Understanding and Accelerating Particle-Based Variational Inference

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ICML 2019

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Introduction

Particle-based Variational Inference Methods (ParVIs):

- Represent the variational distribution q by particles; update the particles to minimize $\mathrm{KL}_p(q)$.
- More flexible than classical VIs; more particle-efficient than MCMCs.

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What is known:

- Stein Variational Gradient Descent (SVGD) [13] simulates the gradient flow (steepest descending curves) of KL_p on $\mathcal{P}_{\mathcal{H}}(\mathcal{X})$ [12].
- The Blob and w-SGLD methods [5] simulate the gradient flow of KL_p on the Wasserstein space $\mathcal{P}_2(\mathcal{X})$.

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What remains unknown:

- Do ParVIs make assumptions when simulating the gradient flow?
 Does one assume stronger than another?
- Is it possible to accelerate the gradient flow?
- Is there a principle for selecting the bandwidth parameter?

Contributions

Findings:

- SVGD approximates the gradient flow on $\mathcal{P}_2(\mathcal{X})$.
- ParVIs approximate the $\mathcal{P}_2(\mathcal{X})$ gradient flow by a compulsory smoothing treatment.
- Various ParVIs either smooth the density or smooth functions, and they are equivalent.

Methods:

- Two novel ParVIs.
- An acceleration framework for general ParVIs.
- A principled bandwidth selection method for the smoothing kernel.

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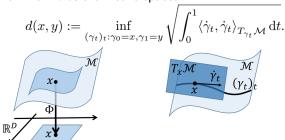
Basic Concepts

Spaces:

- Metric space: a set \mathcal{M} with a distance function $d: \mathcal{M} \times \mathcal{M} \to \mathbb{R}$.
- Riemannian manifold:

A topological space $\mathcal M$ that locally behaves like an Euclidean space (manifold), and there is an inner product $\langle\cdot,\cdot\rangle_{T_x\mathcal M}$ in each of its tangent space $T_x\mathcal M$ (Riemannian).

- Tangent space is the structure of manifolds.
- Riemannian manifolds are metric spaces:



Basic Concepts

Gradient flow $\{(x_t)_t\}$ of a function f: steepest descending curves.

 On metric spaces: various defs ([1], Def. 11.1.1; [18], Def. 23.7), e.g., the Mimimizing Movement Scheme (MMS) ([1], Def. 2.0.6):

$$x_{t+\varepsilon} = \operatorname*{argmin}_{x \in \mathcal{M}} f(x) + \frac{1}{2\varepsilon} d^2(x, x_t).$$

• On Riemannian manifolds: $\dot{x}_t = -\operatorname{grad} f(x_t)$, where:

$$\langle \operatorname{grad} f(x), v \rangle_{T_x \mathcal{M}} = v[f] := \sum_i v^i \partial_i f, \forall v \in T_x \mathcal{M},$$

which is equivalent to:

grad
$$f(x) = \max_{v \in T_x \mathcal{M}, ||v||_{T_x \mathcal{M}} = 1} \frac{\mathrm{d}}{\mathrm{d}t} f(x_t).$$

It coincides with MMS on Riemannian manifolds.

 $\mathcal{P}_2(\mathcal{X}) := \{ q: \text{ distribution on } \mathcal{X} \mid \exists x_0 \in \mathcal{X} \text{ s.t. } \mathbb{E}_q[d(x_0, x)^2] < +\infty \}.$ Consider Euclidean support space $\mathcal{X} = \mathbb{R}^D$ afterwards.

• $\mathcal{P}_2(\mathcal{X})$ as a metric space ([18], Def 6.4):

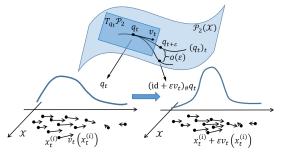
$$d_W(q,p) := \left(\inf_{\pi \in \Pi(q,p)} \mathbb{E}_{\pi(x,y)}[d(x,y)^2]\right)^{1/2},$$

where

$$\Pi(q,p) := \bigg\{\pi\colon \text{distribution on } \mathcal{X}\times\mathcal{X} \bigg| \int_{\mathcal{X}} \pi(x,y)\,\mathrm{d}y = q(x), \\ \int_{\mathcal{X}} \pi(x,y)\,\mathrm{d}x = p(y) \bigg\}.$$

