Stein Variational Gradient Descent with Multiple Kernels

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Abstract
Bayesian inference is an important research area in cognitive computation due to its ability to reason under uncertainty in machine learning. As a representative algorithm, Stein variational gradient descent (SVGD) and its variants have shown promising successes in approximate inference for complex distributions. In practice, we notice that the kernel used in SVGD-based methods has a decisive effect on the empirical performance. Radial basis function (RBF) kernel with median heuristics is a common choice in previous approaches, but unfortunately, this has proven to be sub-optimal. Inspired by the paradigm of Multiple Kernel Learning (MKL), our solution to this flaw is using a combination of multiple kernels to approximate the optimal kernel, rather than a single one which may limit the performance and flexibility. Specifically, we first extend Kernelized Stein Discrepancy (KSD) to its multiple kernels view called Multiple Kernelized Stein Discrepancy (MKSD) and then leverage MKSD to construct a general algorithm Multiple Kernel SVGD (MK-SVGD). Further, MK-SVGD can automatically assign a weight to each kernel without any other parameters, which means that our method not only gets rid of optimal kernel dependence but also maintains computational efficiency. Experiments on various tasks and models demonstrate that our proposed method consistently matches or outperforms the competing methods.

Keywords Bayesian inference · Approximate inference · SVGD · Multiple Kernel Learning · Stein Methods

Introduction
Bayesian inference is a powerful mechanism aiming at systematically reasoning under uncertainty in machine learning, with broad applications to various areas that involve probabilistic modeling. As such, Bayesian inference is a plausible model for natural cognition [1, 2]. The process of finding out the inference can be called cognitive computing [3]. The core concern of Bayesian inference is the posterior distribution of model parameters, which is yet typically computationally intractable for complex models. Hence, enormous approaches have emerged for approximating posterior distribution, roughly including two branches, sampling-based approaches (e.g., Markov Chain Monte Carlo (MCMC) [4–6]), and optimization-based approaches (e.g., Variational Inference (VI) [7, 8]). With the asymptotic convergence guaranteed, MCMC directly approximates the posterior distribution with the drawn samples but converges slowly in practice due to undesirable auto-correlation between samples. By contrast, VI uses a simpler distribution for approximation by minimizing their Kullback-Leibler (KL) divergence, which is efficient and suitable for large dataset scenarios. Under this circumstance, the pre-defined form of the simple distribution greatly affects the accuracy and computational cost of the approximation.

Recently, one combines the advantages of sampling-based and optimization-based approaches, yielding a novel approximation method called Stein variational gradient descent (SVGD) [9]. It can be either considered as a particle-based sampling approach [10–13] or as a non-parametric variational inference algorithm [14]. Specifically, SVGD applies an iteratively transformed set of particles to fit the posterior distribution by minimizing the KL divergence, which is performed with deterministic functional gradient descent. The finally obtained particles can be viewed as samples drawn from the posterior distribution. This method does not require explicit selection of a specific parameter family, thus circumventing
the problem of balancing accuracy and computational cost. Meanwhile, since SVGD conducts with deterministic gradient updates, it converges fast and has a series of variants [15–17].

Despite both theoretical guarantees and practically fast, we notice that the performance of SVGD and its variants crucially depends on the choice of the kernel. First, the kernel used in SVGD guides the transformed direction of the particles, which refers to the direction of the steepest descent in the local average derived by weighting the contribution of all particles [18]. Then, it also can capture the underlying geometry of the target distribution, making flow the particles along with the support of the target distribution [19]. Hence, the kernel should be specified cautiously and vary according to tasks. However, we find that SVGD and most of its variants generally choose the Radial Basis Function (RBF) with median heuristics as the kernel [9, 17, 20]. As a commonly used kernel, RBF is simple but has limited expression ability. The current heuristic median method is not good enough at choosing the proper bandwidth for a kernel. And we also show the performance of SVGD with RBF is unstable, as shown in Fig. 2 of the experimental section. Therefore, to better play the role of the kernel function in SVGD and its variants, some more complex kernels need to be considered.

To this end, we propose a new general algorithm called Multiple Kernel SVGD (MK-SVGD), which is inspired by the paradigm of multiple kernel learning. We first introduce a new discrepancy definition named Multiple Kernelized Stein Discrepancy (MKSD), extending the Kernelized Stein Discrepancy (KSD) to multi-kernel form. Then, based on the MKSD, we present the flexible algorithm MK-SVGD, where the optimal kernel is approximated by weighted multiple kernels instead of a single one. Importantly, the optimal weight of each kernel is learned automatically without additional parameters. It means that MK-SVGD not only improves the ability of expression but also holds computational efficiency.

In summary, our main contributions are as follows:

• We introduce a new discrepancy definition named MKSD, which can be regarded as a multi-kernel version of KSD. When using the optimal weight vector, we obtain its salable variant called maxMKSD.

• We propose a general algorithm MK-SVGD based on the defined MKSD. MK-SVGD uses a combined kernel for approximation, where each kernel is assigned a weight to measure its significance. This can better capture the underlying geometry structure of the target distribution. In addition, the optimal weight of each kernel is learned automatically in MK-SVGD.

• We evaluate the MK-SVGD on both synthetic and real-world data of several different tasks, including Multivariate Gaussian, Bayesian logistic regression, and Bayesian neural networks. Experimental results have demonstrated the effectiveness of our proposed method.

The rest of the paper is organized as follows. We first briefly review the KSD and SVGD in Backgrounds. Then, we present the proposed method MKSD and MK-SVGD in SVGD with Multiple Kernel. After that, we introduce some related research in Related Works, and the experiments are performed in Experiments. Finally, we summarize our work and point out the direction of future work in Conclusion.

Backgrounds

For a better statement and explanation, we briefly introduce some concepts and algorithms, namely Kernelized Stein Discrepancy (KSD) and Stein variational gradient descent (SVGD), which are the basis of our proposed method. Note that vectors are denoted by bold lowercase letters; matrices are denoted by upper-case letters; sets are denoted by calligraphic letters throughout this paper.

