

---

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

---

Anonymous Author(s)

Affiliation

Address

email

## Abstract

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

## 15 1 Introduction

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

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

17 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.

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

31 The success of the MISO method rests upon the efficient minimization of surrogates such as convex  
32 functions, see [Mairal, 2015, Section 2.3]. In many applications of interest, the natural surrogate  
33 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 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. In summary, our contributions are:

- 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 conducted 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, see Theorem 1.

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 [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). Section 4 presents numerical applications including parameter inference for logistic regression with missing data and variational inference for two types of Bayesian neural networks. The proofs of theoretical results are reported as Supplement.

**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, which 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 [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 the assumptions (H1, H2):

**H1.** For all  $i \in \llbracket 1, n \rrbracket$  and  $\bar{\theta} \in \Theta$ ,  $\hat{\mathcal{L}}_i(\theta; \bar{\theta})$  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  $\theta = \bar{\theta}$ .

**H2.** 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  $\Theta_\epsilon = \{\theta \in \mathbb{R}^d, \inf_{\theta' \in \Theta} \|\theta - \theta'\| < \epsilon\}$  is an  $\epsilon$ -neighborhood set of  $\Theta$ . Moreover, for some constant  $L$ , the gradient satisfies

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

We remark that H1 is a common assumption used for surrogate functions, see [Mairal, 2015, Section 2.3]. H2 can be satisfied when the difference function  $\hat{e}(\theta; \{\bar{\theta}_i\}_{i=1}^n)$  is  $L$ -smooth, i.e.,  $\hat{e}$  is differentiable on  $\Theta$  and its gradient  $\nabla \hat{e}$  is  $L$ -Lipschitz,  $\forall \theta \in \Theta$ . H2 can be implied by applying [Razaviyayn et al., 2013, Proposition 1].

The inequality (3) implies  $\hat{\mathcal{L}}_i(\theta; \bar{\theta}) \geq \mathcal{L}_i(\theta) > -\infty$  for any  $\theta \in \Theta$ . The MISO method is an incremental version of the MM method, as summarized by Algorithm 1, which shows that the MISO method maintains an iteratively updated set of surrogate upper-bound functions  $\{\mathcal{A}_i^k(\theta)\}_{i=1}^n$  and updates the iterate via minimizing the average of the surrogate functions.

Particularly, only one out of the  $n$  surrogate functions is updated at each iteration [cf. Line 5] and the sum function  $\frac{1}{n} \sum_{i=1}^n \mathcal{A}_i^{k+1}(\theta)$  is designed to be ‘easy to optimize’, which, for example, can be a sum of quadratic functions. As such, the MISO method is suitable for large-scale optimization as the computation cost per iteration is independent of  $n$ . Under H1, H2, it was shown that the MISO method converges almost surely to a stationary point of (1) [Mairal, 2015, Prop. 3.1].

We now consider the case when the surrogate functions  $\hat{\mathcal{L}}_i(\theta; \bar{\theta})$  are intractable. Let  $Z$  be a measurable 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 function and  $\mu_i$  a  $\sigma$ -finite measure. We consider surrogate functions which satisfy H1, H2 and that can be expressed as an expectation, i.e.:

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

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

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

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

and we summarize the proposed MISSO method in Algorithm 2. Compared to the MISO method, there is a crucial difference in that the MISSO method involves two types of randomness. The first level of randomness comes from the selection of  $i_k$  in Line 5. The second level of randomness stems from the set of Monte 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 iterate  $\theta^{(k)}$ . We now discuss two applications of the MISSO method.

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

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

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  $\mathcal{L}_i(\theta) := -\log g_i(\theta)$ .

---

**Algorithm 1** The MISO method [Mairal, 2015].

---

- 1: **Input:** initialization  $\theta^{(0)}$ .
- 2: Initialize the surrogate function as  $\mathcal{A}_i^0(\theta) := \hat{\mathcal{L}}_i(\theta; \theta^{(0)})$ ,  $i \in \llbracket 1, n \rrbracket$ .
- 3: **for**  $k = 0, 1, \dots, K_{\max}$  **do**
- 4: Pick  $i_k$  uniformly from  $\llbracket 1, n \rrbracket$ .
- 5: Update  $\mathcal{A}_i^{k+1}(\theta)$  as:

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

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

---

**Algorithm 2** The MISSO method.

---

- 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**  $k = 0, 1, \dots, K_{\max}$  **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**
- 

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 H1 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 H2 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  $p(w|y, x)$ :

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

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. 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  $\hat{\mathcal{L}}_i(\theta; \bar{\theta})$  satisfies H1, H2. 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.  $\theta \in \Theta$

149 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  
150 et al., 2015, Proposition 1], the gradient of  $-r_i(\cdot)$  in (10) is:

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

151 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  
152  $\bar{\theta}$ . In addition, for most cases, the term  $\nabla d(\bar{\theta})$  can be evaluated in closed form as the gradient of the  
153 KL between the prior distribution  $\pi(\cdot)$  and the variational candidate  $q(\cdot, \theta)$ .

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

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

### 156 3 Convergence Analysis

157 We now provide asymptotic and non-asymptotic convergence results our method. Assume:

158 **H3.** For all  $i \in \llbracket 1, n \rrbracket$ ,  $\bar{\theta} \in \Theta$ ,  $z_i \in \mathbf{Z}$ ,  $r_i(\cdot; \bar{\theta}, z_i)$  is convex on  $\Theta$  and is lower bounded.

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

161 **H4.** For the samples  $\{z_{i,m}\}_{m=1}^M$ , there exist finite constants  $C_r$  and  $C_{gr}$  such that

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

162

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

163 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  
164 initial distribution  $\xi_i(\cdot; \bar{\theta})$ , transition kernel  $\Pi_{i, \bar{\theta}}$ , and stationary distribution  $p_i(\cdot; \bar{\theta})$ .

165 **Some intuitions behind the controlling terms:** It is common in statistical and optimization prob-  
166 lems, to deal with the manipulation and the control of random variables indexed by sets with an  
167 infinite number of elements. Here, the controlled random variable is an image of a continuous func-  
168 tion defined as  $r_i(\theta; \bar{\theta}, z_{i,m}) - \hat{\mathcal{L}}_i(\theta; \bar{\theta})$  for all  $z \in \mathbf{Z}$  and for fixed  $(\theta, \bar{\theta}) \in \Theta^2$ . To characterize  
169 such control, we will have recourse to the notion of metric entropy (or bracketing number) as de-  
170 veloped in [Van der Vaart, 2000, Vershynin, 2018, Wainwright, 2019]. A collection of results from  
171 those references gives intuition behind our assumption H4, which is classical in empirical processes.  
172 In [Vershynin, 2018, Theorem 8.2.3], the authors recall the uniform law of large numbers:

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

173 where  $\mathcal{F}$  is a class of  $L$ -Lipschitz functions. Moreover, in [Vershynin, 2018, Theorem 8.1.3 ]  
174 and [Wainwright, 2019, Theorem 5.22], the application of the Dudley inequality yields:

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

175 where  $\mathcal{N}(\mathcal{F}, \|\cdot\|_{\infty}, \varepsilon)$  is the bracketing number and  $\varepsilon$  denotes the level of approximation (the brack-  
176 eting number goes to infinity when  $\varepsilon \rightarrow 0$ ). Finally, in [Van der Vaart, 2000, p.271, Example],  
177  $\mathcal{N}(\mathcal{F}, \|\cdot\|_{\infty}, \varepsilon)$  is bounded from above for a class of parametric functions  $\mathcal{F} = f_{\theta} : \theta \in \Theta$ :

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

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

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

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

184 where  $g_+(\bar{\theta}) := \max\{0, g(\bar{\theta})\}$ ,  $g_-(\bar{\theta}) := -\min\{0, g(\bar{\theta})\}$  denote the positive and negative part of  
 185  $g(\bar{\theta})$ , respectively. Note that  $\bar{\theta}$  is a stationary point if and only if  $g_-(\bar{\theta}) = 0$  [Fletcher et al., 2002].  
 186 Furthermore, suppose that the sequence  $\{\theta^{(k)}\}_{k \geq 0}$  has a limit point  $\bar{\theta}$  that is a stationary point,  
 187 then one has  $\lim_{k \rightarrow \infty} g_-(\theta^{(k)}) = 0$ . Thus, the sequence  $\{\theta^{(k)}\}_{k \geq 0}$  is said to satisfy an *asymptotic*  
 188 *stationary point condition*. This is equivalent to [Mairal, 2015, Definition 2.4].

189 To facilitate our analysis, we define  $\tau_i^k$  as the iteration index where the  $i$ -th function is last accessed  
 190 in the MISSO method prior to iteration  $k$ ,  $\tau_{i_k}^{k+1} = k$  for instance. We define:

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

191 We first establish a non-asymptotic convergence rate for the MISSO method:

**Theorem 1.** *Under H1-H4. 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:*

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

192 Note that  $\Delta_{(K_{\max})}$  is finite for any  $K_{\max} \in \mathbb{N}$ . As expected, the MISSO method converges to a sta-  
 193 tionary point of (1) asymptotically and at a sublinear rate  $\mathbb{E}[g_-(\theta^{(K)})] \leq \mathcal{O}(\sqrt{1/K_{\max}})$ . Furthermore, we  
 194 remark that the MISO method can be analyzed in Theorem 1 as a special case of the MISSO method  
 195 satisfying  $C_r = C_{\text{gr}} = 0$ . In this case, while the asymptotic convergence is well known from [Mairal,  
 196 2015] [cf. H4], Eq. (16) gives a non-asymptotic rate of  $\mathbb{E}[g_-(\theta^{(K)})] \leq \mathcal{O}(\sqrt{nL/K_{\max}})$  which is new to  
 197 our best knowledge. Next, we show that under an additional assumption on the sequence of batch  
 198 size  $M_{(k)}$ , the MISSO method converges almost surely to a stationary point:

**Theorem 2.** *Under H1-H4. 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.,  $\lim_{k \rightarrow \infty} g_-(\theta^{(k)}) \stackrel{a.s.}{=} 0$ .*
2. *the objective value  $\mathcal{L}(\theta^{(k)})$  converges a.s. to a finite number  $\underline{\mathcal{L}}$ , i.e.,  $\lim_{k \rightarrow \infty} \mathcal{L}(\theta^{(k)}) \stackrel{a.s.}{=} \underline{\mathcal{L}}$ .*

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

## 201 4 Numerical Experiments

### 202 4.1 Binary logistic regression with missing values

203 This application follows **Example 1** described in Section 2. We consider a binary regression setup,  
 204  $((y_i, z_i), i \in \llbracket n \rrbracket)$  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. This dataset includes information from the first stage of the trauma, namely initial observations on the patient's accident site to the last stage being intense care at the hospital and counts more than 200 variables measured for more than 7 000 patients. Since the dataset considered is heterogeneous – coming from multiple sources with frequently missed entries – we apply the latent data model described in (17) to *predict the risk of a severe hemorrhage* which is one of the main cause of death after a major trauma.

