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

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Abstract

To be completed

2 1 Introduction

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

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

- where Θ is a convex, compact, and closed subset of \mathbb{R}^p , and for any $i \in [1, n]$, the function \mathcal{L}_i :
- $\mathbb{R}^p \to \mathbb{R}$ is bounded from below and is (possibly) non-convex and non-smooth.
- Notations We denote $[1, n] = \{1, \dots, n\}$. Unless otherwise specified, $\|\cdot\|$ denotes the standard
- 7 Euclidean norm and $\langle \cdot | \cdot \rangle$ is the inner product in Euclidean space. For any function $f: \Theta \to \mathbb{R}$,
- 8 $f'(\theta, d)$ is the directional derivative of f at θ along the direction d, i.e.,

$$f'(\boldsymbol{\theta}, \boldsymbol{d}) := \lim_{t \to 0^+} \frac{f(\boldsymbol{\theta} + t\boldsymbol{d}) - f(\boldsymbol{\theta})}{t} . \tag{2}$$

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

10 2 MISSO Algorithm

- 11 For any $i \in [\![1,n]\!]$, we consider a surrogate function $\widehat{\mathcal{L}}_i(\boldsymbol{\theta}; \overline{\boldsymbol{\theta}})$ which satisfies
- 12 **S1.** For all $i \in [1, n]$ and $\overline{\theta} \in \Theta$, the function $\widehat{\mathcal{L}}_i(\theta; \overline{\theta})$ is convex w.r.t. θ , and it holds

$$\widehat{\mathcal{L}}_i(\boldsymbol{\theta}; \overline{\boldsymbol{\theta}}) \ge \mathcal{L}_i(\boldsymbol{\theta}), \ \forall \ \boldsymbol{\theta} \in \Theta \ , \tag{3}$$

- where the equality holds when $\theta = \overline{\theta}$.
- 14 **S2.** For any $\overline{\boldsymbol{\theta}}_i \in \Theta$, $i \in [\![1,n]\!]$ and some $\epsilon > 0$, the difference function $\widehat{e}(\boldsymbol{\theta}; \{\overline{\boldsymbol{\theta}}_i\}_{i=1}^n) :=$
- 15 $\frac{1}{n}\sum_{i=1}^{n}\widehat{\mathcal{L}}_{i}(\boldsymbol{\theta};\overline{\boldsymbol{\theta}}_{i}) \mathcal{L}(\boldsymbol{\theta})$ is defined for all $\boldsymbol{\theta} \in \Theta_{\epsilon}$ and differentiable for all $\boldsymbol{\theta} \in \Theta$, where
- 16 $\Theta_{\epsilon} = \{ \theta \in \mathbb{R}^d, \inf_{\theta' \in \Theta} \|\theta \theta'\| < \epsilon \}$ is an ϵ -neighborhood set of Θ . Moreover, for some constant
- 17 L, the gradient satisfies

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

Algorithm 1 MISSO method

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

$$\widetilde{\mathcal{A}}_{i}^{0}(\boldsymbol{\theta}) := \widetilde{\mathcal{L}}_{i}(\boldsymbol{\theta}; \boldsymbol{\theta}^{(0)}, \{z_{i,m}^{(0)}\}_{m-1}^{M_{(k)}}), \ i \in [1, n]. \tag{7}$$

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

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

- Set $\theta^{(k+1)} \in \arg\min_{\theta \in \Theta} \widetilde{\mathcal{L}}^{(k+1)}(\theta) := \frac{1}{n} \sum_{i=1}^{n} \widetilde{\mathcal{A}}_{i}^{k+1}(\theta)$.
- Let Z be a measurable set, $p_i: Z \times \Theta \to \mathbb{R}_+$ be a pdf, $r_i: \Theta \times \Theta \times Z \to \mathbb{R}$ be a measurable
- function and μ_i be a σ -finite measure, we consider surrogate functions which satisfy S1, S2 that can
- be expressed as an expectation:

$$\widehat{\mathcal{L}}_{i}(\boldsymbol{\theta}; \overline{\boldsymbol{\theta}}) := \int_{\mathbf{Z}} r_{i}(\boldsymbol{\theta}; \overline{\boldsymbol{\theta}}, z_{i}) p_{i}(z_{i}; \overline{\boldsymbol{\theta}}) \mu_{i}(dz_{i}) \quad \forall \ (\boldsymbol{\theta}, \overline{\boldsymbol{\theta}}) \in \Theta \times \Theta \ . \tag{5}$$

- The MISSO method replaces the expectation in (5) by Monte Carlo integration and then optimizes 21
- (1) incrementally.
- Denote by $M \in \mathbb{N}$ the Monte Carlo batch size and let $z_m \in \mathbb{Z}$, m = 1, ..., M be a set of samples.
- To this end, we define

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

and we summarize the proposed MISSO method in Algorithm 1.

3 Convergence Analysis 26

- We provide non-asymptotic convergence bound for the MISSO method.
- **H1.** For all $i \in [1, n]$, $\overline{\theta} \in \Theta$, $z_i \in Z$, the measurable function $r_i(\theta; \overline{\theta}, z_i)$ is convex in θ and is 28
- lower bounded.
- **H2.** For all $i \in [1, n]$, $(\theta, \overline{\theta}) \in \Theta^2$, $z_i \in Z$ we assume the existence of an majorizing function $m_r : Z \to \mathbb{R}$ and a constant $C_r < \infty$ such that:

$$\sup_{M>0} \frac{1}{\sqrt{M}} \sum_{m=1}^{M} \left\{ r_i(\boldsymbol{\theta}; \overline{\boldsymbol{\theta}}, z_{i,m}) - \widehat{\mathcal{L}}_i(\boldsymbol{\theta}; \overline{\boldsymbol{\theta}}) \right\} < m_{\mathsf{r}}(z_i) \quad and \quad \mathbb{E}_{\overline{\boldsymbol{\theta}}} \left[m_{\mathsf{r}}(z_i) | \mathcal{F} \right] < C_{\mathsf{r}}$$
 (9)