Preliminary For any $a_i \in \mathbb{R}$, $x_i \in \mathbb{R}^d$ and a symmetric function $k : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$, if we have $\sum a_i k(x_i, x) \geq 0$, then $k$ is a positive definite kernel. A Reproducing Kernel Hilbert Space (RKHS) $\mathcal{H}_k$ is associated with the specific positive definite kernel $k(x, x')$, and consists the closure of functions of form

$$f(x) = \sum_i a_i k(x, x_i), \quad \forall a_i \in \mathbb{R}, \quad x_i \in \mathbb{R}^d.$$  (1)

Let $g = \sum \beta_i k(x, x_i)$, the equipped inner product of the RKHS $\mathcal{H}_k$ is $(f, g)_{\mathcal{H}} = \sum a_i \beta_j k(x_i, x_j)$ and norm is $\|f\|^2_{\mathcal{H}} = \sum a_i a_j k(x_i, x_j)$. See [21] or [22] for more details.

Kernelized Stein Discrepancy All following advanced approaches start from Stein methods [23, 24] and RHKS theory. Stein methods provide a series of tools to bound the distance between two probability distributions with respect to a specific probability metric. Targeting KSD, we would like to review the whole inference process beginning from Stein Identity. Let $p(x)$ be a probability density function, which is positive and continuously differentiable supported on $\mathbb{R}^d$. Stein Identity says that for any smooth vector function $\phi(x) = [\phi_1(x), \ldots, \phi_d(x)]^T$, we have

$$\mathbb{E}_p[A_p \phi(x)] = \mathbb{E}_p[s_p(x) \phi(x)^T + \nabla_x \phi(x)] = 0,$$  (2)

where $s_p(x) = \nabla_x \log p(x)$ called Score function and $A_p$ is a linear functional operator on $\phi$ called Stein operator. Assuming $\lim_{||x|| \to \infty} p(x) \phi(x) = 0$, we can easily check the correctness using integration by parts. With the holding of Stein Identity, we call that $\phi$ is in the Stein class of function $p$.

Now we can introduce another probability density function $q(x)$, which is also positive and continuously
differentiable supported on \( \mathbb{R}^d \) like \( p(x) \). If we directly replace the first \( p(x) \) in Eq. (2) with \( q(x) \), say consider \( E_q[A_p \phi(x)] \) where the expectation of \( A_p \phi(x) \) is now under \( q(x) \), then the Stein Identity would no longer hold for most general function \( \phi \). Formally, this can be easily checked by
\[
E_q[A_p \phi(x)] = E_q[(s_p(x) - s_q(x)) \phi(x)]^	op,
\]
where \( s_p \) and \( s_q \) are score functions of \( p(x) \) and \( q(x) \) respectively. We notice that Eq. (3) no longer equals 0 unless \( s_p = s_q \), which implies \( p = q \). This gives us the possibility to measure the difference between two distributions. Given a proper function set \( \mathcal{F} \), Stein Divergence (SD) measures the difference between \( p(x) \) and \( q(x) \) as
\[
D_\mathcal{F}(q||p) : \max_{\phi \in \mathcal{F}} \{ E_{x \sim q}[A_p \phi(x)] \},
\]
which means that the Stein Divergence is the maximum violation of Stein Identity in function set \( \mathcal{F} \). Therefore, choosing a proper function set \( \mathcal{F} \) is vital. Traditional methods are generally difficult to optimize or require special considerations [25]. Conversely, Kernelized Stein Discrepancy (KSD) solves this problem by taking function set \( \mathcal{F} \) to the unit ball of an RKHS, in which the optimization has a closed-form solution. Specifically, KSD is defined as
\[
S(q||p) : \max_{\phi \in \mathcal{H}} \{ E_{x \sim q}[A_p \phi(x)] \}, \text{ s.t. } \|\phi\|_{\mathcal{H}} \leq 1
\]
where \( \mathcal{H} \) is an RKHS associated with a kernel \( k(x, x') \), which is in the Stein class of \( p(x) \). According to [9] and [21], the optimal solution of Eq. (5) is
\[
\phi(x) = \phi^*(x)/\|\phi^*\|_{\mathcal{H}}^2, \quad \text{where, } \hat{\phi}^*(\cdot) = E_{x \sim q}[A_p k(x, \cdot)].
\]

Substitute the optimal solution into Eq. (5), the \( S(q||p) \) is \( \|\phi^*\|_{\mathcal{H}}^2 \).

**Stein Variational Gradient Descent** Let \( p(x) \) defined in above be our target distribution. Stein Variational Gradient Descent (SVGD) tends to approximate \( p(x) \) with a set of particles \( \{x_i\}_{i=1}^n \) in the sense that
\[
E_p[f(x)] = \lim_{n \to \infty} \frac{1}{n} \sum_{i=1}^n f(x_i),
\]
where \( f \) can be any test function. To achieve this, SVGD randomly samples a collection of particles from a simple initial distribution (e.g., Standard normal distribution) and then iteratively updates them by a deterministic map
\[
T(x_i) = x_i + \epsilon \phi^*(x_i), \quad \forall i = 1, \cdots, n,
\]
where \( \phi^*: \mathbb{R}^d \to \mathbb{R}^d \) is the perturbations driving the particles to cover the target distribution \( p(x) \) and \( \epsilon \) is a small step size. Assuming \( z = T(x) \) as \( x \sim q(x) \), the optimal perturbation \( \phi^* \) can be obtained by solving the optimization problem as follow,
\[
\phi^* = \arg\max_{\phi \in \mathcal{F}} \left\{ -\frac{d}{d\epsilon} \text{KL}(q_{[\epsilon]}||p) \bigg|_{\epsilon=0} \right\},
\]
where \( \mathcal{F} \) is the candidate perturbation function set. The key observation is that
\[
-\frac{d}{d\epsilon} \text{KL}(q_{[\epsilon]}||p) \bigg|_{\epsilon=0} = \nabla_x \text{log } p(x) \phi(x)^	op + \nabla_x \phi(x)
\]
which is exactly the objective function in Eq. (3). Following the inference form Eqs. (3) to (6), we can obtain the optimal perturbations by restricting the set of \( \mathcal{F} \) to the unit ball of an RKHS \( \mathcal{H} \) as follow
\[
\phi^*(\cdot) \propto E_{x \sim q}[A_p k(x, \cdot)] = E_{x \sim q}\left[ \nabla_x \log p(x) k(x, \cdot) + \nabla_x k(x, \cdot) \right],
\]
where \( k \) is the positive definite kernel associated with RKHS \( \mathcal{H} \). In practice, SVGD iteratively updates particles \( \{x_i\}_{i=1}^n \) by \( x_i \leftarrow x_i + \epsilon \phi^*(x_i) \), where,
\[
\phi^*(x_i) = \frac{1}{n} \sum_{j=1}^n \left[ \nabla_{x_j} \log p(x_j) k(x_j, x_i) + \nabla_{x_j} k(x_j, x_i) \right].
\]

The different parts in the Eq. (12) play different roles: the first part drives the particles to the high probability of target distribution, while the second part acts as a repulsive force to separate different particles to cover the entire density area.

