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# MISSO: Minimization by Incremental Stochastic Surrogate Optimization for Large Scale Nonconvex and Nonsmooth Problems

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## Abstract

Many constrained, nonconvex and nonsmooth optimization problems can be tackled using the Majorization-Minimization (MM) method which alternates between constructing a surrogate function which upper bounds the objective function, and then minimizing this surrogate. For problems which minimize a finite sum of functions, a stochastic version of the MM method selects a batch of functions at random at each iteration and optimizes the accumulated surrogate. However, in many cases of interest such as variational inference for latent variable models, the surrogate functions are expressed as an expectation. In this contribution, we propose a doubly stochastic MM method based on Monte Carlo approximation of these stochastic surrogates. We establish asymptotic and non-asymptotic convergence of our scheme in a constrained, nonconvex, nonsmooth optimization setting. We apply our new framework for inference of logistic regression model with missing data and for variational inference of Bayesian variants of LeNet-5 and Resnet-18 on respectively the MNIST and CIFAR-10 datasets.

## 1 Introduction

We consider the *constrained* minimization problem of a finite sum of functions:

$$\min_{\theta \in \Theta} \mathcal{L}(\theta) := \frac{1}{n} \sum_{i=1}^n \mathcal{L}_i(\theta), \quad (1)$$

where  $\Theta$  is a convex, compact, and closed subset of  $\mathbb{R}^p$ , and for any  $i \in \llbracket 1, n \rrbracket$ , the function  $\mathcal{L}_i : \mathbb{R}^p \rightarrow \mathbb{R}$  is bounded from below and is (possibly) nonconvex and nonsmooth.

To tackle the optimization problem (1), a popular approach is to apply the majorization-minimization (MM) method which iteratively minimizes a majorizing surrogate function. A large number of existing procedures fall into this general framework, for instance gradient-based or proximal methods or the Expectation-Maximization (EM) algorithm [McLachlan and Krishnan, 2008] and some variational Bayes inference techniques [Jordan et al., 1999]; see for example [Razaviyayn et al., 2013] and [Lange, 2016] and the references therein. When the number of terms  $n$  in (1) is large, the vanilla MM method may be intractable because it requires to construct a surrogate function for all the  $n$  terms  $\mathcal{L}_i$  at each iteration. Here, a remedy is to apply the Minimization by Incremental Surrogate Optimization (MISO) method proposed by Mairal [2015], where the surrogate functions are updated incrementally. The MISO method can be interpreted as a combination of MM and ideas which have emerged for variance reduction in stochastic gradient methods [Schmidt et al., 2017]. An extended analysis of MISO has been proposed in [Qian et al., 2019].

The success of the MISO method rests upon the efficient minimization of surrogates such as convex functions, see [Mairal, 2015, Section 2.3]. In many applications of interest, the natural surrogate

functions are intractable, yet they are defined as expectation of tractable functions. For instance, this is the case for inference in latent variable models via maximum likelihood [McLachlan and Krishnan, 2008]. Another application is variational inference, [Ghahramani, 2015], in which the goal is to approximate the posterior distribution of parameters given the observations; see for example [Neal, 2012, Blundell et al., 2015, Polson et al., 2017, Rezende et al., 2014, Li and Gal, 2017].

This paper fills the gap in the literature by proposing a new method called *Minimization by Incremental Stochastic Surrogate Optimization (MISSO)*, designed for the nonconvex and nonsmooth finite sum optimization, with a finite-time convergence guarantee. Our work aims at formulating a *generic class* of incremental stochastic surrogate methods for nonconvex optimization and building the theory to understand its behavior. In particular, we provide convergence guarantees for stochastic EM and Variational Inference-type methods, under mild conditions. Our contributions can be summarized as follows.

- We propose a unifying framework of analysis for incremental stochastic surrogate optimization when the surrogates are defined as expectations of tractable functions. The proposed MISSO method is built on the Monte Carlo integration of the intractable surrogate function, *i.e.*, a doubly stochastic surrogate optimization scheme.
- We present an incremental update of the commonly used variational inference and Monte-Carlo EM methods as special cases of our newly introduced framework. The analysis of those two algorithms is thus done under this unifying framework of analysis.
- We establish both asymptotic and non-asymptotic convergence for the MISSO method. In particular, the MISSO method converges almost surely to a stationary point and in  $\mathcal{O}(n/\epsilon)$  iterations to an  $\epsilon$ -stationary point.

In Section 2, we review the techniques for incremental minimization of finite sum functions based on the MM principle; specifically, we review the MISO method as introduced in [Mairal, 2015], and present a class of surrogate functions expressed as an expectation over a latent space. The MISSO method is then introduced for the latter class of intractable surrogate functions requiring approximation. In Section 3, we provide the asymptotic and non-asymptotic convergence analysis for the MISSO method (and of the MISO [Mairal, 2015] one as a special case). Finally, Section 4 presents numerical applications to illustrate our findings including parameter inference for logistic regression with missing data and variational inference for two types of Bayesian neural networks.

**Notations.** We denote  $\llbracket 1, n \rrbracket = \{1, \dots, n\}$ . Unless otherwise specified,  $\|\cdot\|$  denotes the standard Euclidean norm and  $\langle \cdot | \cdot \rangle$  is the inner product in the Euclidean space. For any function  $f : \Theta \rightarrow \mathbb{R}$ ,  $f'(\theta, d)$  is the directional derivative of  $f$  at  $\theta$  along the direction  $d$ , *i.e.*,

$$f'(\theta, d) := \lim_{t \rightarrow 0^+} \frac{f(\theta + td) - f(\theta)}{t}. \quad (2)$$

The directional derivative is assumed to exist for the functions introduced throughout this paper.