Similar to [Jiang et al., 2018], we select  $p = 16$  influential quantitative measurements, on  $n = 6384$  patients. For the Monte Carlo sampling of  $z_{i,\text{mis}}$ , required while running MISSO, we run a Metropolis-Hastings algorithm with the target distribution  $p(\cdot|z_{i,\text{obs}}, y_i; \theta^{(k)})$ .

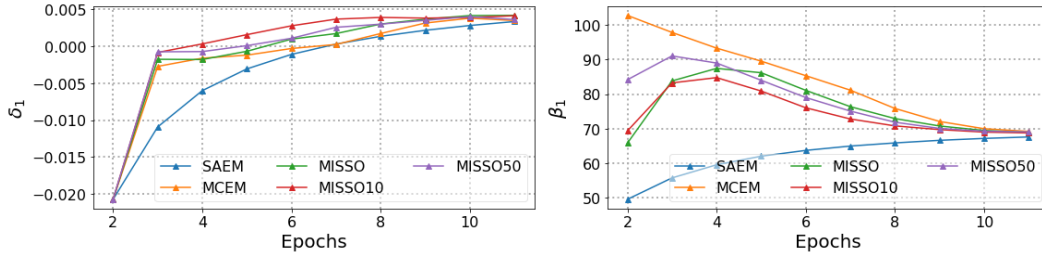


Figure 1: Convergence of first component of the vector of parameters  $\delta$  and  $\beta$  for the SAEM, the MCEM and the MISSO methods. The convergence is plotted against No. of passes over the data.

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

238 **Bayesian LeNet-5 on MNIST [LeCun et al., 1998]:** We apply the MISSO method to fit a Bayesian  
 239 variant of LeNet-5 [LeCun et al., 1998]. We train this network on the MNIST dataset [LeCun,  
 240 1998]. The training set is composed of  $n = 55\,000$  handwritten digits,  $28 \times 28$  images. Each  
 241 image is labelled with its corresponding number (from zero to nine). Under the prior distribution  
 242  $\pi$ , see (8), the weights are assumed independent and identically distributed according to  $\mathcal{N}(0, 1)$ .  
 243 We also assume that  $q(\cdot; \theta) \equiv \mathcal{N}(\mu, \sigma^2 \mathbf{I})$ . The variational posterior parameters are thus  $\theta = (\mu, \sigma)$   
 244 where  $\mu = (\mu_\ell, \ell \in \llbracket d \rrbracket)$  where  $d$  is the number of weights in the neural network. We use the  
 245 re-parametrization as  $w = t(\theta, z) = \mu + \sigma z$  with  $z \sim \mathcal{N}(0, \mathbf{I})$ .

246 **Bayesian ResNet-18 [He et al., 2016] on CIFAR-10 [Krizhevsky et al., 2012]:** We train here the  
 247 Bayesian variant of the ResNet-18 neural network introduced in [He et al., 2016] on CIFAR-10. The  
 248 latter dataset is composed of  $n = 60\,000$  handwritten digits,  $32 \times 32$  colour images in 10 classes,  
 249 with 6 000 images per class. As in the previous example, the weights are assumed independent and  
 250 identically distributed according to  $\mathcal{N}(0, \mathbf{I})$ . Standard hyperparameters values found in the literature,  
 251 such as the annealing constant or the number of MC samples, were used for the benchmark methods.  
 252 For better efficiency and lower variance, the Flipout estimator [Wen et al., 2018] is used.

253 **Experiment Results:** We compare the convergence of the *Monte Carlo variants* of the follow-  
 254 ing state of the art optimization algorithms — the ADAM [Kingma and Ba, 2015], the Momen-  
 255 tum [Sutskever et al., 2013] and the SAG [Schmidt et al., 2017] methods versus the *Bayes by Back-*  
 256 *prop* (BBB) [Blundell et al., 2015] and our proposed MISSO method. For all these methods, the  
 257 loss function (10) and its gradients were computed by Monte Carlo integration based on the re-  
 258 parametrization described above. The mini-batch of indices and MC samples are respectively set to  
 259 128 and  $M_{(k)} = k$ . The learning rates are set to  $10^{-3}$  for LeNet-5 and  $10^{-4}$  for Resnet-18.

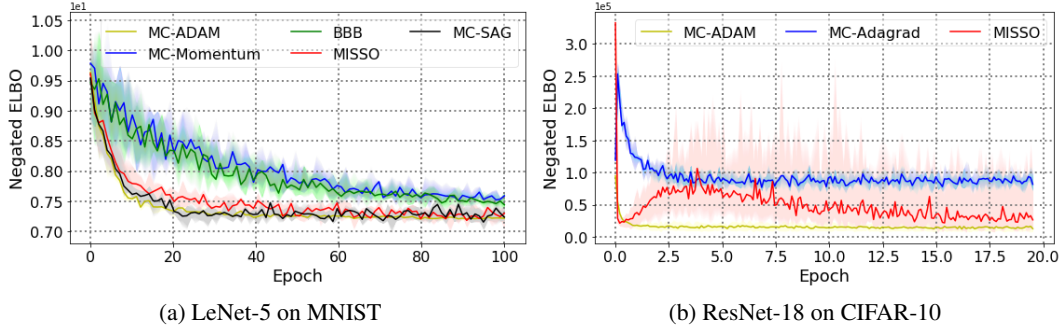


Figure 2: Negated ELBO versus epochs elapsed for fitting (a) Bayesian LeNet-5 on MNIST and (b) Bayesian ResNet-18 on CIFAR-10. The solid curve is obtained from averaging over 5 independent runs of the methods, and the shaded area represents the standard deviation.

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

## 270 5 Conclusion

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



## References

- M. Abadi, A. Agarwal, P. Barham, E. Brevdo, Z. Chen, C. Citro, G. Corrado, A. Davis, J. Dean, M. Devin, S. Ghemawat, I. Goodfellow, A. Harp, G. Irving, M. Isard, Y. Jia, R. Jozefowicz, L. Kaiser, M. Kudlur, J. Levenberg, D. Mané, R. Monga, S. Moore, D. Murray, C. Olah, M. Schuster, J. Shlens, B. Steiner, I. Sutskever, K. Talwar, P. Tucker, V. Vanhoucke, V. Vasudevan, F. Viégas, O. Vinyals, P. Warden, M. Wattenberg, M. Wicke, Y. Yu, and X. Zheng. TensorFlow: Large-scale machine learning on heterogeneous systems, 2015. URL <https://www.tensorflow.org/>. Software available from tensorflow.org.
- C. M. Bishop. *Pattern recognition and machine learning*. springer, 2006.
- D. M. Blei, A. Kucukelbir, and J. D. McAuliffe. Variational inference: A review for statisticians. *Journal of the American Statistical Association*, 112(518):859–877, 2017. doi: 10.1080/01621459.2017.1285773. URL <https://doi.org/10.1080/01621459.2017.1285773>.
- C. Blundell, J. Cornebise, K. Kavukcuoglu, and D. Wierstra. Weight uncertainty in neural network. In *International Conference on Machine Learning*, pages 1613–1622, 2015.
- B. Delyon, M. Lavielle, and E. Moulines. Convergence of a stochastic approximation version of the em algorithm. *Ann. Statist.*, 27(1):94–128, 03 1999. doi: 10.1214/aos/1018031103. URL <https://doi.org/10.1214/aos/1018031103>.
- J. V. Dillon, I. Langmore, D. Tran, E. Brevdo, S. Vasudevan, D. Moore, B. Patton, A. Alemi, M. D. Hoffman, and R. A. Saurous. Tensorflow distributions. *CoRR*, abs/1711.10604, 2017. URL <http://arxiv.org/abs/1711.10604>.
- R. Fletcher, N. I. Gould, S. Leyffer, P. L. Toint, and A. Wächter. Global convergence of a trust-region sqp-filter algorithm for general nonlinear programming. *SIAM Journal on Optimization*, 13(3):635–659, 2002.
- S. Ghadimi and G. Lan. Stochastic first-and zeroth-order methods for nonconvex stochastic programming. *SIAM Journal on Optimization*, 23(4):2341–2368, 2013.
- Z. Ghahramani. Probabilistic machine learning and artificial intelligence. *Nature*, 521(7553):452–459, May 2015. doi: 10.1038/nature14541. URL <https://www.ncbi.nlm.nih.gov/pubmed/26017444/>. On Probabilistic models.
- K. He, X. Zhang, S. Ren, and J. Sun. Deep residual learning for image recognition. In *Proceedings of the IEEE conference on computer vision and pattern recognition*, pages 770–778, 2016.
- W. Jiang, J. Josse, and M. Lavielle. Logistic regression with missing covariates—parameter estimation, model selection and prediction. 2018.
- M. I. Jordan, Z. Ghahramani, T. S. Jaakkola, and L. K. Saul. An introduction to variational methods for graphical models. *Mach. Learn.*, 37(2):183–233, Nov. 1999. ISSN 0885-6125. doi: 10.1023/A:1007665907178. URL <https://doi.org/10.1023/A:1007665907178>.
- D. P. Kingma and J. Ba. Adam: A method for stochastic optimization. In *3rd International Conference on Learning Representations, ICLR 2015, San Diego, CA, USA, May 7-9, 2015, Conference Track Proceedings*, 2015. URL <http://arxiv.org/abs/1412.6980>.
- D. P. Kingma and M. Welling. Auto-encoding variational bayes. In *2nd International Conference on Learning Representations, ICLR 2014, Banff, AB, Canada, April 14-16, 2014, Conference Track Proceedings*, 2014. URL <http://arxiv.org/abs/1312.6114>.
- A. Krizhevsky, I. Sutskever, and G. E. Hinton. Imagenet classification with deep convolutional neural networks. In *Advances in neural information processing systems*, pages 1097–1105, 2012.
- K. Lange. *MM Optimization Algorithms*. SIAM-Society for Industrial and Applied Mathematics, USA, 2016. ISBN 1611974399, 9781611974393.
- Y. LeCun. The mnist database of handwritten digits. <http://yann.lecun.com/exdb/mnist/>, 1998.

324 Y. LeCun, L. Bottou, Y. Bengio, P. Haffner, et al. Gradient-based learning applied to document  
325 recognition. *Proceedings of the IEEE*, 86(11):2278–2324, 1998.

326 Y. Li and Y. Gal. Dropout inference in bayesian neural networks with alpha-divergences. In *Proceed-*  
327 *ings of the 34th International Conference on Machine Learning-Volume 70*, pages 2052–2061.  
328 JMLR. org, 2017.

329 J. Mairal. Incremental majorization-minimization optimization with application to large-scale ma-  
330 chine learning. *SIAM J. Optim.*, 25(2):829–855, 2015. ISSN 1052-6234. doi: 10.1137/  
331 140957639. URL <https://doi.org/10.1137/140957639>.