- where \mathcal{F} is the filtration of the total randomness and we denoted by $\mathbb{E}_{\overline{\theta}}[\cdot]$ the expectation w.r.t. a
- Markov chain $\{z_{i,m}\}_{m=1}^{M}$ with initial distribution $\xi_i(\cdot; \overline{\theta})$, transition kernel $P_{i,\overline{\theta}}$, and stationary
- distribution $p_i(\cdot; \overline{\theta})$. Besides,

$$\sup_{M>0} \frac{1}{\sqrt{M}} \sum_{m=1}^{M} \left\{ \frac{\widehat{\mathcal{L}}_{i}'(\boldsymbol{\theta}, \boldsymbol{\theta} - \overline{\boldsymbol{\theta}}; \overline{\boldsymbol{\theta}}) - r_{i}'(\boldsymbol{\theta}, \boldsymbol{\theta} - \overline{\boldsymbol{\theta}}; \overline{\boldsymbol{\theta}}, z_{i,m})}{\|\overline{\boldsymbol{\theta}} - \boldsymbol{\theta}\|} \right\} < m_{\mathsf{gr}}(z_{i}) \quad and \quad \mathbb{E}_{\overline{\boldsymbol{\theta}}} \left[m_{\mathsf{gr}}(z_{i}) | \mathcal{F} \right] < C_{\mathsf{gr}}$$

$$\tag{10}$$

Some intuitions behind the control terms: It is actually common in statistical and optimization 35 problems, to deal with the manipulation and the control of random variables indexed by sets with 36 an infinite number of elements. here, the random variable we control is an image of a continuous 37 function noted $v: \mathsf{Z} \to \mathbb{R}$ and defined as $v(z) := r_i(\boldsymbol{\theta}; \overline{\boldsymbol{\theta}}, z_{i,m}) - \widehat{\mathcal{L}}_i(\boldsymbol{\theta}; \overline{\boldsymbol{\theta}})$ for all $z \in \mathsf{Z}$ and for 38 fixed $(\theta, \hat{\theta}) \in \Theta^2$. To characterize such control, we will have recourse to the notion of metric entropy 39 (or covering number of bracketing number) as developed in [Van der Vaart, 2000, Vershynin, 2018, 40 Wainwright, 2019]. A collection of results from those books gives intuition behind our assumption 41 H 2, classical in empirical process: 42

In [Vershynin, 2018], the authors recall the uniform law of large numbers by stating that for $(X_i, i \in [1, M])$ random variables taking values in (0, 1), we have:

$$\mathbb{E}\sup_{f\in\mathcal{F}}\left|\frac{1}{M}\sum_{i=1}^{M}f\left(X_{i}\right)-\mathbb{E}f(X)\right|\leq\frac{CL}{\sqrt{M}}\tag{11}$$

Moreover, in [Vershynin, 2018] and [Wainwright, 2019], the application of the Dudley's inequality yields: $N_{l1}\left(\varepsilon\|m\|_{P,r},\mathcal{F},L_r(P)\right)\leq K\left(\frac{\dim\Theta}{\varepsilon}\right)^d$, every $0<\varepsilon<\dim\Theta$

$$\mathbb{E}\sup_{f} |X_f| = \operatorname{Esup}_{f \in \mathcal{F}} |X_f - X_0| \le \frac{1}{\sqrt{M}} \int_0^1 \sqrt{\log \mathcal{N}(\mathcal{F}, \|\cdot\|_{\infty}, \varepsilon)} d\varepsilon \tag{12}$$

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

$$\mathcal{N}(\mathcal{F}, \|\cdot\|_{\infty}, \varepsilon) \le K \left(\frac{\operatorname{diam}\Theta}{\varepsilon}\right)^d, \quad \text{every} \quad 0 < \varepsilon < \operatorname{diam}\Theta$$
 (13)

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.

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

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

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

57 Also, denote

$$\widehat{\mathcal{L}}^{(k)}(\boldsymbol{\theta}) := \frac{1}{n} \sum_{i=1}^{n} \widehat{\mathcal{L}}_{i}(\boldsymbol{\theta}; \boldsymbol{\theta}^{(\tau_{i}^{k})}), \quad \widehat{e}^{(k)}(\boldsymbol{\theta}) := \widehat{\mathcal{L}}^{(k)}(\boldsymbol{\theta}) - \mathcal{L}(\boldsymbol{\theta}).$$
 (15)

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

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

$$\Delta_{(K_{\text{max}})} := 2nL\mathbb{E}[\widetilde{\mathcal{L}}^{(0)}(\boldsymbol{\theta}^{(0)}) - \widetilde{\mathcal{L}}^{(K_{\text{max}})}(\boldsymbol{\theta}^{(K_{\text{max}})})] + \sum_{k=0}^{K_{\text{max}}-1} \frac{4LC_{\text{r}}}{\sqrt{M_{(k)}}}, \tag{16}$$

Then we have following non-asymptotic bounds:

$$\mathbb{E}\left[\|\nabla \widehat{e}^{(K)}(\boldsymbol{\theta}^{(K)})\|^2\right] \le \frac{\Delta_{(K_{\text{max}})}}{K_{\text{max}}} \tag{17}$$

$$\mathbb{E}[g_{-}(\boldsymbol{\theta}^{(K)})] \le \sqrt{\frac{\Delta_{(K_{\text{max}})}}{K_{\text{max}}}} + \frac{C_{\text{gr}}}{K_{\text{max}}} \sum_{k=0}^{K_{\text{max}}-1} M_{(k)}^{-1/2}.$$
 (18)

- 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 $\mathbb{E}[g_{-}^{(K)}] \leq \mathcal{O}(\sqrt{1/K_{\text{max}}})$. 63
- Furthermore, we remark that the MISO method can be analyzed in Theorem 1 as a special case 64
- of the MISSO method satisfying $C_r = C_{gr} = 0$. In this case, while the asymptotic convergence 65
- is well known from [Mairal, 2015] [cf. H2], Eq. (17) gives a non-asymptotic rate of $\mathbb{E}[g_-^{(K)}] \leq$
- $\mathcal{O}(\sqrt{nL/K_{\mathsf{max}}})$ which is new to our best knowledge. 67
- Next, we show that under an additional assumption on the sequence of batch size $M_{(k)}$, the MISSO 68
- method converges almost surely to a stationary point: 69
- **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: 70
- 71
- 1. the negative part of the stationarity measure converges almost surely to zero, 72 i.e., $\lim_{k\to\infty} g_{-}(\theta^{(k)}) = 0$ a.s.. 73
- 2. the objective value $\mathcal{L}(\boldsymbol{\theta}^{(k)})$ converges almost surely to a finite number $\underline{\mathcal{L}}$, 74 i.e., $\lim_{k\to\infty} \mathcal{L}(\boldsymbol{\theta}^{(k)}) = \underline{\mathcal{L}} a.s.$. 75
- In particular, the first result above shows that the sequence $\{\theta^{(k)}\}_{k\geq 0}$ produced by the MISSO 76 method satisfies an asymptotic stationary point condition.

