Stein Variational Gradient Descent with Matrix-Valued Kernels

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Overview

Stein Variational Gradient Descent (SVGD) (Liu and Wang, 2016)

- Given a target distribution p, find $q := \{x_i\}_{i=1}^n$ to approximate p.
- Iteratively move q towards the target p by minimizing KL:

$$\min_{\phi\in\mathcal{F}} \mathrm{KL}(q_{[\epsilon\phi]} \,\|\, p) - \mathrm{KL}(q \,\|\, p), \quad \text{with,}$$

$$q_{[\epsilon\phi]} \text{ is the empirical distribution of } \{x_i' = x_i + \underbrace{\epsilon\phi(x_i)}_{\text{incremental updates}}\}_{i=1}^n.$$

- Closed-form updates by taking $\mathcal{F}$ to be the unit ball of a RKHS.

Key limitations:

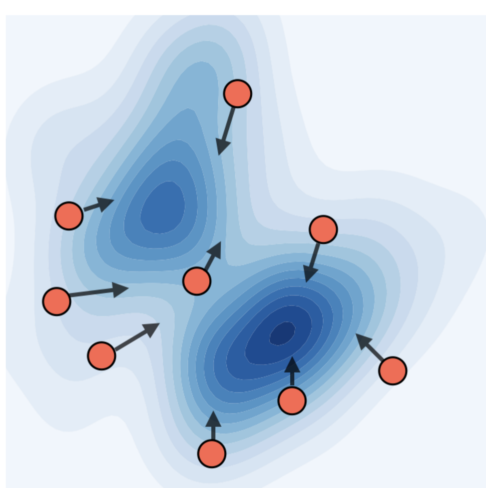
- Scalar-valued kernels; cannot encode potential correlations between different coordinates.

Our work:

- A generalization of SVGD with matrix-valued kernels.
- Improve SVGD by leveraging geometric information.

SVGD with scalar-valued kernels

- Finding the optimal transformation ϕ^* such that $\mathrm{KL}(q\|p)$ decreases as fast as possible:



$$\phi^* = \arg\max_{\phi\in\mathcal{F}} \left\{ -\frac{d}{d\epsilon}\mathrm{KL}(q_{[\epsilon\phi]}\|p)\Big|_{\epsilon=0} \right\},$$

$$= \arg\max_{\phi\in\mathcal{F}} \left\{ \mathbb{E}_{x\sim q}[\mathcal{P}^\top\phi(x)] \right\},$$

where $\underbrace{\mathcal{P}^\top\phi(x) := \nabla_x \log p(x)^\top\phi(x) + \nabla_x^\top\phi(x)}_{\text{Stein operator}}.$

- Taking $\mathcal{F}$ to be the unit ball of a RKHS $\mathcal{H}_k^d := \overbrace{\mathcal{H}_k \times \cdots \times \mathcal{H}_k}^{d}$ associated with kernel $k(x,x')$ (e.g. $k(x,x') = \exp(-\frac{(x-x')^2}{2h^2})$),

$$\phi_k^*(\cdot) \propto \mathbb{E}_{x\sim q}[k(\cdot,x)\nabla_x \log p(x) + \nabla_x k(\cdot,x)].$$

Why matrix-valued kernels

- Improve SVGD with preconditioning

$$x_i = x_i + \epsilon \overbrace{\underbrace{P}_{\text{preconditioning matrix}} \quad \phi_k^*(x_i)}^{\text{A unified approach?}}$$

- Matrix-valued kernels

$$\underbrace{K: \mathcal{X}\times\mathcal{X} \to \mathbb{R}^{d\times d}}_{\text{Matrix-valued}} \qquad \underbrace{k: \mathcal{X}\times\mathcal{X} \to \mathbb{R}^1}_{\text{scalar-valued}}.$$