332 G. J. McLachlan and T. Krishnan. *The EM algorithm and extensions*. Wiley Series in Probabil-  
333 ity and Statistics. Wiley-Interscience [John Wiley & Sons], Hoboken, NJ, second edition, 2008.  
334 ISBN 978-0-471-20170-0. doi: 10.1002/9780470191613. URL [https://doi.org/10.1002/](https://doi.org/10.1002/9780470191613)  
335 [9780470191613](https://doi.org/10.1002/9780470191613).

336 S. P. Meyn and R. L. Tweedie. *Markov chains and stochastic stability*. Springer Science & Business  
337 Media, 2012.

338 R. M. Neal. *Bayesian learning for neural networks*, volume 118. Springer Science & Business  
339 Media, 2012.

340 J. Paisley, D. Blei, and M. Jordan. Variational bayesian inference with stochastic search. In *ICML*.  
341 icml.cc / Omnipress, 2012.

342 N. G. Polson, V. Sokolov, et al. Deep learning: a bayesian perspective. *Bayesian Analysis*, 12(4):  
343 1275–1304, 2017.

344 X. Qian, A. Sailanbayev, K. Mishchenko, and P. Richtárik. Miso is making a comeback with better  
345 proofs and rates. *arXiv preprint arXiv:1906.01474*, 2019.

346 M. Razaviyayn, M. Hong, and Z.-Q. Luo. A unified convergence analysis of block successive  
347 minimization methods for nonsmooth optimization. *SIAM Journal on Optimization*, 23(2):1126–  
348 1153, 2013.

349 D. J. Rezende, S. Mohamed, and D. Wierstra. Stochastic backpropagation and approximate in-  
350 ference in deep generative models. In *International Conference on Machine Learning*, pages  
351 1278–1286, 2014.

352 M. Schmidt, N. Le Roux, and F. Bach. Minimizing finite sums with the stochastic average gradient.  
353 *Mathematical Programming*, 162(1-2):83–112, 2017.

354 I. Sutskever, J. Martens, G. Dahl, and G. Hinton. On the importance of initialization and momentum  
355 in deep learning. In *International conference on machine learning*, pages 1139–1147, 2013.

356 A. W. Van der Vaart. *Asymptotic statistics*, volume 3. Cambridge university press, 2000.

357 R. Vershynin. *High-dimensional probability: An introduction with applications in data science*,  
358 volume 47. Cambridge university press, 2018.

359 M. J. Wainwright. *High-dimensional statistics: A non-asymptotic viewpoint*, volume 48. Cambridge  
360 University Press, 2019.

361 G. C. G. Wei and M. A. Tanner. A monte carlo implementation of the em algorithm and the poor  
362 man’s data augmentation algorithms. *Journal of the American Statistical Association*, 85(411):  
363 699–704, 1990. doi: 10.1080/01621459.1990.10474930. URL [https://www.tandfonline.](https://www.tandfonline.com/doi/abs/10.1080/01621459.1990.10474930)  
364 [com/doi/abs/10.1080/01621459.1990.10474930](https://www.tandfonline.com/doi/abs/10.1080/01621459.1990.10474930).

365 Y. Wen, P. Vicol, J. Ba, D. Tran, and R. Grosse. Flipout: Efficient pseudo-independent weight  
366 perturbations on mini-batches. *arXiv preprint arXiv:1803.04386*, 2018.

## 367 A Proof of Theorem 1

368 **Theorem.** Under H1-H4. For any  $K_{\max} \in \mathbb{N}$ , let  $K$  be an independent discrete r.v. drawn uniformly  
 369 from  $\{0, \dots, K_{\max} - 1\}$  and define the following quantity:

$$\Delta_{(K_{\max})} := 2nL\mathbb{E}[\tilde{\mathcal{L}}^{(0)}(\boldsymbol{\theta}^{(0)}) - \tilde{\mathcal{L}}^{(K_{\max})}(\boldsymbol{\theta}^{(K_{\max})})] + \sum_{k=0}^{K_{\max}-1} \frac{4LC_r}{\sqrt{M_{(k)}}},$$

370 Then we have following non-asymptotic bounds:

$$\mathbb{E}[\|\nabla \hat{\mathcal{L}}^{(K)}(\boldsymbol{\theta}^{(K)})\|^2] \leq \frac{\Delta_{(K_{\max})}}{K_{\max}}, \quad \mathbb{E}[g_-(\boldsymbol{\theta}^{(K)})] \leq \sqrt{\frac{\Delta_{(K_{\max})}}{K_{\max}}} + \frac{C_{gr}}{K_{\max}} \sum_{k=0}^{K_{\max}-1} M_{(k)}^{-1/2}.$$

371 **Proof** We begin by recalling the definition

$$\tilde{\mathcal{L}}^{(k)}(\boldsymbol{\theta}) := \frac{1}{n} \sum_{i=1}^n \tilde{\mathcal{A}}_i^k(\boldsymbol{\theta}).$$

372 Notice that

$$\begin{aligned} \tilde{\mathcal{L}}^{(k+1)}(\boldsymbol{\theta}) &= \frac{1}{n} \sum_{i=1}^n \tilde{\mathcal{L}}_i(\boldsymbol{\theta}; \boldsymbol{\theta}^{(\tau_i^{k+1})}, \{z_{i,m}^{(\tau_i^{k+1})}\}_{m=1}^{M_{(\tau_i^{k+1})}}) \\ &= \tilde{\mathcal{L}}^{(k)}(\boldsymbol{\theta}) + \frac{1}{n} (\tilde{\mathcal{L}}_{i_k}(\boldsymbol{\theta}; \boldsymbol{\theta}^{(k)}, \{z_{i_k,m}^{(k)}\}_{m=1}^{M_{(k)}}) - \tilde{\mathcal{L}}_{i_k}(\boldsymbol{\theta}; \boldsymbol{\theta}^{(\tau_{i_k}^k)}, \{z_{i_k,m}^{(\tau_{i_k}^k)}\}_{m=1}^{M_{(\tau_{i_k}^k)}})). \end{aligned}$$

373 Furthermore, we recall that

$$\hat{\mathcal{L}}^{(k)}(\boldsymbol{\theta}) := \frac{1}{n} \sum_{i=1}^n \hat{\mathcal{L}}_i(\boldsymbol{\theta}; \boldsymbol{\theta}^{(\tau_i^k)}), \quad \hat{\mathcal{e}}^{(k)}(\boldsymbol{\theta}) := \hat{\mathcal{L}}^{(k)}(\boldsymbol{\theta}) - \mathcal{L}(\boldsymbol{\theta}).$$

374 Due to H2, we have

$$\|\nabla \hat{\mathcal{e}}^{(k)}(\boldsymbol{\theta}^{(k)})\|^2 \leq 2L\hat{\mathcal{e}}^{(k)}(\boldsymbol{\theta}^{(k)}). \quad (18)$$

375 To prove the first bound in (16), using the optimality of  $\boldsymbol{\theta}^{(k+1)}$ , one has

$$\begin{aligned} \tilde{\mathcal{L}}^{(k+1)}(\boldsymbol{\theta}^{(k+1)}) &\leq \tilde{\mathcal{L}}^{(k+1)}(\boldsymbol{\theta}^{(k)}) \\ &= \tilde{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)}) + \frac{1}{n} (\tilde{\mathcal{L}}_{i_k}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(k)}, \{z_{i_k,m}^{(k)}\}_{m=1}^{M_{(k)}}) - \tilde{\mathcal{L}}_{i_k}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(\tau_{i_k}^k)}, \{z_{i_k,m}^{(\tau_{i_k}^k)}\}_{m=1}^{M_{(\tau_{i_k}^k)}})) \end{aligned} \quad (19)$$

376 Let  $\mathcal{F}_k$  be the filtration of random variables up to iteration  $k$ , i.e.,  $\{i_{\ell-1}, \{z_{i_{\ell-1},m}^{(\ell-1)}\}_{m=1}^{M_{(\ell-1)}}, \boldsymbol{\theta}^{(\ell)}\}_{\ell=1}^k$ .

377 We observe that the conditional expectation evaluates to

$$\begin{aligned} &\mathbb{E}_{i_k} [\mathbb{E}[\tilde{\mathcal{L}}_{i_k}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(k)}, \{z_{i_k,m}^{(k)}\}_{m=1}^{M_{(k)}}) | \mathcal{F}_k, i_k] | \mathcal{F}_k] \\ &= \mathcal{L}(\boldsymbol{\theta}^{(k)}) + \mathbb{E}_{i_k} [\mathbb{E}[\frac{1}{M_{(k)}} \sum_{m=1}^{M_{(k)}} r_{i_k}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(k)}, z_{i_k,m}^{(k)}) - \tilde{\mathcal{L}}_{i_k}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(k)}) | \mathcal{F}_k, i_k] | \mathcal{F}_k] \\ &\leq \mathcal{L}(\boldsymbol{\theta}^{(k)}) + \frac{C_r}{\sqrt{M_{(k)}}}, \end{aligned}$$

378 where the last inequality is due to H4. Moreover,

$$\mathbb{E}[\tilde{\mathcal{L}}_{i_k}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(\tau_{i_k}^k)}, \{z_{i_k,m}^{(\tau_{i_k}^k)}\}_{m=1}^{M_{(\tau_{i_k}^k)}}) | \mathcal{F}_k] = \frac{1}{n} \sum_{i=1}^n \tilde{\mathcal{L}}_i(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(\tau_i^k)}, \{z_{i,m}^{(\tau_i^k)}\}_{m=1}^{M_{(\tau_i^k)}}) = \tilde{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)}).$$

379 Taking the conditional expectations on both sides of (19) and re-arranging terms give:

$$\tilde{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)}) - \mathcal{L}(\boldsymbol{\theta}^{(k)}) \leq n\mathbb{E}[\tilde{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)}) - \tilde{\mathcal{L}}^{(k+1)}(\boldsymbol{\theta}^{(k+1)}) | \mathcal{F}_k] + \frac{C_r}{\sqrt{M_{(k)}}} \quad (20)$$

Proceeding from (20), we observe the following lower bound for the left hand side

$$\begin{aligned}
\tilde{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)}) - \mathcal{L}(\boldsymbol{\theta}^{(k)}) &\stackrel{(a)}{=} \tilde{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)}) - \widehat{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)}) + \widehat{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)}) \\
&\stackrel{(b)}{\geq} \tilde{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)}) - \widehat{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)}) + \frac{1}{2L} \|\nabla \widehat{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)})\|^2 \\
&= \underbrace{\frac{1}{n} \sum_{i=1}^n \left\{ \frac{1}{M_{(\tau_i^k)}} \sum_{m=1}^{M_{(\tau_i^k)}} r_i(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(\tau_i^k)}, z_{i,m}^{(\tau_i^k)}) - \widehat{\mathcal{L}}_i(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(\tau_i^k)}) \right\}}_{:= -\delta^{(k)}(\boldsymbol{\theta}^{(k)})} + \frac{1}{2L} \|\nabla \widehat{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)})\|^2
\end{aligned}$$

where (a) is due to  $\widehat{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)}) = 0$  [cf. H1], (b) is due to (18) and we have defined the summation in the last equality as  $-\delta^{(k)}(\boldsymbol{\theta}^{(k)})$ . Substituting the above into (20) yields

$$\frac{\|\nabla \widehat{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)})\|^2}{2L} \leq n \mathbb{E}[\tilde{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)}) - \tilde{\mathcal{L}}^{(k+1)}(\boldsymbol{\theta}^{(k+1)}) | \mathcal{F}_k] + \frac{C_r}{\sqrt{M_{(k)}}} + \delta^{(k)}(\boldsymbol{\theta}^{(k)}) \quad (21)$$