## 2 Incremental Minimization of Finite Sum Nonconvex Functions

The objective function in (1) is composed of a finite sum of possibly nonsmooth and nonconvex functions. A popular approach here is to apply the MM method. The MM method tackles (1) through alternating between two steps — (i) minimizing a *surrogate* function which upper bounds the original objective function; and (ii) updating the surrogate function to tighten the upper bound.

As mentioned in the Introduction, the MISO method proposed by Mairal [2015] is developed as an iterative scheme that only updates the surrogate functions *partially* at each iteration. Formally, for any  $i \in \llbracket 1, n \rrbracket$ , we consider a surrogate function  $\hat{\mathcal{L}}_i(\theta; \bar{\theta})$  which satisfies

**S1.** For all  $i \in \llbracket 1, n \rrbracket$  and  $\bar{\theta} \in \Theta$ , the function  $\hat{\mathcal{L}}_i(\theta; \bar{\theta})$  is convex w.r.t.  $\theta$ , and it holds

$$\hat{\mathcal{L}}_i(\theta; \bar{\theta}) \geq \mathcal{L}_i(\theta), \quad \forall \theta \in \Theta, \quad (3)$$

where the equality holds when  $\theta = \bar{\theta}$ .

**S2.** For any  $\bar{\theta}_i \in \Theta$ ,  $i \in \llbracket 1, n \rrbracket$  and some  $\epsilon > 0$ , the difference function  $\hat{e}(\theta; \{\bar{\theta}_i\}_{i=1}^n) := \frac{1}{n} \sum_{i=1}^n \hat{\mathcal{L}}_i(\theta; \bar{\theta}_i) - \mathcal{L}(\theta)$  is defined for all  $\theta \in \Theta_\epsilon$  and differentiable for all  $\theta \in \Theta$ , where

79  $\Theta_\epsilon = \{\theta \in \mathbb{R}^d, \inf_{\theta' \in \Theta} \|\theta - \theta'\| < \epsilon\}$  is an  $\epsilon$ -neighborhood set of  $\Theta$ . Moreover, for some constant  
80  $L$ , the gradient satisfies

$$\|\nabla \hat{e}(\theta; \{\bar{\theta}_i\}_{i=1}^n)\|^2 \leq 2L \hat{e}(\theta; \{\bar{\theta}_i\}_{i=1}^n), \forall \theta \in \Theta. \quad (4)$$

81 **S1** is a common condition used for surrogate optimization, see [Mairal, 2015, Section 2.3]. Mean-  
82 while, **S2** can be satisfied when the difference function  $\hat{e}(\theta; \{\bar{\theta}_i\}_{i=1}^n)$  is  $L$ -smooth for all  $\theta \in \mathbb{R}^d$ ,  
83 where the condition can be implied through applying [Razaviyayn et al., 2013, Proposition 1].

84 The inequality (3) implies  $\hat{\mathcal{L}}_i(\theta; \bar{\theta}) \geq \mathcal{L}_i(\theta) >$   
85  $-\infty$  for any  $\theta \in \Theta$ . The MISO method is  
86 an incremental version of the MM method, as  
87 summarized by Algorithm 1. As seen in the  
88 pseudo code, the MISO method maintains an iter-  
89 atively updated set of surrogate upper-bound  
90 functions  $\{\mathcal{A}_i^k(\theta)\}_{i=1}^n$  and updates the iterate  
91 through minimizing the average of the surro-  
92 gate functions.

93 Particularly, only one out of the  $n$  sur-  
94rogate functions is updated at each iter-  
95ation [cf. Line 5] and the sum function  
96  $\frac{1}{n} \sum_{i=1}^n \mathcal{A}_i^{k+1}(\theta)$  is designed to be ‘easy to  
97 optimize’, for example, it can be a sum of  
98 quadratic functions. As such, the MISO method  
99 is suitable for large-scale optimization as the computation cost per iteration is independent of  $n$ .  
100 Moreover, under **S1**, **S2**, it was shown that the MISO method converges almost surely to a stationary  
101 point of (1) [Mairal, 2015, Prop. 3.1].

102 We now consider the case when the surrogate functions  $\hat{\mathcal{L}}_i(\theta; \bar{\theta})$  are intractable. Let  $Z$  be a mea-  
103 surable set,  $p_i : Z \times \Theta \rightarrow \mathbb{R}_+$  a probability density function,  $r_i : \Theta \times \Theta \times Z \rightarrow \mathbb{R}$  a measurable  
104 function and  $\mu_i$  a  $\sigma$ -finite measure. We consider surrogate functions which satisfy **S1**, **S2** and that  
105 can be expressed as an expectation, i.e.:

$$\hat{\mathcal{L}}_i(\theta; \bar{\theta}) := \int_Z r_i(\theta; \bar{\theta}, z_i) p_i(z_i; \bar{\theta}) \mu_i(dz_i) \quad \forall (\theta, \bar{\theta}) \in \Theta \times \Theta. \quad (5)$$

106 Plugging (5) into the MISO method is not feasible since the update step in Step 6 involves a mini-  
107 mization of an expectation. Several motivating examples of (1) are given in Section 2.