**SVGD with Multiple Kernel**

In this section, we introduce our proposed new method step by step in the following order: Firstly, we intuitively analyze the role of the kernel in Kernelized Stein Discrepancy (KSD) and its importance. Then combined with Multiple Kernel Learning (MKL), we propose a new discrepancy definition to address these issues, named Multiple Kernelized Stein Discrepancy (MKSD). After that, we leverage MKSD to construct a general algorithm based on SVGD, which is called Multiple Kernel SVGD (MK-SVGD). Finally, we simply analyze the time consumption of our algorithm.

**Intuition**

Before moving on to more details, we first give an intuitive analysis of the kernel selection issue in KSD and its variants. We notice that the role of the kernel is mainly reflected in the following two aspects: guiding the particles to the direction of
the steepest descent in the local average by weighting the contribution of each particle [18] and flowing the particles along with the support of the target distribution [19]. Therefore, selecting a suitable kernel is crucial, and the optimal kernel varies by task. In practice, RBF kernel with median heuristics is a common choice but mostly sub-optimal. Some other complex kernels, such as deep kernels [26], might be preferred but not easy to use. To this end, we propose a new optimal kernel approximation method based on multiple kernel learning (MKL), which utilizes a more powerful combined kernel instead of a single one. We also introduce a weight for each kernel to measure its importance. It is worth noting that the weights can be automatically assigned without additional parameters. In short, our method not only gets rid of optimal kernel dependence but also maintains computational effectiveness.

**Multiple Kernelized Stein Discrepancy**

For a better elaboration, we first briefly introduce the basic concepts of Multiple Kernel Learning (MKL). Simply put, MKL [26–32] provides an automatic way to learn the optimal combination of base kernels. The goal of MKL is to maximize a generalized performance measure by finding an optimal base kernel functions combination. In general, MKL-based methods outperform single-kernel ones due to the better feature representation ability and flexibility [33].

Considering the computational efficiency, we use a linear way that combines the kernels as

\[
k_w(x, x') = \sum_{i} w_i k_i(x, x'), \quad \text{s.t.} \quad w \in \mathbb{R}^m_+, ||w||_2 = 1
\]

where \(m\) is the number of base kernels and \(w\) is the weight vector. Referring to Backgrounds, we know that the kernel in KSD or SVGD is required to be in the Stein class for smooth densities in a proper sense. Some commonly used kernels meet the requirements, such as RBF kernel \(k(x, x') = \exp(-\frac{1}{2}||x-x'||^2)\). Therefore, it is first necessary to check the suitability of the multi-kernel, that is, whether it belongs to the Stein class for smooth densities in \(\mathcal{X} = \mathbb{R}^d\).

**Proposition 1** (Multi-kernel in Stein class) Assume a sequence of kernels \(k_i(x, x')\) are in the Stein class, then we have \(k_w(x, x') = \sum_{i} w_i k_i(x, x')\) is in the Stein class for any \(w \in \mathbb{R}^m_+.\) See proof in Appendix B.

According to Proposition 1, we know that the multi-kernel is eligible as long as its base kernels are in the Stein class of smooth densities in \(\mathcal{X} = \mathbb{R}^d\) and the weight vector \(w\) is non-negative. This means that the correctness of our algorithm has a theoretical guarantee. Now, it is natural to take advantage of the multi-kernel to extend the generalization of KSD. Specifically, we propose a new discrepancy based on KSD by directly replacing a single kernel with a multi-kernel, called Multiple Kernelized Stein Discrepancy (MKSD). The formal definition is as follows:

**Definition 1** (Multiple Kernelized Stein Discrepancy) Assume \(q(x)\) and \(p(x)\) are continuously differentiable densities supported on \(\mathcal{X} \subseteq \mathbb{R}^d\) and a sequence of base kernels \(k_i(x, x')\) are in the Stein class of \(q(x)\). By defining

\[
\mu_p(x, x') = \mathbb{E}_{x \sim q}[s_p(x)\nabla_k k_i(x, x')^\top s_q(x') + \nabla_q k_i(x, x') s_p(x') + \text{Tr}(\nabla_{xx} k_i(x, x'))]
\]

where \(\text{Tr}\) represents the trace of the matrix, \(s_p\) and \(s_q\) are score function of \(p(x)\) and \(q(x)\) respectively, then we have

\[
\mu_p^w(x, x') = \mathbb{E}_{x \sim q}[\sum_{i} w_i \mu_i^p(x, x')] = \sum_{i} w_i \mathbb{E}_{x \sim q}[^p \mu_i(x, x')]
\]

Finally, we reach the definition of MKSD as follows:

\[
\mathbb{S}_{k_w}(q\|p) = \mathbb{E}_{x \sim q}[\mu^w_p(x, x')] = \sum_{i} w_i \mathbb{S}_{k_i}(q\|p)
\]

where \(\mathbb{S}_{k_i}(q\|p)\) is the KSD corresponding to the base kernel \(k_i\).

From Eq. (14) in Definition 1, we note that MKSD is defined as the linear combination of KSDs corresponding to the base kernel. In addition, the weight of each KSD is exactly the weight of the corresponding base kernel in the multi-kernel. The advantage of this definition is that it is straightforward to extend while maintaining efficiency. To consider MKSD as a discrepancy metric, however, we need some more qualitative verification, which is done in Proposition 2. Moreover, a corollary about the maximum MKSD is given in Corollary 1.