Observe the following upper bound on the total expectations:

$$\mathbb{E}[\delta^{(k)}(\boldsymbol{\theta}^{(k)})] \leq \mathbb{E}\left[\frac{1}{n} \sum_{i=1}^n \frac{C_r}{\sqrt{M_{(\tau_i^k)}}}\right],$$

which is due to H4. It yields

$$\mathbb{E}[\|\nabla \widehat{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)})\|^2] \leq 2nL \mathbb{E}[\tilde{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)}) - \tilde{\mathcal{L}}^{(k+1)}(\boldsymbol{\theta}^{(k+1)})] + \frac{2LC_r}{\sqrt{M_{(k)}}} + \frac{1}{n} \sum_{i=1}^n \mathbb{E}\left[\frac{2LC_r}{\sqrt{M_{(\tau_i^k)}}}\right]$$

Finally, for any  $K_{\max} \in \mathbb{N}$ , we let  $K$  be a discrete r.v. that is uniformly drawn from  $\{0, 1, \dots, K_{\max} - 1\}$ . Using H4 and taking total expectations lead to

$$\begin{aligned}
\mathbb{E}[\|\nabla \widehat{\mathcal{L}}^{(K)}(\boldsymbol{\theta}^{(K)})\|^2] &= \frac{1}{K_{\max}} \sum_{k=0}^{K_{\max}-1} \mathbb{E}[\|\nabla \widehat{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)})\|^2] \\
&\leq \frac{2nL \mathbb{E}[\tilde{\mathcal{L}}^{(0)}(\boldsymbol{\theta}^{(0)}) - \tilde{\mathcal{L}}^{(K_{\max})}(\boldsymbol{\theta}^{(K_{\max})})]}{K_{\max}} + \frac{2LC_r}{K_{\max}} \sum_{k=0}^{K_{\max}-1} \mathbb{E}\left[\frac{1}{\sqrt{M_{(k)}}} + \frac{1}{n} \sum_{i=1}^n \frac{1}{\sqrt{M_{(\tau_i^k)}}}\right] \quad (22)
\end{aligned}$$

For all  $i \in [1, n]$ , the index  $i$  is selected with a probability equal to  $\frac{1}{n}$  when conditioned independently on the past. We observe:

$$\mathbb{E}[M_{(\tau_i^k)}^{-1/2}] = \sum_{j=1}^k \frac{1}{n} \left(1 - \frac{1}{n}\right)^{j-1} M_{(k-j)}^{-1/2} \quad (23)$$

Taking the sum yields:

$$\begin{aligned}
\sum_{k=0}^{K_{\max}-1} \mathbb{E}[M_{(\tau_i^k)}^{-1/2}] &= \sum_{k=0}^{K_{\max}-1} \sum_{j=1}^k \frac{1}{n} \left(1 - \frac{1}{n}\right)^{j-1} M_{(k-j)}^{-1/2} = \sum_{k=0}^{K_{\max}-1} \sum_{l=0}^{k-1} \frac{1}{n} \left(1 - \frac{1}{n}\right)^{k-(l+1)} M_{(l)}^{-1/2} \\
&= \sum_{l=0}^{K_{\max}-1} M_{(l)}^{-1/2} \sum_{k=l+1}^{K_{\max}-1} \frac{1}{n} \left(1 - \frac{1}{n}\right)^{k-(l+1)} \leq \sum_{l=0}^{K_{\max}-1} M_{(l)}^{-1/2} \quad (24)
\end{aligned}$$

where the last inequality is due to upper bounding the geometric series. Plugging this back into (22) yields

$$\begin{aligned}
\mathbb{E}[\|\nabla \widehat{\mathcal{L}}^{(K)}(\boldsymbol{\theta}^{(K)})\|^2] &= \frac{1}{K_{\max}} \sum_{k=0}^{K_{\max}-1} \mathbb{E}[\|\nabla \widehat{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)})\|^2] \\
&\leq \frac{2nL \mathbb{E}[\tilde{\mathcal{L}}^{(0)}(\boldsymbol{\theta}^{(0)}) - \tilde{\mathcal{L}}^{(K_{\max})}(\boldsymbol{\theta}^{(K_{\max})})]}{K_{\max}} + \frac{1}{K_{\max}} \sum_{k=0}^{K_{\max}-1} \frac{4LC_r}{\sqrt{M_{(k)}}} = \frac{\Delta_{(K_{\max})}}{K_{\max}}.
\end{aligned}$$

392 This concludes our proof for the first inequality in (16).

393 To prove the second inequality of (16), we define the shorthand notations  $g^{(k)} := g(\boldsymbol{\theta}^{(k)})$ ,  $g_-^{(k)} :=$   
 394  $-\min\{0, g^{(k)}\}$ ,  $g_+^{(k)} := \max\{0, g^{(k)}\}$ . We observe that

$$\begin{aligned} g^{(k)} &= \inf_{\boldsymbol{\theta} \in \Theta} \frac{\mathcal{L}'(\boldsymbol{\theta}^{(k)}, \boldsymbol{\theta} - \boldsymbol{\theta}^{(k)})}{\|\boldsymbol{\theta}^{(k)} - \boldsymbol{\theta}\|} \\ &= \inf_{\boldsymbol{\theta} \in \Theta} \left\{ \frac{\frac{1}{n} \sum_{i=1}^n \widehat{\mathcal{L}}'_i(\boldsymbol{\theta}^{(k)}, \boldsymbol{\theta} - \boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(\tau_i^k)})}{\|\boldsymbol{\theta}^{(k)} - \boldsymbol{\theta}\|} - \frac{\langle \nabla \widehat{e}^{(k)}(\boldsymbol{\theta}^{(k)}) | \boldsymbol{\theta} - \boldsymbol{\theta}^{(k)} \rangle}{\|\boldsymbol{\theta}^{(k)} - \boldsymbol{\theta}\|} \right\} \\ &\geq -\|\nabla \widehat{e}^{(k)}(\boldsymbol{\theta}^{(k)})\| + \inf_{\boldsymbol{\theta} \in \Theta} \frac{\frac{1}{n} \sum_{i=1}^n \widehat{\mathcal{L}}'_i(\boldsymbol{\theta}^{(k)}, \boldsymbol{\theta} - \boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(\tau_i^k)})}{\|\boldsymbol{\theta}^{(k)} - \boldsymbol{\theta}\|} \end{aligned}$$

395 where the last inequality is due to the Cauchy-Schwarz inequality and we have defined  
 396  $\widehat{\mathcal{L}}'_i(\boldsymbol{\theta}, \boldsymbol{d}; \boldsymbol{\theta}^{(\tau_i^k)})$  as the directional derivative of  $\widehat{\mathcal{L}}_i(\cdot; \boldsymbol{\theta}^{(\tau_i^k)})$  at  $\boldsymbol{\theta}$  along the direction  $\boldsymbol{d}$ . Moreover,  
 397 for any  $\boldsymbol{\theta} \in \Theta$ ,

$$\begin{aligned} &\frac{1}{n} \sum_{i=1}^n \widehat{\mathcal{L}}'_i(\boldsymbol{\theta}^{(k)}, \boldsymbol{\theta} - \boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(\tau_i^k)}) \\ &= \underbrace{\widetilde{\mathcal{L}}^{(k)'}(\boldsymbol{\theta}^{(k)}, \boldsymbol{\theta} - \boldsymbol{\theta}^{(k)}) - \widetilde{\mathcal{L}}^{(k)'}(\boldsymbol{\theta}^{(k)}, \boldsymbol{\theta} - \boldsymbol{\theta}^{(k)})}_{\geq 0} + \frac{1}{n} \sum_{i=1}^n \widehat{\mathcal{L}}'_i(\boldsymbol{\theta}^{(k)}, \boldsymbol{\theta} - \boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(\tau_i^k)}) \\ &\geq \frac{1}{n} \sum_{i=1}^n \left\{ \widehat{\mathcal{L}}'_i(\boldsymbol{\theta}^{(k)}, \boldsymbol{\theta} - \boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(\tau_i^k)}) - \frac{1}{M_{(\tau_i^k)}} \sum_{m=1}^{M_{(\tau_i^k)}} r'_i(\boldsymbol{\theta}^{(k)}, \boldsymbol{\theta} - \boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(\tau_i^k)}, z_{i,m}^{(\tau_i^k)}) \right\} \end{aligned}$$

398 where the inequality is due to the optimality of  $\boldsymbol{\theta}^{(k)}$  and the convexity of  $\widetilde{\mathcal{L}}^{(k)}(\boldsymbol{\theta})$  [cf. H3]. Denoting  
 399 a scaled version of the above term as:

$$\epsilon^{(k)}(\boldsymbol{\theta}) := \frac{\frac{1}{n} \sum_{i=1}^n \left\{ \frac{1}{M_{(\tau_i^k)}} \sum_{m=1}^{M_{(\tau_i^k)}} r'_i(\boldsymbol{\theta}^{(k)}, \boldsymbol{\theta} - \boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(\tau_i^k)}, z_{i,m}^{(\tau_i^k)}) - \widehat{\mathcal{L}}'_i(\boldsymbol{\theta}^{(k)}, \boldsymbol{\theta} - \boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(\tau_i^k)}) \right\}}{\|\boldsymbol{\theta}^{(k)} - \boldsymbol{\theta}\|}.$$

400 We have

$$g^{(k)} \geq -\|\nabla \widehat{e}^{(k)}(\boldsymbol{\theta}^{(k)})\| + \inf_{\boldsymbol{\theta} \in \Theta} (-\epsilon^{(k)}(\boldsymbol{\theta})) \geq -\|\nabla \widehat{e}^{(k)}(\boldsymbol{\theta}^{(k)})\| - \sup_{\boldsymbol{\theta} \in \Theta} |\epsilon^{(k)}(\boldsymbol{\theta})|. \quad (25)$$

401 Since  $g^{(k)} = g_+^{(k)} - g_-^{(k)}$  and  $g_+^{(k)} g_-^{(k)} = 0$ , this implies

$$g_-^{(k)} \leq \|\nabla \widehat{e}^{(k)}(\boldsymbol{\theta}^{(k)})\| + \sup_{\boldsymbol{\theta} \in \Theta} |\epsilon^{(k)}(\boldsymbol{\theta})|. \quad (26)$$