 $\mathcal{P}_2(\mathcal{X}) := \big\{ q \colon \text{distribution on } \mathcal{X} \mid \exists x_0 \in \mathcal{X} \text{ s.t. } \mathbb{E}_q[d(x_0, x)^2] < +\infty \big\}.$

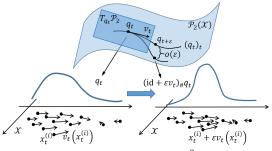
ullet \mathcal{P}_2 as a Riemannian manifold [17, 18, 1] $(\mathcal{X}=\mathbb{R}^D)$:



• Tangent vector $\partial_t q_t$ on $\mathcal{P}_2(\mathcal{X}) \Longleftrightarrow$ Vector field v_t on \mathcal{X} . $\{x^{(i)}\}_{i=1}^N \sim q_t \Longrightarrow \{x^{(i)} + \varepsilon v_t(x^{(i)})\}_{i=1}^N \sim (\operatorname{id} + \varepsilon v_t)_\# q_t = q_{t+\varepsilon} + o(\varepsilon)$. ([1], Prop 8.1.8)

 $\mathcal{P}_2(\mathcal{X}) := \{ q: \text{ distribution on } \mathcal{X} \mid \exists x_0 \in \mathcal{X} \text{ s.t. } \mathbb{E}_q[d(x_0, x)^2] < +\infty \}.$

ullet \mathcal{P}_2 as a Riemannian manifold [17, 18, 1] ($\mathcal{X}=\mathbb{R}^D$):



- Tangent space: $T_q \mathcal{P}_2 := \overline{\{\nabla \varphi \mid \varphi \in C_c^\infty\}}^{\mathcal{L}_q^2}$ $\mathcal{L}_a^2 := \{u : \mathbb{R}^D \to \mathbb{R}^D \mid \int_{\mathcal{V}} \|u(x)\|_2^2 \, \mathrm{d}q < \infty\}, \ \varphi : \mathbb{R}^D \to \mathbb{R}.$ ([18], Thm 13.8; [1], Thm 8.3.1, Def 8.4.1, Prop 8.4.5)
- Riemannian metric: $\langle v, u \rangle_{T_a \mathcal{P}_2} := \int_{\mathcal{V}} v(x) \cdot u(x) \, q(x) \, \mathrm{d}x$. (consistent with the Wasserstein distance d_W [3])

$$\mathcal{P}_2(\mathcal{X}) := \left\{ q: \text{ distribution on } \mathcal{X} \mid \exists x_0 \in \mathcal{X} \text{ s.t. } \mathbb{E}_q[d(x_0, x)^2] < +\infty \right\}.$$

- Gradient flow on $\mathcal{P}_2(\mathcal{X})$ for $\mathrm{KL}_p(q) := \mathbb{E}_q[\log(q/p)]$:
 - $\mathcal{P}_2(\mathcal{X})$ as a Riemannian manifold:

$$v^{\mathsf{GF}} := -\operatorname{grad} \mathrm{KL}_p(q) = -\nabla \left(\frac{\delta}{\delta q} \mathrm{KL}_p(q)\right) = \nabla \log p - \nabla \log q.$$
([18], Thm 23.18; [1], Example 11.1.2)

• Minimizing Movement Scheme (MMS) ([1], Def. 2.0.6):

$$q_{t+\varepsilon} = \operatorname*{argmin}_{q \in \mathcal{P}_2(\mathcal{X})} \mathrm{KL}_p(q) + \frac{1}{2\varepsilon} d_W^2(q, q_t).$$

They coincide under the Riemannian structure.

([18], Prop. 23.1, Rem. 23.4; [1], Thm. 11.1.6; [8], Lem. 2.7)

Remark 1

The Langevin dynamics $dx = \nabla \log p(x) dt + \sqrt{2} dB_t(x)$ (B_t is the Brownian motion) is also the gradient flow of KL_p on $\mathcal{P}_2(\mathcal{X})$ [9].

Particle-Based Variational Inference Methods (ParVIs)

Stein Variational Gradient Descent (SVGD) [13]:

$$\begin{split} v^{\mathsf{SVGD}}(\cdot) &:= \left. \max_{v \in \mathcal{H}^D, \|v\|_{\mathcal{H}^D} = 1} - \frac{\mathrm{d}}{\mathrm{d}\varepsilon} \mathrm{KL}_p \big(\!(\mathrm{id} + \! \varepsilon v)_\# q\big) \right|_{\varepsilon = 0} \\ &= \mathbb{E}_{q(x)}[K(x, \cdot) \nabla \log p(x) + \nabla_x K(x, \cdot)], \end{split}$$

where \mathcal{H} is the reproducing kernel Hilbert space (RKHS) of kernel K.

