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

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Abstract

Many constrained, non-convex 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, non-convex, non-smooth optimization setting. We apply our new framework for inference of logistic regression model with missing covariates 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 Θ 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) non-convex and non-smooth.

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 in both the convex and nonconvex case has recently 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. This for example the case for inference in latent variable models. 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)* which is designed for the finite sum optimization with a finite-time convergence guarantee. Our contributions can be summarized as follows.

- We propose a unifying framework of analysis for incremental stochastic surrogate optimization when the surrogates are defined by 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 ϵ -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 covariates 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 Euclidean space. For any function $f : \Theta \rightarrow \mathbb{R}$, $f'(\theta, d)$ is the directional derivative of f at θ 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 Non-convex Functions

The objective function in (1) is composed of a finite sum of possibly non-smooth and non-convex 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. θ , 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 $\Theta_\epsilon = \{\theta \in \mathbb{R}^d, \inf_{\theta' \in \Theta} \|\theta - \theta'\| < \epsilon\}$ is an ϵ -neighborhood set of Θ . Moreover, for some constant L , the gradient satisfies

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

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

81 The inequality (3) implies $\widehat{\mathcal{L}}_i(\theta; \bar{\theta}) \geq \mathcal{L}_i(\theta) >$
 82 $-\infty$ for any $\theta \in \Theta$. The MISO method is
 83 an incremental version of the MM method, as
 84 summarized by Algorithm 1. As seen in the
 85 pseudo code, the MISO method maintains an iter-
 86 atively updated set of surrogate upper-bound
 87 functions $\{\mathcal{A}_i^k(\theta)\}_{i=1}^n$ and updates the iterate
 88 through minimizing the average of the surro-
 89 gate functions.

90 Particularly, only one out of the n sur-
 91rogate functions is updated at each iter-
 92ation [cf. Line 5] and the sum function
 93 $\frac{1}{n} \sum_{i=1}^n \mathcal{A}_i^{k+1}(\theta)$ is designed to be ‘easy to
 94 optimize’, for example, it can be a sum of
 95 quadratic functions. As such, the MISO method
 96 is suitable for large-scale optimization as the computation cost per iteration is independent of n .
 97 Moreover, under **S1**, **S2**, it was shown that the MISO method converges almost surely to a stationary
 98 point of (1) [Mairal, 2015, Proposition 3.1].

99 We now consider the case when the surrogate functions $\widehat{\mathcal{L}}_i(\theta; \bar{\theta})$ are intractable. Let Z be a measur-
 100 able set, $p_i : Z \times \Theta \rightarrow \mathbb{R}_+$ be a pdf, $r_i : \Theta \times \Theta \times Z \rightarrow \mathbb{R}$ be a measurable function and μ_i be a
 101 σ -finite measure, we consider surrogate functions which satisfy **S1**, **S2** that can be expressed as an
 102 expectation:

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

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

105 We propose the *Minimization by Incremental Stochastic Surrogate Optimization* (MISSO) method
 106 which replaces the expectation in (5) by *Monte Carlo* integration and then optimizes (1) incremen-
 107 tally. Denote by $M \in \mathbb{N}$ the Monte Carlo batch size and let $z_m \in Z$, $m = 1, \dots, M$ be a set of
 108 samples. These samples can be drawn (**Case 1**) i.i.d. from the distribution $p_i(\cdot; \bar{\theta})$ or (**Case 2**)
 109 from a Markov chain with the stationary distribution $p_i(\cdot; \bar{\theta})$; see Section 3 for illustrations. To this
 110 end, we define

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

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

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

$$g_i(\theta) := \int_Z f_i(z_i, \theta) \mu_i(dz_i), \quad i \in \llbracket 1, n \rrbracket \quad (9)$$

121 denote the incomplete data likelihood, i.e., the marginal likelihood of the observations. For
 122 ease of notations, the dependence on the observations is made implicit. The maximum likeli-
 123 hood (ML) estimation problem takes $\mathcal{L}_i(\theta)$ to be the i th negated incomplete data log-likelihood
 124 $\mathcal{L}_i(\theta) := -\log g_i(\theta)$.

Algorithm 1 MISO method [Mairal, 2015]

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

$$\mathcal{A}_{i_k}^{k+1}(\theta) = \begin{cases} \widehat{\mathcal{L}}_{i_k}(\theta; \theta^{(k)}), & \text{if } i = i_k \\ \mathcal{A}_{i_k}^k(\theta), & \text{otherwise.} \end{cases}$$
 - 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**
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Algorithm 2 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

$$\tilde{\mathcal{A}}_i^0(\theta) := \tilde{\mathcal{L}}_i(\theta; \theta^{(0)}, \{z_{i,m}^{(0)}\}_{m=1}^{M_{(0)}}), \quad i \in \llbracket 1, n \rrbracket. \quad (7)$$

- 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 $p_{i_k}(\cdot; \theta^{(k)})$.
- 7: Update the individual surrogate functions recursively as:

$$\tilde{\mathcal{A}}_i^{k+1}(\theta) = \begin{cases} \tilde{\mathcal{L}}_i(\theta; \theta^{(k)}, \{z_{i,m}^{(k)}\}_{m=1}^{M_{(k)}}), & \text{if } i = i_k \\ \tilde{\mathcal{A}}_i^k(\theta), & \text{otherwise.} \end{cases} \quad (8)$$

- 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**
-

125 Assume without loss of generality that $g_i(\theta) \neq 0$ for all $\theta \in \Theta$, we define by $p_i(z_i, \theta) :=$
 126 $f_i(z_i, \theta)/g_i(\theta)$ the conditional distribution of the latent variable z_i given the observation y_i . A sur-
 127 rogate function $\hat{\mathcal{L}}_i(\theta; \bar{\theta})$ satisfying S1 can be obtained through writing $f_i(z_i, \theta) = \frac{f_i(z_i, \theta)}{p_i(z_i, \bar{\theta})} p_i(z_i, \bar{\theta})$
 128 and applying the Jensen inequality:

$$\hat{\mathcal{L}}_i(\theta; \bar{\theta}) = \int_{\mathcal{Z}} \underbrace{\log(p_i(z_i, \bar{\theta})/f_i(z_i, \theta))}_{=r_i(\theta; \bar{\theta}, z_i)} p_i(z_i, \bar{\theta}) \mu_i(dz_i), \quad (10)$$

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

131 **Example 2: Variational Inference.** Let $((x_i, y_i), i \in \llbracket 1, n \rrbracket)$ be i.i.d. input-output pairs and $w \in$
 132 $\mathcal{W} \subseteq \mathbb{R}^d$ be a latent variable. When conditioned on the input $x = (x_i, i \in \llbracket 1, n \rrbracket)$, the joint
 133 distribution of $y = (y_i, i \in \llbracket 1, n \rrbracket)$ and w is given by:

$$p(y, w|x) = \pi(w) \prod_{i=1}^n p(y_i|x_i, w). \quad (11)$$

134 Our goal is to compute the posterior distribution $p(w|y, x)$. In most cases, the posterior distribution
 135 $p(w|y, x)$ is intractable and is approximated using a family of parametric distributions, $\{q(w, \theta), \theta \in$
 136 $\Theta\}$. The variational inference (VI) problem [Blei et al., 2017] boils down to minimizing the KL
 137 divergence between $q(w, \theta)$ and the posterior distribution $p(w|y, x)$, as follows:

$$\min_{\theta \in \Theta} \mathcal{L}(\theta) := \text{KL}(q(w; \theta) || p(w|y, x)) := \mathbb{E}_{q(w; \theta)} [\log(q(w; \theta)/p(w|y, x))] . \quad (12)$$

138 Using (11), we decompose $\mathcal{L}(\theta) = n^{-1} \sum_{i=1}^n \mathcal{L}_i(\theta) + \text{const.}$ where:

$$\mathcal{L}_i(\theta) := -\mathbb{E}_{q(w; \theta)} [\log p(y_i|x_i, w)] + \frac{1}{n} \mathbb{E}_{q(w; \theta)} [\log q(w; \theta)/\pi(w)] = r_i(\theta) + d(\theta). \quad (13)$$

139 Directly optimizing the finite sum objective function in (12) can be difficult. First, with $n \gg 1$,
 140 evaluating the objective function $\mathcal{L}(\theta)$ requires a full pass over the entire dataset. Second, for some
 141 complex models, the expectations in (13) can be intractable even if we assume a simple parametric
 142 model for $q(w; \theta)$. Assume that \mathcal{L}_i is L-smooth, i.e., \mathcal{L}_i is differentiable on Θ and its gradient $\nabla \mathcal{L}_i$
 143 is L-Lipschitz. We apply the MISSO method with a quadratic surrogate function defined as:

$$\hat{\mathcal{L}}_i(\theta; \bar{\theta}) := \mathcal{L}_i(\bar{\theta}) + \langle \nabla_{\theta} \mathcal{L}_i(\bar{\theta}) | \theta - \bar{\theta} \rangle + \frac{L}{2} \|\bar{\theta} - \theta\|^2. \quad (14)$$

