Kernel Selection for Stein Variational Gradient Descent

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Abstract

Stein variational gradient descent (SVGD) and its variants have shown promising successes in approximate inference for complex distributions. However, their empirical performance depends crucially on the choice of optimal kernel. Unfortunately, RBF kernel with median heuristics is a common choice in previous approaches which has been proved sub-optimal. Inspired by the paradigm of multiple kernel learning, our solution to this issue is using a combination of multiple kernels to approximate the optimal kernel instead of a single one which may limit the performance and flexibility. To do so, we extend Kernelized Stein Discrepancy (KSD) to its multiple kernel view called Multiple Kernelized Stein Discrepancy (MKSD). Further, we leverage MKSD to construct a general algorithm based on SVGD, which be called Multiple Kernel SVGD (MK-SVGD). Besides, we automatically assign a weight to each kernel without any other parameters. The proposed method not only gets rid of optimal kernel dependence but also maintains computational effectiveness. Experiments on various tasks and models show the effectiveness of our method.

Keywords: Approximate inference, Kernel Selection, SVGD, multiple kernel learning

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1. Introduction

Bayesian inference is a powerful tool for modeling complex data and reasoning with uncertainty, but computing the posterior distribution is always an intractable challenge. In the current study, there are mainly two proposed methods to solve this problem. One is the sampling-based method, the other is the Variational Inference method (VIs). As a representative of the sampling-based method, Markov Chain Monte Carlo (MCMC) can directly sample in the posterior and has been widely used. (e.g. [1]; [2]). While due to undesirable auto-correlation between samples, they tend to converge slowly in practice despite asymptotically guaranteed. By comparison, Variational Inference leverage a certain simpler distribution family to approximate target distribution by minimizing their Kullback-Leibler (KL) divergence. One crucial and tricky problem in Variational Inference is to choose a distribution family, which would affect both the accuracy and computational cost (e.g. [3]; [4]).

In this paper, we put eyes on Stein variational gradient descent (SVGD) [5], which locates in somewhere between the variational inference and sampling-based methods, and it can be either regarded as a non-parametric variational inference algorithm or a particle-based sampling method [6]. Put merely, SVGD randomly initializes a collection of particles by sampling from a Gaussian distribution and then leverages efficient deterministic dynamics iteratively to transform the particles closer to the target distribution, which would finally converge after several iterations. The particles finally obtained by SVGD can be regarded as samples sampled from the target distribution. It combines the advantages of MCMC, which does not confine the approximation within a parametric family, and variational inference, which converges fast due to deterministic updates that utilize the gradient. We will introduce SVGD [5] in detail in Section 2.
Despite both practically fast and theoretical guaranteed, we notice that the performance of SVGD and its variants crucially relies on the optimal kernel choice. The kernel used in SVGD performs a weighted average of the contribution of all particles to the current particle, so that the current particle moves to the direction of the steepest descent in the local average. It also flows the particles along with the support of the target distribution. Hence, selecting an optimal kernel to capture the underlying geometry of the target distribution, and through the particles effectively to the support of target distribution is crucial.

However, RBF kernel with median heuristic is a common choice in practice [5], [7], [8]. We argue that the expression ability of a single RBF kernel is weak, and the current heuristic median method is not good enough at bandwidth selection. In other words, this kernel is sub-optimal [6]. Therefore, we tested the performance of SVGD with different types of the kernel, such as RBFs with different bandwidths $h$. See more details in Experiments part. Results are drawn in Figure 1 from which we can see that the performance of SVGD is unstable. Inspired by multiple kernel learning, we approximate the optimal kernel by using a combined kernel instead of a single one. Combined with KSD, We purpose a new distance, named MKSD. Furthermore, we leverage MKSD to construct a general algorithm based on SVGD, which be called Multiple Kernel SVGD (MK-SVGD). Moreover, the optimal weight for each kernel can automatically be assigned without any other parameter. Thus, MK-SVGD not only gets rid of optimal kernel dependence but also maintains computational effectiveness.

Figure 1: Bayesian Logistic regression results of SVGD with different kernel on the Covtype dataset.
In summary, our contributions are as follows:

- We propose a more general discrepancy definition, named MKSD, which can be regarded as a multi-kernel version of KSD. Along with its salable variant called maxMKSD using an optimal weight vector.