Example: Separable kernels

· $K(x,x') = k(x,x')B$, where $B \in \mathbb{R}^{d\times d}$. It is easy to see that the corresponding optimal SVGD update is

$$\phi_K^*(\cdot) = B\phi_k^*(\cdot).$$

SVGD with Matrix-valued Kernels

- Let $\mathcal{F}$ be a unit ball of $\mathcal{H}_K$ with matrix-valued kernels, we have

$$\phi_K^*(\cdot) \propto \mathbb{E}_{x\sim q}[K(\cdot,x)\nabla_x \log p(x) + K(\cdot,x)\nabla_x],$$

$$\text{with,} \quad \underbrace{(K(\cdot,x)\nabla_x)_\ell}_{\ell-\text{th element}} = \sum_{m=1}^d \nabla_{x^m} K_{\ell,m}(\cdot,x).$$

Main Algorithm

- **Initialize** a set of particles $\{x_i^0\}_{i=1}^n$;
- **While** NOT converge; do

$$x_i \leftarrow x_i + \frac{\epsilon}{n}\sum_{j=1}^n \left[K(x_i,x_j)\nabla_{x_j}\log p(x_j) + K(x_i,x_j)\nabla_{x_j}\right].$$

Connections with other variants of SVGD

- Vanilla SVGD Liu and Wang, 16

$$K(x,x') = k(x,x')I.$$

- Graphical SVGD Wang et al., 18, Zhuo et al., 18

$$K(x,x') = \mathrm{diag}\left(\left\{k_\ell(x,x')\right\}_{\ell=1}^d\right).$$

- Gradient-free SVGD Han et al., 18:

$$K(x,x') = k(x,x')w(x)w(x')I, \quad w(x) = \frac{\rho(x)}{p(x)}.$$

Practical Choices of Matrix-Valued Kernels

Matrix-SVGD (average)

- Constant preconditioning matrix with RBF kernel:

$$K_Q(x,x') = Q^{-1}\exp\left(-\frac{1}{2h}\|x-x'\|_Q^2\right),$$

$$\text{with } \|x-x'\|_Q^2 = (x-x')^\top Q(x-x').$$

- $Q = \mathrm{Avg}[H(x_1),\cdots,H(x_n)]$, e.g. H: Hessian.

Matrix SVGD (mixture)

- Mixture preconditioning matrix with RBF kernel:

$$K(x,x') = \sum_{\ell=1}^m K_{Q_\ell}(x,x')w_\ell(x)w_\ell(x'),$$

where Q_ℓ as preconditioning of anchor point z_ℓ.

- We set the anchor points to be particles themselves.
- We take $w_\ell(x)$ as the Gaussian mixture probability:

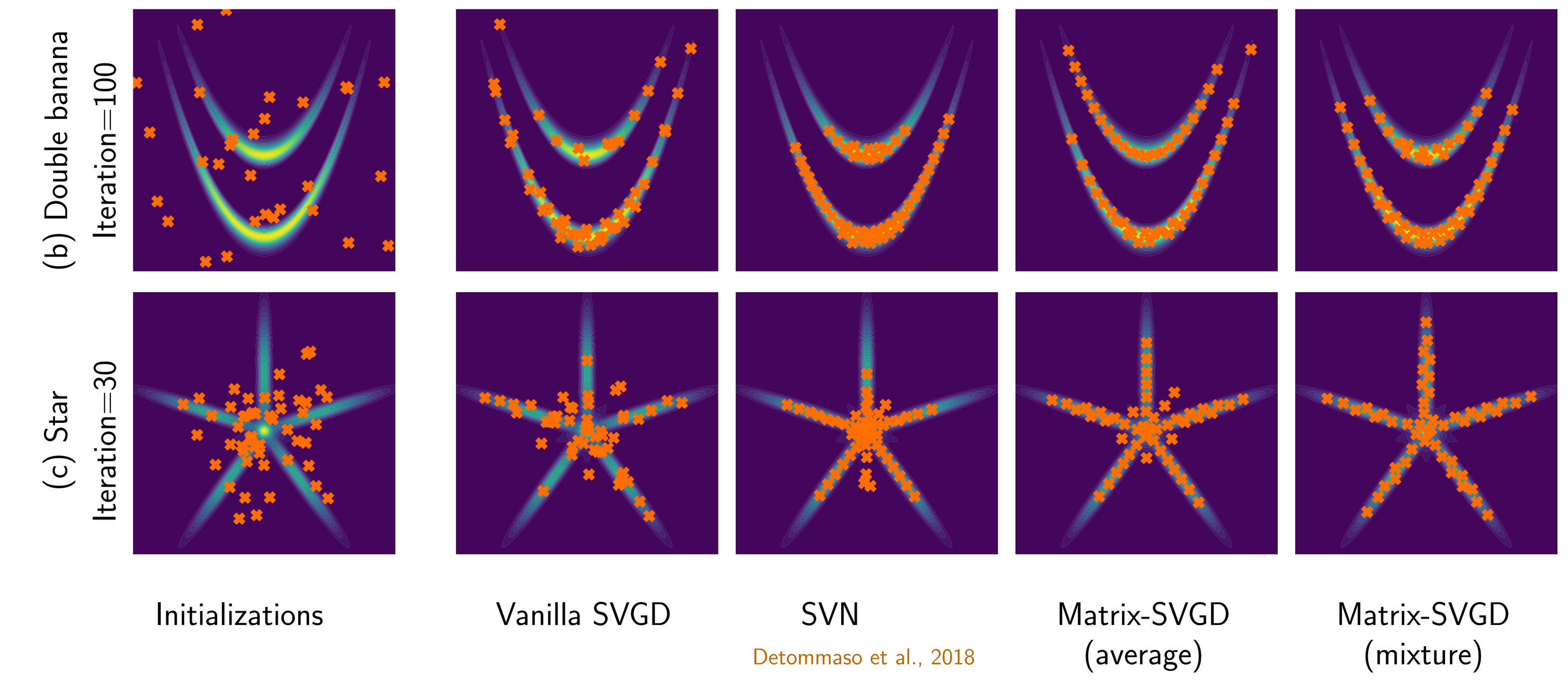
$$w_\ell(x) = \frac{\mathcal{N}(x; z_\ell, Q_\ell^{-1})}{\sum_{\ell'=1}^m \mathcal{N}(x; z_{\ell'}, Q_{\ell'}^{-1})},$$

$$\mathcal{N}(x; z_\ell, Q_\ell^{-1}) := \frac{1}{Z_\ell}\exp\left(-\frac{1}{2}\|x-z_\ell\|_Q^2\right).$$

Experiments

Two-Dimensional Toy Examples

- Search the best learning rate for all algorithms exhaustively.



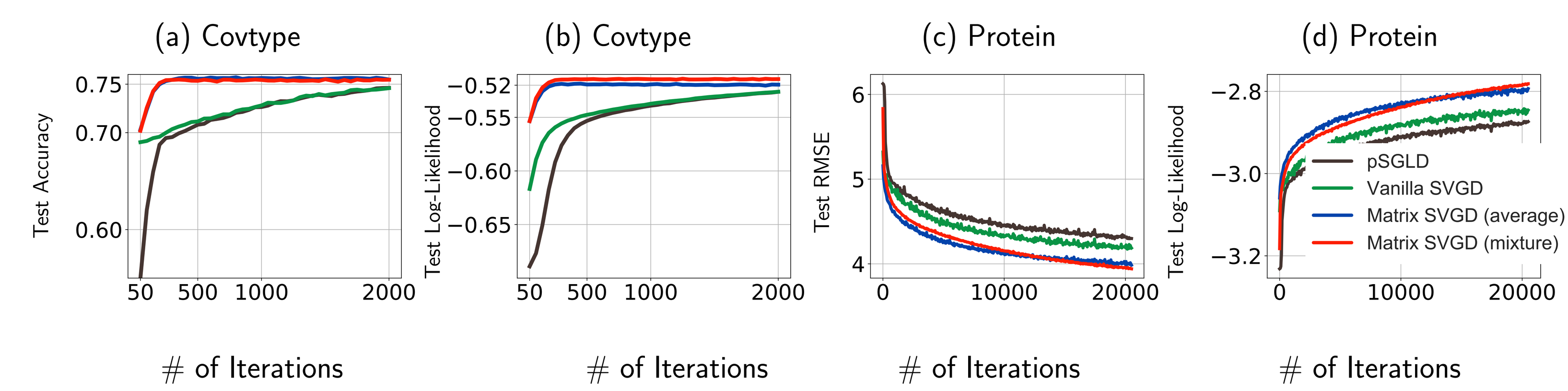
Bayesian Neural Network Regression

- Matrix-SVGD (mixture) generally performs the best among all algorithms.