- v^{SVGD} is the gradient flow of KL_p on a kernel-related distribution manifold $\mathcal{P}_{\mathcal{H}}$ [12].
- Blob (w-SGLD-B) [5]:

$$\begin{split} v^{\mathsf{Blob}} &:= - \nabla \big(\frac{\delta}{\delta q} \mathbb{E}_q[\log(\tilde{q}/p)] \big) \\ &= \nabla \log p - \nabla \log \tilde{q} - \nabla \big((q/\tilde{q}) * K \big), \\ \tilde{q} &:= q * K. \end{split}$$

Particle-Based Variational Inference Methods (ParVIs)

• Particle Optimization (PO) [4]: using MMS; estimate d_W by solving the dual optimal transport problem.

$$x_k^{(i)} = x_{k-1}^{(i)} + \varepsilon(v^{\text{SVGD}}(x_{k-1}^{(i)}) + \mathcal{N}(0, \sigma^2 I)) + \mu(x_{k-1}^{(i)} - x_{k-2}^{(i)}).$$

• $w\text{-}\mathsf{SGLD}$ [5]: using MMS; estimate d_W by solving the primal problem. Similar update rule.

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SVGD Approximates $\mathcal{P}_2(\mathcal{X})$ Gradient Flow

Reformulate $v^{\rm GF}$ as:

$$v^{\mathsf{GF}} = \max_{v \in \mathcal{L}_q^2, \|v\|_{\mathcal{L}_q^2} = 1} \langle v^{\mathsf{GF}}, v \rangle_{\mathcal{L}_q^2}. \tag{1}$$

We find:

Theorem 2 (v^{SVGD} approximates v^{GF})

$$v^{\text{SVGD}} = \max_{v \in \mathcal{H}^D, ||v||_{\mathcal{H}^D} = 1} \langle v^{\text{GF}}, v \rangle_{\mathcal{L}_q^2}.$$

- ullet \mathcal{H}^D is a subspace of \mathcal{L}^2_q , so $v^{ ext{SVGD}}$ is the projection of $v^{ ext{GF}}$ on \mathcal{H}^D .
- The $\mathcal{P}_{\mathcal{H}}(\mathcal{X})$ -gradient-flow interpretation of SVGD: $\mathcal{P}_{\mathcal{H}}(\mathcal{X})$ is not a very nice manifold.
- All ParVIs approximate the $\mathcal{P}_2(\mathcal{X})$ gradient flow.

ParVIs Approximate $\mathcal{P}_2(\mathcal{X})$ Gradient Flow by Smoothing

Smoothing Functions

ullet SVGD restricts the optimization domain \mathcal{L}_q^2 to $\mathcal{H}^D.$

Theorem 3 $(\mathcal{H}^D \text{ smooths } \mathcal{L}^2_q)$

For $\mathcal{X} = \mathbb{R}^D$, a Gaussian kernel K on \mathcal{X} and an absolutely continuous q, the vector-valued RKHS \mathcal{H}^D of K is isometrically isomorphic to the closure $\mathcal{G} := \overline{\{\phi * K : \phi \in \mathcal{C}_c^\infty\}}^{\mathcal{L}_q^2}$.

$$\overline{\mathcal{C}_c^\infty}^{\mathcal{L}_q^2}=\mathcal{L}_q^2$$
 ([11], Thm. 2.11) $\Longrightarrow \mathcal{G}$ is roughly the kernel-smoothed \mathcal{L}_q^2 .

 PO solves the dual problem by restricting the optimization domain of Lipschitz functions to quadratic functions.

ParVIs Approximate $\mathcal{P}_2(\mathcal{X})$ Gradient Flow by Smoothing

Smoothing the Density

• Blob partially smooths the density.

$$v^{\mathrm{GF}} = -\nabla \big(\frac{\delta}{\delta q}\mathbb{E}_q[\log(q/p)]\big) \Longrightarrow v^{\mathrm{Blob}} = -\nabla \big(\frac{\delta}{\delta q}\mathbb{E}_q[\log(\tilde{q}/p)]\big).$$

• w-SGLD adds an entropy regularizer in the primal objective function.

