Minimization by Incremental Stochastic Surrogate with Application to Bayesian Deep Learning

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Problem Statement

We are interested in the constrained minimization of a large sum of nonconvex functions defined as:

$$\min_{\theta \in \Theta} \left[f(\theta) \triangleq \sum_{i=1}^{N} f_i(\theta) \right] \tag{1}$$

Beforehand, let $\mathcal{T}(\Theta)$ be a neighborhood of Θ and assume that:

M 1. *For all $i \in [\![N]\!]$, f_i is continuously differentiable on $\mathcal{T}(\Theta)$.*

M 2. *For all $i \in [\![N]\!]$, f_i is bounded from below, i.e. there exist a constant $M_i \in \mathbb{R}$ such as for all $\theta \in \Theta$, $f_i(\theta) \geq M_i$.*

For any $\theta \in \Theta$ and $i \in [\![N]\!]$, we say, following (Mairal, 2015) that a function $f_{i,\theta} : \mathbb{R}^p \to \mathbb{R}$ is a surrogate of f_i at θ if the following properties are satisfied:

- the function $\vartheta \to f_{i,\theta}(\vartheta)$ is continuously differentiable on $\mathcal{T}(\Theta)$
- for all $\vartheta \in \Theta$, $f_{i,\theta}(\vartheta) \geq f_i(\vartheta)$, $f_{i,\theta}(\theta) = f_i(\theta)$ and $\nabla f_{i,\theta}(\vartheta)\big|_{\vartheta=\theta} = \nabla f_i(\vartheta)\big|_{\vartheta=\theta}$.

The gap $f_{i,\theta} - f_i$ plays a key role in the convergence analysis and we require this error to be L-smooth for some constant $L > 0$ Denote by $\langle \cdot, \cdot \rangle$ the scalar product, we also introduce the following stationary point condition:

Definition 1. (Asymptotic Stationary Point Condition)
A sequence $(\theta^k)_{k\geq 0}$ satisfies the asymptotic stationary point condition if

$$\liminf_{k\to\infty} \inf_{\theta\in\Theta} \frac{\langle \nabla f(\theta^k), \theta - \theta^k \rangle}{\|\theta - \theta^k\|_2} \geq 0. \tag{2}$$

MISO Scheme

The incremental scheme of (Mairal, 2015) computes surrogate functions, at each iteration of the algorithm, for a mini-batch of components:

Algorithm 1 MISO algorithm

Initialization: given an initial parameter estimate θ^0, for all $i \in [\![N]\!]$ compute a surrogate function $\vartheta \to f_{i,\theta^0}(\vartheta)$.

Iteration k: given the current estimate θ^{k-1}:

1. Pick a set I_k uniformly on $\{A \subset [\![N]\!], \mathrm{card}(A) = p\}$
2. For all $i \in I_k$ and compute $\vartheta \to f_{i,\theta^{k-1}}(\vartheta)$, a surrogate of f_i at θ^{k-1}.
3. Set $\theta^k \in \arg\min_{\vartheta\in\Theta} \sum_{i=1}^N a_i^k(\vartheta)$ where $a_i^k(\vartheta)$ are defined recursively as follows:

$$a_i^k(\vartheta) \triangleq \begin{cases} f_{i,\theta^{k-1}}(\vartheta) & \text{if } i \in I_k \\ a_i^{k-1}(\vartheta) & \text{otherwise} \end{cases} \tag{3}$$

MISSO Scheme

- Case when the surrogate functions computed in Algorithm 1 **are not tractable**.
- Assume that the surrogate can be expressed as an integral over a set of latent variables $z = (z_i \in \mathsf{Z}_i, i \in [\![N]\!]) \in \mathsf{Z}$ where $\mathsf{Z} = \times_{i=1}^N \mathsf{Z}_i$ where Z_i is a subset of $\mathbb{R}^{m_i}$.