4 Numerical Experiments

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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 $z_i=[z_{i,\mathrm{mis}},z_{i,\mathrm{obs}}]$ is not fully observed where we denote by $z_{i,\mathrm{mis}}$ the missing values and $z_{i,\mathrm{obs}}$ the observed covariate. It is assumed that $(z_i,i\in \llbracket n\rrbracket)$ are i.i.d. and marginally distributed according to $\mathcal{N}(\boldsymbol{\beta},\Omega)$ 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:

$$p_i(y_i|z_i) = S(\boldsymbol{\delta}^{\top}\bar{z}_i)^{y_i} \left(1 - S(\boldsymbol{\delta}^{\top}\bar{z}_i)\right)^{1 - y_i}$$
(19)

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

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

MISSO update: At the k-th iteration, and after the initialization, for all $i \in [n]$, of the latent variables $(z_i^{(0)})$, the MISSO algorithm consists in picking an index i_k uniformly on [n], completing the observations by sampling a Monte Carlo batch $\{z_{i_k, \min, m}^{(k)}\}_{m=1}^{M_{(k)}}$ of missing values from the conditional distribution $p(z_{i_k, \min}|z_{i_k, \text{obs}}, y_{i_k}; \boldsymbol{\theta}^{(k-1)})$ using an MCMC sampler and computing the estimated parameters as follows:

$$\boldsymbol{\beta}^{(k)} = \arg\min_{\beta \in \Theta} \frac{1}{n} \sum_{i=1}^{n} \tilde{\mathcal{L}}_{i}^{(2)}(\beta, \Omega^{(k)}, \theta^{(\tau_{i}^{k})}, \{z_{i,m}\}_{m=1}^{M_{(\tau_{i}^{k})}}) = \frac{1}{n} \sum_{i=1}^{n} \frac{1}{M_{(\tau_{i}^{k})}} \sum_{m=1}^{M_{(\tau_{i}^{k})}} z_{i,m}^{(k)}$$

$$\boldsymbol{\Omega}^{(k)} = \arg\min_{\Omega \in \Theta} \frac{1}{n} \sum_{i=1}^{n} \tilde{\mathcal{L}}_{i}^{(2)}(\beta^{(k)}, \Omega, \theta^{(\tau_{i}^{k})}, \{z_{i,m}\}_{m=1}^{M_{(\tau_{i}^{k})}}) = \frac{1}{n} \sum_{i=1}^{n} \frac{1}{M_{(\tau_{i}^{k})}} \sum_{m=1}^{M_{(\tau_{i}^{k})}} z_{i,m}^{(k)}(z_{i,m}^{(k)})^{\top} - \boldsymbol{\beta}^{(k)}(\boldsymbol{\beta}^{(k)})^{\top}$$

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

$$(20)$$

where $z_{i,m}^{(k)}=(z_{i,\text{mis},m}^{(k)},z_{i,\text{obs}})$ is composed of a simulated and an observed part and $\tilde{D}^{(k)}=\frac{1}{n}\sum_{i=1}^n \tilde{D}_i^{(\tau_i^k)}$ and $\tilde{H}^{(k)}=\frac{1}{n}\sum_{i=1}^n \tilde{H}_i^{(\tau_i^k)}$. Besides, $\tilde{\mathcal{L}}_i^{(1)}(\beta,\Omega,\overline{\pmb{\theta}},\{z_m\}_{m=1}^M)$ and $\tilde{\mathcal{L}}_i^{(2)}(\beta,\Omega,\overline{\pmb{\theta}},\{z_m\}_{m=1}^M)$ are defined as MC approximation of $\hat{\mathcal{L}}_i^{(1)}(\beta,\Omega,\overline{\pmb{\theta}})$ and $\hat{\mathcal{L}}_i^{(2)}(\beta,\Omega,\overline{\pmb{\theta}})$, for all $i\in \llbracket n \rrbracket$.

Fitting a logistic regression model on the TraumaBase dataset We apply the MISSO method

99 See Appendix ?? for more explanation.

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to fit a logistic regression model on the TraumaBase (http://traumabase.eu) dataset, which 101 consists of data collected from 15 trauma centers in France, covering measurements on patients 102 from the initial to last stage of trauma. 103 Similar to [Jiang et al., 2018], we select p=16 influential quantitative measurements, described 104 in Appendix ??, on n = 6384 patients, and we adopt the logistic regression model with missing 105 covariates in (19) to predict the risk of a severe hemorrhage which is one of the main cause of 106 death after a major trauma. Note as the dataset considered is heterogeneous - coming from multiple 107 sources with frequently missed entries - we apply the latent data model described in the above. For the Monte-Carlo sampling of $z_{i, mis}$, we run a Metropolis Hastings algorithm with the target distribution $p(\cdot|z_{i,\text{obs}},y_i;\boldsymbol{\theta}^{(k)})$ whose procedure is detailed in Appendix ??.

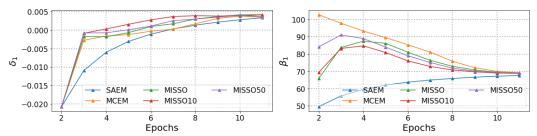


Figure 1: Convergence of first component of the vector of parameters δ and β for the SAEM, the MCEM and the MISSO methods. The convergence is plotted against the number of passes over the data.

We compare in Figure 1 the convergence behavior of the estimated parameters β using SAEM [Delyon et al., 1999] (with stepsize $\gamma_k = 1/k$), 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 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 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

At iteration k, minimizing the sum of stochastic surrogates defined as in (6) and (??) yields the 120 following MISSO update — step (i) pick a function index i_k uniformly on [n]; 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 121

$$\mu_{\ell}^{(k)} = \frac{1}{n} \sum_{i=1}^{n} \mu_{\ell}^{(\tau_{i}^{k})} - \frac{\gamma}{n} \sum_{i=1}^{n} \hat{\delta}_{\mu_{\ell}, i}^{(k)} \quad \text{and} \quad \sigma^{(k)} = \frac{1}{n} \sum_{i=1}^{n} \sigma^{(\tau_{i}^{k})} - \frac{\gamma}{n} \sum_{i=1}^{n} \hat{\delta}_{\sigma, i}^{(k)} , \qquad (21)$$

 $\text{ where } \hat{\pmb{\delta}}_{\mu_\ell,i}^{(k)} = \hat{\pmb{\delta}}_{\mu_\ell,i}^{(k-1)} \text{ and } \hat{\pmb{\delta}}_{\sigma,i}^{(k)} = \hat{\pmb{\delta}}_{\sigma,i}^{(k-1)} \text{ for } i \neq i_k \text{ and:}$

