in \mathbb{R}^p$ such that for each $k \in \mathbb{N}$, $\tilde{\mathbf{v}}_k \in \text{conv}(\mathbf{v}_k, \dots, \mathbf{v}_{N_k})$ such that $\tilde{\mathbf{v}}_k$ converges strongly in $L^2([0, T], \mathbb{R}^p)$ hence pointwise almost everywhere in $[0, T]$. Using (23) and the fact that countable intersection of full measure sets has full measure, we have for almost all $t \in [0, T]$

$$\begin{aligned} \mathbf{v}(t) &= \lim_{k \rightarrow \infty} \tilde{\mathbf{v}}_k(t) \in \lim_{k \rightarrow \infty} -\text{conv}\left(\bigcup_{j=k}^{N_k} D^{\delta(\tau_j+t)}(\mathbf{w}_j(t))\right) \\ &\subset \lim_{k \rightarrow \infty} -\text{conv}\left(\bigcup_{j=k}^{N_k} D^{\delta(\tau_j+t) + \|\mathbf{w}_j - \mathbf{z}\|_\infty}(\mathbf{z}(t))\right) \\ &= -\text{conv}\left(\frac{1}{n} \sum_{i=1}^n D_i(\mathbf{z}(t))\right) = -D(\mathbf{z}(t)). \end{aligned}$$

where we have used (21), the fact that $\lim_{\delta \rightarrow 0} D^\delta = \frac{1}{n} \sum_{i=1}^n D_i$ pointwise since each D_i has closed graph and the definition of D . Using (24), this shows that for almost all $t \in [0, T]$,

$$\dot{\mathbf{z}}(t) = \mathbf{v}(t) \in -D(\mathbf{z}(t)).$$

Using [7, Theorem 4.1], this shows that \mathbf{w} is an asymptotic pseudo trajectory. \square

C Lemmas and additional proofs

Lemma 2 *Let a_1, \dots, a_m be vectors in \mathbb{R}^p , then*

$$\left\| \sum_{i=1}^m a_i \right\|^2 \leq m \sum_{i=1}^m \|a_i\|^2$$

Proof : From the triangle inequality, we have

$$\left\| \sum_{i=1}^m a_i \right\|^2 \leq \left(\sum_{i=1}^m \|a_i\| \right)^2$$

Hence it suffices to prove the claim for $p = 1$. Consider the quadratic form on \mathbb{R}^m

$$Q: x \mapsto m \sum_{i=1}^m x_i^2 - \left\| \sum_{i=1}^m x_i \right\|^2.$$

We have

$$Q(x) = m(\|x\|^2 - (x^T e)^2),$$

where $e \in \mathbb{R}^m$ has unit norm and with all entries equal to $1/\sqrt{m}$. The corresponding matrix is $m(I - ee^T)$ which is positive semidefinite. This proves the result. \square

Lemma 3 *Let $(\delta_k)_{k \in \mathbb{N}}$ be a sequence of positive numbers, and $\delta, \beta > 0$. Then for all $m \in \mathbb{N}$*

$$\sum_{i=0}^m \frac{\delta_i}{\delta^2 + \beta \sum_{i=0}^k \delta_i} \leq \frac{1}{\beta} \log \left(1 + \beta \frac{\sum_{i=0}^m \delta_k}{\delta^2} \right)$$

Proof : We have

$$\begin{aligned} \sum_{i=0}^m \frac{\delta_i}{\delta^2 + \beta \sum_{i=0}^k \delta_i} &= \frac{1}{\beta} \sum_{i=0}^m \frac{\delta_i}{\frac{\delta^2}{\beta} + \sum_{i=0}^k \delta_i} \\ &\leq \frac{1}{\beta} \log \left(1 + \beta \frac{\sum_{i=0}^m \delta_i}{\delta^2} \right) \end{aligned}$$

where the last inequality follows from Lemma 6.2 in [21]. \square