$$f_{i,\theta}(\vartheta) \triangleq \int_{\mathsf{Z}_i} r_{i,\theta}(z_i, \vartheta) p_i(z_i, \theta) \mu_i(\mathrm{d}z_i) \quad \text{for all } (\theta, \vartheta) \in \Theta^2. \tag{4}$$

- Our scheme is based on the computation, at each iteration, of stochastic auxiliary functions for a mini-batch of components. For $i \in [\![N]\!]$, the auxiliary function, noted $\hat{f}_{i,\theta}(\vartheta)$ is a Monte Carlo approximation of the surrogate function $f_{i,\theta}(\vartheta)$ defined by (4) such that:

$$\hat{f}_{i,\theta}(\vartheta) \triangleq \frac{1}{M} \sum_{m=0}^{M-1} r_{i,\theta}(z_i^m, \vartheta) \quad \text{for all } (\theta, \vartheta) \in \Theta^2 \tag{5}$$

where $\{z_i^m\}_{m=0}^{M-1}$ is a Monte Carlo batch.

Algorithm 2 MISSO algorithm

Initialization: given an initial parameter estimate θ^0, for all $i \in [\![N]\!]$ compute the function $\vartheta \to \hat{f}_{i,\theta^0}(\vartheta)$ defined by (5).

Iteration k: given the current estimate θ^{k-1}:

1. Pick a set I_k uniformly on $\{A \subset [\![N]\!], \mathrm{card}(A) = p\}$
2. For all $i \in I_k$, sample a Monte Carlo batch $\{z_i^{k,m}\}_{m=0}^{M_k-1}$ from $p_i(z_i, \theta^{k-1})$.
3. For all $i \in I_k$, compute the function $\vartheta \to \hat{f}_{i,\theta^{k-1}}(\vartheta)$ defined by (5).
4. Set $\theta^k \in \arg\min_{\vartheta\in\Theta} \sum_{i=1}^N \hat{a}_i^k(\vartheta)$ where $\hat{a}_i^k(\vartheta)$ are defined recursively as follows:

$$\hat{a}_i^k(\vartheta) \triangleq \begin{cases} \hat{f}_{i,\theta^{k-1}}(\vartheta) & \text{if } i \in I_k \\ \hat{a}_i^{k-1}(\vartheta) & \text{otherwise} \end{cases} \tag{6}$$

Convergence Guarantees Assumptions

Whether we use Markov Chain Monte Carlo or direct simulation, we need to control the supremum norm of the fluctuations of the Monte Carlo approximation. Let $i \in [\![N]\!]$, $\{j_i(z_i, \vartheta), z_i \in \mathsf{Z}_i, \vartheta \in \Theta\}$ be a family of measurable functions, λ_i a probability measure on $\mathsf{Z}_i \times \mathcal{Z}_i$. We define:

$$C_i(j_i) \triangleq \sup_{\theta\in\Theta} \sup_{M>0} M^{-1/2} \mathbb{E}_{i,\theta} \left[\sup_{\vartheta\in\Theta} \left| \sum_{m=0}^{M-1} \left\{ j_i(z_i^m, \vartheta) - \int_{\mathsf{Z}_i} j_i(z_i, \vartheta) p_i(z_i, \theta) \lambda_i(\mathrm{d}z_i) \right\} \right| \right] \tag{7}$$

M 3. *For all $i \in [\![N]\!]$ and $\theta \in \Theta$:*

$$\lim_{k\to\infty} C_i(r_{i,\theta}) < \infty \quad \textit{and} \quad \lim_{k\to\infty} C_i(\nabla r_{i,\theta}) < \infty. \tag{8}$$

M 4. *$\{M_k\}_{k\geq 0}$ is a non deacreasing sequence of integers which satisfies $\sum_{k=0}^{\infty} M_k^{-1/2} < \infty$.*

Theorem: MISSO Convergence Guarantees

Assume **M1-M4**. Let $\left(\theta^k\right)_{k\geq 1}$ be a sequence generated from $\theta^0 \in \Theta$ by the iterative application described by Algorithm 2. Then:

(i) $\left(f(\theta^k)\right)_{k\geq 1}$ converges almost surely.