108 We propose the *Minimization by Incremental Stochastic Surrogate Optimization* (MISSO) method  
109 which replaces the expectation in (5) by *Monte Carlo* integration and then optimizes the objective  
110 function (1) in an incremental manner. Denote by  $M \in \mathbb{N}$  the Monte Carlo batch size and let  
111  $\{z_m \in Z\}_{m=1}^M$  be a set of samples. These samples can be drawn (**Case 1**) i.i.d. from the distribution  
112  $p_i(\cdot; \bar{\theta})$  or (**Case 2**) from a Markov chain with stationary distribution  $p_i(\cdot; \bar{\theta})$ ; see Section 3 for  
113 illustrations. To this end, we define the stochastic surrogate as follows:

$$\tilde{\mathcal{L}}_i(\theta; \bar{\theta}, \{z_m\}_{m=1}^M) := \frac{1}{M} \sum_{m=1}^M r_i(\theta; \bar{\theta}, z_m), \quad (6)$$

114 and we summarize the proposed MISSO method in Algorithm 2. As seen, the procedure is similar  
115 to the MISO method but it involves two types of randomness. The first level of randomness comes  
116 from the selection of  $i_k$  in Line 5. The second level of randomness stems from the set of Monte-  
117 Carlo approximated functions  $\tilde{\mathcal{A}}_i^k(\theta)$  used in lieu of  $\mathcal{A}_i^k(\theta)$  in Line 6 when optimizing for the next  
118 iterate  $\theta^{(k)}$ . We now discuss two applications of the MISSO method.

119 **Example 1: Maximum Likelihood Estimation for Latent Variable Model.** Latent variable mod-  
120 els [Bishop, 2006] are constructed by introducing unobserved (latent) variables which help explain  
121 the observed data. We consider  $n$  independent observations  $((y_i, z_i), i \in \llbracket n \rrbracket)$  where  $y_i$  is observed  
122 and  $z_i$  is latent. In this incomplete data framework, define  $\{f_i(z_i, \theta), \theta \in \Theta\}$  to be the complete  
123 data likelihood models, i.e., the joint likelihood of the observations and latent variables. Let

$$g_i(\theta) := \int_Z f_i(z_i, \theta) \mu_i(dz_i), \quad i \in \llbracket 1, n \rrbracket, \quad \theta \in \Theta$$

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**Algorithm 2** MISSO method
 

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- 1: **Input:** initialization  $\theta^{(0)}$ ; a sequence of non-negative numbers  $\{M_{(k)}\}_{k=0}^{\infty}$ .
- 2: For all  $i \in \llbracket 1, n \rrbracket$ , draw  $M_{(0)}$  Monte-Carlo samples with the stationary distribution  $p_i(\cdot; \theta^{(0)})$ .
- 3: Initialize the surrogate function as

$$\tilde{\mathcal{A}}_i^0(\theta) := \tilde{\mathcal{L}}_i(\theta; \theta^{(0)}, \{z_{i,m}^{(0)}\}_{m=1}^{M_{(0)}}), \quad i \in \llbracket 1, n \rrbracket.$$

- 4: **for**  $k = 0, 1, \dots$  **do**
- 5:   Pick a function index  $i_k$  uniformly on  $\llbracket 1, n \rrbracket$ .
- 6:   Draw  $M_{(k)}$  Monte-Carlo samples with the stationary distribution  $p_i(\cdot; \theta^{(k)})$ .
- 7:   Update the individual surrogate functions recursively as:

$$\tilde{\mathcal{A}}_i^{k+1}(\theta) = \begin{cases} \tilde{\mathcal{L}}_i(\theta; \theta^{(k)}, \{z_{i,m}^{(k)}\}_{m=1}^{M_{(k)}}), & \text{if } i = i_k \\ \tilde{\mathcal{A}}_i^k(\theta), & \text{otherwise.} \end{cases}$$

- 8:   Set  $\theta^{(k+1)} \in \arg \min_{\theta \in \Theta} \tilde{\mathcal{L}}^{(k+1)}(\theta) := \frac{1}{n} \sum_{i=1}^n \tilde{\mathcal{A}}_i^{k+1}(\theta)$ .
  - 9: **end for**
- 

denote the incomplete data likelihood, *i.e.*, the marginal likelihood of the observations  $y_i$ . For ease of notations, the dependence on the observations is made implicit. The maximum likelihood (ML) estimation problem sets the individual objective function  $\mathcal{L}_i(\theta)$  to be the  $i$ -th negated incomplete data log-likelihood  $\mathcal{L}_i(\theta) := -\log g_i(\theta)$ .

Assume, without loss of generality, that  $g_i(\theta) \neq 0$  for all  $\theta \in \Theta$ . We define by  $p_i(z_i, \theta) := f_i(z_i, \theta)/g_i(\theta)$  the conditional distribution of the latent variable  $z_i$  given the observations  $y_i$ . A surrogate function  $\hat{\mathcal{L}}_i(\theta; \bar{\theta})$  satisfying S1 can be obtained through writing  $f_i(z_i, \theta) = \frac{f_i(z_i, \theta)}{p_i(z_i, \bar{\theta})} p_i(z_i, \bar{\theta})$  and applying the Jensen inequality:

$$\hat{\mathcal{L}}_i(\theta; \bar{\theta}) = \int_{\mathcal{Z}} \underbrace{\log(p_i(z_i, \bar{\theta})/f_i(z_i, \theta))}_{=r_i(\theta; \bar{\theta}, z_i)} p_i(z_i, \bar{\theta}) \mu_i(dz_i). \quad (7)$$

We note that S2 can also be verified for common distribution models. We can apply the MISSO method following the above specification of  $r_i(\theta; \bar{\theta}, z_i)$  and  $p_i(z_i, \bar{\theta})$ .