- Using the newly defined MKSD, we further expand it to vanilla SVGD and get a more general algorithm MK-SVGD. Unlike SVGD and its variants, our algorithm approximates the optimal kernel by using a combined kernel stead of a single one, which can better capture the underlying geometry structure of the target distribution. In addition, MK-SVGD automatically learn an optimal weight for each kernel without any other parameter. This means that it not only get rid of optimal kernel dependence but also maintains computational efficiency.

- We test the newly proposed method on different tasks and models. Specifically, we first test our algorithm on a simple toy example in multivariate Gaussian then move on to some challenge tasks concluding Bayesian logistic regression and Bayesian neural networks. Experiments results show the effectiveness of our method.

The organization of the paper is as follows. Section 2 briefly reviews the KSD and SVGD. Section 3 introduces MKSD and MK-SVGD, which is our main contribution. Some related research will be discussed in Section 4 and Section 5 presents the experiments. Finally, we summarize our work and point out the direction of future work in Section 6.

2. Background

Notation and Preliminary Throughout this paper, vectors in \( \mathbb{R}^d \) are denoted by bold lowercase letters (e.g., \( \mathbf{x} \)). A positive definite kernel function \( k : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R} \) is symmetric and \( \sum_{ij} \alpha_i k(\mathbf{x}_i, \mathbf{x}_j) \alpha_j \geq 0 \) for any \( \alpha_i \subset \mathbb{R} \) and \( \mathbf{x}_i \subset \mathbb{R}^d \). The reproducing kernel Hilbert space (RKHS) \( \mathcal{H}_k \) realted to \( k(\mathbf{x}, \mathbf{x}') \) includes functions of from

\[
f(\mathbf{x}) = \sum_i \alpha_i k(\mathbf{x}, \mathbf{x}_i), \quad \forall \alpha_i \subset \mathbb{R}, \quad \mathbf{x}_i \subset \mathbb{R}^d
\] (1)
equipped with inner product $\langle f, g \rangle_H = \sum_{ij} \alpha_i \beta_j k(x_i, x_j)$ for $g = \sum_j \beta_j k(x, x_j)$ and RKHS norm $\|f\|^2_H = \sum_{ij} \alpha_i \alpha_j k(x_i, x_j)$. See [9] or [10] for more detail.

**KSD and SVGD** Before presenting the proposed method, we first introduce some basic concepts and algorithms, namely Kernelized Stein Discrepancy (KSD) and Stein variational gradient descent (SVGD). See more detail in [5] or [11].

Denote probability density function $p(x)$ as our target distribution, which is positive and continuously differentiable supported on $\mathbb{R}^d$. SVGD tends to obtain a collection of particles $\{x_i\}_{i=1}^n$, which can be regarded as samples drawn from $p(x)$. Then for any test function $T$, we can use them to approximate $p(x)$ in the sense that

$$\mathbb{E}_p[T(x)] = \lim_{n \to \infty} \frac{1}{n} \sum_{i=1}^n T(x_i) \quad (2)$$

To achieve this, SVGD randomly sampling a collection of particles $\{x_i\}_{i=1}^n$ from a simple distribution (e.g. standard normal distribution), and iteratively updating them according to a deterministic transformation

$$x_i \leftarrow x_i + \epsilon \phi^*(x_i), \quad \forall i = 1, \cdots, n \quad (3)$$

where $\phi^* : \mathbb{R}^d \to \mathbb{R}^d$ is a chosen velocity field to drive the particles covering the target distribution and $\epsilon$ is step size. As $x \sim q$, the distribution of updated particles $x' = x + \epsilon \phi(x)$ is denoted as $q[\epsilon \phi]$. Then we can obtain the optimal choice of $\phi$ by solving the optimization problem as follow:

$$\phi^* = \arg \max_{\phi \in \mathcal{F}} \left\{ -\frac{d}{d\epsilon} \text{KL}(q[\epsilon \phi] \| p) \bigg|_{\epsilon = 0} \right\} \quad (4)$$

where $\mathcal{F}$ is the candidate velocity fields. With a specific velocity field $\mathcal{F}$, we can get the optimal $\phi$ by maximizing the decreasing rate of the KL divergence between the particle distribution and the target distribution. The key observation is that

$$-\frac{d}{d\epsilon} \text{KL}(q[\epsilon \phi] \| p) \bigg|_{\epsilon = 0} = \mathbb{E}_{x \sim q} [A_p^\top \phi(x)], \quad A_p^\top \phi(x) = \nabla_x \log p(x)^\top \phi(x) + \nabla^\top_x \phi(x) \quad (5)$$