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

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

with
$$d(\boldsymbol{\theta}) = n^{-1} \sum_{\ell=1}^{d} \left(-\log(\sigma) + (\sigma^2 + \mu_{\ell}^2)/2 - 1/2 \right)$$
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Bayesian LeNet-5 on MNIST [LeCun et al., 1998]: This application follows Example 2 de-125 scribed in Section 2. We apply the MISSO method to fit a Bayesian variant of LeNet-5 [LeCun et al., 1998] (see Appendix ??). 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 (??), the weights are assumed independent and identically distributed according to $\mathcal{N}(0,1)$. We also assume that $q(\cdot; \boldsymbol{\theta}) \equiv \mathcal{N}(\mu, \sigma^2 \mathbf{I})$. The variational posterior parameters are thus $\boldsymbol{\theta} = (\mu, \sigma)$ where $\mu = (\mu_\ell, \ell \in [\![d]\!])$ where d is the number of weights in the neural network. We use the re-parametrization as $w = t(\boldsymbol{\theta}, z) = \mu + \sigma z$ with $z \sim \mathcal{N}(0, \mathbf{I})$.

We describe in Table ?? the architecture of the Convolutional Neural Network introduced in [LeCun 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

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 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 [?] is preferred than a simple reparametrization trick for ResNet-18.

layer type	Output Size	ResNet-18	nonlinearity
conv1	$112 \times 112 \times 64$	7×7 , 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	$14\times14\times256$	$ \begin{pmatrix} 3 \times 3, 256 \\ 3 \times 3, 256 \end{pmatrix} \times 2 $	ReLU
conv5x	$7\times7\times512$	$\begin{pmatrix} 3 \times 3, 512 \\ 3 \times 3, 512 \end{pmatrix} imes 2$	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

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 (??) 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 ??. 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 $M_{(k)} = k$.

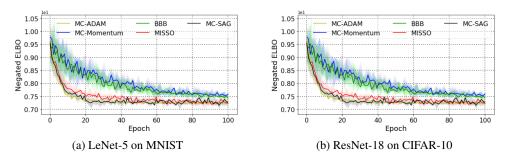


Figure 2: (a) Negated ELBO versus epochs elapsed for fitting the Bayesian LeNet-5 on MNIST using different algorithms. (b) ELBO versus epochs elapsed for fitting the Bayesian ResNet-18 on CIFAR-10 using different algorithms. The solid curve is obtained from averaging over 5 independent runs of the methods,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

Figure 2 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.

References

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206 A Proof of Theorem 1

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

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

209 Then we have following non-asymptotic bounds:

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

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

$$\widetilde{\mathcal{L}}^{(k)}(\boldsymbol{\theta}) := \frac{1}{n} \sum_{i=1}^{n} \widetilde{\mathcal{A}}_{i}^{k}(\boldsymbol{\theta}). \tag{22}$$

211 Notice that

$$\widetilde{\mathcal{L}}^{(k+1)}(\boldsymbol{\theta}) = \frac{1}{n} \sum_{i=1}^{n} \widetilde{\mathcal{L}}_{i}(\boldsymbol{\theta}; \boldsymbol{\theta}^{(\tau_{i}^{k+1})}, \{z_{i,m}^{(\tau_{i}^{k+1})}\}_{m=1}^{M_{(\tau_{i}^{k+1})}})
= \widetilde{\mathcal{L}}^{(k)}(\boldsymbol{\theta}) + \frac{1}{n} (\widetilde{\mathcal{L}}_{i_{k}}(\boldsymbol{\theta}; \boldsymbol{\theta}^{(k)}, \{z_{i_{k},m}^{(k)}\}_{m=1}^{M_{(k)}}) - \widetilde{\mathcal{L}}_{i_{k}}(\boldsymbol{\theta}; \boldsymbol{\theta}^{(\tau_{i_{k}}^{k})}, \{z_{i_{k},m}^{(\tau_{i_{k}}^{k})}\}_{m=1}^{M_{(\tau_{i_{k}}^{k})}})).$$
(23)

212 Furthermore, we recall that

$$\widehat{\mathcal{L}}^{(k)}(\boldsymbol{\theta}) := \frac{1}{n} \sum_{i=1}^{n} \widehat{\mathcal{L}}_{i}(\boldsymbol{\theta}; \boldsymbol{\theta}^{(\tau_{i}^{k})}), \quad \widehat{e}^{(k)}(\boldsymbol{\theta}) := \widehat{\mathcal{L}}^{(k)}(\boldsymbol{\theta}) - \mathcal{L}(\boldsymbol{\theta}). \tag{24}$$

213 Due to S2, we have

$$\|\nabla \widehat{e}^{(k)}(\boldsymbol{\theta}^{(k)})\|^2 \le 2L\widehat{e}^{(k)}(\boldsymbol{\theta}^{(k)}). \tag{25}$$

To prove the first bound in (17), using the optimality of $\theta^{(k+1)}$, one has

$$\widetilde{\mathcal{L}}^{(k+1)}(\boldsymbol{\theta}^{(k+1)}) \leq \widetilde{\mathcal{L}}^{(k+1)}(\boldsymbol{\theta}^{(k)}) \\
= \widetilde{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)}) + \frac{1}{n} \left(\widetilde{\mathcal{L}}_{i_k}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(k)}, \{z_{i_k,m}^{(k)}\}_{m=1}^{M_{(k)}}) - \widetilde{\mathcal{L}}_{i_k}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(\tau_{i_k}^k)}, \{z_{i_k,m}^{(\tau_{i_k}^k)}\}_{m=1}^{M_{(\tau_{i_k}^k)}}) \right)$$
(26)