**Proposition 2** (MKSD as Discrepancy) Assume a sequence \(k_i(x, x')\) are integrally strictly positive definite, and \(q, p\) are continuous densities with \(\mathbb{E}_q[\mu_p^w(x, x')] < \infty\) for all \(w \in \mathbb{R}^m_+,\) we have \(\mathbb{S}_{k_w}(q\|p) \geq 0\) and \(\mathbb{S}_{k_w}(q\|p) = 0\) if and only if \(q = p\). See proof in Appendix B.

**Corollary 1** (maxMKSD) Assume the conditions in Definition 1 are satisfied. Then
MKSD_{max}(q, p) = \max_{w \in \mathbb{R}^n, ||w||_1 = 1} S_{k_w}(q\|p)

is equal to 0 if and only if p = q a.e.

### SVGD with Multiple Kernels

As mentioned in Eq. (12), the role of the kernel in guiding particle update in SVGD is mainly reflected in the following two aspects: Pushing each particle towards the high probability areas of target distribution by weighting the gradient direction of each particle in the first term; Acting as a repulsive force that spreads the particle along with target distribution and doesn’t collapse into the local modes in the second terms. Take RBF kernel $k(x, x') = \exp(-\frac{1}{h}\|x - x'\|^2)$ as an example. The corresponding repulsion force term is $E_{x \sim q}[\nabla_x k(x, x')] = E_{x \sim q}[\frac{\partial}{\partial x} k(x, x')]$, driving point $x$ away from its neighboring point $x'$ which has a large $k(x, x')$. Besides, the bandwidth $h$ plays its role in turning the smoothness of the repulsive force term, e.g., the repulsive term vanishes when $h \to 0$. Therefore, if bandwidth $h$ can be adjusted according to the current surrounding of particles, the kernel could better capture the underlying geometry structure of the target distribution $p(x)$. Then each particle can efficiently spread the target distribution.

To this end, we propose a more general algorithm, Multiple Kernel Stein Variational Gradient Descent (MK-SVGD). The key idea is to combine the different kernels with self-adjusted weights to approximate the optimal kernel and thus get rid of the dependence on the single kernel, which may limit the performance and flexibility. As a result, our algorithm can dynamically perform kernel selection during SVGD updates. Next, we will introduce MK-SVGD in detail.

Let $\phi_w : \mathbb{R}^d \to \mathbb{R}^d$ be a perturbation function in the unit ball of a general RKHS $H_{k_w}$ equipped with the multiple kernels $k_w(x, x') = \sum_i w_i k_i(x, x')$. Then moving the particles through the transition function $T_{k_w}(x) = x + \epsilon\phi_w(x)$. Assuming $q_{|T_{k_w}}(z)$ as the density of $z = T_{k_w}(x)$ when $x \sim q(x)$, the steepest descent direction $\phi_w^*(\cdot)$ can be obtained by solving the optimization problem as follow,

$$\phi_w^* = \arg \max_{\phi_w \in H_{k_w}} \left\{ -\frac{d}{d\epsilon} KL(q_{|T_{k_w}}||p) \bigg|_{\epsilon=0} \right\}.$$  

Similar to Eq. (10), we have

$$-\frac{d}{d\epsilon} KL(q_{|T_{k_w}}||p) \bigg|_{\epsilon=0} = \nabla_x \log p(x)\phi_w(x)^T + \nabla_x \phi_w(x)$$

$$= E_{x \sim q}[A_i\phi_w(x)] - S_{k_w}(q\|p).$$  

From Eq. (17), we know that the gradient of KL divergence with respect to $\epsilon$ in Eq. (16) is exactly the negative MKSD. Therefore, with weight vector $w$, the steepest descent direction is

$$\phi_w^*(\cdot) = E_{x \sim q}[A_i k_w(x, \cdot)] = \sum_i w_i E_{x \sim q}[A_i k_i(x, \cdot)] = \sum_i w_i \phi_i^*(\cdot),$$  

where $\phi_i^*(\cdot)$ denotes the optimal direction related to $i$-th base kernel. In other words, given a weight vector $w$, the optimal update direction is jointly determined by the steepest descent direction of each base kernel. In practice, MK-SVGD iteratively updates particles by $x \leftarrow x + \epsilon\phi_w^*(x)$, where

$$\phi_w^*(x) = \sum_{i=1}^m w_i \sum_{j=1}^n \left[ \nabla_j \log p(x_j) k_i(x_j, x) + \nabla_j k_i(x_j, x) \right].$$  

Next, we focus on weight vector $w$. As mentioned before, the weight vector is vital to choosing the final direction for each particle by linearly combining the base kernels. In the different particles surrounding, the optimal combination of base kernels is also different, so we need to update the weight vector as the particles move. Formally, we need to find a set of weights that maximize MKSD, which is exactly the problem explained in Corollary 1. Therefore, the problem can be turned into an optimization problem about $w$, as

$$w^* = \arg \max_w S_{k_w}(q\|p) = \arg \max_w \left\{ w_i, S_{k_i}(q\|p) \right\}.$$  

This is a straightforward optimization problem, and the maximum is achieved when

$$w_i = \sqrt{S_{k_i}(q\|p)/ \sum_i S_{k_i}(q\|p)} = \frac{||\phi_i||_{H_{k_i}}}{\sqrt{\sum_i ||\phi_i||_{H_{k_i}}^2}}.$$  

Combining all the above steps results in a more general and powerful algorithm, Multiple Kernel Stein Variational Gradient Descent (MK-SVGD), which is clearly summarized in Algorithm 1.

### Algorithm 1: Multiple Kernel Stein Variational Gradient Descent

**Input:** Particles $(x_i)_{i=1}^n$, initial from simple prior distribution $q$; A sequence kernel function $(k_i)_{i=1}^m$; Weight vector $(w_i)_{i=1}^m$, initialized with $\frac{1}{m}$; Step size $\epsilon$; Iteration number $T$.