144 It is easily checked that $\hat{\mathcal{L}}_i(\theta; \bar{\theta})$ satisfies S1, S2.

145 To compute the gradient $\nabla \mathcal{L}_i(\bar{\theta})$, we apply the re-parametrization technique suggested in [Paisley
 146 et al., 2012, Kingma and Welling, 2014, Blundell et al., 2015]. Let $t : \mathbb{R}^d \times \Theta \mapsto \mathbb{R}^d$ be a differen-
 147 tiable function w.r.t. $\theta \in \Theta$ which is designed such that the law of $w = t(z, \bar{\theta})$, where $z \sim \mathcal{N}_d(0, \mathbf{I})$,
 148 is $q(\cdot, \bar{\theta})$. By [Blundell et al., 2015, Proposition 1], the gradient of $-r_i(\cdot)$ in (13) is:

$$\nabla_{\theta} \mathbb{E}_{q(w; \bar{\theta})} [\log p(y_i | x_i, w)] = \mathbb{E}_{z \sim \mathcal{N}_d(0, \mathbf{I})} [\mathbf{J}_{\theta}^t(z, \bar{\theta}) \nabla_w \log p(y_i | x_i, w) \big|_{w=t(z, \bar{\theta})}], \quad (15)$$

149 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 θ evaluated at
 150 $\bar{\theta}$. In addition, for most cases, the term $\nabla d(\bar{\theta})$ can be evaluated in closed form.

$$r_i(\theta; \bar{\theta}, z) := \left\langle \nabla_{\theta} d(\bar{\theta}) - \mathbf{J}_{\theta}^t(z, \bar{\theta}) \nabla_w \log p(y_i | x_i, w) \big|_{w=t(z, \bar{\theta})} \mid \theta - \bar{\theta} \right\rangle + \frac{L}{2} \|\theta - \bar{\theta}\|^2. \quad (16)$$

151 Finally, using (14) and (16), the surrogate function (6) is given by $\tilde{\mathcal{L}}_i(\theta; \bar{\theta}, \{z_m\}_{m=1}^M) :=$
 152 $M^{-1} \sum_{m=1}^M r_i(\theta; \bar{\theta}, z_m)$ where $\{z_m\}_{m=1}^M$ is an i.i.d sample from $\mathcal{N}(0, \mathbf{I})$.

153 3 Convergence Analysis

154 We provide non-asymptotic convergence bound for the MISSO method.

155 **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 θ and is
 156 lower bounded.

157 We are particularly interested in the *constrained optimization* setting where Θ is a bounded set. To
 158 this end, we control the supremum norm of the of the above approximation as:

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

$$C_r := \sup_{\bar{\theta} \in \Theta} \sup_{M > 0} \frac{1}{\sqrt{M}} \mathbb{E}_{\bar{\theta}} \left[\sup_{\theta \in \Theta} \left| \sum_{m=1}^M \left\{ r_i(\theta; \bar{\theta}, z_{i,m}) - \hat{\mathcal{L}}_i(\theta; \bar{\theta}) \right\} \right| \right] \quad (17)$$

$$C_{gr} := \sup_{\bar{\theta} \in \Theta} \sup_{M > 0} \sqrt{M} \mathbb{E}_{\bar{\theta}} \left[\sup_{\theta \in \Theta} \left| \frac{1}{M} \sum_{m=1}^M \frac{\hat{\mathcal{L}}'_i(\theta, \theta - \bar{\theta}; \bar{\theta}) - r'_i(\theta, \theta - \bar{\theta}; \bar{\theta}, z_{i,m})}{\|\bar{\theta} - \theta\|} \right|^2 \right] \quad (18)$$

161 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
 162 initial distribution $\xi_i(\cdot; \bar{\theta})$, transition kernel $P_{i, \bar{\theta}}$, and stationary distribution $p_i(\cdot; \bar{\theta})$.

163 **Some intuitions behind the controlling terms:** It is actually common in statistical and optimization
 164 problems, to deal with the manipulation and the control of random variables indexed by sets with
 165 an infinite number of elements. here, the random variable we control is an image of a continuous
 166 function noted $v : \mathbf{Z} \rightarrow \mathbb{R}$ and defined as $v(z) := r_i(\theta; \bar{\theta}, z_{i,m}) - \hat{\mathcal{L}}_i(\theta; \bar{\theta})$ for all $z \in \mathbf{Z}$ and for
 167 fixed $(\theta, \hat{\theta}) \in \Theta^2$. To characterize such control, we will have recourse to the notion of metric entropy
 168 (or covering number of bracketing number) as developed in [Van der Vaart, 2000, Vershynin, 2018,
 169 Wainwright, 2019]. A collection of results from those books gives intuition behind our assumption
 170 **H 2**, classical in empirical process: In [Vershynin, 2018, Theorem 8.2.3], the authors recall the
 171 uniform law of large numbers by stating that for $(z_{i,m}, i \in \llbracket 1, M \rrbracket)$ random variables in $(0, 1)$, we
 172 have, for a class of L -Lipschitz functions:

$$\mathbb{E} \left[\sup_{f \in \mathcal{F}} \left| \frac{1}{M} \sum_{i=1}^M f(z_{i,m}) - \mathbb{E}[f(z_i)] \right| \right] \leq \frac{CL}{\sqrt{M}} \quad (19)$$

173 Moreover, in [Vershynin, 2018, Theorem 8.1.3] and [Wainwright, 2019, Theorem 5.22], the appli-
 174 cation of the Dudley's inequality yields:

$$\mathbb{E} \left[\sup_{f \in \mathcal{F}} |X_f - X_0| \right] \leq \frac{1}{\sqrt{M}} \int_0^1 \sqrt{\log \mathcal{N}(\mathcal{F}, \|\cdot\|_{\infty}, \varepsilon)} d\varepsilon \quad (20)$$

where $\mathcal{N}(\mathcal{F}, \|\cdot\|_\infty, \varepsilon)$ is the bracketing number and ε denotes the level of approximation (the bracketing number goes to infinity when $\varepsilon \rightarrow 0$). Finally, in [Van der Vaart, 2000, p.271, Example], this bracketing number is bounded from above for a class of parametric function $\mathcal{F} = f_\theta : \theta \in \Theta$ on a bounded set $\Theta \subset \mathbb{R}$ as:

$$\mathcal{N}(\mathcal{F}, \|\cdot\|_\infty, \varepsilon) \leq K \left(\frac{\text{diam } \Theta}{\varepsilon} \right)^d, \quad \text{every } 0 < \varepsilon < \text{diam } \Theta \quad (21)$$

It is worth contrasting the exponential dependence of this metric entropy on the dimension d . The authors acknowledge that this is a dramatic manifestation of the curse of dimensionality happening when sampling is needed. Nevertheless, the dependence on the dimension highly depends on the class of functions \mathcal{F} , corresponding to the class of surrogate functions in our work, as smaller bounds on these controlling terms can be derived for simpler class, such as quadratic functions.

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

$$g(\bar{\theta}) := \inf_{\theta \in \Theta} \frac{\mathcal{L}'(\bar{\theta}, \theta - \bar{\theta})}{\|\bar{\theta} - \theta\|} \quad \text{and} \quad g(\bar{\theta}) = g_+(\bar{\theta}) - g_-(\bar{\theta}), \quad (22)$$

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

Also, denote

$$\hat{\mathcal{L}}^{(k)}(\theta) := \frac{1}{n} \sum_{i=1}^n \hat{\mathcal{L}}_i(\theta; \theta^{(\tau_i^k)}), \quad \hat{e}^{(k)}(\theta) := \hat{\mathcal{L}}^{(k)}(\theta) - \mathcal{L}(\theta). \quad (23)$$

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

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:*

$$\Delta_{(K_{\max})} := 2n\mathbb{E}[\tilde{\mathcal{L}}^{(0)}(\theta^{(0)}) - \tilde{\mathcal{L}}^{(K_{\max})}(\theta^{(K_{\max})})] + \sum_{k=0}^{K_{\max}-1} \frac{4LC_r}{\sqrt{M_{(k)}}}, \quad (24)$$

Then we have following non-asymptotic bounds:

$$\mathbb{E}[\|\nabla \hat{e}^{(K)}(\theta^{(K)})\|^2] \leq \frac{\Delta_{(K_{\max})}}{K_{\max}} \quad (25)$$

$$\mathbb{E}[g_-(\theta^{(K)})] \leq \sqrt{\frac{\Delta_{(K_{\max})}}{K_{\max}}} + \frac{C_{\text{gr}}}{K_{\max}} \sum_{k=0}^{K_{\max}-1} M_{(k)}^{-1/2}. \quad (26)$$

Note that $\Delta_{(K_{\max})}$ is finite for any $K_{\max} \in \mathbb{N}$. As expected, the MISSO method converges to a stationary point of (1) asymptotically and at a sublinear rate $\mathbb{E}[g_-(\theta^{(K)})] \leq \mathcal{O}(\sqrt{1/K_{\max}})$.