402 Consider the above inequality when  $k = K$ , i.e., the random index, and taking total expectations on  
 403 both sides gives

$$\mathbb{E}[g_-^{(K)}] \leq \mathbb{E}[\|\nabla \widehat{e}^{(K)}(\boldsymbol{\theta}^{(K)})\|] + \mathbb{E}[\sup_{\boldsymbol{\theta} \in \Theta} \epsilon^{(K)}(\boldsymbol{\theta})]$$

404 We note that

$$\left( \mathbb{E}[\|\nabla \widehat{e}^{(K)}(\boldsymbol{\theta}^{(K)})\|] \right)^2 \leq \mathbb{E}[\|\nabla \widehat{e}^{(K)}(\boldsymbol{\theta}^{(K)})\|^2] \leq \frac{\Delta(K_{\max})}{K_{\max}},$$

405 where the first inequality is due to the convexity of  $(\cdot)^2$  and the Jensen's inequality, and

$$\begin{aligned} \mathbb{E}[\sup_{\boldsymbol{\theta} \in \Theta} \epsilon^{(K)}(\boldsymbol{\theta})] &= \frac{1}{K_{\max}} \sum_{k=0}^{K_{\max}} \mathbb{E}[\sup_{\boldsymbol{\theta} \in \Theta} \epsilon^{(k)}(\boldsymbol{\theta})] \stackrel{(a)}{\leq} \frac{C_{\text{gr}}}{K_{\max}} \sum_{k=0}^{K_{\max}-1} \mathbb{E}\left[\frac{1}{n} \sum_{i=1}^n M_{(\tau_i^k)}^{-1/2}\right] \\ &\stackrel{(b)}{\leq} \frac{C_{\text{gr}}}{K_{\max}} \sum_{k=0}^{K_{\max}-1} M_{(k)}^{-1/2} \end{aligned}$$

406 where (a) is due to H4 and (b) is due to (24). This implies

$$\mathbb{E}[g_-^{(K)}] \leq \sqrt{\frac{\Delta(K_{\max})}{K_{\max}}} + \frac{C_{\text{gr}}}{K_{\max}} \sum_{k=0}^{K_{\max}-1} M_{(k)}^{-1/2},$$

407 and concludes the proof of the theorem.  $\square$



## B Proof of Theorem 2

**Theorem.** Under H1-H4. 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 almost surely to zero, i.e.,  $\lim_{k \rightarrow \infty} g_{-}(\boldsymbol{\theta}^{(k)}) = 0$  a.s..
2. the objective value  $\mathcal{L}(\boldsymbol{\theta}^{(k)})$  converges almost surely to a finite number  $\underline{\mathcal{L}}$ , i.e.,  $\lim_{k \rightarrow \infty} \mathcal{L}(\boldsymbol{\theta}^{(k)}) = \underline{\mathcal{L}}$  a.s..

**Proof** We apply the following auxiliary lemma which proof can be found in Appendix C for the readability of the current proof:

**Lemma 1.** Let  $(V_k)_{k \geq 0}$  be a non negative sequence of random variables such that  $\mathbb{E}[V_0] < \infty$ . Let  $(X_k)_{k \geq 0}$  a non negative sequence of random variables and  $(E_k)_{k \geq 0}$  be a sequence of random variables such that  $\sum_{k=0}^{\infty} \mathbb{E}[|E_k|] < \infty$ . If for any  $k \geq 1$ :

$$V_k \leq V_{k-1} - X_{k-1} + E_{k-1} \quad (27)$$

then:

(i) for all  $k \geq 0$ ,  $\mathbb{E}[V_k] < \infty$  and the sequence  $(V_k)_{k \geq 0}$  converges a.s. to a finite limit  $V_{\infty}$ .

(ii) the sequence  $(\mathbb{E}[V_k])_{k \geq 0}$  converges and  $\lim_{k \rightarrow \infty} \mathbb{E}[V_k] = \mathbb{E}[V_{\infty}]$ .

(iii) the series  $\sum_{k=0}^{\infty} X_k$  converges almost surely and  $\sum_{k=0}^{\infty} \mathbb{E}[X_k] < \infty$ .

We proceed from (19) by re-arranging terms and observing that

$$\begin{aligned} \widehat{\mathcal{L}}^{(k+1)}(\boldsymbol{\theta}^{(k+1)}) &\leq \widehat{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)}) - \frac{1}{n} (\widehat{\mathcal{L}}_{i_k}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(\tau_{i_k}^k)}) - \widehat{\mathcal{L}}_{i_k}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(k)})) \\ &\quad - (\widetilde{\mathcal{L}}^{(k+1)}(\boldsymbol{\theta}^{(k+1)}) - \widehat{\mathcal{L}}^{(k+1)}(\boldsymbol{\theta}^{(k+1)})) + (\widetilde{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)}) - \widehat{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)})) \\ &\quad + \frac{1}{n} (\widetilde{\mathcal{L}}_{i_k}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(k)}, \{z_{i_k, m}^{(k)}\}_{m=1}^{M_{(k)}}) - \widehat{\mathcal{L}}_{i_k}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(k)})) \\ &\quad + \frac{1}{n} (\widehat{\mathcal{L}}_{i_k}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(\tau_{i_k}^k)}) - \widetilde{\mathcal{L}}_{i_k}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(\tau_{i_k}^k)}, \{z_{i_k, m}^{(\tau_{i_k}^k)}\}_{m=1}^{M_{(\tau_{i_k}^k)}})) \end{aligned}$$

Our idea is to apply Lemma 1. Under H1, the finite sum of surrogate functions  $\widehat{\mathcal{L}}^{(k)}(\boldsymbol{\theta})$ , defined in (15), is lower bounded by a constant  $c_k > -\infty$  for any  $\boldsymbol{\theta}$ . To this end, we observe that

$$V_k := \widehat{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)}) - \inf_{k \geq 0} c_k \geq 0 \quad (28)$$

is a non-negative random variable.

Secondly, under H1, the following random variable is non-negative

$$X_k := \frac{1}{n} (\widehat{\mathcal{L}}_{i_k}(\boldsymbol{\theta}^{(\tau_{i_k}^k)}; \boldsymbol{\theta}^{(k)}) - \widehat{\mathcal{L}}_{i_k}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(k)})) \geq 0. \quad (29)$$

Thirdly, we define

$$\begin{aligned} E_k &= -(\widetilde{\mathcal{L}}^{(k+1)}(\boldsymbol{\theta}^{(k+1)}) - \widehat{\mathcal{L}}^{(k+1)}(\boldsymbol{\theta}^{(k+1)})) + (\widetilde{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)}) - \widehat{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)})) \\ &\quad + \frac{1}{n} (\widetilde{\mathcal{L}}_{i_k}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(k)}, \{z_{i_k, m}^{(k)}\}_{m=1}^{M_{(k)}}) - \widehat{\mathcal{L}}_{i_k}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(k)})) \\ &\quad + \frac{1}{n} (\widehat{\mathcal{L}}_{i_k}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(\tau_{i_k}^k)}) - \widetilde{\mathcal{L}}_{i_k}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(\tau_{i_k}^k)}, \{z_{i_k, m}^{(\tau_{i_k}^k)}\}_{m=1}^{M_{(\tau_{i_k}^k)}})). \end{aligned} \quad (30)$$

Note that from the definitions (28), (29), (30), we have  $V_{k+1} \leq V_k - X_k + E_k$  for any  $k \geq 1$ .

Under H4, we observe that

$$\mathbb{E}[|\widetilde{\mathcal{L}}_{i_k}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(k)}, \{z_{i_k, m}^{(k)}\}_{m=1}^{M_{(k)}}) - \widehat{\mathcal{L}}_{i_k}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(k)})|] \leq C_r M_{(k)}^{-1/2}$$

$$\mathbb{E} \left[ \left| \widehat{\mathcal{L}}_{i_k}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(\tau_{i_k}^k)}) - \widetilde{\mathcal{L}}_{i_k}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(\tau_{i_k}^k)}, \{z_{i_k, m}^{(\tau_{i_k}^k)}\}_{m=1}^{M_{(\tau_{i_k}^k)}}) \right| \right] \leq C_r \mathbb{E} \left[ M_{(\tau_{i_k}^k)}^{-1/2} \right]$$

$$\mathbb{E} \left[ |\widetilde{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)}) - \widehat{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)})| \right] \leq \frac{1}{n} \sum_{i=1}^n C_r \mathbb{E} \left[ M_{(\tau_i^k)}^{-1/2} \right]$$

Therefore,

$$\mathbb{E} [|E_k|] \leq \frac{C_r}{n} \left( M_{(k)}^{-1/2} + \mathbb{E} \left[ M_{(\tau_{i_k}^k)}^{-1/2} + \sum_{i=1}^n \{ M_{(\tau_i^k)}^{-1/2} + M_{(\tau_{i+1}^k)}^{-1/2} \} \right] \right)$$

Using (24) and the assumption on the sequence  $\{M_{(k)}\}_{k \geq 0}$ , we obtain that

$$\sum_{k=0}^{\infty} \mathbb{E} [|E_k|] < \frac{C_r}{n} (2 + 2n) \sum_{k=0}^{\infty} M_{(k)}^{-1/2} < \infty.$$

Therefore, the conclusions in Lemma 1 hold. Precisely, we have  $\sum_{k=0}^{\infty} X_k < \infty$  and

$\sum_{k=0}^{\infty} \mathbb{E} [X_k] < \infty$  almost surely. Note that this implies

$$\begin{aligned} \infty &> \sum_{k=0}^{\infty} \mathbb{E} [X_k] = \frac{1}{n} \sum_{k=0}^{\infty} \mathbb{E} [\widehat{\mathcal{L}}_{i_k}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(\tau_{i_k}^k)}) - \widehat{\mathcal{L}}_{i_k}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(k)})] \\ &= \frac{1}{n} \sum_{k=0}^{\infty} \mathbb{E} [\widehat{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)}) - \mathcal{L}(\boldsymbol{\theta}^{(k)})] = \frac{1}{n} \sum_{k=0}^{\infty} \mathbb{E} [\widehat{e}^{(k)}(\boldsymbol{\theta}^{(k)})] \end{aligned}$$

Since  $\widehat{e}^{(k)}(\boldsymbol{\theta}^{(k)}) \geq 0$ , the above implies

$$\lim_{k \rightarrow \infty} \widehat{e}^{(k)}(\boldsymbol{\theta}^{(k)}) = 0 \quad \text{a.s.} \quad (31)$$

and subsequently applying (18), we have  $\lim_{k \rightarrow \infty} \|\widehat{e}^{(k)}(\boldsymbol{\theta}^{(k)})\| = 0$  almost surely. Finally, it follows from (18) and (26) that

$$\lim_{k \rightarrow \infty} g_-^{(k)} \leq \lim_{k \rightarrow \infty} \sqrt{2L} \sqrt{\widehat{e}^{(k)}(\boldsymbol{\theta}^{(k)})} + \lim_{k \rightarrow \infty} \sup_{\boldsymbol{\theta} \in \Theta} |\epsilon^{(k)}(\boldsymbol{\theta})| = 0, \quad (32)$$

where the last equality holds almost surely due to the fact that  $\sum_{k=0}^{\infty} \mathbb{E} [\sup_{\boldsymbol{\theta} \in \Theta} |\epsilon^{(k)}(\boldsymbol{\theta})|] < \infty$ . This concludes the asymptotic convergence of the MISSO method.