That is, the objective in Eq.(4) is a linear combination function of $\phi$ and the linear operator $A_p$ is called Stein Operator. Based on the Stein operator, we can see the RHS
of Eq. (5) equals zero if $p = q$:

$$E_p[A_p \phi] = E_p[\nabla_x \log p(x)^\top \phi(x) + \nabla_x^\top \phi(x)] = 0$$  \hspace{1cm} (6)

This is the so-called Stein Identity which can be easily checked using integration by parts. Therefore, the optimization in Eq. (4) turns into

$$D_F(q || p) \overset{\text{def}}{=} \max_{\phi \in \mathcal{F}} \left\{ E_{x \sim q} \left[ A_p^\top \phi(x) \right] \right\}$$  \hspace{1cm} (7)

This is Stein Discrepancy. Some existing work directly optimize Stein Discrepancy, e.g. ([12], [13], [14]). Here the choice of candidate velocity fields $\mathcal{F}$ determines the Stein discrepancy’s discrimination ability and computational tractability, so it is very critical. In vanilla SVGD, $\mathcal{F}$ is chosen as the unit ball of a RKHS $\mathcal{H}$ associated with a positive definite kernel $k(x, x')$, that is $\mathcal{F} = \{ \phi \in \mathcal{H} : \| \phi \|_\mathcal{H} \leq 1 \}$. This choice of $\mathcal{F}$ makes it possible to consider velocity fields in infinite dimensional function spaces while still obtaining computationally tractable solution. Under this setting, we can get Kernelized Stein Discrepancy (KSD), which is defined as

$$S(q || p) \overset{\text{def}}{=} \max_{\phi \in \mathcal{H}} \left\{ E_{x \sim q} \left[ A_p^\top \phi(x) \right] \right\}, \text{ s.t. } \| \phi \|_\mathcal{H} \leq 1$$  \hspace{1cm} (8)

Some advanced work optimizes and learns KSD, such as [15] and [16]. Combining equations Eq. (5) and Eq. (8), we can quickly get a closed-form solution to Eq. (4):

$$\phi^*(\cdot) \propto E_{x \sim q} [A_k(x, \cdot)] = E_{x \sim q} [\nabla_x \log p(x) k(x, \cdot) + \nabla_x k(x, \cdot)]$$  \hspace{1cm} (9)

where $k$ is the positive definite kernel associated with RKHS $\mathcal{H}_0$. Such $\phi$ provides the optimal update direction for all particles to approximate target distribution.

In practice, SVGD iteratively update particles $\{x_i\}_{i=1}^n$ by $x_i \leftarrow x_i + \epsilon \phi^*(x_i)$, where,

$$\phi^*(x_i) = \frac{1}{n} \sum_{j=1}^n \left[ \nabla_{x_j} \log p(x_j) k(x_j, x_i) + \nabla_{x_j} k(x_j, x_i) \right]$$  \hspace{1cm} (10)

The different parts of the Eq. (10) 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.
3. SVGD with Multiple Kernel

This section introduces guidance for kernel selection to achieve our goals. First, we intuitively analyze the issue of kernel selection in Kernelized Stein Discrepancy (KSD). Then combined with Multiple Kernel Learning (MKL) to propose a new distance 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 be called Multiple Kernel SVGD (MK-SVGD). Finally, we simply analyze the time consumption of our algorithm.