**Output:** Final particles $(x_i)_{i=1}^n$, that represents the target distribution $p(x)$

For $t = 1$ to $T$

for $1 \leq i \leq n$ do

Update particles

Update all particles $(x_i)_{i=1}^n$ by $x_i \leftarrow x_i + \epsilon\phi_i(x_i)$ and calculate $S_{k_i}(q\|p)$ using Eq. (19)

Update weight vector $w$

Use weight vector $(w_i)_{i=1}^m$ using Eq. (21)

end

Finally, we simply analyze the time complexity of our algorithm. From [9], we know that the major computation bottleneck in iterative procedure of SVGD lies on calculating the gradient $\nabla_x \log p(x)$ for all the points $(x_i)_{i=1}^n$. Therefore,
the introduction of multi-kernel in our algorithm does not significantly increase the time consumption. For example, if we use multiple RBF kernels $k(x, x') = \exp(-\frac{1}{2}||x - x'||_2^2)$ with different bandwidth $h$, the term $||x - x'||_2^2$ is shared by each kernel. In other words, we only need to compute the rest part for the kernels with different $h$, and the time consumption is linearly increased compared to SVGD, which is $O(mn^2)$. Additional speedup methods, such as mini-batch, also can be obtained similar to SVGD.

### Related Works

As a pioneering work, SVGD is a very attractive algorithm. Therefore, many exciting and effective works have been proposed based on SVGD in the machine learning community. Generally speaking, the works related to SVGD are mainly concentrated in two research lines. One is to combine SVGD with other models or embed SVGD into other models, such as [34–38]. Another major concern is the improvement or generalization of the vanilla SVGD algorithm, such as [15–17, 39–41]. Next, we will briefly introduce several representatives works in these two directions.

In the first case, SVGD is often used as a part of the model. For example, in work [34], SVGD was used to train stochastic neural networks with the purpose of drawing samples from the target distribution for probability inference. Based on SVGD, a new learning method for variational auto-encoders (VAEs) is proposed in [35]. Another work [36] proposes an algorithm to directly estimate the score function of the implicitly defined distribution, which is similar to the main framework of SVGD.

Our work is an extension of the vanilla SVGD, which belongs to the second case. There also exist many works in the second case. Using a surrogate gradient to replace the true gradient in SVGD, [15] proposes a gradient-free SVGD that focuses on the target distributions with intractable gradients. Besides, in work [20], the authors extend the idea of gradient-free SVGD to discrete distribution and solve the limitation that original SVGD can only work under continuous distribution. Another work [16] accelerates and generalizes the SVGD algorithm to approximate a Newton-like iteration in function space by including second-order information. The Scaled Hessian kernel is proposed using second-order information. Furthermore, the work [17] leverages a more general matrix-valued kernel to generate SVGD for flexibly incorporating preconditioning information. Note that, Our method is intrinsically different from [17]. The work [17] introduces the optimization problem to vector-valued RKHS with matrix-valued kernels, while our method focuses on leveraging the effectiveness of Multiple Kernel Learning, which optimizes the objective in real-valued RKHS.

### Experiments

To evaluate the performance of MK-SVGD, we conduct sufficient experiments on both synthetic and real-world data for several different tasks. Information of all datasets is summarized in Table 1. Firstly, we test our algorithm on a multivariate Gaussian distribution as a toy example and then move on to a series of more challenging tasks concluding with Bayesian logistic regression and Bayesian neural networks. For a fair comparison, we adopt basic experimental settings similar to [9]. We select RBF kernels with different bandwidths as the basic components of the multi-kernel. Specifically, to provide a wider range of scales, we use 10 RBFs with a ratio of 0.1 between each adjacent bandwidth $h$. Besides, the bandwidth range varies for different experiments, and the specific settings are described in each experiment section. All particles are randomly sampled from the prior unless otherwise specified. The step size updating is controlled by AdaGrad [42].

The comparison methods involved in the experiment are summarized as follows,

- **Probabilistic back-propagation (PBP)** [43], a classic scalable method for learning Bayesian neural networks. It is also the only non-SVGD-based method in the comparison methods, using the implementation by [9];
- **Vanilla SVGD**, the baseline of SVGD-based methods and code is also available on [9];
- **Matrix-SVGD**, a recent advanced SVGD-based method, uses the constant preconditioning matrix kernel, including Matrix-SVGD (average) and Matrix-SVGD (mixture) and using the code in [17];
- **MK-SVGD**, Multiple Kernel SVGD, our new proposed method.

### Multivariate Gaussian

We start our experiments with a toy example simulating a multivariate Gaussian distribution. Given a target distribution

| Dataset    | Number of Attributes | Number of Instances |
|------------|----------------------|--------------------|
| Covtype    | 54                   | 581012             |
| Boston     | 14                   | 506                |
| Combined   | 5                    | 9568               |
| Concrete   | 10                   | 1030               |
| Wine       | 12                   | 4898               |
| Yacht      | 7                    | 308                |

Table 1: Datasets used in our experiments. Covtype, used in Bayesian Logistic Regression; Other datasets, used in Bayesian Neural Networks.
we use MK-SVGD to get a set of particles that cover the target distribution nicely. Note that the parameters of target distribution settings are randomly chosen. In detail, we firstly initialize 500 particles randomly sampling from a standard normal distribution \( N(\mathbf{x};0,\mathbf{I}) \) which is far away from the target distribution. Then the particles are updated through MK-SVGD by 200 epochs. In addition, the bandwidths of 10 RBF kernels are in the range of \([2^{-2}, 2^{-3}, \ldots, 2^{11}]\).

Results After particles updating, we get the final set of particles, which can be viewed as sampling samples from the target distribution. Figure 1a shows the final results, from which we can see that the particle group fits the target distribution well. According to the weight distribution of each kernel shown in Fig. 1b, we find that the kernels with bandwidth \( h = 1 \) and \( h = 2 \) play a major role. Further, we calculate the mean of each variable of the final particle group over ten random runs, and the value is \([-0.68792629, 0.80107447]\), which is pretty close to the groundtruth.