$$d_W^2(\{x^{(i)}\}_{i=1}^N, \{y^{(j)}\}_{j=1}^N) \approx \min_{\pi_{ij}} \sum_{i,j} \pi_{ij} d_{ij}^2 + \lambda \sum_{i,j} \pi_{ij} \log \pi_{ij},$$

s.t.
$$\sum_i \pi_{ij} = 1/N, \sum_j \pi_{ij} = 1/N.$$

ParVIs Approximate $\mathcal{P}_2(\mathcal{X})$ Gradient Flow by Smoothing

- Equivalence:
 - Smoothing-function objective = $\mathbb{E}_q[L(v)]$, $L: \mathcal{L}_q^2 \to L_q^2$ linear.

$$\Longrightarrow \mathbb{E}_{\tilde{q}}[L(v)] = \mathbb{E}_{q*K}[L(v)] = \mathbb{E}_{q}[L(v)*K] = \mathbb{E}_{q}[L(v*K)].$$

• Necessity: $\operatorname{grad} \operatorname{KL}_p(q)$ undefined at $q = \hat{q} := \frac{1}{N} \sum_{i=1}^N \delta_{r(i)}$.

Theorem 4 (Necessity of smoothing for SVGD)

For $q = \hat{q}$ and $v \in \mathcal{L}_n^2$, problem (1):

$$\max_{v \in \mathcal{L}_p^2, \|v\|_{\mathcal{L}_p^2} = 1} \langle v^{\mathsf{GF}}, v \rangle_{\mathcal{L}_{\hat{q}}^2},$$

has no optimal solution. In fact the supremum of the objective is infinite, indicating that a maximizing sequence of v tends to be ill-posed.

ParVIs rely on the smoothing assumption! No free lunch!

New ParVIs with Smoothing

Gradient Flow with Smoothed Density (GFSD):
 Fully smooth the density:

$$v^{\mathsf{GFSD}} := \nabla \log p - \nabla \log \tilde{q}.$$

Gradient Flow with Smoothed test Functions (GFSF):

$$v^{\mathsf{GF}} = \nabla \log p - \nabla \log q$$

$$\implies v^{\mathsf{GF}} = \nabla \log p + \operatorname*{argmin}_{u \in \mathcal{L}^2} \max_{\substack{\phi \in \mathcal{C}_c^{\infty}, \\ \|\phi\|_{\mathcal{L}^2_a} = 1}} \left(\mathbb{E}_q[\phi \cdot u - \nabla \cdot \phi] \right)^2.$$

Smooth ϕ : take ϕ from \mathcal{H}^D :

$$v^{\mathsf{GFSF}} := \nabla \log p + \underset{u \in \mathcal{L}^2}{\operatorname{argmin}} \max_{\substack{\phi \in \mathcal{H}^D, \\ \|\phi\|_{\mathcal{H}^D} = 1}} \left(\mathbb{E}_q[\phi \cdot u - \nabla \cdot \phi] \right)^2.$$

Solution:
$$\hat{v}^{\text{GFSF}} = \hat{g} + \hat{K}'\hat{K}^{-1}$$
. (Note $\hat{v}^{\text{SVGD}} = \hat{v}^{\text{GFSF}}\hat{K}$.)
 $\hat{g}_{:,i} = \nabla_{x^{(i)}} \log p(x^{(i)})$, $\hat{K}_{ij} = K(x^{(i)}, x^{(j)})$, $\hat{K}'_{:,i} = \sum_{i} \nabla_{x^{(j)}} K(x^{(j)}, x^{(i)})$.

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Nesterov's Acceleration Methods on Riemannian Manifolds

 $r_k \in \mathcal{P}_2(\mathcal{X})$: auxiliary variable. $v_k := -\operatorname{grad} \operatorname{KL}(r_k)$.

• Riemannian Accelerated Gradient (RAG) [14] (with simplification):

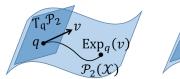
$$\begin{cases} q_k = \operatorname{Exp}_{r_{k-1}}(\varepsilon v_{k-1}), \\ r_k = \operatorname{Exp}_{q_k} \left[-\Gamma_{r_{k-1}}^{q_k} \left(\frac{k-1}{k} \operatorname{Exp}_{r_{k-1}}^{-1}(q_{k-1}) - \frac{k+\alpha-2}{k} \varepsilon v_{k-1} \right) \right]. \end{cases}$$