Furthermore, we remark that the MISO method can be analyzed in Theorem 1 as a special case of the MISSO method satisfying $C_r = C_{\text{gr}} = 0$. In this case, while the asymptotic convergence is well known from [Mairal, 2015] [cf. H2], Eq. (25) gives a non-asymptotic rate of $\mathbb{E}[g_-(\theta^{(K)})] \leq \mathcal{O}(\sqrt{nL/K_{\max}})$ which is new to our best knowledge.

Next, we show that under an additional assumption on the sequence of batch 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 almost surely to zero, i.e., $\lim_{k \rightarrow \infty} g_-(\theta^{(k)}) = 0$ a.s..
2. the objective value $\mathcal{L}(\theta^{(k)})$ converges almost surely to a finite number $\underline{\mathcal{L}}$, i.e., $\lim_{k \rightarrow \infty} \mathcal{L}(\theta^{(k)}) = \underline{\mathcal{L}}$ a.s..

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

4 Numerical Experiments

4.1 Binary logistic regression with missing values

This application follows **Example 1** described in Section 2. We consider a binary regression setup, $((y_i, z_i), i \in \llbracket n \rrbracket)$ 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 Ω 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:

$$p_i(y_i|z_i) = S(\delta^\top \bar{z}_i)^{y_i} (1 - S(\delta^\top \bar{z}_i))^{1-y_i} \quad (27)$$

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

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

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. Details on the surrogate functions and the parameters updates are given in (84) and 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 (27) to predict the risk of a severe hemorrhage which is one of the main cause of death after a major trauma. Note as the dataset considered is heterogeneous – coming from multiple sources with frequently missed entries – we apply the latent data model described in the above. For the Monte-Carlo sampling of $z_{i,\text{mis}}$, we run a Metropolis Hastings algorithm with the target distribution $p(\cdot|z_{i,\text{obs}}, y_i; \theta^{(k)})$ whose procedure is detailed in Appendix D.1.2.

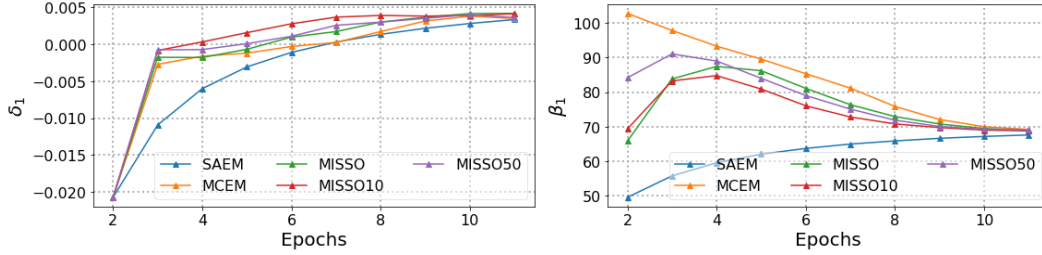


Figure 1: Convergence of first component of the vector of parameters δ and β for the SAEM, the MCCEM and the MISSO methods. The convergence is plotted against No. of passes over the data.

We compare in Figure 1 the convergence behavior of the estimated parameters β using SAEM [Delyon et al., 1999] (with stepsize $\gamma_k = 1/k$), MCCEM [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 function (MISSO), 10% (MISSO10) and 50% (MISSO50) of the functions per iteration. From Figure 1, the MISSO method converges to a static value with less number of epochs than the MCCEM, 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 (13) to fit Bayesian Neural Networks on different datasets. At iteration k , minimizing the sum of stochastic surrogates defined as in (6) and (16) 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 as

$$\mu_\ell^{(k)} = \frac{1}{n} \sum_{i=1}^n \mu_\ell^{(\tau_i^k)} - \frac{\gamma}{n} \sum_{i=1}^n \hat{\delta}_{\mu_\ell, i}^{(k)}, \quad (28)$$

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:

$$\hat{\delta}_{\mu_\ell, i_k}^{(k)} = -\frac{1}{M(k)} \sum_{m=1}^{M(k)} \nabla_w \log p(y_{i_k} | x_{i_k}, w) \Big|_{w=t(\theta^{(k-1)}, z_m^{(k)})} + \nabla_{\mu_\ell} d(\theta^{(k-1)}),$$

with $d(\theta) = n^{-1} \sum_{\ell=1}^d (-\log(\sigma) + (\sigma^2 + \mu_\ell^2)/2 - 1/2)$.

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, 28×28 images. Each image is labelled with its corresponding number (from zero to nine). Under the prior distribution π , see (11), 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, 32×32 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 $\mathcal{N}(0, 1)$. The source code used as a backbone here can be found in the TensorFlow Probability Github repo (https://github.com/tensorflow/probability/blob/master/tensorflow_probability/examples/cifar10_bnn.py) where the default hyperparameters, as the L 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 preferred than a simple reparametrization trick for ResNet-18.

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 (13) 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 $M(k) = k$.

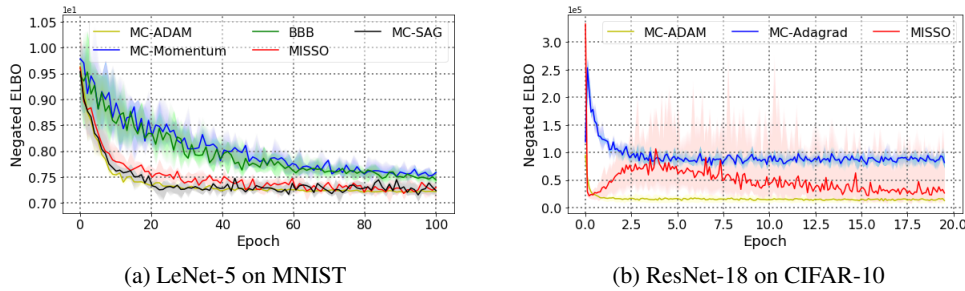


Figure 2: (a) Negated ELBO versus epochs elapsed for fitting the Bayesian LeNet-5 on MNIST using different algorithms. (b) ELBO versus epochs elapsed for fitting the Bayesian ResNet-18 on CIFAR-10 using different algorithms. The solid curve is obtained from averaging over 5 independent runs of the methods, 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 (see Table 2) 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. Figure 2(b) also highlights high variance of the MISSO estimator which would then benefit from variance reduction methods, being for now just an incremental one. We leave that research direction open for the sake of clarity of our paper.

5 Conclusion

We present a unifying framework for minimizing a non-convex 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 non-convex 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 CNNs on benchmark datasets.

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385 A Proof of Theorem 1

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

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

388 Then we have following non-asymptotic bounds:

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

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

$$\tilde{\mathcal{L}}^{(k)}(\boldsymbol{\theta}) := \frac{1}{n} \sum_{i=1}^n \tilde{\mathcal{A}}_i^k(\boldsymbol{\theta}). \quad (29)$$

390 Notice that

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

391 Furthermore, we recall that

$$\hat{\mathcal{L}}^{(k)}(\boldsymbol{\theta}) := \frac{1}{n} \sum_{i=1}^n \hat{\mathcal{L}}_i(\boldsymbol{\theta}; \boldsymbol{\theta}^{(\tau_i^k)}), \quad \hat{e}^{(k)}(\boldsymbol{\theta}) := \hat{\mathcal{L}}^{(k)}(\boldsymbol{\theta}) - \mathcal{L}(\boldsymbol{\theta}). \quad (31)$$

392 Due to S2, we have

$$\|\nabla \hat{e}^{(k)}(\boldsymbol{\theta}^{(k)})\|^2 \leq 2L\hat{e}^{(k)}(\boldsymbol{\theta}^{(k)}). \quad (32)$$

393 To prove the first bound in (25), using the optimality of $\boldsymbol{\theta}^{(k+1)}$, one has

$$\begin{aligned} \tilde{\mathcal{L}}^{(k+1)}(\boldsymbol{\theta}^{(k+1)}) &\leq \tilde{\mathcal{L}}^{(k+1)}(\boldsymbol{\theta}^{(k)}) \\ &= \tilde{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)}) + \frac{1}{n} (\tilde{\mathcal{L}}_{i_k}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(k)}, \{z_{i_k,m}^{(k)}\}_{m=1}^{M_{(k)}}) - \tilde{\mathcal{L}}_{i_k}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(\tau_{i_k}^k)}, \{z_{i_k,m}^{(\tau_{i_k}^k)}\}_{m=1}^{M_{(\tau_{i_k}^k)}})) \end{aligned} \quad (33)$$