Bayesian Logistic Regression

We then evaluate MK-SVGD on more complex models and real data. As for the model, we firstly consider a binary classification problem based on the Bayesian logistic regression. Denote the dataset as \( D = \{(\mathbf{x}_j, y_j)\}_{j=1}^N \) where \( \mathbf{x}_j \) is the feature vector, \( y_j \in \{0, 1\} \) is the corresponding binary label and \( N \) is the number of data points. Then a Bayesian logistic regression model for binary classification defines as follows

\[
p(\theta | D) \propto p(D | \theta) p(\theta)
\]

with

\[
p(D | \theta) = \prod_{j=1}^N \left[ y_j \sigma(\theta^\top \mathbf{x}_j) + (1 - y_j) \sigma(-\theta^\top \mathbf{x}_j) \right],
\]

where \( \sigma(*) \) is a standard logistic function, defined as \( \sigma(*) : 1/(1 + \exp(-*)) \), and the prior of \( \theta \) is a Gaussian distribution \( p_0(\theta | a) = N(\mathbf{0}; a^{-1}) \) with \( p(a) = \text{Gamma}(a,a) \). The value of the hyperparameters \( a \) and \( b \) in Gamma distribution are set to 0 and 0.01, respectively. Our interest is using MK-SVGD to generate a set of samples \( \{\theta_i\}_{i=1}^n \) to approximate the posterior distribution \( p(\theta | D) \). After that, we can use the particles group to predict the class labels of test data points.

As for the dataset, we use the Covtype, which is a binary dataset with 581,012 data points, and each data point has 54 features. And the dataset analyzed during the current task is available in this repository\(^1\). We select 20% of the dataset for testing and the rest for training. For all training processes, we use AdaGrad optimizer with a learning rate of 0.05 for both \( \theta \) and \( \mathbf{w} \). The mini-batch size is 100. We use \( n = 100 \) particles for all methods. Unlike toy example in Sec. 5.1, we select bandwidth of 10 RBF kernels in the range of \([2^2, 2^3, \ldots, 2^{11}]\). All results are averaged on ten random trials.

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\(^1\) https://www.csie.ntu.edu.tw/~cjlin/libsvmtools/datasets/binary.html
Results  Figure 2 show the results of MK-SVGD and vanilla SVGD with different kernels in two aspects: Test accuracy and Test log-likelihood. Specifically, we compare MK-SVGD with five vanilla SVGDs with different bandwidths, which are $h = 2^0$, $h = 2^4$, $h = 2^8$, $h = 2^{12}$ and median heuristics way. We can see that the final results of our algorithm are better than vanilla SVGD on both test accuracy and test log-likelihood. Moreover, it can be clearly seen that our algorithm results are more stable, while the convergence speed is slightly slower due to the mixture process of multi-kernel.

Bayesian Neural Networks  

Finally, we test our algorithm on Bayesian neural network regression on several UCI datasets, which are all available in this repository. All datasets information used in our experiments is summarized in Table 1. For all datasets, we use a neural network with one hidden layer with 50 units and ReLU activation functions. We initialize the network weights using isotropic Gaussian prior and do not scale the input of the output layer. We perform ten random trials for all results and then take the average. As the experimental setup remains the same, the results for PBP are obtained from [9] directly. All methods use $n = 20$ particles. All datasets are randomly selected 90% for training, and the rest are used for testing. For the weight of the kernel, we use gradient descent or AgaGrad for different datasets. The mini-batch size is 100. In addition, we select bandwidth of 10 RBF kernels in the range of $[2^{-4}, 2^{-3}, \ldots, 2^5]$.

Results  We compare MK-SVGD with vanilla SVGD, probabilistic back-propagation (PBP), Matrix-SVGD(average), and Matrix-SVGD(mixture) in terms of the Root Mean Square Error(RMSE) and the log-likelihood on test data. All results are shown in Tables 2 and 3 respectively. We can see our algorithm yields better performance than other methods in most cases.

Table 2  Average Test RMSE

| Dataset | PB | Vanilla SVGD | Matrix-SVGD(average) | Matrix-SVGD (mixture) | MK-SVGD |
|---------|----|-------------|---------------------|----------------------|--------|
| Boston  | 2.977 ± 0.093 | 2.957 ± 0.099 | 2.898 ± 0.184 | 2.717 ± 0.166 | 2.703 ± 0.263 |
| Combined | 4.052 ± 0.031 | 4.033 ± 0.033 | 4.056 ± 0.033 | 4.029 ± 0.033 | 4.013 ± 0.053 |
| Concrete | 5.506 ± 0.103 | 5.324 ± 0.104 | 4.869 ± 0.124 | **4.721 ± 0.111** | 5.162 ± 0.219 |
| Wine | 0.614 ± 0.008 | 0.609 ± 0.010 | 0.637 ± 0.008 | 0.637 ± 0.009 | **0.601 ± 0.050** |
| Yacht | 0.778 ± 0.042 | 0.864 ± 0.052 | 2.750 ± 0.125 | 2.961 ± 0.074 | **0.688 ± 0.100** |

2  https://archive.ics.uci.edu/ml/datasets.php
Table 3  Average Log-Likelihood

| Dataset  | PBP       | Vanilla SVGD | Matrix-SVGD (average) | Matrix-SVGD (mixture) | MK-SVGD   |
|----------|-----------|--------------|-----------------------|-----------------------|-----------|
| Boston   | −2.579 ± 0.052 | −2.504 ± 0.029 | −2.669 ± 0.141        | −2.861 ± 0.207        | −2.474 ± 0.070 |
| Combined | −2.819 ± 0.008 | −2.815 ± 0.008 | −2.824 ± 0.009        | −2.817 ± 0.009        | −2.835 ± 0.035  |
| Concrete | −3.137 ± 0.021 | −3.082 ± 0.018 | −3.150 ± 0.054        | −3.207 ± 0.071        | −3.080 ± 0.031  |
| Wine     | −0.931 ± 0.014 | −0.925 ± 0.014 | −0.980 ± 0.016        | −0.988 ± 0.018        | −0.902 ± 0.040  |
| Yacht    | −1.221 ± 0.044 | −1.225 ± 0.042 | −2.390 ± 0.452        | −2.475 ± 0.067        | −1.199 ± 0.053  |

Conclusion

In this work, we define a new discrepancy metric MKSD, and then propose a more general and efficient algorithm MK-SVGD based on MKSD. Taking advantage of MKL, MK-SVGD gets rid of the dependence on the optimal kernel choice in SVGD-based methods with single kernel. Moreover, MK-SVGD can automatically learn a weight vector to adjust the importance of each base kernel without any other parameters, which guarantees computational efficiency. Experiments on different data and models show the effectiveness of our algorithm.

In the future, we will consider other forms of kernels that are not limited to RBF kernel, such as linear kernel and polynomial kernel. In addition, it is also worth exploring how to combine kernels better. Finally, we will also consider how to apply the obtained optimal kernel to downstream tasks.