**Example 2: Variational Inference.** Let  $((x_i, y_i), i \in \llbracket 1, n \rrbracket)$  be i.i.d. input-output pairs and  $w \in \mathcal{W} \subseteq \mathbb{R}^d$  be a latent variable. When conditioned on the input data  $x = (x_i, i \in \llbracket 1, n \rrbracket)$ , the joint distribution of  $y = (y_i, i \in \llbracket 1, n \rrbracket)$  and  $w$  is given by:

$$p(y, w|x) = \pi(w) \prod_{i=1}^n p(y_i|x_i, w). \quad (8)$$

Our goal is to compute the posterior distribution  $p(w|y, x)$ . In most cases, the posterior distribution  $p(w|y, x)$  is intractable and is approximated using a family of parametric distributions,  $\{q(w, \theta), \theta \in \Theta\}$ . The variational inference (VI) problem [Blei et al., 2017] boils down to minimizing the Kullback-Leibler (KL) divergence between  $q(w, \theta)$  and the posterior distribution  $p(w|y, x)$ , as follows:

$$\min_{\theta \in \Theta} \mathcal{L}(\theta) := \text{KL}(q(w; \theta) || p(w|y, x)) := \mathbb{E}_{q(w; \theta)} [\log(q(w; \theta)/p(w|y, x))] . \quad (9)$$

Using (8), we decompose  $\mathcal{L}(\theta) = n^{-1} \sum_{i=1}^n \mathcal{L}_i(\theta) + \text{const.}$  where:

$$\mathcal{L}_i(\theta) := -\mathbb{E}_{q(w; \theta)} [\log p(y_i|x_i, w)] + \frac{1}{n} \mathbb{E}_{q(w; \theta)} [\log q(w; \theta)/\pi(w)] := r_i(\theta) + d(\theta). \quad (10)$$

Directly optimizing the finite sum objective function in (9) can be difficult. First, with  $n \gg 1$ , evaluating the objective function  $\mathcal{L}(\theta)$  requires a full pass over the entire dataset. Second, for some complex models, the expectations in (10) can be intractable even if we assume a simple parametric model for  $q(w; \theta)$ . Assume that  $\mathcal{L}_i$  is L-smooth, *i.e.*,  $\mathcal{L}_i$  is differentiable on  $\Theta$  and its gradient  $\nabla \mathcal{L}_i$  is L-Lipschitz. We apply the MISSO method with a quadratic surrogate function defined as:

$$\hat{\mathcal{L}}_i(\theta; \bar{\theta}) := \mathcal{L}_i(\bar{\theta}) + \langle \nabla_{\theta} \mathcal{L}_i(\bar{\theta}) | \theta - \bar{\theta} \rangle + \frac{L}{2} \|\bar{\theta} - \theta\|^2, \quad (\theta, \bar{\theta}) \in \Theta^2. \quad (11)$$

It is easily checked that the quadratic function  $\widehat{\mathcal{L}}_i(\theta; \bar{\theta})$  satisfies S1, S2. To compute the gradient  $\nabla \mathcal{L}_i(\bar{\theta})$ , we apply the re-parametrization technique suggested in [Paisley et al., 2012, Kingma and Welling, 2014, Blundell et al., 2015]. Let  $t : \mathbb{R}^d \times \Theta \mapsto \mathbb{R}^d$  be a differentiable function w.r.t.  $\theta \in \Theta$  which is designed such that the law of  $w = t(z, \bar{\theta})$  is  $q(\cdot, \bar{\theta})$ , where  $z \sim \mathcal{N}_d(0, \mathbf{I})$ . By [Blundell et al., 2015, Proposition 1], the gradient of  $-r_i(\cdot)$  in (10) is:

$$\nabla_{\theta} \mathbb{E}_{q(w; \bar{\theta})} [\log p(y_i | x_i, w)] = \mathbb{E}_{z \sim \mathcal{N}_d(0, \mathbf{I})} [\mathbf{J}_{\theta}^t(z, \bar{\theta}) \nabla_w \log p(y_i | x_i, w) \big|_{w=t(z, \bar{\theta})}] , \quad (12)$$

where for each  $z \in \mathbb{R}^d$ ,  $\mathbf{J}_{\theta}^t(z, \bar{\theta})$  is the Jacobian of the function  $t(z, \cdot)$  with respect to  $\theta$  evaluated at  $\bar{\theta}$ . In addition, for most cases, the term  $\nabla d(\bar{\theta})$  can be evaluated in closed form as the gradient of the KL between the prior distribution  $\pi(\cdot)$  and the variational candidate  $q(\cdot, \bar{\theta})$ .

$$r_i(\theta; \bar{\theta}, z) := \left\langle \nabla_{\theta} d(\bar{\theta}) - \mathbf{J}_{\theta}^t(z, \bar{\theta}) \nabla_w \log p(y_i | x_i, w) \big|_{w=t(z, \bar{\theta})} \mid \theta - \bar{\theta} \right\rangle + \frac{L}{2} \|\theta - \bar{\theta}\|^2 . \quad (13)$$

Finally, using (11) and (13), the surrogate function (6) is given by  $\tilde{\mathcal{L}}_i(\theta; \bar{\theta}, \{z_m\}_{m=1}^M) := M^{-1} \sum_{m=1}^M r_i(\theta; \bar{\theta}, z_m)$  where  $\{z_m\}_{m=1}^M$  are i.i.d samples drawn from  $\mathcal{N}(0, \mathbf{I})$ .