Finally, we prove that  $\mathcal{L}(\boldsymbol{\theta}^{(k)})$  converges almost surely. As a consequence of Lemma 1, it is clear that  $\{V_k\}_{k \geq 0}$  converges almost surely and so is  $\{\widehat{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)})\}_{k \geq 0}$ , i.e., we have  $\lim_{k \rightarrow \infty} \widehat{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)}) = \underline{\mathcal{L}}$ . Applying (31) implies that

$$\underline{\mathcal{L}} = \lim_{k \rightarrow \infty} \widehat{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)}) = \lim_{k \rightarrow \infty} \mathcal{L}(\boldsymbol{\theta}^{(k)}) \quad \text{a.s.}$$

This shows that  $\mathcal{L}(\boldsymbol{\theta}^{(k)})$  converges almost surely to  $\underline{\mathcal{L}}$ .  $\square$

## C Proof of Lemma 1

**Lemma.** Let  $(V_k)_{k \geq 0}$  be a non negative sequence of random variables such that  $\mathbb{E}[V_0] < \infty$ . Let  $(X_k)_{k \geq 0}$  a non negative sequence of random variables and  $(E_k)_{k \geq 0}$  be a sequence of random variables such that  $\sum_{k=0}^{\infty} \mathbb{E}[|E_k|] < \infty$ . If for any  $k \geq 1$ :

$$V_k \leq V_{k-1} - X_{k-1} + E_{k-1}$$

then:

(i) for all  $k \geq 0$ ,  $\mathbb{E}[V_k] < \infty$  and the sequence  $(V_k)_{k \geq 0}$  converges a.s. to a finite limit  $V_{\infty}$ .

(ii) the sequence  $(\mathbb{E}[V_k])_{k \geq 0}$  converges and  $\lim_{k \rightarrow \infty} \mathbb{E}[V_k] = \mathbb{E}[V_{\infty}]$ .

(iii) the series  $\sum_{k=0}^{\infty} X_k$  converges almost surely and  $\sum_{k=0}^{\infty} \mathbb{E}[X_k] < \infty$ .

455 **Proof** We first show that for all  $k \geq 0$ ,  $\mathbb{E}[V_k] < \infty$ . Note indeed that:

$$0 \leq V_k \leq V_0 - \sum_{j=1}^k X_j + \sum_{j=1}^k E_j \leq V_0 + \sum_{j=1}^k E_j \quad (33)$$

456 showing that  $\mathbb{E}[V_k] \leq \mathbb{E}[V_0] + \mathbb{E}\left[\sum_{j=1}^k E_j\right] < \infty$ .

457 Since  $0 \leq X_k \leq V_{k-1} - V_k + E_k$  we also obtain for all  $k \geq 0$ ,  $\mathbb{E}[X_k] < \infty$ . Moreover, since

458  $\mathbb{E}\left[\sum_{j=1}^{\infty} |E_j|\right] < \infty$ , the series  $\sum_{j=1}^{\infty} E_j$  converges a.s. We may therefore define:

$$W_k = V_k + \sum_{j=k+1}^{\infty} E_j \quad (34)$$

459 Note that  $\mathbb{E}[|W_k|] \leq \mathbb{E}[V_k] + \mathbb{E}\left[\sum_{j=k+1}^{\infty} |E_j|\right] < \infty$ . For all  $k \geq 1$ , we get:

$$\begin{aligned} W_k &\leq V_{k-1} - X_k + \sum_{j=k}^{\infty} E_j \leq W_{k-1} - X_k \leq W_{k-1} \\ \mathbb{E}[W_k] &\leq \mathbb{E}[W_{k-1}] - \mathbb{E}[X_k] \end{aligned} \quad (35)$$

460 Hence the sequences  $(W_k)_{k \geq 0}$  and  $(\mathbb{E}[W_k])_{k \geq 0}$  are non increasing. Since for all  $k \geq 0$ ,  $W_k \geq$

461  $-\sum_{j=1}^{\infty} |E_j| > -\infty$  and  $\mathbb{E}[W_k] \geq -\sum_{j=1}^{\infty} \mathbb{E}[|E_j|] > -\infty$ , the (random) sequence  $(W_k)_{k \geq 0}$

462 converges a.s. to a limit  $W_{\infty}$  and the (deterministic) sequence  $(\mathbb{E}[W_k])_{k \geq 0}$  converges to a limit  $w_{\infty}$ .

463 Since  $|W_k| \leq V_0 + \sum_{j=1}^{\infty} |E_j|$ , the Fatou lemma implies that:

$$\mathbb{E}[\liminf_{k \rightarrow \infty} |W_k|] = \mathbb{E}[|W_{\infty}|] \leq \liminf_{k \rightarrow \infty} \mathbb{E}[|W_k|] \leq \mathbb{E}[V_0] + \sum_{j=1}^{\infty} \mathbb{E}[|E_j|] < \infty \quad (36)$$

464 showing that the random variable  $W_{\infty}$  is integrable.

465 In the sequel, set  $U_k \triangleq W_0 - W_k$ . By construction we have for all  $k \geq 0$ ,  $U_k \geq 0$ ,  $U_k \leq U_{k+1}$  and

466  $\mathbb{E}[U_k] \leq \mathbb{E}[|W_0|] + \mathbb{E}[|W_k|] < \infty$  and by the monotone convergence theorem, we get:

$$\lim_{k \rightarrow \infty} \mathbb{E}[U_k] = \mathbb{E}[\lim_{k \rightarrow \infty} U_k] \quad (37)$$

467 Finally, we have:

$$\lim_{k \rightarrow \infty} \mathbb{E}[U_k] = \mathbb{E}[W_0] - w_{\infty} \quad \text{and} \quad \mathbb{E}[\lim_{k \rightarrow \infty} U_k] = \mathbb{E}[W_0] - \mathbb{E}[W_{\infty}] \quad (38)$$

468 showing that  $\mathbb{E}[W_{\infty}] = w_{\infty}$  and concluding the proof of (ii). Moreover, using (35) we have that

469  $W_k \leq W_{k-1} - X_k$  which yields:

$$\begin{aligned} \sum_{j=1}^{\infty} X_j &\leq W_0 - W_{\infty} < \infty \\ \sum_{j=1}^{\infty} \mathbb{E}[X_j] &\leq \mathbb{E}[W_0] - w_{\infty} < \infty \end{aligned} \quad (39)$$

470 which concludes the proof of the lemma.  $\square$

## 471 D Details about the Numerical Experiments

### 472 D.1 Binary Logistic Regression on the Traumabase

#### 473 D.1.1 Traumabase quantitative variables

474 The list of the 16 quantitative variables we use in our experiments are as follows — *age, weight,*  
 475 *height, BMI (Body Mass Index), the Glasgow Coma Scale, the Glasgow Coma Scale motor com-*  
 476 *ponent, the minimum systolic blood pressure, the minimum diastolic blood pressure, the maximum*  
 477 *number of heart rate (or pulse) per unit time (usually a minute), the systolic blood pressure at ar-*  
 478 *rival of ambulance, the diastolic blood pressure at arrival of ambulance, the heart rate at arrival*  
 479 *of ambulance, the capillary Hemoglobin concentration, the oxygen saturation, the fluid expansion*  
 480 *colloids, the fluid expansion cristalloids, the pulse pressure for the minimum value of diastolic and*  
 481 *systolic blood pressure, the pulse pressure at arrival of ambulance.*

#### 482 D.1.2 Metropolis-Hastings algorithm

483 During the simulation step of the MISSO method, the sampling from the target distribution  
 484  $\pi(z_{i,\text{mis}}; \theta) := p(z_{i,\text{mis}} | z_{i,\text{obs}}, y_i; \theta)$  is performed using a Metropolis-Hastings (MH) algo-  
 485 rithm [Meyn and Tweedie, 2012] with proposal distribution  $q(z_{i,\text{mis}}; \delta) := p(z_{i,\text{mis}} | z_{i,\text{obs}}; \delta)$  where  
 486  $\theta = (\beta, \Omega)$  and  $\delta = (\xi, \Sigma)$ . The parameters of the Gaussian conditional distribution of  $z_{i,\text{mis}} | z_{i,\text{obs}}$   
 487 read:

$$\begin{aligned}\xi &= \beta_{\text{mis}} + \Omega_{\text{mis},\text{obs}} \Omega_{\text{obs},\text{obs}}^{-1} (z_{i,\text{obs}} - \beta_{\text{obs}}) , \\ \Sigma &= \Omega_{\text{mis},\text{mis}} + \Omega_{\text{mis},\text{obs}} \Omega_{\text{obs},\text{obs}}^{-1} \Omega_{\text{obs},\text{mis}}\end{aligned}$$

488 where we have used the Schur Complement of  $\Omega_{\text{obs},\text{obs}}$  in  $\Omega$  and noted  $\beta_{\text{mis}}$  (resp.  $\beta_{\text{obs}}$ ) the missing  
 489 (resp. observed) elements of  $\beta$ . The MH algorithm is summarized in Algorithm 3.

---

#### Algorithm 3 MH algorithm

---

```

1: Input: initialization  $z_{i,\text{mis},0} \sim q(z_{i,\text{mis}}; \delta)$ 
2: for  $m = 1, \dots, M$  do
3:   Sample  $z_{i,\text{mis},m} \sim q(z_{i,\text{mis}}; \delta)$ 
4:   Sample  $u \sim \mathcal{U}([0, 1])$ 
5:   Calculate the ratio  $r = \frac{\pi(z_{i,\text{mis},m}; \theta) / q(z_{i,\text{mis},m}; \delta)}{\pi(z_{i,\text{mis},m-1}; \theta) / q(z_{i,\text{mis},m-1}; \delta)}$ 
6:   if  $u < r$  then
7:     Accept  $z_{i,\text{mis},m}$ 
8:   else
9:      $z_{i,\text{mis},m} \leftarrow z_{i,\text{mis},m-1}$ 
10:  end if
11: end for
12: Output:  $z_{i,\text{mis},M}$ 

```

---

#### 490 D.1.3 MISSO Update

491 **Choice of surrogate function for MISO:** We recall the MISO deterministic surrogate defined in  
 492 (7):

$$\hat{\mathcal{L}}_i(\theta; \bar{\theta}) = \int_{\mathcal{Z}} \log(p_i(z_{i,\text{mis}}, \bar{\theta}) / f_i(z_{i,\text{mis}}, \theta)) p_i(z_{i,\text{mis}}, \bar{\theta}) \mu_i(dz_i) .$$

493 where  $\theta = (\delta, \beta, \Omega)$  and  $\bar{\theta} = (\bar{\delta}, \bar{\beta}, \bar{\Omega})$ . We adapt it to our missing covariates problem and decom-  
 494 pose the surrogate function defined above into an observed and a missing part.