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

216 We observe that the conditional expectation evaluates to

$$\mathbb{E}_{i_{k}} \left[\mathbb{E} \left[\widetilde{\mathcal{L}}_{i_{k}}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(k)}, \{z_{i_{k},m}^{(k)}\}_{m=1}^{M_{(k)}}) | \mathcal{F}_{k}, i_{k} \right] | \mathcal{F}_{k} \right] \\
= \mathcal{L}(\boldsymbol{\theta}^{(k)}) + \mathbb{E}_{i_{k}} \left[\mathbb{E} \left[\frac{1}{M_{(k)}} \sum_{m=1}^{M_{(k)}} r_{i_{k}}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(k)}, z_{i_{k},m}^{(k)}) - \widehat{\mathcal{L}}_{i_{k}}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(k)}) | \mathcal{F}_{k}, i_{k} \right] | \mathcal{F}_{k} \right] \\
\leq \mathcal{L}(\boldsymbol{\theta}^{(k)}) + \frac{C_{r}}{\sqrt{M_{(k)}}}, \tag{27}$$

where the last inequality is due to H2. Moreover,

$$\mathbb{E}\left[\widetilde{\mathcal{L}}_{i_k}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(\tau_{i_k}^k)}, \{z_{i_k,m}^{(\tau_{i_k}^k)}\}_{m=1}^{M_{(\tau_{i_k}^k)}}) | \mathcal{F}_k\right] = \frac{1}{n} \sum_{i=1}^n \widetilde{\mathcal{L}}_i(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(\tau_i^k)}, \{z_{i,m}^{(\tau_i^k)}\}_{m=1}^{M_{(\tau_i^k)}}) = \widetilde{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)}).$$
(28)

Taking the conditional expectations on both sides of (26) and re-arranging terms give:

$$\widetilde{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)}) - \mathcal{L}(\boldsymbol{\theta}^{(k)}) \le n \mathbb{E} \left[\widetilde{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)}) - \widetilde{\mathcal{L}}^{(k+1)}(\boldsymbol{\theta}^{(k+1)}) | \mathcal{F}_k \right] + \frac{C_{\mathsf{r}}}{\sqrt{M_{(k)}}}$$
(29)

219 Proceeding from (29), we observe the following lower bound for the left hand side

$$\widetilde{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)}) - \mathcal{L}(\boldsymbol{\theta}^{(k)}) \stackrel{(a)}{=} \widetilde{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)}) - \widehat{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)}) + \widehat{e}^{(k)}(\boldsymbol{\theta}^{(k)})$$

$$\stackrel{(b)}{\geq} \widetilde{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)}) - \widehat{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)}) + \frac{1}{2L} \|\nabla \widehat{e}^{(k)}(\boldsymbol{\theta}^{(k)})\|^{2}$$

$$= \underbrace{\frac{1}{n} \sum_{i=1}^{n} \left\{ \frac{1}{M_{(\tau_{i}^{k})}} \sum_{m=1}^{M_{(\tau_{i}^{k})}} r_{i}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(\tau_{i}^{k})}, z_{i,m}^{(\tau_{i}^{k})}) - \widehat{\mathcal{L}}_{i}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(\tau_{i}^{k})}) \right\}}_{:=-\delta^{(k)}(\boldsymbol{\theta}^{(k)})} + \frac{1}{2L} \|\nabla \widehat{e}^{(k)}(\boldsymbol{\theta}^{(k)})\|^{2}$$

$$(30)$$

where (a) is due to $\hat{e}^{(k)}(\boldsymbol{\theta}^{(k)}) = 0$ [cf. S1], (b) is due to (25) and we have defined the summation in the last equality as $-\delta^{(k)}(\boldsymbol{\theta}^{(k)})$. Substituting the above into (29) yields

$$\frac{\|\nabla \widehat{e}^{(k)}(\boldsymbol{\theta}^{(k)})\|^2}{2L} \le n\mathbb{E}\left[\widetilde{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)}) - \widetilde{\mathcal{L}}^{(k+1)}(\boldsymbol{\theta}^{(k+1)})|\mathcal{F}_k\right] + \frac{C_{\mathsf{r}}}{\sqrt{M_{(k)}}} + \delta^{(k)}(\boldsymbol{\theta}^{(k)}) \tag{31}$$

Observe the following upper bound on the total expectations:

$$\mathbb{E}\left[\delta^{(k)}(\boldsymbol{\theta}^{(k)})\right] \le \mathbb{E}\left[\frac{1}{n}\sum_{i=1}^{n}\frac{C_{\mathsf{r}}}{\sqrt{M_{(\tau_{i}^{k})}}}\right],\tag{32}$$

223 which is due to H2. It yields

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

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

$$\mathbb{E}[\|\nabla \widehat{e}^{(K)}(\boldsymbol{\theta}^{(K)})\|^{2}] = \frac{1}{K_{\text{max}}} \sum_{k=0}^{K_{\text{max}}-1} \mathbb{E}[\|\nabla \widehat{e}^{(k)}(\boldsymbol{\theta}^{(k)})\|^{2}] \\
\leq \frac{2nL\mathbb{E}[\widetilde{\mathcal{L}}^{(0)}(\boldsymbol{\theta}^{(0)}) - \widetilde{\mathcal{L}}^{(K_{\text{max}})}(\boldsymbol{\theta}^{(K_{\text{max}})})]}{K_{\text{max}}} + \frac{2LC_{\text{r}}}{K_{\text{max}}} \sum_{k=0}^{K_{\text{max}}-1} \mathbb{E}\Big[\frac{1}{\sqrt{M_{(k)}}} + \frac{1}{n} \sum_{i=1}^{n} \frac{1}{\sqrt{M_{(\tau_{i}^{k})}}}\Big]$$
(33)

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:

$$\mathbb{E}[M_{(\tau_i^k)}^{-1/2}] = \sum_{j=1}^k \frac{1}{n} \left(1 - \frac{1}{n}\right)^{j-1} M_{(k-j)}^{-1/2}$$
(34)

228 Taking the sum yields:

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

$$(35)$$

where the last inequality is due to upper bounding the geometric series. Plugging this back into (33)
 yields

$$\mathbb{E}[\|\nabla \widehat{e}^{(K)}(\boldsymbol{\theta}^{(K)})\|^{2}] = \frac{1}{K_{\text{max}}} \sum_{k=0}^{K_{\text{max}}-1} \mathbb{E}[\|\nabla \widehat{e}^{(k)}(\boldsymbol{\theta}^{(k)})\|^{2}] \\
\leq \frac{2nL\mathbb{E}[\widetilde{\mathcal{L}}^{(0)}(\boldsymbol{\theta}^{(0)}) - \widetilde{\mathcal{L}}^{(K_{\text{max}})}(\boldsymbol{\theta}^{(K_{\text{max}})})]}{K_{\text{max}}} + \frac{1}{K_{\text{max}}} \sum_{k=0}^{K_{\text{max}}-1} \frac{4LC_{\text{r}}}{\sqrt{M_{(k)}}} = \frac{\Delta_{(K_{\text{max}})}}{K_{\text{max}}}.$$
(36)