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

395 We observe that the conditional expectation evaluates to

$$\begin{aligned} \mathbb{E}_{i_k} [\mathbb{E}[\tilde{\mathcal{L}}_{i_k}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(k)}, \{z_{i_k,m}^{(k)}\}_{m=1}^{M_{(k)}}) | \mathcal{F}_k, i_k] | \mathcal{F}_k] \\ = \mathcal{L}(\boldsymbol{\theta}^{(k)}) + \mathbb{E}_{i_k} [\mathbb{E}[\frac{1}{M_{(k)}} \sum_{m=1}^{M_{(k)}} r_{i_k}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(k)}, z_{i_k,m}^{(k)}) - \hat{\mathcal{L}}_{i_k}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(k)}) | \mathcal{F}_k, i_k] | \mathcal{F}_k] \\ \leq \mathcal{L}(\boldsymbol{\theta}^{(k)}) + \frac{C_r}{\sqrt{M_{(k)}}}, \end{aligned} \quad (34)$$

396 where the last inequality is due to H2. Moreover,

$$\mathbb{E}[\tilde{\mathcal{L}}_{i_k}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(\tau_{i_k}^k)}, \{z_{i_k,m}^{(\tau_{i_k}^k)}\}_{m=1}^{M_{(\tau_{i_k}^k)}}) | \mathcal{F}_k] = \frac{1}{n} \sum_{i=1}^n \tilde{\mathcal{L}}_i(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(\tau_i^k)}, \{z_{i,m}^{(\tau_i^k)}\}_{m=1}^{M_{(\tau_i^k)}}) = \tilde{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)}). \quad (35)$$

397 Taking the conditional expectations on both sides of (33) and re-arranging terms give:

$$\tilde{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)}) - \mathcal{L}(\boldsymbol{\theta}^{(k)}) \leq n\mathbb{E}[\tilde{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)}) - \tilde{\mathcal{L}}^{(k+1)}(\boldsymbol{\theta}^{(k+1)}) | \mathcal{F}_k] + \frac{C_r}{\sqrt{M_{(k)}}} \quad (36)$$

398 Proceeding from (36), we observe the following lower bound for the left hand side

$$\begin{aligned}
& \tilde{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)}) - \mathcal{L}(\boldsymbol{\theta}^{(k)}) \stackrel{(a)}{=} \tilde{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)}) - \hat{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)}) + \hat{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)}) \\
& \stackrel{(b)}{\geq} \tilde{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)}) - \hat{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)}) + \frac{1}{2L} \|\nabla \hat{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)})\|^2 \\
& = \frac{1}{n} \sum_{i=1}^n \left\{ \frac{1}{M_{(\tau_i^k)}} \sum_{m=1}^{M_{(\tau_i^k)}} r_i(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(\tau_i^k)}, z_{i,m}^{(\tau_i^k)}) - \hat{\mathcal{L}}_i(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(\tau_i^k)}) \right\} + \frac{1}{2L} \|\nabla \hat{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)})\|^2 \\
& \quad \underbrace{\hspace{10em}}_{:= -\delta^{(k)}(\boldsymbol{\theta}^{(k)})}
\end{aligned} \tag{37}$$

399 where (a) is due to $\hat{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)}) = 0$ [cf. S1], (b) is due to (32) and we have defined the summation in
400 the last equality as $-\delta^{(k)}(\boldsymbol{\theta}^{(k)})$. Substituting the above into (36) yields

$$\frac{\|\nabla \hat{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)})\|^2}{2L} \leq n \mathbb{E}[\tilde{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)}) - \tilde{\mathcal{L}}^{(k+1)}(\boldsymbol{\theta}^{(k+1)}) | \mathcal{F}_k] + \frac{C_r}{\sqrt{M_{(k)}}} + \delta^{(k)}(\boldsymbol{\theta}^{(k)}) \tag{38}$$

401 Observe the following upper bound on the total expectations:

$$\mathbb{E}[\delta^{(k)}(\boldsymbol{\theta}^{(k)})] \leq \mathbb{E}\left[\frac{1}{n} \sum_{i=1}^n \frac{C_r}{\sqrt{M_{(\tau_i^k)}}}\right], \tag{39}$$

402 which is due to H2. It yields

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

403 Finally, for any $K_{\max} \in \mathbb{N}$, we let K be a discrete r.v. that is uniformly drawn from $\{0, 1, \dots, K_{\max} -$
404 $1\}$. Using H2 and taking total expectations lead to

$$\begin{aligned}
\mathbb{E}[\|\nabla \hat{\mathcal{L}}^{(K)}(\boldsymbol{\theta}^{(K)})\|^2] &= \frac{1}{K_{\max}} \sum_{k=0}^{K_{\max}-1} \mathbb{E}[\|\nabla \hat{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)})\|^2] \\
&\leq \frac{2nL \mathbb{E}[\tilde{\mathcal{L}}^{(0)}(\boldsymbol{\theta}^{(0)}) - \tilde{\mathcal{L}}^{(K_{\max})}(\boldsymbol{\theta}^{(K_{\max})})]}{K_{\max}} + \frac{2LC_r}{K_{\max}} \sum_{k=0}^{K_{\max}-1} \mathbb{E}\left[\frac{1}{\sqrt{M_{(k)}}} + \frac{1}{n} \sum_{i=1}^n \frac{1}{\sqrt{M_{(\tau_i^k)}}}\right]
\end{aligned} \tag{40}$$

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

$$\mathbb{E}[M_{(\tau_i^k)}^{-1/2}] = \sum_{j=1}^k \frac{1}{n} \left(1 - \frac{1}{n}\right)^{j-1} M_{(k-j)}^{-1/2} \tag{41}$$

407 Taking the sum yields:

$$\begin{aligned}
\sum_{k=0}^{K_{\max}-1} \mathbb{E}[M_{(\tau_i^k)}^{-1/2}] &= \sum_{k=0}^{K_{\max}-1} \sum_{j=1}^k \frac{1}{n} \left(1 - \frac{1}{n}\right)^{j-1} M_{(k-j)}^{-1/2} = \sum_{k=0}^{K_{\max}-1} \sum_{l=0}^{k-1} \frac{1}{n} \left(1 - \frac{1}{n}\right)^{k-(l+1)} M_{(l)}^{-1/2} \\
&= \sum_{l=0}^{K_{\max}-1} M_{(l)}^{-1/2} \sum_{k=l+1}^{K_{\max}-1} \frac{1}{n} \left(1 - \frac{1}{n}\right)^{k-(l+1)} \leq \sum_{l=0}^{K_{\max}-1} M_{(l)}^{-1/2}
\end{aligned} \tag{42}$$

408 where the last inequality is due to upper bounding the geometric series. Plugging this back into (40)
409 yields

$$\begin{aligned}
\mathbb{E}[\|\nabla \hat{\mathcal{L}}^{(K)}(\boldsymbol{\theta}^{(K)})\|^2] &= \frac{1}{K_{\max}} \sum_{k=0}^{K_{\max}-1} \mathbb{E}[\|\nabla \hat{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)})\|^2] \\
&\leq \frac{2nL \mathbb{E}[\tilde{\mathcal{L}}^{(0)}(\boldsymbol{\theta}^{(0)}) - \tilde{\mathcal{L}}^{(K_{\max})}(\boldsymbol{\theta}^{(K_{\max})})]}{K_{\max}} + \frac{1}{K_{\max}} \sum_{k=0}^{K_{\max}-1} \frac{4LC_r}{\sqrt{M_{(k)}}} = \frac{\Delta_{(K_{\max})}}{K_{\max}}.
\end{aligned} \tag{43}$$

410 This concludes our proof for the first inequality in (25).

411 To prove the second inequality of (25), we define the shorthand notations $g^{(k)} := g(\boldsymbol{\theta}^{(k)})$, $g_-^{(k)} :=$
 412 $-\min\{0, g^{(k)}\}$, $g_+^{(k)} := \max\{0, g^{(k)}\}$. We observe that

$$\begin{aligned} g^{(k)} &= \inf_{\boldsymbol{\theta} \in \Theta} \frac{\mathcal{L}'(\boldsymbol{\theta}^{(k)}, \boldsymbol{\theta} - \boldsymbol{\theta}^{(k)})}{\|\boldsymbol{\theta}^{(k)} - \boldsymbol{\theta}\|} \\ &= \inf_{\boldsymbol{\theta} \in \Theta} \left\{ \frac{\frac{1}{n} \sum_{i=1}^n \widehat{\mathcal{L}}'_i(\boldsymbol{\theta}^{(k)}, \boldsymbol{\theta} - \boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(\tau_i^k)})}{\|\boldsymbol{\theta}^{(k)} - \boldsymbol{\theta}\|} - \frac{\langle \nabla \widehat{e}^{(k)}(\boldsymbol{\theta}^{(k)}) | \boldsymbol{\theta} - \boldsymbol{\theta}^{(k)} \rangle}{\|\boldsymbol{\theta}^{(k)} - \boldsymbol{\theta}\|} \right\} \\ &\geq -\|\nabla \widehat{e}^{(k)}(\boldsymbol{\theta}^{(k)})\| + \inf_{\boldsymbol{\theta} \in \Theta} \frac{\frac{1}{n} \sum_{i=1}^n \widehat{\mathcal{L}}'_i(\boldsymbol{\theta}^{(k)}, \boldsymbol{\theta} - \boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(\tau_i^k)})}{\|\boldsymbol{\theta}^{(k)} - \boldsymbol{\theta}\|} \end{aligned} \quad (44)$$