Dataset	Test RMSE: Vanilla SVGD	Test RMSE: Matrix-SVGD (average)	Test RMSE: Matrix-SVGD (mixture)	Test Log-Likelihood: Vanilla SVGD	Test Log-Likelihood: Matrix-SVGD (average)	Test Log-Likelihood: Matrix-SVGD (mixture)
Boston	$2.785_{\pm 0.169}$	$2.898_{\pm 0.184}$	$\mathbf{2.717_{\pm 0.166}}$	$-2.706_{\pm 0.158}$	$\mathbf{-2.669_{\pm 0.141}}$	$-2.861_{\pm 0.207}$
Concrete	$5.027_{\pm 0.116}$	$4.869_{\pm 0.124}$	$\mathbf{4.721_{\pm 0.111}}$	$\mathbf{-3.064_{\pm 0.034}}$	$-3.150_{\pm 0.054}$	$-3.207_{\pm 0.071}$
Energy	$0.889_{\pm 0.024}$	$\mathbf{0.795_{\pm 0.025}}$	$0.868_{\pm 0.025}$	$-1.315_{\pm 0.020}$	$\mathbf{-1.135_{\pm 0.026}}$	$-1.249_{\pm 0.036}$
Kin8nm	$0.093_{\pm 0.001}$	$0.092_{\pm 0.001}$	$\mathbf{0.090_{\pm 0.001}}$	$0.964_{\pm 0.012}$	$0.956_{\pm 0.011}$	$\mathbf{0.975_{\pm 0.011}}$
Naval	$0.004_{\pm 0.000}$	$0.001_{\pm 0.000}$	$\mathbf{0.000_{\pm 0.000}}$	$4.312_{\pm 0.087}$	$5.383_{\pm 0.081}$	$\mathbf{5.639_{\pm 0.048}}$
Combined	$4.088_{\pm 0.033}$	$4.056_{\pm 0.033}$	$\mathbf{4.029_{\pm 0.033}}$	$-2.832_{\pm 0.009}$	$-2.824_{\pm 0.009}$	$\mathbf{-2.817_{\pm 0.009}}$
Wine	$0.645_{\pm 0.009}$	$\mathbf{0.637_{\pm 0.008}}$	$\mathbf{0.637_{\pm 0.009}}$	$-0.997_{\pm 0.019}$	$\mathbf{-0.980_{\pm 0.016}}$	$-0.988_{\pm 0.018}$
Protein	$4.186_{\pm 0.017}$	$3.997_{\pm 0.018}$	$\mathbf{3.852_{\pm 0.014}}$	$-2.846_{\pm 0.003}$	$-2.796_{\pm 0.004}$	$\mathbf{-2.755_{\pm 0.003}}$
Year	$8.686_{\pm 0.010}$	$8.637_{\pm 0.005}$	$\mathbf{8.594_{\pm 0.009}}$	$-3.577_{\pm 0.002}$	$-3.569_{\pm 0.001}$	$\mathbf{-3.561_{\pm 0.002}}$

SVGD Acceleration

- (a)-(b) Results of Bayesian Logistic regression on the Covtype dataset.
- (c)-(d) Average test RMSE and log-likelihood vs. training batches on the Protein dataset for Bayesian neural regression.



Classification With Recurrent Neural Networks

Method	MR (Pang & Lee, 05)	CR (Hu & Liu, 04)	SUBJ (Pang & Lee, 04)	MPQA (Wiebe et al., 05)
SGLD	20.52	18.65	7.66	11.24
pSGLD Li et al., 16	19.75	17.50	6.99	10.80
Vanilla SVGD	19.73	18.07	6.67	**10.58**
Matrix-SVGD (average)	19.22	17.29	6.76	10.79
Matrix-SVGD (mixture)	**19.09**	**17.13**	**6.59**	10.71

Table: Sentence classification erros measured with four benchmarks.

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