3.1. Intuition and Multiple Kernelized Stein Discrepancy

Intuition. Before moving to the details, we give a brief overview of the intuition on how to tackle the kernel selection issue of KSD and its application. First, we notice that the kernel moves the particles to the direction of the steepest descent in the local average by weighting the contribution of each particle, and it also flows the particles along with the support of the target distribution. Hence, selecting the optimal kernel to capture the underlying geometry of the target distribution, and through the particles effectively to the support of target distribution is crucial. (17), (18). In practice, RBF kernel with median heuristics is a common choice but the sub-optimal. And better kernels, e.g. deep kernels might be preferred but not easy to use. Inspired by multiple kernel learning, our algorithm approximates the optimal kernel by using a combined kernel stead of a single one to track this problem. Then the optimal weight for each kernel can automatically be assigned without any other parameter. Thus, the above two steps not only get rid of optimal kernel dependence but also maintain the computational effectiveness.

Multiple kernel learning (MKL) provides an way to automatically learn the optimal combination of different base kernels. (19), (20), (21), (22). In other words, the goal of MKL is to maximize a generalized performance measure by finding an optimal basic kernel functions combination. In general, the MKL performs better than the single-kernel method (23). According to different needs and tasks, there are many ways to combine kernels. For the convenience of calculation, we combine the kernels in a
linear way. That is,

\[ k_w(x, x') = \sum_{i} w_i k_i(x, x') \quad \text{s.t.} \quad w \in \mathbb{R}_+^m, \|w\|_2 = 1 \quad (11) \]

where \( m \) is the number of kernel used to combined, and \( w_j \) is the weight of kernel \( k_j \). From [5], we know that kernel used in SVGD should in the Stein class for smooth densities in a proper sense (See definition in Appendix A.2). Some commonly used kernels meet the requirements, such as RBF kernel \( k(x, x') = \exp\left(-\frac{1}{h} \|x - x'\|_2^2\right) \). In other words, the RBF kernel is in the Stein Class of smooth densities in \( \mathcal{X} = \mathbb{R}^d \).

**Proposition 3.1.** (MK 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 \( w \in \mathbb{R}_+^m \).

Assume every single kernel we used to combine is in the Stein class of smooth densities in \( \mathcal{X} = \mathbb{R}^d \) in MK-SVGD. Then according to Proposition 3.1 (See proof in Appendix B), we could say that the combined multiple kernels are strictly positive definite too. This means that we have a theoretical guarantee for the correctness of our algorithm.

Now It is natural to take advantage of multiple kernels to extend the generalization of KSD. We replace the single kernel in KSD with a combination of multiple kernels. As a result, it is straightforward to define a multiple kernels version of KSD, called Multiple Kernelized Stein Discrepancy (MKSD).

**Theorem 3.2.** (MKSD) Assume \( q(x) \) and \( p(x) \) are continuous differentiable densities supported on \( \mathcal{X} \subseteq \mathbb{R}^D \) and a sequence of \( k_i(x, x') \) are in the Stein class of \( q(x) \). By define \( u_p^i(x, x') = s_p(x)^T k_i(x, x') s_p(x') + s_p(x)^T \nabla_{x'} k_i(x, x') + \)
\[ \nabla x k_i(x, x')^\top s_q(x') + \text{Tr}(\nabla x x' k_i(x, x')), \] we have

\[ u_w^p(x, x') = s_p(x)^\top k_w(x, x') s_p(x') + s_p(x)^\top \nabla x k_w(x, x') + \text{Tr}(\nabla x x' k_w(x, x')) \]

\[ \sum_i w_i u_p^i(x, x') \]

then

\[ S_{k_w}(q, p) = E_{x, x' \sim q}[u_w^p(x, x')] = \sum_i w_i E_{x, x' \sim q}[u_p^i(x, x')] = \sum_i w_i S_{k_i}(q, p). \]

(12)

where \( s_p(x) = \nabla x \log p(x) \) and \( s_q(x) \) accordingly, and \( S_{k_i}(q, p) \) is the KSD corresponding different kernel \( k_i \).

**Proposition 3.3.** (MKSD as a discrepancy) Assume a sequence \( k_i(x, x') \) are integrally strictly positive definite, and \( q, p \) are continuous densities with \( E_q(x)[u_w^p(x, x')] < \infty \) for all \( w \in \mathbb{R}_m^+ \), we have \( S_{k_w}(q, p) \geq 0 \) and \( S_{k_w}(q, p) = 0 \) if and only if \( q = p \).