### 3 Convergence Analysis

We now provide asymptotic and non-asymptotic convergence results for the MISSO method

**H1.** For all  $i \in \llbracket 1, n \rrbracket$ ,  $\bar{\theta} \in \Theta$ ,  $z_i \in \mathbf{Z}$ , the measurable function  $r_i(\theta; \bar{\theta}, z_i)$  is convex in  $\theta$  and is lower bounded.

We are particularly interested in the *constrained optimization* setting where  $\Theta$  is a bounded set. To this end, we control the supremum norm of the MC approximation, introduced in (6), as:

**H2.** For the samples  $\{z_{i,m}\}_{m=1}^M$ , there exists finite constants  $C_r$  and  $C_{gr}$  such that

$$C_r := \sup_{\bar{\theta} \in \Theta} \sup_{M > 0} \frac{1}{\sqrt{M}} \mathbb{E}_{\bar{\theta}} \left[ \sup_{\theta \in \Theta} \left| \sum_{m=1}^M \left\{ r_i(\theta; \bar{\theta}, z_{i,m}) - \widehat{\mathcal{L}}_i(\theta; \bar{\theta}) \right\} \right| \right]$$

$$C_{gr} := \sup_{\bar{\theta} \in \Theta} \sup_{M > 0} \sqrt{M} \mathbb{E}_{\bar{\theta}} \left[ \sup_{\theta \in \Theta} \left| \frac{1}{M} \sum_{m=1}^M \frac{\widehat{\mathcal{L}}'_i(\theta, \theta - \bar{\theta}; \bar{\theta}) - r'_i(\theta, \theta - \bar{\theta}; \bar{\theta}, z_{i,m})}{\|\bar{\theta} - \theta\|} \right|^2 \right]$$

for all  $i \in \llbracket 1, n \rrbracket$ , and we denoted by  $\mathbb{E}_{\bar{\theta}}[\cdot]$  the expectation w.r.t. a Markov chain  $\{z_{i,m}\}_{m=1}^M$  with initial distribution  $\xi_i(\cdot; \bar{\theta})$ , transition kernel  $P_{i, \bar{\theta}}$ , and stationary distribution  $p_i(\cdot; \bar{\theta})$ .

**Some intuitions behind the controlling terms:** It is actually common in statistical and optimization problems, to deal with the manipulation and the control of random variables indexed by sets with an infinite number of elements. Here, the controlled random variable is an image of a continuous function defined as  $r_i(\theta; \bar{\theta}, z_{i,m}) - \widehat{\mathcal{L}}_i(\theta; \bar{\theta})$  for all  $z \in \mathbf{Z}$  and for fixed  $(\theta, \bar{\theta}) \in \Theta^2$ . To characterize such control, we will have recourse to the notion of metric entropy (or bracketing number) as developed in [Van der Vaart, 2000, Vershynin, 2018, Wainwright, 2019]. A collection of results from those references gives intuition behind our assumption H2, which is classical in empirical processes. In [Vershynin, 2018, Theorem 8.2.3], the authors recall the uniform law of large numbers for a class of  $L$ -Lipschitz functions:

$$\mathbb{E} \left[ \sup_{f \in \mathcal{F}} \left| \frac{1}{M} \sum_{i=1}^M f(z_{i,m}) - \mathbb{E}[f(z_i)] \right| \right] \leq \frac{CL}{\sqrt{M}} \quad \text{for all } z_{i,m}, i \in \llbracket 1, M \rrbracket .$$

Moreover, in [Vershynin, 2018, Theorem 8.1.3] and [Wainwright, 2019, Theorem 5.22], the application of the Dudley's inequality yields:

$$\mathbb{E} \left[ \sup_{f \in \mathcal{F}} |X_f - X_0| \right] \leq \frac{1}{\sqrt{M}} \int_0^1 \sqrt{\log \mathcal{N}(\mathcal{F}, \|\cdot\|_{\infty}, \varepsilon)} d\varepsilon ,$$

where  $\mathcal{N}(\mathcal{F}, \|\cdot\|_{\infty}, \varepsilon)$  is the bracketing number and  $\varepsilon$  denotes the level of approximation (the bracketing number goes to infinity when  $\varepsilon \rightarrow 0$ ). Finally, in [Van der Vaart, 2000, p.271, Example],

181  $\mathcal{N}(\mathcal{F}, \|\cdot\|_\infty, \varepsilon)$  is bounded from above for a class of parametric functions  $\mathcal{F} = f_\theta : \theta \in \Theta$  on a  
 182 bounded set  $\Theta \subset \mathbb{R}$  :

$$\mathcal{N}(\mathcal{F}, \|\cdot\|_\infty, \varepsilon) \leq K \left( \frac{\text{diam } \Theta}{\varepsilon} \right)^d, \quad \text{every } 0 < \varepsilon < \text{diam } \Theta.$$

183 The authors acknowledge that those bounds are a dramatic manifestation of the curse of dimension-  
 184 ality happening when sampling is needed. Nevertheless, the dependence on the dimension highly  
 185 depends on the class of surrogate functions  $\mathcal{F}$  used in our scheme, as smaller bounds on these con-  
 186 trolling terms can be derived for simpler class of functions, such as quadratic functions.