413 where the last inequality is due to the Cauchy-Schwarz inequality and we have defined
 414 $\widehat{\mathcal{L}}'_i(\boldsymbol{\theta}, \boldsymbol{d}; \boldsymbol{\theta}^{(\tau_i^k)})$ as the directional derivative of $\widehat{\mathcal{L}}_i(\cdot; \boldsymbol{\theta}^{(\tau_i^k)})$ at $\boldsymbol{\theta}$ along the direction \boldsymbol{d} . Moreover,
 415 for any $\boldsymbol{\theta} \in \Theta$,

$$\begin{aligned} &\frac{1}{n} \sum_{i=1}^n \widehat{\mathcal{L}}'_i(\boldsymbol{\theta}^{(k)}, \boldsymbol{\theta} - \boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(\tau_i^k)}) \\ &= \underbrace{\widetilde{\mathcal{L}}^{(k)'}(\boldsymbol{\theta}^{(k)}, \boldsymbol{\theta} - \boldsymbol{\theta}^{(k)}) - \widetilde{\mathcal{L}}^{(k)'}(\boldsymbol{\theta}^{(k)}, \boldsymbol{\theta} - \boldsymbol{\theta}^{(k)})}_{\geq 0} + \frac{1}{n} \sum_{i=1}^n \widehat{\mathcal{L}}'_i(\boldsymbol{\theta}^{(k)}, \boldsymbol{\theta} - \boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(\tau_i^k)}) \\ &\geq \frac{1}{n} \sum_{i=1}^n \left\{ \widehat{\mathcal{L}}'_i(\boldsymbol{\theta}^{(k)}, \boldsymbol{\theta} - \boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(\tau_i^k)}) - \frac{1}{M_{(\tau_i^k)}} \sum_{m=1}^{M_{(\tau_i^k)}} r'_i(\boldsymbol{\theta}^{(k)}, \boldsymbol{\theta} - \boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(\tau_i^k)}, z_{i,m}^{(\tau_i^k)}) \right\} \end{aligned} \quad (45)$$

416 where the inequality is due to the optimality of $\boldsymbol{\theta}^{(k)}$ and the convexity of $\widetilde{\mathcal{L}}^{(k)}(\boldsymbol{\theta})$ [cf. H1]. Denoting
 417 a scaled version of the above term as:

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

418 We have

$$g^{(k)} \geq -\|\nabla \widehat{e}^{(k)}(\boldsymbol{\theta}^{(k)})\| + \inf_{\boldsymbol{\theta} \in \Theta} (-\epsilon^{(k)}(\boldsymbol{\theta})) \geq -\|\nabla \widehat{e}^{(k)}(\boldsymbol{\theta}^{(k)})\| - \sup_{\boldsymbol{\theta} \in \Theta} |\epsilon^{(k)}(\boldsymbol{\theta})|. \quad (46)$$

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

$$g_-^{(k)} \leq \|\nabla \widehat{e}^{(k)}(\boldsymbol{\theta}^{(k)})\| + \sup_{\boldsymbol{\theta} \in \Theta} |\epsilon^{(k)}(\boldsymbol{\theta})|. \quad (47)$$

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

$$\mathbb{E}[g_-^{(K)}] \leq \mathbb{E}[\|\nabla \widehat{e}^{(K)}(\boldsymbol{\theta}^{(K)})\|] + \mathbb{E}[\sup_{\boldsymbol{\theta} \in \Theta} \epsilon^{(K)}(\boldsymbol{\theta})] \quad (48)$$

422 We note that

$$\left(\mathbb{E}[\|\nabla \widehat{e}^{(K)}(\boldsymbol{\theta}^{(K)})\|] \right)^2 \leq \mathbb{E}[\|\nabla \widehat{e}^{(K)}(\boldsymbol{\theta}^{(K)})\|^2] \leq \frac{\Delta(K_{\max})}{K_{\max}}, \quad (49)$$

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

$$\begin{aligned} \mathbb{E}[\sup_{\boldsymbol{\theta} \in \Theta} \epsilon^{(K)}(\boldsymbol{\theta})] &= \frac{1}{K_{\max}} \sum_{k=0}^{K_{\max}} \mathbb{E}[\sup_{\boldsymbol{\theta} \in \Theta} \epsilon^{(k)}(\boldsymbol{\theta})] \stackrel{(a)}{\leq} \frac{C_{\text{gr}}}{K_{\max}} \sum_{k=0}^{K_{\max}-1} \mathbb{E}\left[\frac{1}{n} \sum_{i=1}^n M_{(\tau_i^k)}^{-1/2}\right] \\ &\stackrel{(b)}{\leq} \frac{C_{\text{gr}}}{K_{\max}} \sum_{k=0}^{K_{\max}-1} M_{(k)}^{-1/2} \end{aligned} \quad (50)$$

424 where (a) is due to H2 and (b) is due to (42). This implies

$$\mathbb{E}[g_-^{(K)}] \leq \sqrt{\frac{\Delta(K_{\max})}{K_{\max}}} + \frac{C_{\text{gr}}}{K_{\max}} \sum_{k=0}^{K_{\max}-1} M_{(k)}^{-1/2}, \quad (51)$$

425 and concludes the proof of the theorem. \square

426 B Proof of Theorem 2

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

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

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

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

$$V_k \leq V_{k-1} - X_{k-1} + E_{k-1} \quad (52)$$

438 then:

439 (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_{∞} .

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

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

442 We proceed from (33) by re-arranging terms and observing that

$$\begin{aligned} \widehat{\mathcal{L}}^{(k+1)}(\boldsymbol{\theta}^{(k+1)}) &\leq \widehat{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)}) - \frac{1}{n} (\widehat{\mathcal{L}}_{i_k}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(\tau_{i_k}^k)}) - \widehat{\mathcal{L}}_{i_k}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(k)})) \\ &\quad - (\widetilde{\mathcal{L}}^{(k+1)}(\boldsymbol{\theta}^{(k+1)}) - \widehat{\mathcal{L}}^{(k+1)}(\boldsymbol{\theta}^{(k+1)})) + (\widetilde{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)}) - \widehat{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)})) \\ &\quad + \frac{1}{n} (\widetilde{\mathcal{L}}_{i_k}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(k)}, \{z_{i_k, m}^{(k)}\}_{m=1}^{M_{(k)}}) - \widehat{\mathcal{L}}_{i_k}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(k)})) \\ &\quad + \frac{1}{n} (\widehat{\mathcal{L}}_{i_k}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(\tau_{i_k}^k)}) - \widetilde{\mathcal{L}}_{i_k}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(\tau_{i_k}^k)}, \{z_{i_k, m}^{(\tau_{i_k}^k)}\}_{m=1}^{M_{(\tau_{i_k}^k)}})) \end{aligned} \quad (53)$$

443 Our idea is to apply Lemma 1. Under S1, the finite sum of surrogate functions $\widehat{\mathcal{L}}^{(k)}(\boldsymbol{\theta})$, defined in
 444 (23), is lower bounded by a constant $c_k > -\infty$ for any $\boldsymbol{\theta}$. To this end, we observe that

$$V_k := \widehat{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)}) - \inf_{k \geq 0} c_k \geq 0 \quad (54)$$

445 is a non-negative random variable.