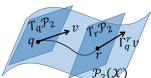
• Riemannian Nesterov's method (RNes) [20] (with simplification):

$$\begin{cases}
q_k = \operatorname{Exp}_{r_{k-1}}(\varepsilon v_{k-1}), \\
r_k = \operatorname{Exp}_{q_k} \left\{ c_1 \operatorname{Exp}_{q_k}^{-1} \left[\operatorname{Exp}_{r_{k-1}} \left((1 - c_2) \operatorname{Exp}_{r_{k-1}}^{-1} (q_{k-1}) + c_2 \operatorname{Exp}_{r_{k-1}}^{-1} (q_k) \right) \right] \right\}.
\end{cases}$$

Required:

- Exponential map $\operatorname{Exp}_q:T_q\mathcal{P}_2(\mathcal{X})\to\mathcal{P}_2(\mathcal{X})$ and its inverse.
- Parallel transport $\Gamma_q^r: T_q\mathcal{P}_2(\mathcal{X}) \to T_r\mathcal{P}_2(\mathcal{X}).$





Leveraging the Riemannian Structure of $\mathcal{P}_2(\mathcal{X})$

- Exponential map ([18], Coro. 7.22; [1], Prop. 8.4.6; [8], Prop. 2.1): $\operatorname{Exp}_q(v) = (\operatorname{id} + v)_\# q, \text{ i.e., } \{x^{(i)}\}_i \sim q \Rightarrow \{x^{(i)} + v(x^{(i)})\}_i \sim \operatorname{Exp}_q(v).$
- Inverse exponential map: require the optimal transport map.
 - Sinkhorn methods [6, 19] appear costly and unstable.
 - Make approximations when $\{x^{(i)}\}_i$ and $\{y^{(i)}\}_i$ are pairwise close: $d(x^{(i)},y^{(i)})\ll\min\big\{\min_{j\neq i}d(x^{(i)},x^{(j)}),\min_{j\neq i}d(y^{(i)},y^{(j)})\big\}.$

Proposition 5 (Inverse exponential map)

For pairwise close samples $\{x^{(i)}\}_i$ of q and $\{y^{(i)}\}_i$ of r, we have $(\operatorname{Exp}_q^{-1}(r))(x^{(i)}) \approx y^{(i)} - x^{(i)}$.

- Parallel transport
 - Hard to implement analytical results [15, 16].
 - Use Schild's ladder method [7, 10] for approximation.

Proposition 6 (Parallel transport)

For pairwise close samples $\{x^{(i)}\}_i$ of q and $\{y^{(i)}\}_i$ of r, we have $(\Gamma_q^r(v))(y^{(i)}) \approx v(x^{(i)})$, $\forall v \in T_q \mathcal{P}_2$.