187 **Stationarity measure.** As problem (1) is a constrained optimization task, we consider the following  
 188 stationarity measure:

$$g(\bar{\theta}) := \inf_{\theta \in \Theta} \frac{\mathcal{L}'(\bar{\theta}, \theta - \bar{\theta})}{\|\bar{\theta} - \theta\|} \quad \text{and} \quad g(\bar{\theta}) = g_+(\bar{\theta}) - g_-(\bar{\theta}), \quad (14)$$

189 where  $g_+(\bar{\theta}) := \max\{0, g(\bar{\theta})\}$ ,  $g_-(\bar{\theta}) := -\min\{0, g(\bar{\theta})\}$  denote the positive and negative part of  
 190  $g(\bar{\theta})$ , respectively. Note that  $\bar{\theta}$  is a stationary point if and only if  $g_-(\bar{\theta}) = 0$  [Fletcher et al., 2002].  
 191 Also, denote

$$\widehat{\mathcal{L}}^{(k)}(\theta) := \frac{1}{n} \sum_{i=1}^n \widehat{\mathcal{L}}_i(\theta; \theta^{(\tau_i^k)}), \quad \widehat{e}^{(k)}(\theta) := \widehat{\mathcal{L}}^{(k)}(\theta) - \mathcal{L}(\theta), \quad \overline{M}_{(k)} := \sum_{k=0}^{K_{\max}-1} M_{(k)}^{-1/2}. \quad (15)$$

192 We first establish a non-asymptotic convergence rate for the MISSO method using a random termi-  
 193 nation number  $K$  as in [Ghadimi and Lan, 2013]:

**Theorem 1.** *Under S1, S2, H1, H2. For any  $K_{\max} \in \mathbb{N}$ , let  $K$  be an independent discrete r.v. drawn uniformly from  $\{0, \dots, K_{\max} - 1\}$  and define the following quantity:*

$$\Delta_{(K_{\max})} := 2nL\mathbb{E}[\widehat{\mathcal{L}}^{(0)}(\theta^{(0)}) - \widehat{\mathcal{L}}^{(K_{\max})}(\theta^{(K_{\max})})] + 4LC_r\overline{M}_{(k)}.$$

*Then we have following non-asymptotic bounds:*

$$\mathbb{E}[\|\nabla \widehat{e}^{(K)}(\theta^{(K)})\|^2] \leq \frac{\Delta_{(K_{\max})}}{K_{\max}} \quad \text{and} \quad \mathbb{E}[g_-(\theta^{(K)})] \leq \sqrt{\frac{\Delta_{(K_{\max})}}{K_{\max}}} + \frac{C_{\text{gr}}}{K_{\max}} \overline{M}_{(k)}. \quad (16)$$

194 Note that  $\Delta_{(K_{\max})}$  is finite for any  $K_{\max} \in \mathbb{N}$ . As expected, the MISSO method converges to a sta-  
 195 tionary point of (1) asymptotically and at a sublinear rate  $\mathbb{E}[g_-(\theta^{(K)})] \leq \mathcal{O}(\sqrt{1/K_{\max}})$ . Furthermore, we  
 196 remark that the MISSO method can be analyzed in Theorem 1 as a special case of the MISSO method  
 197 satisfying  $C_r = C_{\text{gr}} = 0$ . In this case, while the asymptotic convergence is well known from [Mairal,  
 198 2015] [cf. H2], Eq. (16) gives a non-asymptotic rate of  $\mathbb{E}[g_-(\theta^{(K)})] \leq \mathcal{O}(\sqrt{nL/K_{\max}})$  which is new to  
 199 our best knowledge. Next, we show that under an additional assumption on the sequence of batch  
 200 size  $M_{(k)}$ , the MISSO method converges almost surely to a stationary point:

**Theorem 2.** *Under S1, S2, H1, H2. In addition, assume that  $\{M_{(k)}\}_{k \geq 0}$  is a non-decreasing sequence of integers which satisfies  $\sum_{k=0}^{\infty} M_{(k)}^{-1/2} < \infty$ . Then:*

1. *the negative part of the stationarity measure converges a.s. to zero, i.e.,  $\lim_{k \rightarrow \infty} g_-(\theta^{(k)}) \stackrel{\text{a.s.}}{=} 0$ .*
2. *the objective value  $\mathcal{L}(\theta^{(k)})$  converges a.s. to a finite number  $\underline{\mathcal{L}}$ , i.e.,  $\lim_{k \rightarrow \infty} \mathcal{L}(\theta^{(k)}) \stackrel{\text{a.s.}}{=} \underline{\mathcal{L}}$ .*

201 In particular, the first result above shows that the sequence  $\{\theta^{(k)}\}_{k \geq 0}$  produced by the MISSO  
 202 method satisfies an *asymptotic stationary point condition*.

## 203 4 Numerical Experiments

### 204 4.1 Binary logistic regression with missing values

205 This application follows **Example 1** described in Section 2. We consider a binary regression setup,  
 206  $((y_i, z_i), i \in \llbracket n \rrbracket)$  where  $y_i \in \{0, 1\}$  is a binary response and  $z_i = (z_{i,j} \in \mathbb{R}, j \in \llbracket p \rrbracket)$  is a covariate



vector. The vector of covariates  $z_i = [z_{i,\text{mis}}, z_{i,\text{obs}}]$  is not fully observed where we denote by  $z_{i,\text{mis}}$  the missing values and  $z_{i,\text{obs}}$  the observed covariate. It is assumed that  $(z_i, i \in \llbracket n \rrbracket)$  are i.i.d. and marginally distributed according to  $\mathcal{N}(\beta, \Omega)$  where  $\beta \in \mathbb{R}^p$  and  $\Omega$  is a positive definite  $p \times p$  matrix. We define the conditional distribution of the observations  $y_i$  given  $z_i = (z_{i,\text{mis}}, z_{i,\text{obs}})$  as:

$$p_i(y_i|z_i) = S(\delta^\top \bar{z}_i)^{y_i} (1 - S(\delta^\top \bar{z}_i))^{1-y_i}, \quad (17)$$

where for  $u \in \mathbb{R}$ ,  $S(u) = 1/(1+e^{-u})$ ,  $\delta = (\delta_0, \dots, \delta_p)$  are the logistic parameters and  $\bar{z}_i = (1, z_i)$ . Here,  $\theta = (\delta, \beta, \Omega)$  is the parameter to estimate. For  $i \in \llbracket n \rrbracket$ , the complete log-likelihood reads:

$$\log f_i(z_{i,\text{mis}}, \theta) \propto y_i \delta^\top \bar{z}_i - \log(1 + \exp(\delta^\top \bar{z}_i)) - \frac{1}{2} \log(|\Omega|) + \frac{1}{2} \text{Tr}(\Omega^{-1}(z_i - \beta)(z_i - \beta)^\top).$$

**Fitting a logistic regression model on the TraumaBase dataset:** We apply the MISSO method to fit a logistic regression model on the TraumaBase (<http://traumabase.eu>) dataset, which consists of data collected from 15 trauma centers in France, covering measurements on patients from the initial to last stage of trauma. Extended implementation details are given in Appendix D.1.3.

Similar to [Jiang et al., 2018], we select  $p = 16$  influential quantitative measurements, described in Appendix D.1.1, on  $n = 6384$  patients, and we adopt the logistic regression model with missing covariates in (17) to predict the risk of a severe hemorrhage which is one of the main cause of death after a major trauma. For the Monte-Carlo sampling of  $z_{i,\text{mis}}$ , required while running MISSO, we run a Metropolis Hastings algorithm with the target distribution  $p(\cdot|z_{i,\text{obs}}, y_i; \theta^{(k)})$ .

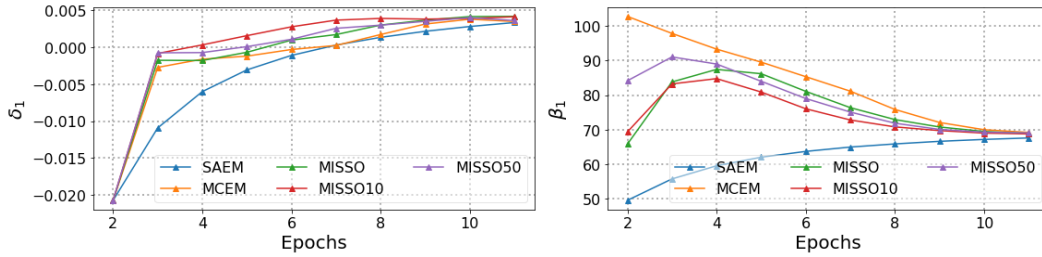


Figure 1: Convergence of first component of the vector of parameters  $\delta$  and  $\beta$  for the SAEM, the MCEM and the MISSO methods. The convergence is plotted against No. of passes over the data.

We compare in Figure 1 the convergence behavior of the estimated parameters  $\delta$  and  $\beta$  using SAEM [Delyon et al., 1999] (with stepsize  $\gamma_k = 1/k$ ), MCEM [Wei and Tanner, 1990] and the proposed MISSO method. For the MISSO method, we set the batch size to  $M_{(k)} = 10 + k^2$  and we examine with selecting different number of functions in Line 5 in the method – the default settings with 1 (MISSO), 10% (MISSO10) and 50% (MISSO50) minibatches per iteration. From Figure 1, the MISSO method converges to a static value with less number of epochs than the MCEM, SAEM methods. It is worth noting that the difference among the MISSO runs for different number of selected functions demonstrates a variance-cost tradeoff.

## 4.2 Training Bayesian CNN using MISSO

This application follows Example 2 described in Section 2. We use variational inference and the ELBO loss (10) to fit Bayesian Neural Networks on different datasets. At iteration  $k$ , minimizing the sum of stochastic surrogates defined as in (6) and (13) yields the following MISSO update — step (i) pick a function index  $i_k$  uniformly on  $\llbracket n \rrbracket$ ; step (ii) sample a Monte Carlo batch  $\{z_m^{(k)}\}_{m=1}^{M_{(k)}}$  from  $\mathcal{N}(0, \mathbf{I})$ ; and step (iii) update the parameters, with  $\tilde{w} = t(\theta^{(k-1)}, z_m^{(k)})$ , as

$$\mu_\ell^{(k)} = \hat{\mu}_\ell^{(\tau^k)} - \frac{\gamma}{n} \sum_{i=1}^n \hat{\delta}_{\mu_\ell, i}^{(k)} \quad \text{and} \quad \hat{\delta}_{\mu_\ell, i_k}^{(k)} = -\frac{1}{M_{(k)}} \sum_{m=1}^{M_{(k)}} \nabla_w \log p(y_{i_k}|x_{i_k}, \tilde{w}) + \nabla_{\mu_\ell} d(\theta^{(k-1)}),$$

where  $\hat{\mu}_\ell^{(\tau^k)} = \frac{1}{n} \sum_{i=1}^n \mu_\ell^{(\tau^k)}$  and  $d(\theta) = n^{-1} \sum_{\ell=1}^d (-\log(\sigma) + (\sigma^2 + \mu_\ell^2)/2 - 1/2)$ .