**Corollary 3.4.** (maxMKSD) Assume the conditions in Theorem 3.2 are satisfied. Then

\[ MKSD_{\text{max}}(q, p) = \max_{w \in \mathbb{R}_m^+} \frac{1}{||w||_2} S_{k_w}(q, p) \]

is equal to 0 if and only if \( p = q \text{ a.e.} \)

3.2. SVGD with Multiple Kernels

We first explained the roles played by \( w \) and \( k_i(x, x') \). We notice the kernel plays a critical role in driving particles to the posterior in two different way: Pushing each particle towards the high probability areas of target distribution by weighting the gradient direction of each particles in the first term; Acting as a repulsive force that spreads the particle along with target distribution and not collapse into the local modes in the second terms.

Take RBF kernel \( k(x, x') = \exp(-\frac{1}{h}||x - x'||_2^2) \) as an example. The repulsive force \( E_{x' \sim q}[\nabla x' k(x, x')] = E_{x' \sim q}[\frac{2}{h}(x - x')k(x, x')] \) drives point \( x \) away from its neighboring point \( x' \) which has large \( k(x, x') \). Here, the bandwidth \( h \) can be viewed as the role for turning the smoothness and repulsive force in the two-term above, eg.
the repulsive term vanishes when $h \to 0$. If bandwidth $h$ can be adjusted according to the current surrounding of particles, the optimal kernel could capture the underlying geometry structure of the target distribution $p(x)$, then each particle can spread the target distribution efficiently.

Hence, the key idea to get rid of the dependence on the single kernel which may limit the performance and flexibility of $\phi(\cdot)$ is to combine the different kernels $k_i(x, x')$ with self-adjusted weights $w$ to approximate the optimal kernel. As a result, it can be seen as kernel selection for the update of SVGD.

We now extend this idea and obtain the multiple kernel version of SVGD. Following the similar recipe of [5], we first consider the connection between the denition of KSD and the steepest descent on the KL divergence, and then derive the optimal perturbation directions. To achieve this, we optimize the perturbation $\phi_w$ in the unit ball of a general RKHS $H_{k_w}$ with the multiple kernels $k_w(x, x) = \sum_i w_i k_i(x, x)$.

**Theorem 3.5.** Let $T_w(x) = x + \epsilon \phi_w(x)$ and $q[T_w](z)$ as the density of $z = T_w(x)$ when $x \sim q(x)$. If the perturbation $\phi_w \in H_{k_w}$ where $H_{k_w}$ is an RKHS equipped with kernel $k_w$ and $\|\phi_w\|_{H_D} \leq D(q, p)$. With weight vector $w$, the steepest descent direction is

$$
\phi^*_w(\cdot) = E_{x \sim q}[A_p k_w(x, \cdot)] = \sum_i w_i E_{x \sim q}[A_p k_i(x, \cdot)] = \sum_i w_i \phi^*_i(\cdot) \quad (14)
$$

and

$$
\nabla, KL(q[T_w]|p)|_{\epsilon = 0} = -E_{x \sim q}[A_p \phi^*_w(x)] = -S_{k_w}(q, p) \quad (15)
$$

where $S_{k_w}(q, p) = E_{x, x' \sim q}[w^w(x, x')] = \sum_i w_i S_{k_i}(q, p)$

The result in Theorem 3.5 suggests that multiple kernels are essentially the consequence of the different changes of variables and yield a gradient update $x \leftarrow x + \epsilon \phi_i(x)$ in different direction, where $\phi_i(x) = E_{x' \sim q}[A_p k_i(x', x)]$.

Next, we focus on weight vector $w$. As we mentioned before, the weight vector linearly combines each kernel, which is vital for choosing the final direction of each particle. To find the optimal combination of weights under the current particles, we need to update the weight vector $w$. In other words, we need to find a set of weight
vector to maximize MKSD, which is the problem explained by Corollary 3.4. Therefore, the problem can be turned into an optimization problem about $w$, as

$$w^* = \arg \max_w S_{w_i}(q\|p) = \arg \max_w \langle w_i, S(q\|p) \rangle$$

where the maximum is achieved when

$$w_i = \sqrt{S_{w_i}(q,p)} / \sum_i S_{w_i}(q,p) = ||\phi_i||_{\mathcal{H}_d} / \sqrt{\sum_i ||\phi_i||_{\mathcal{H}_d}^2}.$$ 