Acceleration Framework for ParVIs

 $\begin{tabular}{ll} \textbf{Algorithm 1} The acceleration framework with Wasserstein Accelerated Gradient (WAG) and Wasserstein Nesterov's method (WNes) \\ \end{tabular}$

```
1: WAG: select acceleration factor \alpha > 3:
      WNes: select or calculate c_1, c_2 \in \mathbb{R}^+;
 2: Initialize \{x_0^{(i)}\}_{i=1}^N distinctly; let y_0^{(i)} = x_0^{(i)};
 3: for k = 1, 2, \dots, k_{\text{max}}, do
          for i=1,\cdots,N, do
 4:
              Find v(y_{k-1}^{(i)}) by SVGD/Blob/GFSD/GFSF;
             x_{i}^{(i)} = y_{i-1}^{(i)} + \varepsilon v(y_{i-1}^{(i)});
 6:
             y_k^{(i)} = x_k^{(i)} + \begin{cases} \text{WAG: } \frac{k-1}{k}(y_{k-1}^{(i)} - x_{k-1}^{(i)}) + \frac{k+\alpha-2}{k}\varepsilon v(y_{k-1}^{(i)}); \\ \text{WNes: } c_1(c_2-1)(x_k^{(i)} - x_k^{(i)}); \end{cases}
 7:
          end for
 8.
 9: end for
10: Return \{x_k^{(i)}\}_{i=1}^N.
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Bandwidth Selection via the Heat Equation

Note

Under the dynamics $dx = -\nabla \log q_t(x) dt$, q_t evolves following the heat equation (HE): $\partial_t q_t(x) = \Delta q_t(x)$.

Smoothing the density: $q_t(x) \approx \tilde{q}(x) = \tilde{q}(x; \{x^{(i)}\}_{i=1}^N)$. Then for $q_{t+\varepsilon}(x)$,

- Due to HE, $q_{t+\varepsilon}(x) \approx \tilde{q}(x) + \varepsilon \Delta \tilde{q}(x)$.
- Due to the effect of the dynamics, updated particles $\{x^{(i)} \varepsilon \nabla \log \tilde{q}(x^{(i)})\}_{i=1}^N$ approximate $q_{t+\varepsilon}$, so $q_{t+\varepsilon}(x) \approx \tilde{q}(x; \{x^{(i)} \varepsilon \nabla \log \tilde{q}(x^{(i)})\}_{i=1}^N)$.

Objective:
$$\sum_{k} \left(\tilde{q}(x^{(k)}) + \varepsilon \Delta \tilde{q}(x^{(k)}) - \tilde{q}(x^{(k)}; \{x^{(i)} - \varepsilon \nabla \log \tilde{q}(x^{(i)})\}_{i=1}^{N}) \right)^{2}.$$

Take $\varepsilon \to 0$, make the objective dimensionless (h/x^2 is dimensionless):

$$\frac{1}{h^{D+2}} \sum_{k} \left[\Delta \tilde{q}(x^{(k)}; \{x^{(i)}\}_i) + \sum_{j} \nabla_{x^{(j)}} \tilde{q}(x^{(k)}; \{x^{(i)}\}_i) \cdot \nabla \log \tilde{q}(x^{(j)}; \{x^{(i)}\}_i) \right]^2.$$

Also applicable to smoothing functions.

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Toy Experiments

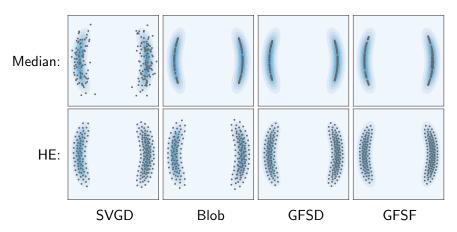


Figure: Comparison of HE (bottom row) with the median method (top row) for bandwidth selection.

Bayesian Logistic Regression (BLR)

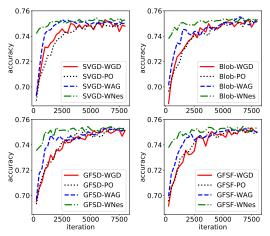


Figure: Acceleration effect of WAG and WNes on BLR on the Covertype dataset, measured by prediction accuracy on test dataset. Each curve is averaged over 10 runs.

Bayesian Neural Networks (BNNs)

Table: Results on BNN on the Kin8nm dataset (one of the UCI datasets [2]). Results are averaged over 20 runs.

Method	Avg. Test RMSE ($ imes 10^{-2}$)			
	SVGD	Blob	GFSD	GFSF
WGD	8.4±0.2	8.2±0.2	8.0±0.3	8.3±0.2
PO	7.8 ± 0.2	8.1 ± 0.2	8.1 ± 0.2	8.0 ± 0.2
WAG	7.0 ± 0.2	$\textbf{7.0}{\pm}\textbf{0.2}$	$7.1 {\pm} 0.1$	7.0 ± 0.1
WNes	$6.9 {\pm} 0.1$	7.0 ± 0.2	$6.9{\pm}0.1$	$6.8 {\pm} 0.1$
Method	Avg. Test LL			
	SVGD	Blob	GFSD	GFSF
WGD	1.042 ± 0.016	1.079 ± 0.021	1.087 ± 0.029	1.044 ± 0.016
PO	1.114 ± 0.022	1.070 ± 0.020	$1.067 {\pm} 0.017$	1.073 ± 0.016
WAG	$1.167{\pm}0.015$	1.169 ± 0.015	$1.167{\pm}0.017$	$1.190 {\pm} 0.014$
WNes	1.171 ± 0.014	$1.168{\pm}0.014$	1.173 ± 0.016	1.193 ± 0.014

Latent Dirichlet Allocation (LDA)

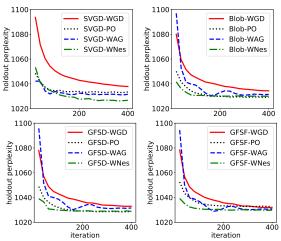


Figure: Acceleration effect of WAG and WNes on LDA. Inference results are measured by the hold-out perplexity. Curves are averaged over 10 runs.

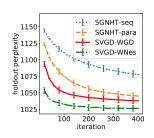


Figure: Comparison of SVGD and SGNHT on LDA, as representatives of ParVIs and MCMCs. Average over 10 runs.

Thank you!



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