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

$$X_k := \frac{1}{n} (\widehat{\mathcal{L}}_{i_k}(\boldsymbol{\theta}^{(\tau_{i_k}^k)}; \boldsymbol{\theta}^{(k)}) - \widehat{\mathcal{L}}_{i_k}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(k)})) \geq 0. \quad (55)$$

447 Thirdly, we define

$$\begin{aligned} E_k &= -(\widetilde{\mathcal{L}}^{(k+1)}(\boldsymbol{\theta}^{(k+1)}) - \widehat{\mathcal{L}}^{(k+1)}(\boldsymbol{\theta}^{(k+1)})) + (\widetilde{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)}) - \widehat{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)})) \\ &\quad + \frac{1}{n} (\widetilde{\mathcal{L}}_{i_k}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(k)}, \{z_{i_k, m}^{(k)}\}_{m=1}^{M_{(k)}}) - \widehat{\mathcal{L}}_{i_k}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(k)})) \\ &\quad + \frac{1}{n} (\widehat{\mathcal{L}}_{i_k}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(\tau_{i_k}^k)}) - \widetilde{\mathcal{L}}_{i_k}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(\tau_{i_k}^k)}, \{z_{i_k, m}^{(\tau_{i_k}^k)}\}_{m=1}^{M_{(\tau_{i_k}^k)}})). \end{aligned} \quad (56)$$

448 Note that from the definitions (54), (55), (56), we have $V_{k+1} \leq V_k - X_k + E_k$ for any $k \geq 1$.

449 Under H2, we observe that

$$\mathbb{E}[|\widetilde{\mathcal{L}}_{i_k}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(k)}, \{z_{i_k, m}^{(k)}\}_{m=1}^{M_{(k)}}) - \widehat{\mathcal{L}}_{i_k}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(k)})|] \leq C_r M_{(k)}^{-1/2} \quad (57)$$

$$\mathbb{E} \left[\left| \widehat{\mathcal{L}}_{i_k}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(\tau_{i_k}^k)}) - \widetilde{\mathcal{L}}_{i_k}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(\tau_{i_k}^k)}, \{z_{i_k, m}^{(\tau_{i_k}^k)}\}_{m=1}^{M_{(\tau_{i_k}^k)}}) \right| \right] \leq C_r \mathbb{E} \left[M_{(\tau_{i_k}^k)}^{-1/2} \right] \quad (58)$$

$$\mathbb{E} \left[\left| \widetilde{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)}) - \widehat{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)}) \right| \right] \leq \frac{1}{n} \sum_{i=1}^n C_r \mathbb{E} \left[M_{(\tau_i^k)}^{-1/2} \right] \quad (59)$$

Therefore,

$$\mathbb{E} [|E_k|] \leq \frac{C_r}{n} \left(M_{(k)}^{-1/2} + \mathbb{E} \left[M_{(\tau_{i_k}^k)}^{-1/2} + \sum_{i=1}^n \{ M_{(\tau_i^k)}^{-1/2} + M_{(\tau_{i+1}^k)}^{-1/2} \} \right] \right) \quad (60)$$

Using (42) and the assumption on the sequence $\{M_{(k)}\}_{k \geq 0}$, we obtain that

$$\sum_{k=0}^{\infty} \mathbb{E} [|E_k|] < \frac{C_r}{n} (2 + 2n) \sum_{k=0}^{\infty} M_{(k)}^{-1/2} < \infty. \quad (61)$$

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

$$\begin{aligned} \infty &> \sum_{k=0}^{\infty} \mathbb{E} [X_k] = \frac{1}{n} \sum_{k=0}^{\infty} \mathbb{E} [\widehat{\mathcal{L}}_{i_k}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(\tau_{i_k}^k)}) - \widehat{\mathcal{L}}_{i_k}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(k)})] \\ &= \frac{1}{n} \sum_{k=0}^{\infty} \mathbb{E} [\widehat{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)}) - \mathcal{L}(\boldsymbol{\theta}^{(k)})] = \frac{1}{n} \sum_{k=0}^{\infty} \mathbb{E} [\widehat{e}^{(k)}(\boldsymbol{\theta}^{(k)})] \end{aligned} \quad (62)$$

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

$$\lim_{k \rightarrow \infty} \widehat{e}^{(k)}(\boldsymbol{\theta}^{(k)}) = 0 \quad \text{a.s.} \quad (63)$$

and subsequently applying (32), we have $\lim_{k \rightarrow \infty} \|\widehat{e}^{(k)}(\boldsymbol{\theta}^{(k)})\| = 0$ almost surely. Finally, it follows from (32) and (47) that

$$\lim_{k \rightarrow \infty} g_-^{(k)} \leq \lim_{k \rightarrow \infty} \sqrt{2L} \sqrt{\widehat{e}^{(k)}(\boldsymbol{\theta}^{(k)})} + \lim_{k \rightarrow \infty} \sup_{\boldsymbol{\theta} \in \Theta} |\epsilon^{(k)}(\boldsymbol{\theta})| = 0, \quad (64)$$

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 (63) implies that

$$\underline{\mathcal{L}} = \lim_{k \rightarrow \infty} \widehat{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)}) = \lim_{k \rightarrow \infty} \mathcal{L}(\boldsymbol{\theta}^{(k)}) \quad \text{a.s.} \quad (65)$$

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_{∞} .

(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 $\sum_{k=0}^{\infty} \mathbb{E}[X_k] < \infty$.

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

$$0 \leq V_k \leq V_0 - \sum_{j=1}^k X_j + \sum_{j=1}^k E_j \leq V_0 + \sum_{j=1}^k E_j \quad (66)$$

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

475 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

476 $\mathbb{E}\left[\sum_{j=1}^{\infty} |E_j|\right] < \infty$, the series $\sum_{j=1}^{\infty} E_j$ converges a.s. We may therefore define:

$$W_k = V_k + \sum_{j=k+1}^{\infty} E_j \quad (67)$$

477 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:

$$\begin{aligned} W_k &\leq V_{k-1} - X_k + \sum_{j=k}^{\infty} E_j \leq W_{k-1} - X_k \leq W_{k-1} \\ \mathbb{E}[W_k] &\leq \mathbb{E}[W_{k-1}] - \mathbb{E}[X_k] \end{aligned} \quad (68)$$

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

479 $-\sum_{j=1}^{\infty} |E_j| > -\infty$ and $\mathbb{E}[W_k] \geq -\sum_{j=1}^{\infty} \mathbb{E}[|E_j|] > -\infty$, the (random) sequence $(W_k)_{k \geq 0}$

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

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

$$\mathbb{E}[\liminf_{k \rightarrow \infty} |W_k|] = \mathbb{E}[|W_{\infty}|] \leq \liminf_{k \rightarrow \infty} \mathbb{E}[|W_k|] \leq \mathbb{E}[V_0] + \sum_{j=1}^{\infty} \mathbb{E}[|E_j|] < \infty \quad (69)$$

482 showing that the random variable W_{∞} is integrable.

483 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

484 $\mathbb{E}[U_k] \leq \mathbb{E}[|W_0|] + \mathbb{E}[|W_k|] < \infty$ and by the monotone convergence theorem, we get:

$$\lim_{k \rightarrow \infty} \mathbb{E}[U_k] = \mathbb{E}[\lim_{k \rightarrow \infty} U_k] \quad (70)$$

485 Finally, we have:

$$\lim_{k \rightarrow \infty} \mathbb{E}[U_k] = \mathbb{E}[W_0] - w_{\infty} \quad \text{and} \quad \mathbb{E}[\lim_{k \rightarrow \infty} U_k] = \mathbb{E}[W_0] - \mathbb{E}[W_{\infty}] \quad (71)$$

486 showing that $\mathbb{E}[W_{\infty}] = w_{\infty}$ and concluding the proof of (ii). Moreover, using (68) we have that

487 $W_k \leq W_{k-1} - X_k$ which yields:

$$\begin{aligned} \sum_{j=1}^{\infty} X_j &\leq W_0 - W_{\infty} < \infty \\ \sum_{j=1}^{\infty} \mathbb{E}[X_j] &\leq \mathbb{E}[W_0] - w_{\infty} < \infty \end{aligned} \quad (72)$$