495 **Surrogate function decomposition** We adapt it to our missing covariates problem and decompose  
 496 the term depending on  $\theta$ , while  $\bar{\theta}$  is fixed, in two following parts leading to

$$\begin{aligned}
 \hat{\mathcal{L}}_i(\theta; \bar{\theta}) &= - \int_{\mathbf{Z}} \log f_i(z_{i,\text{mis}}, z_{i,\text{obs}}, \theta) p_i(z_{i,\text{mis}}, \bar{\theta}) \mu_i(dz_{i,\text{mis}}) \\
 &= - \int_{\mathbf{Z}} \log [p_i(y_i | z_{i,\text{mis}}, z_{i,\text{obs}}, \delta) p_i(z_{i,\text{mis}}, \beta, \Omega)] p_i(z_i, \bar{\theta}) \mu_i(dz_{i,\text{mis}}) \\
 &= - \underbrace{\int_{\mathbf{Z}} \log p_i(y_i | z_{i,\text{mis}}, z_{i,\text{obs}}, \delta) p_i(z_i, \bar{\theta}) \mu_i(dz_{i,\text{mis}})}_{=\hat{\mathcal{L}}_i^{(1)}(\delta, \bar{\theta})} - \underbrace{\int_{\mathbf{Z}} \log p_i(z_{i,\text{mis}}, \beta, \Omega) p_i(z_i, \bar{\theta}) \mu_i(dz_{i,\text{mis}})}_{=\hat{\mathcal{L}}_i^{(2)}(\beta, \Omega, \bar{\theta})}
 \end{aligned} \tag{40}$$

497 The mean  $\beta$  and the covariance  $\Omega$  of the latent structure can be estimated minimizing the sum of  
 498 MISSO surrogates  $\tilde{\mathcal{L}}_i^{(2)}(\beta, \Omega, \bar{\theta}, \{z_m\}_{m=1}^M)$ , defined as MC approximation of  $\hat{\mathcal{L}}_i^{(2)}(\beta, \Omega, \bar{\theta})$ , for all  
 499  $i \in \llbracket n \rrbracket$ , in closed-form expression.

500 We thus keep the surrogate  $\hat{\mathcal{L}}_i^{(2)}(\beta, \Omega, \bar{\theta})$  as it is, and consider the following quadratic approximation  
 501 of  $\hat{\mathcal{L}}_i^{(1)}(\delta, \bar{\theta})$  to estimate the vector of logistic parameters  $\delta$ :

$$\begin{aligned}
 \hat{\mathcal{L}}_i^{(1)}(\bar{\delta}, \bar{\theta}) &- \int_{\mathbf{Z}} \nabla \log p_i(y_i | z_{i,\text{mis}}, z_{i,\text{obs}}, \delta) \big|_{\delta=\bar{\delta}} p_i(z_{i,\text{mis}}, \bar{\theta}) \mu_i(dz_{i,\text{mis}}) (\delta - \bar{\delta}) \\
 &- (\delta - \bar{\delta})/2 \int_{\mathbf{Z}} \nabla^2 \log p_i(y_i | z_{i,\text{mis}}, z_{i,\text{obs}}, \delta) p_i(z_{i,\text{mis}}, \bar{\theta}) p_i(z_{i,\text{mis}}, \bar{\theta}) \mu_i(dz_{i,\text{mis}}) (\delta - \bar{\delta})^\top
 \end{aligned}$$

502 Recall that:

$$\begin{aligned}
 \nabla \log p_i(y_i | z_{i,\text{mis}}, z_{i,\text{obs}}, \delta) &= z_i (y_i - S(\delta^\top z_i)) \\
 \nabla^2 \log p_i(y_i | z_{i,\text{mis}}, z_{i,\text{obs}}, \delta) &= -z_i z_i^\top \dot{S}(\delta^\top z_i)
 \end{aligned}$$

503 where  $\dot{S}(u)$  is the derivative of  $S(u)$ . Note that  $\dot{S}(u) \leq 1/4$  and since, for all  $i \in \llbracket n \rrbracket$ , the  $p \times p$   
 504 matrix  $z_i z_i^\top$  is semi-definite positive we can assume:

505 **L1.** For all  $i \in \llbracket n \rrbracket$  and  $\epsilon > 0$ , there exist, for all  $z_i \in \mathbf{Z}$ , a positive definite matrix  $H_i(z_i) :=$   
 506  $\frac{1}{4}(z_i z_i^\top + \epsilon I_d)$  such that for all  $\delta \in \mathbb{R}^p$ ,  $-z_i z_i^\top \dot{S}(\delta^\top z_i) \leq H_i(z_i)$ .

507 Then, we use, for all  $i \in \llbracket n \rrbracket$ , the following surrogate function to estimate  $\delta$ :

$$\bar{\mathcal{L}}_i^{(1)}(\delta, \bar{\theta}) = \hat{\mathcal{L}}_i^{(1)}(\bar{\delta}, \bar{\theta}) - D_i^\top (\delta - \bar{\delta}) + \frac{1}{2} (\delta - \bar{\delta}) H_i (\delta - \bar{\delta})^\top \tag{41}$$

508 where:

$$\begin{aligned}
 D_i &= \int_{\mathbf{Z}} \nabla \log p_i(y_i | z_{i,\text{mis}}, z_{i,\text{obs}}, \delta) \big|_{\delta=\bar{\delta}} p_i(z_{i,\text{mis}}, \bar{\theta}) \mu_i(dz_{i,\text{mis}}) \\
 H_i &= \int_{\mathbf{Z}} H_i(z_{i,\text{mis}}) p_i(z_{i,\text{mis}}, \bar{\theta}) \mu_i(dz_{i,\text{mis}})
 \end{aligned}$$

509 Finally, at iteration  $k$ , the total surrogate is:

$$\begin{aligned}
 \tilde{\mathcal{L}}^{(k)}(\theta) &= \frac{1}{n} \sum_{i=1}^n \tilde{\mathcal{L}}_i(\theta, \theta^{(\tau_i^k)}, \{z_{i,m}\}_{m=1}^{M(\tau_i^k)}) \\
 &= \frac{1}{n} \sum_{i=1}^n \tilde{\mathcal{L}}_i^{(2)}(\beta, \Omega, \theta^{(\tau_i^k)}, \{z_{i,m}\}_{m=1}^{M(\tau_i^k)}) - \frac{1}{n} \sum_{i=1}^n \bar{D}_i^{(\tau_i^k)} (\delta - \delta^{(\tau_i^k)}) \\
 &\quad + \frac{1}{2n} \sum_{i=1}^n (\delta - \delta^{(\tau_i^k)}) \left\{ \tilde{H}_i^{(\tau_i^k)} \right\} (\delta - \delta^{(\tau_i^k)})^\top
 \end{aligned} \tag{42}$$



510 where for all  $i \in \llbracket n \rrbracket$ :

$$\begin{aligned}\tilde{D}_i^{(\tau_i^k)} &= \frac{1}{M_{(\tau_i^k)}} \sum_{m=1}^{M_{(\tau_i^k)}} z_{i,m}^{(\tau_i^k)} \left( y_i - S(\left( \delta^{(\tau_i^k)} \right)^\top z_{i,m}^{(\tau_i^k)}) \right) \\ \tilde{H}_i^{(\tau_i^k)} &= \frac{1}{4M_{(\tau_i^k)}} \sum_{m=1}^{M_{(\tau_i^k)}} z_{i,m}^{(\tau_i^k)} (z_{i,m}^{(\tau_i^k)})^\top\end{aligned}$$

511 Minimizing the total surrogate (42) boils down to performing a quasi-Newton step. It is perhaps sen-  
512 sible to apply some diagonal loading which is perfectly compatible with the surrogate interpretation  
513 we just gave.

514 The logistic parameters are estimated as follows:

$$\delta^{(k)} = \arg \min_{\delta \in \Theta} \frac{1}{n} \sum_{i=1}^n \tilde{\mathcal{L}}_i^{(1)}(\delta, \theta^{(\tau_i^k)}, \{z_{i,m}\}_{m=1}^{M_{(\tau_i^k)}})$$

515 where  $\tilde{\mathcal{L}}_i^{(1)}(\delta, \theta^{(\tau_i^k)}, \{z_{i,m}\}_{m=1}^{M_{(\tau_i^k)}})$  is the MC approximation of the MISO surrogate defined in  
516 (41) and which leads to the following quasi-Newton step:

$$\delta^{(k)} = \frac{1}{n} \sum_{i=1}^n \delta^{(\tau_i^k)} - (\tilde{H}^{(k)})^{-1} \tilde{D}^{(k)}$$

517 with  $\tilde{D}^{(k)} = \frac{1}{n} \sum_{i=1}^n \tilde{D}_i^{(\tau_i^k)}$  and  $\tilde{H}^{(k)} = \frac{1}{n} \sum_{i=1}^n \tilde{H}_i^{(\tau_i^k)}$ .

518 **MISSO updates:** At the  $k$ -th iteration, and after the initialization, for all  $i \in \llbracket n \rrbracket$ , of the latent  
519 variables  $(z_i^{(0)})$ , the MISSO algorithm consists in picking an index  $i_k$  uniformly on  $\llbracket n \rrbracket$ , complet-  
520 ing the observations by sampling a Monte Carlo batch  $\{z_{i_k, \text{mis}, m}^{(k)}\}_{m=1}^{M_{(k)}}$  of missing values from the  
521 conditional distribution  $p(z_{i_k, \text{mis}} | z_{i_k, \text{obs}}, y_{i_k}; \theta^{(k-1)})$  using an MCMC sampler and computing the  
522 estimated parameters as follows:

$$\begin{aligned}\beta^{(k)} &= \arg \min_{\beta \in \Theta} \frac{1}{n} \sum_{i=1}^n \tilde{\mathcal{L}}_i^{(2)}(\beta, \Omega^{(k)}, \theta^{(\tau_i^k)}, \{z_{i,m}\}_{m=1}^{M_{(\tau_i^k)}}) = \frac{1}{n} \sum_{i=1}^n \frac{1}{M_{(\tau_i^k)}} \sum_{m=1}^{M_{(\tau_i^k)}} z_{i,m}^{(k)} \\ \Omega^{(k)} &= \arg \min_{\Omega \in \Theta} \frac{1}{n} \sum_{i=1}^n \tilde{\mathcal{L}}_i^{(2)}(\beta^{(k)}, \Omega, \theta^{(\tau_i^k)}, \{z_{i,m}\}_{m=1}^{M_{(\tau_i^k)}}) = \frac{1}{n} \sum_{i=1}^n \frac{1}{M_{(\tau_i^k)}} \sum_{m=1}^{M_{(\tau_i^k)}} w_{i,m}^{(k)} \\ \delta^{(k)} &= \frac{1}{n} \sum_{i=1}^n \delta^{(\tau_i^k)} - (\tilde{H}^{(k)})^{-1} \tilde{D}^{(k)}.\end{aligned}\tag{43}$$

523 where  $z_{i,m}^{(k)} = (z_{i, \text{mis}, m}^{(k)}, z_{i, \text{obs}})$  is composed of a simulated and an observed part,  $\tilde{D}^{(k)} =$   
524  $\frac{1}{n} \sum_{i=1}^n \tilde{D}_i^{(\tau_i^k)}$ ,  $\tilde{H}^{(k)} = \frac{1}{n} \sum_{i=1}^n \tilde{H}_i^{(\tau_i^k)}$  and  $w_{i,m}^{(k)} = z_{i,m}^{(k)} (z_{i,m}^{(k)})^\top - \beta^{(k)} (\beta^{(k)})^\top$ . Be-  
525 sides,  $\tilde{\mathcal{L}}_i^{(1)}(\beta, \Omega, \bar{\theta}, \{z_m\}_{m=1}^M)$  and  $\tilde{\mathcal{L}}_i^{(2)}(\beta, \Omega, \bar{\theta}, \{z_m\}_{m=1}^M)$  are defined as MC approximation of  
526  $\hat{\mathcal{L}}_i^{(1)}(\beta, \Omega, \bar{\theta})$  and  $\hat{\mathcal{L}}_i^{(2)}(\beta, \Omega, \bar{\theta})$ , for all  $i \in \llbracket n \rrbracket$  as components of the surrogate function (40).