(ii) $\left(\theta^k\right)_{k\geq 1}$ satisfies the Asymptotic Stationary Point Condition.

Application to Variational Bayesian Inference

- Let $x = (x_i, i \in [\![N]\!])$ and $y = (y_i, i \in [\![N]\!])$ be i.i.d. input-output pairs and w be a global latent variable taking values in W as subset of $\mathbb{R}^J$. A natural decomposition of the joint distribution is:

$$p(y, x, w) = p(w) \prod_{i=1}^{N} p_i(y_i | x_i, w) \tag{9}$$

The goal is to calculate the posterior distribution $p(w|y,x)$**.**

- Variational inference problem boils down to minimizing the following KL divergence:

$$\theta^* = \arg\min_{\theta\in\Theta} \mathrm{KL}(q(w;\theta) \parallel p(w|y,x)) = \arg\min_{\theta\in\Theta} f(\theta) \tag{10}$$

where for all $\theta \in \Theta$, $f(\theta) = \sum_{i=1}^N f_i(\theta)$ with :

$$f_i(\theta) \triangleq -\int_{\mathsf{W}} q(w;\theta) \log p_i(y_i, x_i | w) \mathrm{d}w + \frac{1}{N} \mathrm{KL}(q(w;\theta) \parallel p(w)) = r_i(\theta) + d(\theta) \tag{11}$$

- Define following quadratic surrogate at $\theta \in \Theta$:

$$f_{i,\theta}(\vartheta) \triangleq f_i(\theta) + \nabla f_i(\theta)^\top (\vartheta - \theta) + \frac{L}{2} \|\vartheta - \theta\|_2^2 \tag{12}$$

where $\|\cdot\|_2$ is the ℓ_2-norm and L is an upper bound of the spectral norm of the Hessian of f_i at θ.

- **Reparametrization trick:** We assume that for all $\theta \in \Theta$, the distribution of the random vector $W = t(\theta, e)$ where $e \sim \mathcal{N}_d(0, \mathrm{Id})$ has a density $q(\cdot, \theta)$. Then, following (Proposition 1)blundell:

$$\nabla \int_{\mathsf{W}} \log p_i(y_i, x_i | w) q(w, \theta) \mathrm{d}w = \int_{\mathsf{W}} \mathrm{J}(\theta, e) \nabla \log p_i(y_i, x_i | t(\theta, e)) \phi(e) \mathrm{d}e$$

where for each $e \in \mathbb{R}^d$, $\mathrm{J}(\theta, e)$ is the Jacobian of the function $t(\cdot, e)$ with respect to θ.

- The pair $\left(r_{i,\theta}(e, \vartheta), \phi(e)\right)$ defining $f_{i,\theta}(\vartheta)$ is given by:

$$\begin{aligned} r_{i,\theta}(e, \vartheta) \triangleq & \left(-\log p_i(y_i, x_i | t(\theta, e)) + d(\theta)\right) \\ & + \left(-\mathrm{J}(\theta, e) \nabla \log p_i(y_i, x_i | t(\theta, e)) + \nabla d(\theta)\right)^\top (\vartheta - \theta) + \frac{L}{2} \|\vartheta - \theta\|_2^2 \end{aligned} \tag{13}$$

The MISSO algorithm consists in:

1. Picking a set I_k uniformly on $\{A \subset [\![N]\!], \mathrm{card}(A) = p\}$.
2. Sampling a Monte Carlo batch $\{e^{k,m}\}_{m=0}^{M_k-1}$ from the standard Gaussian distribution.
3. Setting $\theta^k = \theta^{k-1} - \frac{1}{L} \sum_{i=1}^N \hat{a}_i^k$ where $\hat{a}_i^k$ are defined recursively as follows:

$$\hat{a}_i^k \triangleq \begin{cases} -\frac{1}{M_k} \sum_{m=0}^{M_k-1} \mathrm{J}(\theta, e^{k,m}) \nabla_\theta \log p_i(y_i, x_i | t(\theta, e^{k,m})) + \nabla d(\theta^{k-1}) & \text{if } i \in I_k \\ \hat{a}_i^{k-1} & \text{otherwise} \end{cases} \tag{14}$$