488 which concludes the proof of the lemma. \square

D Details about the Numerical Experiments

D.1 Binary Logistic Regression on the Traumabase

D.1.1 Traumabase quantitative variables

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

D.1.2 Metropolis Hastings algorithm

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

$$\begin{aligned} \xi &= \beta_{\text{mis}} + \Omega_{\text{mis},\text{obs}} \Omega_{\text{obs},\text{obs}}^{-1} (z_{i,\text{obs}} - \beta_{\text{obs}}) , \\ \Sigma &= \Omega_{\text{mis},\text{mis}} + \Omega_{\text{mis},\text{obs}} \Omega_{\text{obs},\text{obs}}^{-1} \Omega_{\text{obs},\text{mis}} \end{aligned} \quad (73)$$

where we have used the Schur Complement of $\Omega_{\text{obs},\text{obs}}$ in Ω and noted β_{mis} (resp. β_{obs}) the missing (resp. observed) elements of β . 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:  $z_{i,\text{mis},M}$ 

```

D.1.3 MISSO Update

Choice of surrogate function for MISO: We recall the MISO deterministic surrogate defined in (10):

$$\hat{\mathcal{L}}_i(\theta; \bar{\theta}) = \int_{\mathcal{Z}} \log(p_i(z_{i,\text{mis}}, \bar{\theta}) / f_i(z_{i,\text{mis}}, \theta)) p_i(z_{i,\text{mis}}, \bar{\theta}) \mu_i(dz_i) . \quad (74)$$

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

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

$$\begin{aligned}
 \hat{\mathcal{L}}_i(\theta; \bar{\theta}) &= - \int_{\mathbf{Z}} \log f_i(z_{i,\text{mis}}, z_{i,\text{obs}}, \theta) p_i(z_{i,\text{mis}}, \bar{\theta}) \mu_i(dz_{i,\text{mis}}) \\
 &= - \int_{\mathbf{Z}} \log [p_i(y_i | z_{i,\text{mis}}, z_{i,\text{obs}}, \delta) p_i(z_{i,\text{mis}}, \beta, \Omega)] p_i(z_i, \bar{\theta}) \mu_i(dz_{i,\text{mis}}) \\
 &= - \underbrace{\int_{\mathbf{Z}} \log p_i(y_i | z_{i,\text{mis}}, z_{i,\text{obs}}, \delta) p_i(z_i, \bar{\theta}) \mu_i(dz_{i,\text{mis}})}_{=\hat{\mathcal{L}}_i^{(1)}(\delta, \bar{\theta})} - \underbrace{\int_{\mathbf{Z}} \log p_i(z_{i,\text{mis}}, \beta, \Omega) p_i(z_i, \bar{\theta}) \mu_i(dz_{i,\text{mis}})}_{=\hat{\mathcal{L}}_i^{(2)}(\beta, \Omega, \bar{\theta})}
 \end{aligned} \tag{75}$$

515 The mean β and the covariance Ω of the latent structure can be estimated minimizing the sum of
 516 MISSO surrogates $\hat{\mathcal{L}}_i^{(2)}(\beta, \Omega, \bar{\theta}, \{z_m\}_{m=1}^M)$, defined as MC approximation of $\hat{\mathcal{L}}_i^{(2)}(\beta, \Omega, \bar{\theta})$, for all
 517 $i \in \llbracket n \rrbracket$, in closed-form expression.

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

$$\begin{aligned}
 \hat{\mathcal{L}}_i^{(1)}(\delta, \bar{\theta}) &- \int_{\mathbf{Z}} \nabla \log p_i(y_i | z_{i,\text{mis}}, z_{i,\text{obs}}, \delta) \big|_{\delta=\bar{\delta}} p_i(z_{i,\text{mis}}, \bar{\theta}) \mu_i(dz_{i,\text{mis}}) (\delta - \bar{\delta}) \\
 &- (\delta - \bar{\delta})/2 \int_{\mathbf{Z}} \nabla^2 \log p_i(y_i | z_{i,\text{mis}}, z_{i,\text{obs}}, \delta) p_i(z_{i,\text{mis}}, \bar{\theta}) p_i(z_{i,\text{mis}}, \bar{\theta}) \mu_i(dz_{i,\text{mis}}) (\delta - \bar{\delta})^\top
 \end{aligned} \tag{76}$$

520 Recall that:

$$\begin{aligned}
 \nabla \log p_i(y_i | z_{i,\text{mis}}, z_{i,\text{obs}}, \delta) &= z_i (y_i - S(\delta^\top z_i)) \\
 \nabla^2 \log p_i(y_i | z_{i,\text{mis}}, z_{i,\text{obs}}, \delta) &= -z_i z_i^\top \dot{S}(\delta^\top z_i)
 \end{aligned} \tag{77}$$

521 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 $p \times p$
 522 matrix $z_i z_i^\top$ is semi-definite positive we can assume:

523 **L1.** For all $i \in \llbracket n \rrbracket$ and $\epsilon > 0$, there exist, for all $z_i \in \mathbf{Z}$, a positive definite matrix $H_i(z_i) :=$
 524 $\frac{1}{4}(z_i z_i^\top + \epsilon I_d)$ such that for all $\delta \in \mathbb{R}^p$, $-z_i z_i^\top \dot{S}(\delta^\top z_i) \leq H_i(z_i)$.

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

$$\bar{\mathcal{L}}_i^{(1)}(\delta, \bar{\theta}) = \hat{\mathcal{L}}_i^{(1)}(\delta, \bar{\theta}) - D_i^\top (\delta - \bar{\delta}) + \frac{1}{2} (\delta - \bar{\delta}) H_i (\delta - \bar{\delta})^\top \tag{78}$$

526 where:

$$\begin{aligned}
 D_i &= \int_{\mathbf{Z}} \nabla \log p_i(y_i | z_{i,\text{mis}}, z_{i,\text{obs}}, \delta) \big|_{\delta=\bar{\delta}} p_i(z_{i,\text{mis}}, \bar{\theta}) \mu_i(dz_{i,\text{mis}}) \\
 H_i &= \int_{\mathbf{Z}} H_i(z_{i,\text{mis}}) p_i(z_{i,\text{mis}}, \bar{\theta}) \mu_i(dz_{i,\text{mis}})
 \end{aligned} \tag{79}$$

527 Finally, at iteration k , the total surrogate is:

$$\begin{aligned}
 \tilde{\mathcal{L}}^{(k)}(\theta) &= \frac{1}{n} \sum_{i=1}^n \tilde{\mathcal{L}}_i(\theta, \theta^{(\tau_i^k)}, \{z_{i,m}\}_{m=1}^{M_{(\tau_i^k)}}) \\
 &= \frac{1}{n} \sum_{i=1}^n \tilde{\mathcal{L}}_i^{(2)}(\beta, \Omega, \theta^{(\tau_i^k)}, \{z_{i,m}\}_{m=1}^{M_{(\tau_i^k)}}) - \frac{1}{n} \sum_{i=1}^n \tilde{D}_i^{(\tau_i^k)} (\delta - \delta^{(\tau_i^k)}) \\
 &\quad + \frac{1}{2n} \sum_{i=1}^n (\delta - \delta^{(\tau_i^k)}) \left\{ \tilde{H}_i^{(\tau_i^k)} \right\} (\delta - \delta^{(\tau_i^k)})^\top
 \end{aligned} \tag{80}$$

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

$$\begin{aligned}\tilde{D}_i^{(\tau_i^k)} &= \frac{1}{M_{(\tau_i^k)}} \sum_{m=1}^{M_{(\tau_i^k)}} z_{i,m}^{(\tau_i^k)} \left(y_i - S(\left(\delta^{(\tau_i^k)} \right)^\top z_{i,m}^{(\tau_i^k)}) \right) \\ \tilde{H}_i^{(\tau_i^k)} &= \frac{1}{4M_{(\tau_i^k)}} \sum_{m=1}^{M_{(\tau_i^k)}} z_{i,m}^{(\tau_i^k)} (z_{i,m}^{(\tau_i^k)})^\top\end{aligned}\tag{81}$$

529 Minimizing the total surrogate (80) boils down to performing a quasi-Newton step. It is perhaps sen-
530 sible to apply some diagonal loading which is perfectly compatible with the surrogate interpretation
531 we just gave.

532 The logistic parameters are estimated as follows:

$$\delta^{(k)} = \arg \min_{\delta \in \Theta} \frac{1}{n} \sum_{i=1}^n \tilde{\mathcal{L}}_i^{(1)}(\delta, \theta^{(\tau_i^k)}, \{z_{i,m}\}_{m=1}^{M_{(\tau_i^k)}})\tag{82}$$

533 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
534 (78) and which leads to the following quasi-Newton step:

$$\delta^{(k)} = \frac{1}{n} \sum_{i=1}^n \delta^{(\tau_i^k)} - (\tilde{H}^{(k)})^{-1} \tilde{D}^{(k)}\tag{83}$$

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

536 **MISSO updates:** At the k -th iteration, and after the initialization, for all $i \in \llbracket n \rrbracket$, of the latent