And in this time, MKSD achieve the maxMKSD in Corollary 3.4. The resulting algorithm, Multiple Kernel Stein Variational Gradient Descent (MK-SVGD), is summarised in Algorithm 1:

**Algorithm 1: Multiple Kernel Stein Variational Gradient Descent (MK-SVGD)**

**Input**: Particles $\{x_i\}_{i=1}^n$ initial from prior; Score function of target $s_p(x)$; A sequence kernel function $\{k_j\}_{j=1}^m$; Step size $\epsilon$; Iteration number $T$

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

**for** $t \leq T$ **do**

For each $k_j$ calculate the the steepest direction $\phi_j$ using $\{x^t_i\}_{i=1}^n$ based on Eq.(10):

Find the optimal weight vector $w$ by maximizing Eq.(16) using $\{x^t_i\}_{i=1}^n$ and $\phi_i$;

Summarize the final update direction $\phi^*_w(\cdot)$ using Eq.(14);

Update each particles $x^{t+1}_i = x^t_i + \epsilon \phi^*_w(x^t_i)$.

**end**

Finally, we simply analyze the time complexity of our algorithm. From [5], 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 $\{x^{n-1}_i\}$. Therefore, the introduction of multi-kernels in our algorithm does not significantly increase the time consumption. For example, if we use multiple RBF kernels $k(x, x') = \exp(-\frac{1}{h} \|x - x'\|_2^2)$ with different bandwidth $h$, the term $\|x - x'\|_2^2$ is shared by each kernel. Therefore, we only need to compute the rest part for the kernels with different $h$, and the time consump-
tion is linearly increased compared to the SVGD, which costs $O(mn^2)$. Additional speedup method, such as mini-batch, also can be obtained similar to SVGD.

4. 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 work related to SVGD is mainly concentrated in two directions. One is to combine SVGD with other models or embed SVGD in other models, such as [24], [25], [26]. The other is the improvement or generalization of the vanilla SVGD algorithm, such as [27], [28], [8], [29]. Next, we will briefly introduce several works in these two directions.

For the first case, SVGD is often used as part of the model. For example, in work [24], 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 autoencoders (VAEs) was proposed in [25]. Another work, [26], proposed an algorithm to directly estimates the score function of the implicitly dened 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. For the second case, there also exist many works. Using a surrogate gradient to replace true gradient in SVGD, [27] propose a gradient-free SVGD which focuses on the target distributions with intractable gradient. Furthermore, in work [7], the author extended the idea of gradient-free SVGD to discrete distribution, and solved the limitation that original SVGD can only work under continuous distribution. Another work, [28], accelerated and generalized the SVGD algorithm to approximate a Newton-like iteration in function space by including second-order information. And a Scaled Hessian kernel is proposed using second-order information. Furthermore, the work [8] leverages more general matrix-valued kernels to generate SVGD for exibly incorporating preconditioning information. Note that, Our method is intrinsically different from [8]. [8] introduces the optimization problem to vector-valued RKHS with matrix-valued kernels, while our method focuses on leveraging the effectiveness of MKL, which optimizes
the objective in real-valued RKHS.

5. Experiments

We evaluate MK-SVGD on both synthetic data and real-world examples based on different tasks. We first test our algorithm on a simple toy example in multivariate Gaussian then move on to some challenge tasks concluding Bayesian logistic regression and Bayesian neural networks. The basic settings of our experiments are based on [5]. For all our example, we use multiple RBF kernels with different bandwidth. In detail, we choose 10 RBF kernels \((m = 10)\) to combine, which provides a wide range of options. Furthermore, for a different experiment, we use a different set of bandwidths \(h\). All particles are randomly sampled from the prior unless otherwise specified. AdaGrad([30]) is used for step size.

5.1. Multivariate Gaussian

**Settings** Firstly, We illustrate our method using a Multivariate Gaussian as a toy example. The target distribution is set as

\[
p(x) = \mathcal{N}(x; \mu, \Sigma), \quad \text{where} \quad \mu = [-0.6871, 0.8010], \quad \Sigma = \begin{bmatrix} 0.2260 & 0.1652 \\ 0.1652 & 0.6779 \end{bmatrix}.
\]

(17)

This is a set of parameters we randomly selected. Then we initialize the particles randomly sampling from a standard normal distribution \(\mathcal{N}(x; 0, I)\) which is far away from the target distribution. We use 500 particles and run 200 iterations. In addition, we select bandwidth of 10 RBF kernels in the range of: \([2^{-4}, 2^{-3}, \cdots, 2^5]\).

