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

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Abstract

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

1 Introduction

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

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

where 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) nonconvex and nonsmooth.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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 $x = (x_i, i \in \llbracket 1, n \rrbracket)$, 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 KL divergence between $q(w, \theta)$ and the posterior distribution $p(w|y, x)$, as follows:

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

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

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

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

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

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

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

152 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
 153 $\bar{\theta}$. In addition, for most cases, the term $\nabla d(\bar{\theta})$ can be evaluated in closed form.

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

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 $\{z_m\}_{m=1}^M$ is an i.i.d sample from $\mathcal{N}(0, \mathbf{I})$.

156 3 Convergence Analysis

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

158 **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
 159 lower bounded.

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

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

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

163

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

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

166 **Some intuitions behind the controlling terms:** It is actually common in statistical and optimization
 167 problems, to deal with the manipulation and the control of random variables indexed by sets with
 168 an infinite number of elements. Here, the controlled random variable is an image of a continuous
 169 function 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
 170 such control, we will have recourse to the notion of metric entropy (or bracketing number) as de-
 171 veloped in [Van der Vaart, 2000, Vershynin, 2018, Wainwright, 2019]. A collection of results from
 172 those books gives intuition behind our assumption H 2, which is classical in empirical processes. In
 173 [Vershynin, 2018, Theorem 8.2.3], the authors recall the uniform law of large numbers for a class of
 174 L -Lipschitz functions:

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

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

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

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

179 $\mathcal{N}(\mathcal{F}, \|\cdot\|_\infty, \varepsilon)$ is bounded from above for a class of parametric functions $\mathcal{F} = f_\theta : \theta \in \Theta$ on a
 180 bounded set $\Theta \subset \mathbb{R}$:

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

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

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

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

187 where $g_+(\bar{\theta}) := \max\{0, g(\bar{\theta})\}$, $g_-(\bar{\theta}) := -\min\{0, g(\bar{\theta})\}$ denote the positive and negative part of
 188 $g(\bar{\theta})$, respectively. Note that $\bar{\theta}$ is a stationary point if and only if $g_-(\bar{\theta}) = 0$ [Fletcher et al., 2002].
 189 Also, denote

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

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

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

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

Then we have following non-asymptotic bounds:

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

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 MISSO 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. H2], Eq. (16) gives a non-asymptotic rate of $\mathbb{E}[g_-(\theta^{(K)})] \leq \mathcal{O}(\sqrt{nL/K_{\max}})$ which is new to
 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 S1, S2, H1, H2. In addition, assume that $\{M_{(k)}\}_{k \geq 0}$ is a non-decreasing sequence of integers which satisfies $\sum_{k=0}^{\infty} M_{(k)}^{-1/2} < \infty$. Then:*

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

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 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:

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

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

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

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

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

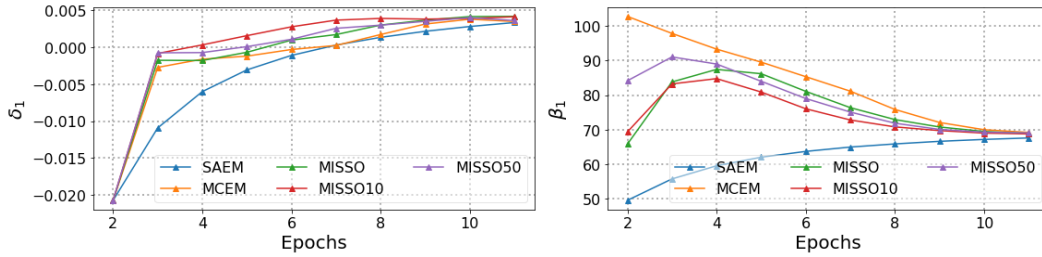


Figure 1: Convergence of first component of the vector of parameters δ and β for the SAEM, the MCEM and the MISSO methods. The convergence is plotted against No. of passes over the data.

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

4.2 Training Bayesian CNN using MISSO

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

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

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

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

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

Bayesian ResNet-18 [He et al., 2016] on CIFAR-10 [Krizhevsky et al., 2012]: We train here the Bayesian variant of the ResNet-18 neural network (see Appendix D.2.2) introduced in [He et al., 2016] on CIFAR-10. The latter dataset is composed of $n = 60\,000$ handwritten digits, 32×32 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 where the default hyperparameters, such as the annealing constant or the number of MC samples, were used for the benchmark methods. For better efficiency and lower variance, the Flipout estimator [Wen et al., 2018] is used.

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

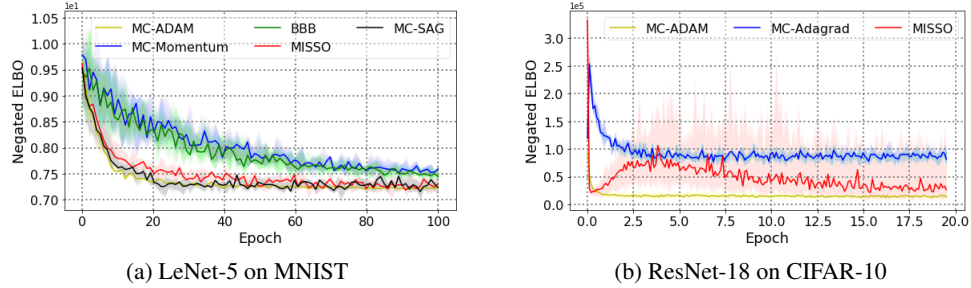


Figure 2: Negated ELBO versus epochs elapsed for fitting (a) Bayesian LeNet-5 on MNIST and (b) Bayesian ResNet-18 on CIFAR-10. The solid curve is obtained from averaging over 5 independent runs of the methods, and the shaded area represents the standard deviation.

Figure 2(a) shows the convergence of the negated evidence lower bound against the number of passes over data (one pass represents an epoch). As observed, the proposed MISSO method outperforms *Bayes by Backprop* and Momentum, while similar convergence rates are observed with the MISSO, ADAM and SAG methods for our experiment on MNIST dataset using a Bayesian variant of LeNet-5. On the other hand, the experiment conducted on CIFAR-10 (Figure 2(b)) using a much larger network, *i.e.*, a Bayesian variant of ResNet-18 (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.

5 Conclusion

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

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367 A Proof of Theorem 1

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

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

370 Then we have following non-asymptotic bounds:

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

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 S2, 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 H2. Moreover,

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

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

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

where (a) is due to $\hat{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)}) = 0$ [cf. S1], (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

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

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 H2. It yields

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

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 H2 and taking total expectations lead to

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

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

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

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. H1]. 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 H2 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 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., $\lim_{k \rightarrow \infty} g_{-}(\boldsymbol{\theta}^{(k)}) = 0$ 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_{∞} .

(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 S1, 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 H2, we observe that

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

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

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

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_{∞} .

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

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_{∞} 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:

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

467 Finally, we have:

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

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) algorithm
 485 [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 Ω and noted β_{mis} (resp. β_{obs}) the missing
 489 (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:  $z_{i,\text{mis},M}$ 

```

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 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 θ , while $\bar{\theta}$ is fixed, in two following parts leading to

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

497 The mean β and the covariance Ω 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 δ :

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

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 δ :

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

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 (5×5)	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

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	$1 \times 1 \times 512$	7×7 average pool	ReLU
fully connected	1000	512×1000 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 μ_ℓ for all $\ell \in \llbracket d \rrbracket$ and σ 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 α and γ , 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: $\gamma = 10^{-3}$, $\rho_1 = 0.9$, $\rho_2 = 0.999$, $\epsilon = 10^{-8}$.