## 527 D.2 Incremental Variational Inference

### 528 D.2.1 Bayesian LeNet-5 Architecture

529 We describe in Table 1 the architecture of the Convolutional Neural Network introduced in [LeCun  
530 et al., 1998] and trained on MNIST:

layer type	width	stride	padding	input shape	nonlinearity
convolution ( $5 \times 5$ )	6	1	0	$1 \times 32 \times 32$	ReLU
max-pooling ( $2 \times 2$ )		2	0	$6 \times 28 \times 28$	
convolution ( $5 \times 5$ )	6	1	0	$1 \times 14 \times 14$	ReLU
max-pooling ( $2 \times 2$ )		2	0	$16 \times 10 \times 10$	
fully-connected	120			400	ReLU
fully-connected	84			120	ReLU
fully-connected	10			84	

Table 1: LeNet-5 architecture

### 531 D.2.2 Bayesian ResNet-18 Architecture

532 We describe in Table 2 the architecture of the Resnet-18 we train on CIFAR-10:

layer type	Output Size	ResNet-18	nonlinearity
conv1	$112 \times 112 \times 64$	$7 \times 7, 64$ , stride 2	ReLU
conv2x	$56 \times 56 \times 64$	$\begin{pmatrix} 3 \times 3, 64 \\ 3 \times 3, 64 \end{pmatrix} \times 2$	ReLU
conv3x	$28 \times 28 \times 128$	$\begin{pmatrix} 3 \times 3, 128 \\ 3 \times 3, 128 \end{pmatrix} \times 2$	ReLU
conv4x	$14 \times 14 \times 256$	$\begin{pmatrix} 3 \times 3, 256 \\ 3 \times 3, 256 \end{pmatrix} \times 2$	ReLU
conv5x	$7 \times 7 \times 512$	$\begin{pmatrix} 3 \times 3, 512 \\ 3 \times 3, 512 \end{pmatrix} \times 2$	ReLU
average pool	$1 \times 1 \times 512$	$7 \times 7$ average pool	ReLU
fully connected	1000	$512 \times 1000$ fully connections	
softmax	1000		

Table 2: ResNet-18 architecture

### 533 D.2.3 Algorithms updates

534 First, we initialize the means  $\mu_\ell^{(0)}$  for  $\ell \in \llbracket d \rrbracket$  and variance estimates  $\sigma^{(0)}$ . At iteration  $k$ , minimizing  
535 the sum of stochastic surrogates defined as in (6) and (13) yields the following MISSO update —  
536 **step (i)** pick a function index  $i_k$  uniformly on  $\llbracket n \rrbracket$ ; **step (ii)** sample a Monte Carlo batch  $\{z_m^{(k)}\}_{m=1}^{M(k)}$   
537 from  $\mathcal{N}(0, \mathbf{I})$ ; and **step (iii)** update the parameters as

$$\mu_\ell^{(k)} = \frac{1}{n} \sum_{i=1}^n \mu_\ell^{(\tau_i^k)} - \frac{\gamma}{n} \sum_{i=1}^n \hat{\delta}_{\mu_\ell, i}^{(k)} \quad \text{and} \quad \sigma^{(k)} = \frac{1}{n} \sum_{i=1}^n \sigma^{(\tau_i^k)} - \frac{\gamma}{n} \sum_{i=1}^n \hat{\delta}_{\sigma, i}^{(k)}, \quad (44)$$

538 where we define the following gradient terms for all  $i \in \llbracket 1, n \rrbracket$ :

$$\begin{aligned} \hat{\delta}_{\mu_\ell, i}^{(k)} &= -\frac{1}{M(k)} \sum_{m=1}^{M(k)} \nabla_w \log p(y_i | x_i, w) \Big|_{w=t(\theta^{(k-1)}, z_m^{(k)})} + \nabla_{\mu_\ell} d(\theta^{(k-1)}), \\ \hat{\delta}_{\sigma, i}^{(k)} &= -\frac{1}{M(k)} \sum_{m=1}^{M(k)} z_m^{(k)} \nabla_w \log p(y_i | x_i, w) \Big|_{w=t(\theta^{(k-1)}, z_m^{(k)})} + \nabla_{\sigma} d(\theta^{(k-1)}). \end{aligned} \quad (45)$$

539 For all benchmark algorithms, we pick, at iteration  $k$ , a function index  $i_k$  uniformly on  $\llbracket n \rrbracket$  and  
540 sample a Monte Carlo batch  $\{z_m^{(k)}\}_{m=1}^{M(k)}$  from the standard Gaussian distribution. The updates of the  
541 parameters  $\mu_\ell$  for all  $\ell \in \llbracket d \rrbracket$  and  $\sigma$  break down as follows:

542 **Monte Carlo SAG update:** Set

$$\mu_\ell^{(k)} = \mu_\ell^{(k-1)} - \frac{\gamma}{n} \sum_{i=1}^n \hat{\delta}_{\mu_\ell, i}^{(k)} \quad \text{and} \quad \sigma^{(k)} = \sigma^{(k-1)} - \frac{\gamma}{n} \sum_{i=1}^n \hat{\delta}_{\sigma, i}^{(k)},$$

543 where  $\hat{\delta}_{\mu_\ell, i}^{(k)} = \hat{\delta}_{\mu_\ell, i}^{(k-1)}$  and  $\hat{\delta}_{\sigma, i}^{(k)} = \hat{\delta}_{\sigma, i}^{(k-1)}$  for  $i \neq i_k$  and are defined by (45) for  $i = i_k$ . The learning  
 544 rate is set to  $\gamma = 10^{-3}$ .

545 **Bayes By Backprop update:** Set

$$\mu_\ell^{(k)} = \mu_\ell^{(k-1)} - \frac{\gamma}{n} \hat{\delta}_{\mu_\ell, i_k}^{(k)} \quad \text{and} \quad \sigma^{(k)} = \sigma^{(k-1)} - \frac{\gamma}{n} \hat{\delta}_{\sigma, i_k}^{(k)},$$

546 where the learning rate  $\gamma = 10^{-3}$ .

547 **Monte Carlo Momentum update:** Set

$$\mu_\ell^{(k)} = \mu_\ell^{(k-1)} + \hat{\mathbf{v}}_{\mu_\ell}^{(k)} \quad \text{and} \quad \sigma^{(k)} = \sigma^{(k-1)} + \hat{\mathbf{v}}_\sigma^{(k)},$$

548 where

$$\hat{\mathbf{v}}_{\mu_\ell, i}^{(k)} = \alpha \hat{\mathbf{v}}_{\mu_\ell}^{(k-1)} - \frac{\gamma}{n} \hat{\delta}_{\mu_\ell, i_k}^{(k)} \quad \text{and} \quad \hat{\mathbf{v}}_\sigma^{(k)} = \alpha \hat{\mathbf{v}}_\sigma^{(k-1)} - \frac{\gamma}{n} \hat{\delta}_{\sigma, i_k}^{(k)},$$

549 where  $\alpha$  and  $\gamma$ , respectively the momentum and the learning rates, are set to  $10^{-3}$ .

550 **Monte Carlo ADAM update:** Set

$$\mu_\ell^{(k)} = \mu_\ell^{(k-1)} - \frac{\gamma}{n} \hat{\mathbf{m}}_{\mu_\ell}^{(k)} / (\sqrt{\hat{\mathbf{m}}_{\mu_\ell}^{(k)}} + \epsilon) \quad \text{and} \quad \sigma^{(k)} = \sigma^{(k-1)} - \frac{\gamma}{n} \hat{\mathbf{m}}_\sigma^{(k)} / (\sqrt{\hat{\mathbf{m}}_\sigma^{(k)}} + \epsilon),$$

551 where

$$\begin{aligned} \hat{\mathbf{m}}_{\mu_\ell}^{(k)} &= \mathbf{m}_{\mu_\ell}^{(k-1)} / (1 - \rho_1^k) \quad \text{with} \quad \mathbf{m}_{\mu_\ell}^{(k)} = \rho_1 \mathbf{m}_{\mu_\ell}^{(k-1)} + (1 - \rho_1) \hat{\delta}_{\mu_\ell, i_k}^{(k)}, \\ \hat{\mathbf{v}}_{\mu_\ell}^{(k)} &= \mathbf{v}_{\mu_\ell}^{(k-1)} / (1 - \rho_2^k) \quad \text{with} \quad \mathbf{v}_{\mu_\ell}^{(k)} = \rho_2 \mathbf{v}_{\mu_\ell}^{(k-1)} + (1 - \rho_2) (\hat{\delta}_{\mu_\ell, i_k}^{(k)})^2 \end{aligned}$$

552 and

$$\begin{aligned} \hat{\mathbf{m}}_\sigma^{(k)} &= \mathbf{m}_\sigma^{(k-1)} / (1 - \rho_1^k) \quad \text{with} \quad \mathbf{m}_\sigma^{(k)} = \rho_1 \mathbf{m}_\sigma^{(k-1)} + (1 - \rho_1) \hat{\delta}_{\sigma, i_k}^{(k)}, \\ \hat{\mathbf{v}}_\sigma^{(k)} &= \mathbf{v}_\sigma^{(k-1)} / (1 - \rho_2^k) \quad \text{with} \quad \mathbf{v}_\sigma^{(k)} = \rho_2 \mathbf{v}_\sigma^{(k-1)} + (1 - \rho_2) (\hat{\delta}_{\sigma, i_k}^{(k)})^2. \end{aligned}$$

553 The hyperparameters are set as follows:  $\gamma = 10^{-3}$ ,  $\rho_1 = 0.9$ ,  $\rho_2 = 0.999$ ,  $\epsilon = 10^{-8}$ .