Appendix A. Definitions

Definition 2 (Strictly Positive Kernel) For any function $f$ that satisfies $0 \leq ||f||_2^2 \leq \infty$, a kernel $k(x, x')$ is said to be integrally strictly positive definition if

$$\int_{\mathcal{X}} f(x)k(x, x')f(x')dx dx' > 0.$$  

Definition 3 (Stein Class) For a smooth function $f : \mathcal{X} \to \mathbb{R}$, then, we can say that $f$ is in the Stein class of $q$ if satisfies

$$\int_{\mathcal{X}} \nabla_q(f(x)q(x))dx = 0$$  

Definition 4 (Kernel in Stein Class) If kernel $k(x, x')$ has continuous second-order partial derivatives, and for any fixed $x$, both $k(x, \cdot)$ and $k(\cdot, x)$ are in the Stein class of $p$, then the kernel $k(x, x')$ said to be in the Stein class of $p$.

Appendix B. Proof

Proof of Proposition 1

Proof For the kernel $k_w(x, x') = \sum_{i=1}^{m} w_i k_i(x, x')$, where $w \in \mathbb{R}_+^m, ||w||_2 = 1$, and $k_i(x, x')$ is in the Stein class. According to Definition 4, we know that $k_i(x, x')$ has continuous second-order partial derivatives. Setting $g$ be the continuous second-order partial, we know that the continuous second-order partial $g$ of multiple kernel $k_w$ is

$$g = \sum_{i=1}^{m} w_i g_i$$

So, the kernel $k_w(x, x') = \sum_{i=1}^{m} w_i k_i(x, x')$, where $w \in \mathbb{R}_+^m, ||w||_2 = 1$, is in the Stein class.

Proof of Proposition 2

Proof We know $\mathbb{S}_k(q||p) \geq 0$ and $\mathbb{S}_k(q||p) = 0$ if and only if $q = p$ a.e. This means $\mathbb{S}_{k_w}(q, p) \geq 0$ and $\mathbb{S}_{k_w}(q, p) = 0$ when $q = p$ a.e. for any $w \in \mathbb{R}_+^m$. Then, we know $\mathbb{S}_{k_w}(q, p) = 0$ if and only if $\mathbb{S}_{k}(q, p) = 0$. Thus $q = p$ a.e.

Appendix C. Comparison to Matrix-SVGD (average)

Although using a similar “mixture” form, our approach is intrinsically different from Matrix-SVGD (average). Next, we will detailedly compare the two methods from theoretical aspect.

To elaborate more clearly, we briefly review the “mixture preconditioning kernel” in the Matrix-SVGD, which has the form of:

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

where $K_Q(x, x')$ is defined as...
\[ K_{\theta}(x,x') := Q_{\epsilon}^{-1/2} K_\theta \left( Q_{\epsilon}^{1/2} x, Q_{\epsilon}^{1/2} x' \right) Q_{\epsilon}^{-1/2}, \]

and \( w_{\epsilon}(x) \) is defined as

\[ w_{\epsilon}(x) = \frac{N(x|z_{\epsilon}, Q_{\epsilon}^{-1})}{\sum_{\epsilon'=1}^{\infty} N(x|z_{\epsilon'}, Q_{\epsilon'}^{-1})}. \]

\( K_\theta \) can be chosen to be the standard RBF kernel and \( N \) is Gaussian distribution.

The kernel used in our method is defined as

\[ k_w(x,x') = \sum_{i} w_i k_i(x,x'), \quad \text{s.t.} \quad w \in \mathbb{R}_+^m, ||w||_2 = 1 \] (28)

as shown in Eq. (13) in “Multiple Kernelized Stein Discrepancy”. Therefore, we can summarize the difference between the two as follows.

- Different RKHS. The Matrix-SVGD introduces the optimization problem to vector-valued RKHS with matrix-valued kernels, while our method focuses on leveraging the effectiveness of Multiple Kernel Learning, which optimizes the objective in scalar-valued RKHS. So, the value of kernel \( K_{\theta}(x,x') \) in Eq. (25) is a matrix while our kernel is still a scalar. The resultant value of the mixture kernel is also different: vector-value for Matrix-SVGD and scalar-value for ours.

- Different roles. In Matrix-SVGD(average), the “mixture” form was introduced to address the intractability of the “Point-wise Preconditioning” matrix, which is done by using a weighted combination of several constant pre-conditioning matrices associated with a set of anchor points. In contrast, taking inspiration from the paradigm of multiple kernel learning, we utilize a more powerful “mixture” kernel instead of a single one to approximate the optimal kernel.

- Different weight’s updating way. According to Eq. (27), we know that the kernel’s weight is the product of two Gaussian mixture probability from the anchor points, in which the weight’s distribution is pre-defined. While in our method, the optimal weight of each kernel is learned automatically, as shown in Eq. (21) in “SVGD with Multiple Kernels”.