- This concludes our proof for the first inequality in (17).
- To prove the second inequality of (17), we define the shorthand notations $g^{(k)}:=g(\pmb{\theta}^{(k)}),\,g_-^{(k)}:=g(\pmb{\theta}^{(k)})$
- 233 $-\min\{0, g^{(k)}\}, g_+^{(k)} := \max\{0, g^{(k)}\}.$ We observe that

$$g^{(k)} = \inf_{\boldsymbol{\theta} \in \Theta} \frac{\mathcal{L}'(\boldsymbol{\theta}^{(k)}, \boldsymbol{\theta} - \boldsymbol{\theta}^{(k)})}{\|\boldsymbol{\theta}^{(k)} - \boldsymbol{\theta}\|}$$

$$= \inf_{\boldsymbol{\theta} \in \Theta} \left\{ \frac{\frac{1}{n} \sum_{i=1}^{n} \widehat{\mathcal{L}}'_{i}(\boldsymbol{\theta}^{(k)}, \boldsymbol{\theta} - \boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(\tau_{i}^{k})})}{\|\boldsymbol{\theta}^{(k)} - \boldsymbol{\theta}\|} - \frac{\left\langle \nabla \widehat{e}^{(k)}(\boldsymbol{\theta}^{(k)}) \mid \boldsymbol{\theta} - \boldsymbol{\theta}^{(k)} \right\rangle}{\|\boldsymbol{\theta}^{(k)} - \boldsymbol{\theta}\|} \right\}$$

$$\geq -\|\nabla \widehat{e}^{(k)}(\boldsymbol{\theta}^{(k)})\| + \inf_{\boldsymbol{\theta} \in \Theta} \frac{\frac{1}{n} \sum_{i=1}^{n} \widehat{\mathcal{L}}'_{i}(\boldsymbol{\theta}^{(k)}, \boldsymbol{\theta} - \boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(\tau_{i}^{k})})}{\|\boldsymbol{\theta}^{(k)} - \boldsymbol{\theta}\|}$$
(37)

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

$$\frac{1}{n} \sum_{i=1}^{n} \widehat{\mathcal{L}}'_{i}(\boldsymbol{\theta}^{(k)}, \boldsymbol{\theta} - \boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(\tau_{i}^{k})}) \\
= \underbrace{\widetilde{\mathcal{L}}^{(k)'}(\boldsymbol{\theta}^{(k)}, \boldsymbol{\theta} - \boldsymbol{\theta}^{(k)})}_{\geq 0} - \widehat{\mathcal{L}}^{(k)'}(\boldsymbol{\theta}^{(k)}, \boldsymbol{\theta} - \boldsymbol{\theta}^{(k)}) + \frac{1}{n} \sum_{i=1}^{n} \widehat{\mathcal{L}}'_{i}(\boldsymbol{\theta}^{(k)}, \boldsymbol{\theta} - \boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(\tau_{i}^{k})}) \\
\geq \frac{1}{n} \sum_{i=1}^{n} \left\{ \widehat{\mathcal{L}}'_{i}(\boldsymbol{\theta}^{(k)}, \boldsymbol{\theta} - \boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(\tau_{i}^{k})}) - \frac{1}{M_{(\tau_{i}^{k})}} \sum_{m=1}^{M_{(\tau_{i}^{k})}} r'_{i}(\boldsymbol{\theta}^{(k)}, \boldsymbol{\theta} - \boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(\tau_{i}^{k})}, \boldsymbol{z}_{i,m}^{(\tau_{i}^{k})}) \right\}$$
(38)

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

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

239 We have

$$g^{(k)} \ge -\|\nabla \widehat{e}^{(k)}(\boldsymbol{\theta}^{(k)})\| + \inf_{\boldsymbol{\theta} \in \Theta} (-\epsilon^{(k)}(\boldsymbol{\theta})) \ge -\|\nabla \widehat{e}^{(k)}(\boldsymbol{\theta}^{(k)})\| - \sup_{\boldsymbol{\theta} \in \Theta} |\epsilon^{(k)}(\boldsymbol{\theta})|. \tag{39}$$

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

$$g_{-}^{(k)} \le \|\nabla \widehat{e}^{(k)}(\boldsymbol{\theta}^{(k)})\| + \sup_{\boldsymbol{\theta} \in \Theta} |\epsilon^{(k)}(\boldsymbol{\theta})|. \tag{40}$$

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

$$\mathbb{E}[g_{-}^{(K)}] \leq \mathbb{E}[\|\nabla \widehat{e}^{(K)}(\boldsymbol{\theta}^{(K)})\|] + \mathbb{E}[\sup_{\boldsymbol{\theta} \in \Theta} \epsilon^{(K)}(\boldsymbol{\theta})] \tag{41}$$

243 We note that

$$\left(\mathbb{E}[\|\nabla \widehat{e}^{(K)}(\boldsymbol{\theta}^{(K)})\|]\right)^{2} \leq \mathbb{E}[\|\nabla \widehat{e}^{(K)}(\boldsymbol{\theta}^{(K)})\|^{2}] \leq \frac{\Delta(K_{\mathsf{max}})}{K_{\mathsf{max}}},\tag{42}$$

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

$$\mathbb{E}[\sup_{\boldsymbol{\theta} \in \Theta} \epsilon^{(K)}(\boldsymbol{\theta})] = \frac{1}{K_{\text{max}}} \sum_{k=0}^{K_{\text{max}}} \mathbb{E}[\sup_{\boldsymbol{\theta} \in \Theta} \epsilon^{(k)}(\boldsymbol{\theta})] \stackrel{(a)}{\leq} \frac{C_{\text{gr}}}{K_{\text{max}}} \sum_{k=0}^{K_{\text{max}}-1} \mathbb{E}\left[\frac{1}{n} \sum_{i=1}^{n} M_{(\tau_{i}^{k})}^{-1/2}\right] \\
\stackrel{(b)}{\leq} \frac{C_{\text{gr}}}{K_{\text{max}}} \sum_{k=0}^{K_{\text{max}}-1} M_{(k)}^{-1/2} \tag{43}$$

where (a) is due to H^2 and (b) is due to (35). This implies

$$\mathbb{E}[g_{-}^{(K)}] \le \sqrt{\frac{\Delta_{(K_{\text{max}})}}{K_{\text{max}}}} + \frac{C_{\text{gr}}}{K_{\text{max}}} \sum_{k=0}^{K_{\text{max}}-1} M_{(k)}^{-1/2}, \tag{44}$$

246 and concludes the proof of the theorem.