**Result** Figure 1 shows the result for 2D toy example and weight distribution of each kernel. We can see that the kernels with bandwidth \(h = 1\) and \(h = 2\) plays a major role. Otherwise, the average numerical result over ten random runs is \([-0.68792629, 0.80107447]\).
5.2. Bayesian Logistic Regression

Settings Following [5], we next test MK-SVGD on Bayesian logistic regression for binary classification, and the setting is the basic same. Denote the dataset as $\mathbf{D} = \{(x_i, y_i)\}_{i=1}^{N}$, where $x_i$ is the feature and $y_i \in \{0, 1\}$ is the corresponding binary label. So the model is

$$p(\theta | \mathbf{D}) \propto p(\mathbf{D} | \theta)p(\theta) \quad (18)$$

$$p(\mathbf{D} | \theta) = \prod_{j=1}^{N} \left[ y_j \sigma (\theta^T x_j) + (1 - y_j) \sigma (-\theta^T x_j) \right] \quad (19)$$

where $\sigma(z)$ is a standard logistic function, defined as $\sigma(z) := \frac{1}{1 + \exp(-z)}$, and the prior is set as a Gaussian distribution $p_0(\theta | \alpha) = \mathcal{N}(\theta; 0, \alpha^{-1})$ and $p(\alpha) = \text{Gamma}(\alpha; a, b)$. We set hyperparameters $a$ and $b$ as $\{0, 0.01\}$. Our interest is using MK-SVGD to generate a set of samples $\{\theta\}_{i=1}^{n}$ to approximate the posterior distribution $p(\theta | \mathbf{D})$. After that, we can use it to predict the test data points class label.

We use the Covtype data set, which has 581,012 data points, and each data point has 54 features. We use 80% of the data set for training and 20% for testing. All results are averaged on 10 random trials. We use Adagrad optimizer for both with the learning rate is 0.05 for both $\theta$ and $w$. The mini-batch size is 100. We use $n = 100$ particles. Unlike toy example in 5.1, we select bandwidth of 10 RBF kernels in the range of: $[2^2, 2^3, \ldots, 2^{11}]$.

Result Figure 2 show the results of MK-SVGD and vanilla SVGD with different
kernels in two aspects: Test accuracy and Test log-likelihood from which one can see that the final result of our algorithm is 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 introduction of multi-kernel.

5.3. Bayesian Neural Networks

Settings Similar to the vanilla SVGD and matrix-SVGD, we test our algorithm on Bayesian neural network regression with almost identity settings. We use several UCI datasets. For most datasets, we use neural network with one hidden layer with 50 units and ReLU activation functions, except that we take 100 for Yacht which relatively large. We initialize the network weights using isotropic Gaussian priors and do not scale the input of the output layer. We perform 10 random trials for all results and then take the average. 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 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) \([31]\) and Matrix-SVGD in terms of the RMSE and the log-likelihood on test data. All results are showed in Table 1. We can see our algorithm yields better performance than other methods in most cases.

| Dataset  | PBP          | Vanilla SVGD | Matrix-SVGD | MK-SVGD  |
|----------|--------------|--------------|-------------|----------|
| Boston   | 2.977 ± 0.093 | 2.957 ± 0.099 | 2.898 ± 0.184 | 2.750 ± 0.316 |
| Combined | 4.052 ± 0.031 | 4.033 ± 0.033 | 4.056 ± 0.033 | 4.029 ± 0.110 |
| Concrete | 5.506 ± 0.103 | 5.324 ± 0.104 | 4.869 ± 0.124 | 5.162 ± 0.219 |
| Wine     | 0.614 ± 0.008 | 0.609 ± 0.010 | 0.637 ± 0.008 | 0.601 ± 0.050 |
| Yacht    | 0.778 ± 0.042 | 0.864 ± 0.052 | 2.750 ± 0.125 | 0.688 ± 0.1000 |