**Bayesian LeNet-5 on MNIST [LeCun et al., 1998]:** We apply the MISSO method to fit a Bayesian variant of LeNet-5 [LeCun et al., 1998] (see Appendix D.2.1). We train this network on the MNIST dataset [LeCun, 1998]. The training set is composed of  $n = 55\,000$  handwritten digits,  $28 \times 28$

images. Each image is labelled with its corresponding number (from zero to nine). Under the prior distribution  $\pi$ , see (8), the weights are assumed independent and identically distributed according to  $\mathcal{N}(0, 1)$ . We also assume that  $q(\cdot; \theta) \equiv \mathcal{N}(\mu, \sigma^2 \mathbf{I})$ . The variational posterior parameters are thus  $\theta = (\mu, \sigma)$  where  $\mu = (\mu_\ell, \ell \in \llbracket d \rrbracket)$  where  $d$  is the number of weights in the neural network. We use the re-parametrization as  $w = t(\theta, z) = \mu + \sigma z$  with  $z \sim \mathcal{N}(0, \mathbf{I})$ .

**Bayesian ResNet-18 [He et al., 2016] on CIFAR-10 [Krizhevsky et al., 2012]:** We train here the Bayesian variant of the ResNet-18 neural network (see Appendix D.2.2) introduced in [He et al., 2016] on CIFAR-10. The latter dataset is composed of  $n = 60\,000$  handwritten digits,  $32 \times 32$  colour images in 10 classes, with 6 000 images per class. As in the previous example, the weights are assumed independent and identically distributed according to  $\mathcal{N}(0, \mathbf{I})$ . The source code used as a backbone here can be found in the TensorFlow Probability Github repo where the default hyperparameters, such as the annealing constant or the number of MC samples, were used for the benchmark methods. For better efficiency and lower variance, the Flipout estimator [Wen et al., 2018] is used.

**Experiment Results:** We compare the convergence of the *Monte Carlo variants* of the following state of the art optimization algorithms — the ADAM [Kingma and Ba, 2015], the Momentum [Sutskever et al., 2013] and the SAG [Schmidt et al., 2017] methods versus the *Bayes by Backprop* (BBB) [Blundell et al., 2015] and our proposed MISSO method. For all these methods, the loss function (10) and its gradients were computed by Monte Carlo integration using Tensorflow Probability library [Dillon et al., 2017], based on the re-parametrization described above. Update rules for each algorithm are performed using their vanilla implementations on TensorFlow [Abadi et al., 2015] as detailed in Appendix D.2.3. We use the following hyperparameters for all runs — the learning rate is  $10^{-3}$ , we run 100 epochs with a mini-batch size of 128 and use the batchsize of  $M_{(k)} = k$ .

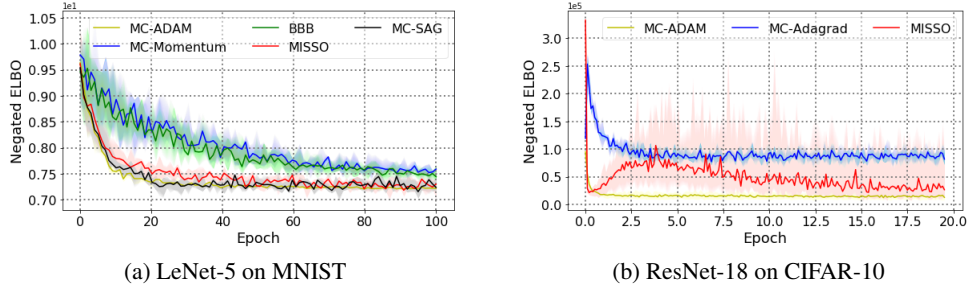


Figure 2: Negated ELBO versus epochs elapsed for fitting (a) Bayesian LeNet-5 on MNIST and (b) Bayesian ResNet-18 on CIFAR-10. The solid curve is obtained from averaging over 5 independent runs of the methods, and the shaded area represents the standard deviation.

Figure 2(a) shows the convergence of the negated evidence lower bound against the number of passes over data (one pass represents an epoch). As observed, the proposed MISSO method outperforms *Bayes by Backprop* and Momentum, while similar convergence rates are observed with the MISSO, ADAM and SAG methods for our experiment on MNIST dataset using a Bayesian variant of LeNet-5. On the other hand, the experiment conducted on CIFAR-10 (Figure 2(b)) using a much larger network, *i.e.*, a Bayesian variant of ResNet-18 showcases the need of a well-tuned adaptive methods to reach better training loss (and also faster). Our MISSO method is similar to the Monte Carlo variant of ADAM but slower than built-in TF optimizer Adagrad. Recall that the purpose of this paper is to provide a common class of optimizers, such as VI, in order to study their convergence behaviors, and not to introduce a novel method outperforming the baselines methods.

## 5 Conclusion

We present a unifying framework for minimizing a nonconvex and nonsmooth finite-sum objective function using incremental surrogates when the latter functions are expressed as an expectation and are intractable. Our approach covers a large class of nonconvex applications in machine learning such as logistic regression with missing values and variational inference. We provide both finite-time and asymptotic guarantees of our incremental stochastic surrogate optimization technique and illustrate our findings training a binary logistic regression with missing covariates to predict hemorrhagic shock and Bayesian variants of two Convolutional Neural Networks on benchmark datasets.



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