247 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., $\lim_{k\to\infty} g_-(\pmb{\theta}^{(k)}) = 0$ a.s..
- 252 2. the objective value $\mathcal{L}(\boldsymbol{\theta}^{(k)})$ converges almost surely to a finite number $\underline{\mathcal{L}}$, i.e., $\lim_{k\to\infty}\mathcal{L}(\boldsymbol{\theta}^{(k)})=\underline{\mathcal{L}}$ 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 $k \geq 1$:

$$V_k \le V_{k-1} - X_{k-1} + E_{k-1} \tag{45}$$

- 259 then:
- (i) for all $k \geq 0$, $\mathbb{E}[V_k] < \infty$ and the sequence $(V_k)_{k>0}$ converges a.s. to a finite limit V_{∞} .
- (ii) the sequence $(\mathbb{E}[V_k])_{k\geq 0}$ converges and $\lim_{k\to\infty}\mathbb{E}[V_k]=\mathbb{E}[V_\infty]$.
- (iii) the series $\sum_{k=0}^{\infty} X_k$ converges almost surely and $\sum_{k=0}^{\infty} \mathbb{E}[X_k] < \infty$.
- 263 We proceed from (26) by re-arranging terms and observing that

$$\widehat{\mathcal{L}}^{(k+1)}(\boldsymbol{\theta}^{(k+1)}) \leq \widehat{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)}) - \frac{1}{n} (\widehat{\mathcal{L}}_{i_{k}}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(\tau_{i_{k}}^{k})}) - \widehat{\mathcal{L}}_{i_{k}}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(k)}))
- (\widetilde{\mathcal{L}}^{(k+1)}(\boldsymbol{\theta}^{(k+1)}) - \widehat{\mathcal{L}}^{(k+1)}(\boldsymbol{\theta}^{(k+1)})) + (\widetilde{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)}) - \widehat{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)}))
+ \frac{1}{n} (\widetilde{\mathcal{L}}_{i_{k}}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(k)}; \{z_{i_{k},m}^{(k)}\}_{m=1}^{M_{(k)}}) - \widehat{\mathcal{L}}_{i_{k}}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(\tau_{i_{k}}^{k})}, \{z_{i_{k},m}^{(\tau_{i_{k}}^{k})}\}_{m=1}^{M_{(\tau_{i_{k}}^{k})}}))
+ \frac{1}{n} (\widehat{\mathcal{L}}_{i_{k}}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(\tau_{i_{k}}^{k})}) - \widetilde{\mathcal{L}}_{i_{k}}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(\tau_{i_{k}}^{k})}, \{z_{i_{k},m}^{(\tau_{i_{k}}^{k})}\}_{m=1}^{M_{(\tau_{i_{k}}^{k})}}))$$
(46)

Our idea is to apply Lemma 1. Under S1, the finite sum of surrogate functions $\widehat{\mathcal{L}}^{(k)}(\theta)$, defined in (15), is lower bounded by a constant $c_k > -\infty$ for any θ . To this end, we observe that

$$V_k := \widehat{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)}) - \inf_{k \ge 0} c_k \ge 0$$
(47)

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

$$X_k := \frac{1}{n} (\widehat{\mathcal{L}}_{i_k}(\boldsymbol{\theta}^{(\tau_{i_k}^k)}; \boldsymbol{\theta}^{(k)}) - \widehat{\mathcal{L}}_{i_k}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(k)})) \ge 0. \tag{48}$$

268 Thirdly, we define

$$E_{k} = -\left(\widetilde{\mathcal{L}}^{(k+1)}(\boldsymbol{\theta}^{(k+1)}) - \widehat{\mathcal{L}}^{(k+1)}(\boldsymbol{\theta}^{(k+1)})\right) + \left(\widetilde{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)}) - \widehat{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)})\right) + \frac{1}{n}\left(\widetilde{\mathcal{L}}_{i_{k}}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(k)}, \{z_{i_{k}, m}^{(k)}\}_{m=1}^{M_{(k)}}) - \widehat{\mathcal{L}}_{i_{k}}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(k)})\right) + \frac{1}{n}\left(\widehat{\mathcal{L}}_{i_{k}}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(\tau_{i_{k}}^{k})}) - \widetilde{\mathcal{L}}_{i_{k}}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(\tau_{i_{k}}^{k})}, \{z_{i_{k}, m}^{(\tau_{i_{k}}^{k})}\}_{m=1}^{M_{(\tau_{i_{k}}^{k})}})\right).$$

$$(49)$$

- Note that from the definitions (47), (48), (49), we have $V_{k+1} \leq V_k X_k + E_k$ for any $k \geq 1$.
- 270 Under H2, we observe that

$$\mathbb{E}\left[|\widehat{\mathcal{L}}_{i_k}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(k)}, \{z_{i_k,m}^{(k)}\}_{m=1}^{M_{(k)}}) - \widehat{\mathcal{L}}_{i_k}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(k)})|\right] \le C_{\mathsf{r}} M_{(k)}^{-1/2}$$
(50)

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$$\mathbb{E}\left[\left|\widehat{\mathcal{L}}_{i_k}(\boldsymbol{\theta}^{(k)};\boldsymbol{\theta}^{(\tau_{i_k}^k)}) - \widetilde{\mathcal{L}}_{i_k}(\boldsymbol{\theta}^{(k)};\boldsymbol{\theta}^{(\tau_{i_k}^k)}, \{z_{i_k,m}^{(\tau_{i_k}^k)}\}_{m=1}^{M_{(\tau_{i_k}^k)}})\right|\right] \le C_{\mathsf{r}} \mathbb{E}\left[M_{(\tau_{i_k}^k)}^{-1/2}\right] \tag{51}$$

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$$\mathbb{E}\left[\left|\widetilde{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)}) - \widehat{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)})\right|\right] \le \frac{1}{n} \sum_{i=1}^{n} C_{\mathsf{r}} \mathbb{E}\left[M_{(\tau^{k})}^{-1/2}\right]$$
(52)

273 Therefore,

$$\mathbb{E}[|E_k|] \le \frac{C_r}{n} \left(M_{(k)}^{-1/2} + \mathbb{E} \left[M_{(\tau_{i,1}^k)}^{-1/2} + \sum_{i=1}^n \left\{ M_{(\tau_{i}^k)}^{-1/2} + M_{(\tau_{i}^{k+1})}^{-1/2} \right\} \right] \right)$$
 (53)

Using (35) and the assumption on the sequence $\{M_{(k)}\}_{k>0}$, we obtain that

$$\sum_{k=0}^{\infty} \mathbb{E}[|E_k|] < \frac{C_{\mathsf{r}}}{n} (2+2n) \sum_{k=0}^{\infty} M_{(k)}^{-1/2} < \infty.$$
 (54)