Table 1: Average Test RMSE.
Table 2: Average Log-Likelihood.

| Dataset | PBP       | Vanilla SVGD | Matrix-SVGD | MK-SVGD |
|---------|-----------|--------------|-------------|---------|
| Boston  | $-2.579 \pm 0.052$ | $-2.504 \pm 0.029$ | $-2.669 \pm 0.141$ | $\mathbf{-2.474 \pm 0.070}$ |
| Combined| $-2.819 \pm 0.008$ | $\mathbf{-2.815 \pm 0.008}$ | $-2.824 \pm 0.009$ | $-2.835 \pm 0.035$ |
| Concrete| $-3.137 \pm 0.021$ | $-3.082 \pm 0.018$ | $-3.150 \pm 0.054$ | $\mathbf{-3.080 \pm 0.031}$ |
| Wine    | $-0.931 \pm 0.014$ | $-0.925 \pm 0.014$ | $-0.980 \pm 0.016$ | $\mathbf{-0.902 \pm 0.040}$ |
| Yacht   | $-1.221 \pm 0.044$ | $-1.225 \pm 0.042$ | $-2.390 \pm 0.452$ | $\mathbf{-1.199 \pm 0.053}$ |

6. Conclusion

In this paper, we propose a new distance definition MKSD, which can be regarded as a multi-kernel version of KSD. Then extend MKSD to SVGD to get a more general algorithm MK-SVGD. So as to get rid of the dependence on the optimal kernel choice of SVGD, while ensuring the computational efficiency of the algorithm. Besides, we automatically assign a weight to each kernel without any other parameters. Experiments on different data and models have proved the effectiveness of our algorithm. For the convenience of the experiment and the guarantee of the calculation efficiency, the kernels used in this article are RBFs with different bandwidth. But the proposed algorithm is also compatible with other kernels, which is reserved for our future work.

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Appendices

Appendix A. Definitions

Definition Appendix A.1. (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 if
\[
\int_X f(x) k(x, x') f(x') dx dx' > 0.
\]

Definition Appendix A.2. (Stein class) For a smooth function \( f : X \to \mathbb{R} \), then, we can say that \( f \) is in the Stein class of \( q \) if satisfies
\[
\int_{x \in X} \nabla_x (f(x) q(x)) dx = 0
\]

Definition Appendix A.3. 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 \( p \).

Definition Appendix A.4. (Kernelized Stein Discrepancy, (KSD)) If the kernel \( k(x, x') \) is in the Stein class of \( q \), and \( q \) and \( p \) are smooth densities. Set
\[
 u_p(x, x') = s_p(x)^\top k(x, x') s_p(x') + s_p(x)^\top \nabla_{x'} k(x, x') +
\]
\[
+ \nabla_x k(x, x')^\top s_p(x') + \text{trace} (\nabla_{x,x'} k(x, x')).
\]
where \( s_p(x) = \nabla_x \log p(x) \) is the score function of \( p \), then the KSD between distribution \( q \) and \( p \) is
\[
S(q, p) = \mathbb{E}_{x, x' \sim q} [u_p(x, x')]
\]
where \( x, x' \) are i.i.d. draws from \( q(x) \). And we have \( S(q, p) \geq 0 \) and \( S(q, p) = 0 \) if and only if \( q = p \).

Appendix B. Proof

Proof of Proposition 3.1
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 Appendix A.3, we know that $k_i(x, x')$ has continuous second order partial derivatives.

Setting $g_i$ be the continuous second order partial, we know that the continuous second order partial $g$ of multiple kernel $k_{w}$ is

$$g = \sum_{i=1}^{m} w_i g_i \quad \text{(B.1)}$$

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.\qed

Proof of Proposition 3.3

Proof. From Definition Appendix A.4, we know $S_{k_i}(q, p) \geq 0$ and $S_{k_i}(q, p) = 0$ if and only if $q = p$ a.e. This means $S_{k_w} \geq 0$ and $S_{k_w}(q, p) = 0$ when $q = p$ a.e. for any $w \in \mathbb{R}_+^m$.

Then, we know $S_{k_w}(q, p) = 0$ if and only if $S_{k_i}(q, p) = 0$. Thus $q = p$ a.e. \qed