537 variables $(z_i^{(0)})$, the MISSO algorithm consists in picking an index i_k uniformly on $\llbracket n \rrbracket$, complet-
538 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
539 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
540 estimated parameters as follows:

$$\begin{aligned}\beta^{(k)} &= \arg \min_{\beta \in \Theta} \frac{1}{n} \sum_{i=1}^n \tilde{\mathcal{L}}_i^{(2)}(\beta, \Omega^{(k)}, \theta^{(\tau_i^k)}, \{z_{i,m}\}_{m=1}^{M_{(\tau_i^k)}}) = \frac{1}{n} \sum_{i=1}^n \frac{1}{M_{(\tau_i^k)}} \sum_{m=1}^{M_{(\tau_i^k)}} z_{i,m}^{(k)} \\ \Omega^{(k)} &= \arg \min_{\Omega \in \Theta} \frac{1}{n} \sum_{i=1}^n \tilde{\mathcal{L}}_i^{(2)}(\beta^{(k)}, \Omega, \theta^{(\tau_i^k)}, \{z_{i,m}\}_{m=1}^{M_{(\tau_i^k)}}) = \frac{1}{n} \sum_{i=1}^n \frac{1}{M_{(\tau_i^k)}} \sum_{m=1}^{M_{(\tau_i^k)}} w_{i,m}^{(k)} \\ \delta^{(k)} &= \frac{1}{n} \sum_{i=1}^n \delta^{(\tau_i^k)} - (\tilde{H}^{(k)})^{-1} \tilde{D}^{(k)}.\end{aligned}\tag{84}$$

541 where $z_{i,m}^{(k)} = (z_{i, \text{mis}, m}^{(k)}, z_{i, \text{obs}})$ is composed of a simulated and an observed part, $\tilde{D}^{(k)} =$
542 $\frac{1}{n} \sum_{i=1}^n \tilde{D}_i^{(\tau_i^k)}$, $\tilde{H}^{(k)} = \frac{1}{n} \sum_{i=1}^n \tilde{H}_i^{(\tau_i^k)}$ and $w_{i,m}^{(k)} = z_{i,m}^{(k)} (z_{i,m}^{(k)})^\top - \beta^{(k)} (\beta^{(k)})^\top$. Be-
543 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
544 $\hat{\mathcal{L}}_i^{(1)}(\beta, \Omega, \bar{\theta})$ and $\hat{\mathcal{L}}_i^{(2)}(\beta, \Omega, \bar{\theta})$, for all $i \in \llbracket n \rrbracket$ as components of the surrogate function (75).

545 D.2 Incremental Variational Inference

546 D.2.1 Bayesian LeNet-5 Architecture

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

layer type	width	stride	padding	input shape	nonlinearity
convolution (5×5)	6	1	0	$1 \times 32 \times 32$	ReLU
max-pooling (2×2)		2	0	$6 \times 28 \times 28$	
convolution (5×5)	6	1	0	$1 \times 14 \times 14$	ReLU
max-pooling (2×2)		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

549 D.2.2 Bayesian ResNet-18 Architecture

550 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	$1 \times 1 \times 512$	7×7 average pool	ReLU
fully connected	1000	512×1000 fully connections	
softmax	1000		

Table 2: ResNet-18 architecture

551 D.2.3 Algorithms updates

552 First, we initialize the means $\mu_\ell^{(0)}$ for $\ell \in \llbracket d \rrbracket$ and variance estimates $\sigma^{(0)}$. At iteration k , minimizing
553 the sum of stochastic surrogates defined as in (6) and (16) yields the following MISSO update —
554 **step (i)** pick a function index i_k uniformly on $\llbracket n \rrbracket$; **step (ii)** sample a Monte Carlo batch $\{z_m^{(k)}\}_{m=1}^{M(k)}$
555 from $\mathcal{N}(0, \mathbf{I})$; and **step (iii)** update the parameters as

$$\mu_\ell^{(k)} = \frac{1}{n} \sum_{i=1}^n \mu_\ell^{(\tau_i^k)} - \frac{\gamma}{n} \sum_{i=1}^n \hat{\delta}_{\mu_\ell, i}^{(k)} \quad \text{and} \quad \sigma^{(k)} = \frac{1}{n} \sum_{i=1}^n \sigma^{(\tau_i^k)} - \frac{\gamma}{n} \sum_{i=1}^n \hat{\delta}_{\sigma, i}^{(k)}, \quad (85)$$

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

$$\begin{aligned} \hat{\delta}_{\mu_\ell, i}^{(k)} &= -\frac{1}{M(k)} \sum_{m=1}^{M(k)} \nabla_w \log p(y_i | x_i, w) \Big|_{w=t(\theta^{(k-1)}, z_m^{(k)})} + \nabla_{\mu_\ell} d(\theta^{(k-1)}), \\ \hat{\delta}_{\sigma, i}^{(k)} &= -\frac{1}{M(k)} \sum_{m=1}^{M(k)} z_m^{(k)} \nabla_w \log p(y_i | x_i, w) \Big|_{w=t(\theta^{(k-1)}, z_m^{(k)})} + \nabla_{\sigma} d(\theta^{(k-1)}). \end{aligned} \quad (86)$$

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

560 **Monte Carlo SAG update:** Set

$$\mu_\ell^{(k)} = \mu_\ell^{(k-1)} - \frac{\gamma}{n} \sum_{i=1}^n \hat{\delta}_{\mu_\ell, i}^{(k)} \quad \text{and} \quad \sigma^{(k)} = \sigma^{(k-1)} - \frac{\gamma}{n} \sum_{i=1}^n \hat{\delta}_{\sigma, i}^{(k)}, \quad (87)$$

561 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 (86) for $i = i_k$. The learning
 562 rate is set to $\gamma = 10^{-3}$.

563 **Bayes By Backprop update:** Set

$$\mu_\ell^{(k)} = \mu_\ell^{(k-1)} - \frac{\gamma}{n} \hat{\delta}_{\mu_\ell, i_k}^{(k)} \quad \text{and} \quad \sigma^{(k)} = \sigma^{(k-1)} - \frac{\gamma}{n} \hat{\delta}_{\sigma, i_k}^{(k)}, \quad (88)$$

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

565 **Monte Carlo Momentum update:** Set

$$\mu_\ell^{(k)} = \mu_\ell^{(k-1)} + \hat{\mathbf{v}}_{\mu_\ell}^{(k)} \quad \text{and} \quad \sigma^{(k)} = \sigma^{(k-1)} + \hat{\mathbf{v}}_\sigma^{(k)}, \quad (89)$$

566 where

$$\hat{\mathbf{v}}_{\mu_\ell, i}^{(k)} = \alpha \hat{\mathbf{v}}_{\mu_\ell}^{(k-1)} - \frac{\gamma}{n} \hat{\delta}_{\mu_\ell, i_k}^{(k)} \quad \text{and} \quad \hat{\mathbf{v}}_\sigma^{(k)} = \alpha \hat{\mathbf{v}}_\sigma^{(k-1)} - \frac{\gamma}{n} \hat{\delta}_{\sigma, i_k}^{(k)}, \quad (90)$$

567 where α and γ , respectively the momentum and the learning rates, are set to 10^{-3} .

568 **Monte Carlo ADAM update:** Set

$$\mu_\ell^{(k)} = \mu_\ell^{(k-1)} - \frac{\gamma}{n} \hat{\mathbf{m}}_{\mu_\ell}^{(k)} / (\sqrt{\hat{\mathbf{m}}_{\mu_\ell}^{(k)}} + \epsilon) \quad \text{and} \quad \sigma^{(k)} = \sigma^{(k-1)} - \frac{\gamma}{n} \hat{\mathbf{m}}_\sigma^{(k)} / (\sqrt{\hat{\mathbf{m}}_\sigma^{(k)}} + \epsilon), \quad (91)$$

569 where

$$\begin{aligned} \hat{\mathbf{m}}_{\mu_\ell}^{(k)} &= \mathbf{m}_{\mu_\ell}^{(k-1)} / (1 - \rho_1^k) \quad \text{with} \quad \mathbf{m}_{\mu_\ell}^{(k)} = \rho_1 \mathbf{m}_{\mu_\ell}^{(k-1)} + (1 - \rho_1) \hat{\delta}_{\mu_\ell, i_k}^{(k)}, \\ \hat{\mathbf{v}}_{\mu_\ell}^{(k)} &= \mathbf{v}_{\mu_\ell}^{(k-1)} / (1 - \rho_2^k) \quad \text{with} \quad \mathbf{v}_{\mu_\ell}^{(k)} = \rho_2 \mathbf{v}_{\mu_\ell}^{(k-1)} + (1 - \rho_2) (\hat{\delta}_{\mu_\ell, i_k}^{(k)})^2 \end{aligned} \quad (92)$$

570 and

$$\begin{aligned} \hat{\mathbf{m}}_\sigma^{(k)} &= \mathbf{m}_\sigma^{(k-1)} / (1 - \rho_1^k) \quad \text{with} \quad \mathbf{m}_\sigma^{(k)} = \rho_1 \mathbf{m}_\sigma^{(k-1)} + (1 - \rho_1) \hat{\delta}_{\sigma, i_k}^{(k)}, \\ \hat{\mathbf{v}}_\sigma^{(k)} &= \mathbf{v}_\sigma^{(k-1)} / (1 - \rho_2^k) \quad \text{with} \quad \mathbf{v}_\sigma^{(k)} = \rho_2 \mathbf{v}_\sigma^{(k-1)} + (1 - \rho_2) (\hat{\delta}_{\sigma, i_k}^{(k)})^2. \end{aligned} \quad (93)$$

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