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

$$\infty > \sum_{k=0}^{\infty} \mathbb{E}[X_k] = \frac{1}{n} \sum_{k=0}^{\infty} \mathbb{E}\left[\widehat{\mathcal{L}}_{i_k}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(\tau_{i_k}^k)}) - \widehat{\mathcal{L}}_{i_k}(\boldsymbol{\theta}^{(k)}; \boldsymbol{\theta}^{(k)})\right]
= \frac{1}{n} \sum_{k=0}^{\infty} \mathbb{E}\left[\widehat{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)}) - \mathcal{L}(\boldsymbol{\theta}^{(k)})\right] = \frac{1}{n} \sum_{k=0}^{\infty} \mathbb{E}\left[\widehat{e}^{(k)}(\boldsymbol{\theta}^{(k)})\right]$$
(55)

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

$$\lim_{k \to \infty} \widehat{e}^{(k)}(\boldsymbol{\theta}^{(k)}) = 0 \quad \text{a.s.}$$
 (56)

and subsequently applying (25), we have $\lim_{k\to\infty} \|\widehat{e}^{(k)}(\boldsymbol{\theta}^{(k)})\| = 0$ almost surely. Finally, it follows from (25) and (40) that

$$\lim_{k \to \infty} g_{-}^{(k)} \le \lim_{k \to \infty} \sqrt{2L} \sqrt{\widehat{e}^{(k)}(\boldsymbol{\theta}^{(k)})} + \lim_{k \to \infty} \sup_{\boldsymbol{\theta} \in \Theta} |\epsilon^{(k)}(\boldsymbol{\theta})| = 0, \tag{57}$$

where the last equality holds almost surely due to the fact that $\sum_{k=0}^{\infty} \mathbb{E}[\sup_{\theta \in \Theta} |\epsilon^{(k)}(\theta)|] < \infty$. This concludes the asymptotic convergence of the MISSO method. 280 281

Finally, we prove that $\mathcal{L}(\theta^{(k)})$ converges almost surely. As a consequence of Lemma 1, it is clear that 282

 $\{V_k\}_{k\geq 0}$ converges almost surely and so is $\{\widehat{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)})\}_{k\geq 0}$, i.e., we have $\lim_{k\to\infty}\widehat{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)})=\underline{\mathcal{L}}$. 283 Applying (56) implies that 284

$$\underline{\mathcal{L}} = \lim_{k \to \infty} \widehat{\mathcal{L}}^{(k)}(\boldsymbol{\theta}^{(k)}) = \lim_{k \to \infty} \mathcal{L}(\boldsymbol{\theta}^{(k)}) \quad \text{a.s.}$$
 (58)

This shows that $\mathcal{L}(\boldsymbol{\theta}^{(k)})$ converges almost surely to $\underline{\mathcal{L}}$. 285

Proof of Lemma 1 286

Lemma. Let $(V_k)_{k>0}$ be a non negative sequence of random variables such that $\mathbb{E}[V_0] < \infty$. 287

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 $k \geq 1$: 288

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

then: 290

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

(ii) the sequence $(\mathbb{E}[V_k])_{k\geq 0}$ converges and $\lim_{k\to\infty}\mathbb{E}[V_k]=\mathbb{E}[V_\infty]$. 292

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

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

$$0 \le V_k \le V_0 - \sum_{j=1}^k X_j + \sum_{j=1}^k E_j \le V_0 + \sum_{j=1}^k E_j$$
 (59)

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

Since $0 \le X_k \le V_{k-1} - V_k + E_k$ we also obtain for all $k \ge 0$, $\mathbb{E}[X_k] < \infty$. Moreover, since $\mathbb{E}\left[\sum_{j=1}^{\infty}|E_j|\right] < \infty$, the series $\sum_{j=1}^{\infty}E_j$ converges a.s. We may therefore define:

$$W_k = V_k + \sum_{j=k+1}^{\infty} E_j \tag{60}$$

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:

$$W_{k} \leq V_{k-1} - X_{k} + \sum_{j=k}^{\infty} E_{j} \leq W_{k-1} - X_{k} \leq W_{k-1}$$

$$\mathbb{E}[W_{k}] \leq \mathbb{E}[W_{k-1}] - \mathbb{E}[X_{k}]$$
(61)

Hence the sequences $(W_k)_{k\geq 0}$ and $(\mathbb{E}[W_k])_{k\geq 0}$ are non increasing. Since for all $k\geq 0, W_k\geq 0$ and $\mathbb{E}[W_k]\geq 0$ are non increasing. Since for all $k\geq 0, W_k\geq 0$ since $(W_k)_{k\geq 0}\geq 0$ and $\mathbb{E}[W_k]\geq 0$ and $\mathbb{E}[W_k]\geq 0$ sequence $(\mathbb{E}[W_k])_{k\geq 0}$ converges a.s. to a limit W_∞ and the (deterministic) sequence $(\mathbb{E}[W_k])_{k\geq 0}$ converges to a limit W_∞ . Since $|W_k|\leq V_0+\sum_{j=1}^\infty |E_j|$, the Fatou lemma implies that:

$$\mathbb{E}[\liminf_{k \to \infty} |W_k|] = \mathbb{E}[|W_\infty|] \le \liminf_{k \to \infty} \mathbb{E}[|W_k|] \le \mathbb{E}[V_0] + \sum_{j=1}^{\infty} \mathbb{E}[|E_j|] < \infty$$
 (62)

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

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

$$\lim_{k \to \infty} \mathbb{E}[U_k] = \mathbb{E}[\lim_{k \to \infty} U_k]$$
(63)

306 Finally, we have:

$$\lim_{k \to \infty} \mathbb{E}[U_k] = \mathbb{E}[W_0] - w_{\infty} \quad \text{and} \quad \mathbb{E}[\lim_{k \to \infty} U_k] = \mathbb{E}[W_0] - \mathbb{E}[W_{\infty}]$$
 (64)

showing that $\mathbb{E}[W_{\infty}] = w_{\infty}$ and concluding the proof of (ii). Moreover, using (61) we have that $W_k \leq W_{k-1} - X_k$ which yields:

$$\sum_{j=1}^{\infty} X_j \le W_0 - W_{\infty} < \infty$$

$$\sum_{j=1}^{\infty} \mathbb{E}[X_j] \le \mathbb{E}[W_0] - w_{\infty} < \infty$$
(65)

which concludes the proof of the lemma.