### References

1. Faix M, Mazer E, Laurent R, Abdallah MO, LeHy R, Lobo J. Cognitive computation: a bayesian machine case study. In: 2015 IEEE 14th International Conference on Cognitive Informatics & Cognitive Computing (ICCI* CC). IEEE. 2015:67-75.
2. Chater N, Oaksford M, Hahn U, Heit E. Bayesian models of cognition. Wiley Interdisciplinary Reviews: Cognitive Science. 2010;16(6):811-23.
3. Knill DC, Richards W. Perception as Bayesian inference. Cambridge University Press. 1996.
4. Neal RM, et al. MCMC using Hamiltonian dynamics. Handbook of markov chain monte carlo. 2011:2(11):2.
5. Hoffman MD, Gelman A. The No-U-Turn sampler: adaptively setting path lengths in Hamiltonian Monte Carlo. J Mach Learn Res. 2014;15(1):1593–623.
6. Zhang R, Li C, Zhang J, Chen C, Wilson AG. Cyclical Stochastic Gradient MCMC for Bayesian Deep Learning. International Conference on Learning Representations. 2020.
7. Kingma DP, Welling M. Auto-encoding variational bayes. arXiv preprint arXiv:1312.6114. 2013.
8. Blei DM, Kucukelbir A, McAuliffe JD. Variational inference: A review for statisticians. J Am Stat Assoc. 2017;112(518):859–77.
9. Liu Q, Wang D. Stein variational gradient descent: A general purpose bayesian inference algorithm. In: Adv Neural Inf Process Syst. 2016;2378-86.
10. Chen C, Zhang R, Wang W, Li B, Chen L. A unified particle-optimization framework for scalable Bayesian sampling. arXiv preprint arXiv:1805.11659. 2018.
11. Liu C, Zhuo J, Cheng P, Zhang R, Zhu J, Carin L. Accelerated first-order methods on the Wasserstein space for Bayesian inference. stat. 2018;1050:4.
12. Zhang J, Zhang R, Carin L, Chen C. Stochastic particle-optimization sampling and the non-asymptotic convergence theory. In: International Conference on Artifical Intelligence and Statistics. PMLR. 2020;1877-87.
13. Zhang C, Li Z, Qian H, Du X. DPVI A Dynamic-Weight Particle-Based Variational Inference Framework. arXiv preprint arXiv:2112.00945. 2021.
14. Liu C, Zhuo J, Cheng P, Zhang R, Zhu J. Understanding and accelerating particle-based variational inference. In: International Conference on Machine Learning. 2019;4082-92.
15. Han J, Liu Q. Stein variational gradient descent without gradient. In: International Conference on Machine Learning. PMLR. 2018;1900-8.
16. Detommaso G, Cui T, Marzouk Y, Spantini A, Scheichl R. A Stein variational Newton method. In: Adv Neural Inf Process Syst. 2018;9169-79.
17. Wang D, Tang Z, Bajaj C, Liu Q. Stein variational gradient descent with matrix-valued kernels. In: Adv Neural Inf Process Syst. 2019;7836-46.
18. Gorham J, Mackey L. Measuring sample quality with kernels. In: International Conference on Machine Learning. PMLR. 2017;1292-301.
19. Hofmann T, Schölkopf B, Smola AJ. Kernel methods in machine learning. The annals of statistics. 2008;1171-220.
20. Han J, Ding F, Liu X, Torressei L, Peng J, Liu Q. Stein variational inference for discrete distributions. In: International Conference on Artificial Intelligence and Statistics. PMLR. 2020;4563-72.
21. Liu Q, Lee J, Jordan M. A kernelized Stein discrepancy for goodness-of-fit tests. In: International conference on machine learning. 2016;276-84.
22. Berlinet A, Thomas-Agnan C. Reproducing kernel Hilbert spaces in probability and statistics. Springer Science & Business Media. 2011.
23. Stein C. A bound for the error in the normal approximation to the distribution of a sum of dependent random variables. In: Proceedings of the sixth Berkeley symposium on mathematical statistics and probability, volume 2: Probability theory. vol.6. University of California Press. 1972;583-603.
24. Barbour AD, Chen LH. Steins (magic) method. arXiv preprint arXiv:1411.1179. 2014.
25. Gorham J. Measuring sample quality with Stein’s method. Stanford University. 2017.
26. Wilson AG, Hu Z, Salakhutdinov R, Xing EP. Deep kernel learning. In: Artificial intelligence and statistics. PMLR. 2016;370-8.
27. Kang Z, Lu X, Yi J, Xu Z. Self-weighted multiple kernel learning for graph-based clustering and semi-supervised classification. In: Proceedings of the 27th International Joint Conference on Artificial Intelligence. 2018;2312-8.
28. Xu Z, Jin R, King I, Lyu M. An extended level method for efficient multiple kernel learning. In: Adv Neural Inf Process Syst. 2009;1825-32.
29. Xu Z, Jin R, Yang H, King I, Lyu MR. Simple and efficient multiple kernel learning by group lasso. In: Proceedings of the 27th international conference on machine learning (ICML-10). Citeseer. 2010;1175-82.
30. Gönen M, Alpayd in E. Multiple kernel learning algorithms. J Mach Learn Res. 2011;12:2211–68.
31. Huang S, Kang Z, Tsang IW, Xu Z. Auto-weighted multi-view clustering via kernelized graph learning. Pattern Recognit. 2019;88:174–84.
32. Zhang Q, Kang Z, Xu Z, Huang S, Fu H. Spaks: Self-paced multiple kernel subspace clustering with feature smoothing regularization. Knowl Based Syst. 2022;109500.
33. Pan Z, Zhang H, Liang C, Li G, Xiao Q, Ding P, et al. Self-Weighted Multi-Kernel Multi-Label Learning for Potential miRNA-Disease Association Prediction. Molecular Therapy-Nucleic Acids. 2019;17:414–23.
34. Feng Y, Wang D, Liu Q. Learning to draw samples with amortized stein variational gradient descent. arXiv preprint arXiv:1707.06626. 2017.
35. Pu Y, Gan Z, Henao R, Li C, Han S, Carin L. Vae learning via stein variational gradient descent. In: Adv Neural Inf Process Syst. 2017;4236-45.
36. Li Y, Turner RE. Gradient estimators for implicit models. arXiv preprint http://arxiv.org/abs/1705.07107.
37. Korba A, Sulim A, Arbel M, Luise G, Gretton A. A non-asymptotic analysis for Stein variational gradient descent. Adv Neural Inf Process Syst. 2020;33:4672–82.
38. Liu X, Tong X, Liu Q. Profiling pareto front with multi-objective stein variational gradient descent. Adv Neural Inf Process Syst. 2021;34.
39. Chen P, Ghattas O. Projected Stein variational gradient descent. Adv Neural Inf Process Syst. 2020;33:1947–58.
40. Jaini P, Holdijk L, Welling M. Learning Equivariant Energy Based Models with Equivariant Stein Variational Gradient Descent. Adv Neural Inf Process Syst. 2021;34.
41. Bu J, Erdogan MA, Ghassemi M, Sun S, Suzuki T, Wu D, et al. Understanding the Variance Collapse of SVGD in High Dimensions. In: International Conference on Learning Representations. 2021.
42. Duchi I, Hazan E, Singer Y. Adaptive subgradient methods for online learning and stochastic optimization. J Mach Learn Res. 2011;12(7).
43. Hernández-Lobato JM, Adams R. Probabilistic backpropagation for scalable learning of bayesian neural networks. In: International Conference On Machine Learning. PMLR. 2015;1861-9.

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