Training a Bayesian Neural Network on MNIST

Settings

- 2-layer bayesian neural network
- Tanh activation function
- Standard Gaussian prior on the weight
- Gaussian variational posterior independent of i and l (layers)

$$p(w) = \mathcal{N}(0, \mathrm{Id})$$
$$p(y_i | x_i, w) = \mathrm{Softmax}(f(x_i, w))$$

- Input layer $d = 784$
- A single hidden layer of $p = 100$ hyperbolic tangent units
- Final softmax output layer with $K = 10$ classes
- MNIST dataset $N = 60\,000$

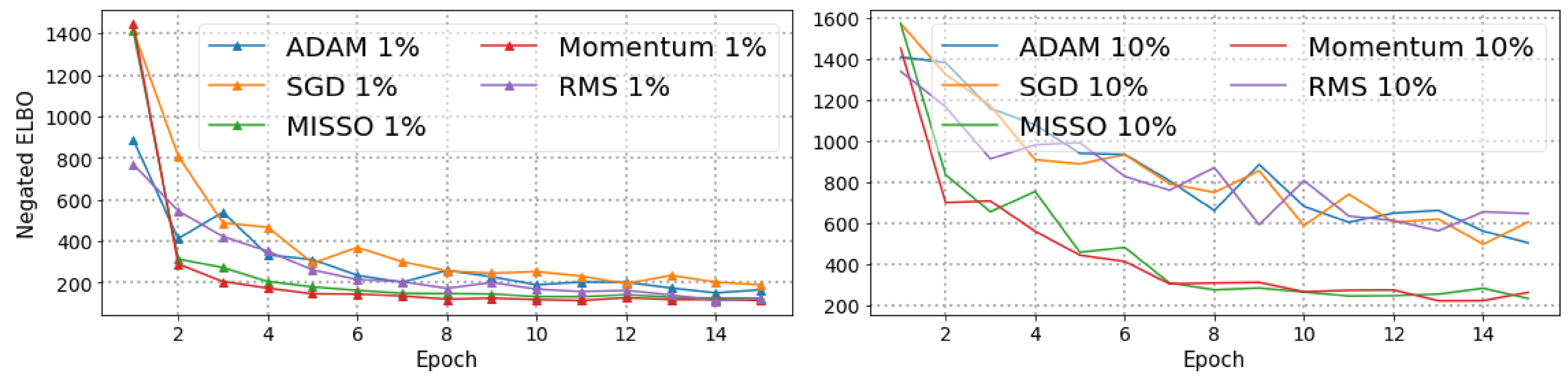

Figure 1: ELBO convergence.

References

(Blundell et al.(2015)Blundell, Cornebise, Kavukcuoglu, and Wierstra) C. Blundell, J. Cornebise, K. Kavukcuoglu, and D. Wierstra. Weight uncertainty in neural networks. In *Proceedings of the 32Nd International Conference on ICML - Volume 37*, ICML'15, pages 1613–1622. JMLR.org, 2015.

(Gal(2016)) Y. Gal. *Uncertainty in Deep Learning*. PhD thesis, University of Cambridge, 2016.

(Le Roux et al.(2012)Le Roux, Schmidt, and Bach) N. Le Roux, M.W. Schmidt, and F. Bach. A stochastic gradient method with an exponential convergence rate for finite training sets. In *NIPS*, pages 2672–2680, 2012.

(Mairal(2015)) J. Mairal. Incremental Majorization-Minimization Optimization with Application to Large-Scale Machine Learning. *SIAM*, 2015.

(Ranganath et al.(2014)Ranganath, Gerrish, and Blei) R. Ranganath, S. Gerrish, and D. Blei. Black Box Variational Inference. *PMLR*, 33:814–822, 2014.