Repulsive Deep Ensembles are Bayesian

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Abstract

Deep ensembles have recently gained popularity in the deep learning community for their conceptual simplicity and efficiency. However, maintaining functional diversity between ensemble members that are independently trained with gradient descent is challenging. This can lead to pathologies when adding more ensemble members, such as a saturation of the ensemble performance, which converges to the performance of a single model. Moreover, this does not only affect the quality of its predictions, but even more so the uncertainty estimates of the ensemble, and thus its performance on out-of-distribution data. We hypothesize that this limitation can be overcome by discouraging different ensemble members from collapsing to the same function. To this end, we introduce a kernelized repulsive term in the update rule of the deep ensembles. We show that this simple modification not only enforces and maintains diversity among the members but, even more importantly, transforms the maximum a posteriori inference into proper Bayesian inference. Namely, we show that the training dynamics of our proposed repulsive ensembles follow a Wasserstein gradient flow of the KL divergence to the true posterior. We study repulsive terms in weight and function space and empirically compare their performance to standard ensembles and Bayesian baselines on synthetic and real-world prediction tasks.

1 Introduction

There have been many recent advances on the theoretical properties of sampling algorithms for approximate Bayesian inference, which changed our interpretation and understanding of them. Particularly worth mentioning is the work of Jordan et al. [38], who reinterpret Markov Chain Monte Carlo (MCMC) as a gradient flow of the KL divergence over the Wasserstein space of probability measures. This new formulation allowed for a deeper understanding of approximate inference methods but also inspired the inception of new and more efficient inference strategies. Following this direction, Liu and Wang [51] recently proposed the Stein Variational Gradient Descent (SVGD) method to perform approximate Wasserstein gradient descent. Conceptually, this method, which belongs to the family of particle-optimization variational inference (POVI), introduces a repulsive force through a kernel acting in the parameter space to evolve a set of samples towards high-density regions of the target distribution without collapsing to a point estimate.

Another method which has achieved great success recently are ensembles of neural networks (so-called deep ensembles), which work well both in terms of predictive performance [42, 80] as well as uncertainty estimation [65], and have also been proposed as a way to perform approximate inference in Bayesian neural networks [82, 36]. That being said, while they might allow for the averaging of predictions over several hypotheses, they do not offer any guarantees for the diversity between those hypotheses nor do they provably converge to the true Bayesian posterior under any meaningful limit. In this work, we show how the introduction of a repulsive term between the members in the ensemble, inspired by SVGD, not only naïvely guarantees the diversity among the members, avoiding their...
collapse in parameter space, but also allows for a reformulation of the method as a gradient flow of the KL divergence in the Wasserstein space of distributions. It thus allows to endow deep ensembles with convergence guarantees to the true Bayesian posterior.

An additional problem is that BNN inference in weight space can lead to degenerate solutions, due to the overparametrization of these models. That is, several samples could have very different weights but map to the same function, thus giving a false sense of diversity in the ensemble. This property, that we will refer to as non-identifiability of neural networks (see Appendix A), can lead to redundancies in the posterior distribution. It implies that methods like MCMC sampling, deep ensembles, and SVGD waste computation in local modes that account for equivalent functions. Predictive distributions approximated using samples from these modes do not improve over a simple point estimate and lead to a poor uncertainty estimation. Following this idea, Wang et al. [76] introduced a new method to extend POVI methods to function space, overcoming this limitation. Here, we also study an update rule that allows for an approximation of the gradient flow of the KL divergence in function space in our proposed repulsive ensembles.

We make the following contributions:

- We derive several different repulsion terms that can be added as regularizers to the gradient updates of deep ensembles to endow them with Bayesian convergence properties.
- We show that these terms approximate Wasserstein gradient flows of the KL divergence and can be used both in weight space and function space.
- We compare these proposed methods theoretically to standard deep ensembles and SVGD and highlight their different guarantees.
- We assess all these methods on synthetic and real-world deep learning tasks and show that our proposed repulsive ensembles can achieve competitive performance and improved uncertainty estimation.

## 2 Repulsive Deep Ensembles

In supervised deep learning, we typically consider a likelihood function \( p(y|f(x; w)) \) (e.g., Gaussian for regression or Categorical for classification) parameterized by a neural network \( f(x; w) \) and training data \( D = \{(x_i, y_i)\}_{i=1}^n \) with \( x \in \mathcal{X} \) and \( y \in \mathcal{Y} \). In Bayesian neural networks (BNNs), we are interested in the posterior distribution of all likely networks given by \( p(w|D) \propto \prod_{i=1}^n p(y_i|f(x_i; w)) p(w) \), where \( p(w) \) is the prior distribution over weights. Crucially, when making a prediction on a test point \( x^* \), in the Bayesian approach we do not only use a single parameter \( \tilde{w} \) to predict \( y^* = f(x^*; \tilde{w}) \), but we marginalize over the whole posterior, thus taking all possible explanations of the data into account:

\[
p(y^*|x^*, D) = \int p(y^*|f(x^*; w)) p(w|D) \, dw \tag{1}
\]
While approximating the posterior of Bayesian neural networks (or sampling from it) is a challenging task, performing maximum a posteriori (MAP) estimation, which corresponds to finding the mode of the posterior, is usually simple. Ensembles of neural networks use the non-convexity of the MAP optimization problem to create a collection of $K$ independent—and possibly different—solutions. Considering $n$ weight configurations of a neural network $\{w_i\}_{i=1}^n$ with $w_i \in \mathbb{R}^d$, the dynamics of the ensemble under the gradient of the posterior lead to the following update rule at iteration $t$:

$$w_i^{t+1} \leftarrow w_i^t + \epsilon_t \phi(w_i^t)$$

with 

$$\phi(w_i^t) = \nabla_{w_i^t} \log p(w_i^t | D),$$

with step size $\epsilon_t$. Ensemble methods have a long history [e.g., 45, 26, 6] and were recently revisited for neural networks [42] and coined deep ensembles. The predictions of the different members are combined to create a predictive distribution by using the solutions to compute the Bayesian model average (BMA) in Eq. (1). Recent works [65] have shown that deep ensembles can outperform some of the Bayesian approaches for uncertainty estimation. Even more recently, Wilson and Izmailov [82] argued that deep ensembles can be considered a compelling approach to Bayesian model averaging. Despite these ideas, the ability of deep ensembles to efficiently average over multiple hypotheses and to explore the functional landscape of the posterior distribution studied in [18] does not guarantee sampling from the right distribution. Indeed, the additional Langevin noise introduced in [77], which is not considered in deep ensembles, is crucial to ensure samples from the true Bayesian posterior.

From a practical standpoint, since the quality of an ensemble hinges on the diversity of its members, many methods were recently proposed to improve this diversity without compromising the individual accuracy. For instance, Wenzel et al. [60] propose hyper-deep ensembles that combine deep networks with different hyperparameters. Similarly, cyclical learning-rate schedules can explore several local minima for the ensemble members [53]. Alternatively, Rame and Cord [67] proposed an information-theoretic framework to avoid redundancy in the members and Oswald et al. [63] studied possible interactions between members based on weight sharing. However, the absence of a constraint that prevents particles from converging to the same mode limits the possibility of improvement by introducing more ensemble members. This means that any hopes to converge to different modes must exclusively rely on:

1. the randomness of the initialization
2. the noise in the estimation of the gradients due to minibatching
3. the number of local optima that might be reached during gradient descent.

Moreover, the recent study of Geiger et al. [25] showed how the empirical test error of the ensemble converges to the one of a single trained model when the number of parameters goes to infinity, leading to deterioration of the performance. In other words, the bigger the model, the harder it is to maintain diversity in the ensemble and avoid collapse to the same solution. This is intuitively due to the fact that bigger models are less sensitive to the initialization. Namely, in order for them to get stuck in a local minimum, they must have second derivatives that are positive simultaneously in all directions. As the number of hidden units gets larger, this becomes less likely.

### 2.1 Repulsive force in weight space

To overcome the aforementioned limitations of standard deep ensembles, we introduce, inspired by SVGD [51], a deep ensemble with members that interact with each other through a repulsive component. Using a kernel function to model this interaction, the single models repel each other by SVGD [51], a deep ensemble with members that interact with each other through a repulsive kernel $R$.

Considering a stationary kernel $k(\cdot, \cdot) : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}$ acting in the parameter space of the neural network, a repulsive term $R$ can be parameterized through its gradient:

$$\phi(w_i) = \nabla_{w_i} \log p(w_i | D) - R \left( \left\{ \nabla_{w_i} k(w_i, w_j) \right\}_{j=1}^n \right).$$

To get an intuition for the behavior of this repulsive term and its gradients, we can consider the RBF kernel $k(w_i, w_j) = \exp \left( -\frac{1}{h} \| w_i - w_j \|^2 \right)$ with lengthscale $h$ and notice how its gradient

$$\nabla_{w_i} k(w_i, w_j) = \frac{2}{h} (w_i - w_j) k(w_i, w_j)$$
drives \( w_i \) away from its neighboring members \( w_j \), thus creating a repulsive effect. Naturally, not all the choices of \( \mathcal{R} \) induce this effect. One of the simplest formulations to obtain it is via a linear combination of the kernel gradients scaled by a positive factor, that is, \( \beta \sum_{j=1}^{n} \nabla w_j k(w_i^t, w_j^t) \) with \( \beta \in \mathbb{R}^+ \). We will see in Section 3 how the choice of \( \beta \) can be justified in order to obtain convergence to the Bayesian posterior together with alternative possible formulations of \( \mathcal{R} \) that preserve this convergence.

### 2.2 Repulsive force in function space

To overcome the aforementioned overparameterization issue, the update in Eq. (3) can be formulated in function space instead of weight space. Let \( f : w \mapsto f(\cdot : w) \) be the map that maps a configuration of weights \( w \in \mathbb{R}^d \) to the corresponding neural network regression function and denote as \( f_i := f(\cdot : w_i) \) the function with a certain configuration of weights \( w_i \). We can now consider \( n \) particles in function space \( \{f_i\}_{i=1}^{n} \) with \( f \in \mathcal{F} \) and model their interaction with a general positive definite kernel \( k(\cdot, \cdot) \). We also consider the implicit functional likelihood \( p(y|x, f) \), determined by the measure \( p(y|x, w) \) in the weight space, as well as the functional prior \( p(f) \), which can either be defined separately (e.g., using a GP) or modeled as a push-forward measure of the weight-space prior \( p(w) \). Together, they determine the posterior in function space \( p(f|D) \). The functional evolution of a particle can then be written as:

\[
 f_i^{t+1} \leftarrow f_i^t + \epsilon_t \phi(f_i^t) \\
 \text{with} \quad \phi(f_i^t) = \nabla f_i^t \log p(f_i^t|D) - \mathcal{R} \left( \{ \nabla f_i^t k(f_i^t, f_j^t) \}_{j=1}^{n} \right). \tag{4}
\]

However, computing the update in function space is neither tractable nor practical, which is why two additional considerations are needed. The first one regards the infinite dimensionality of function space, which we circumvent using a canonical projection into a subspace:

**Definition 1 (Canonical projection).** For any \( A \subset \mathcal{X} \), we define \( \pi_A : \mathbb{R}^\mathcal{X} \to \mathbb{R}^A \) as the canonical projection onto \( A \), that is, \( \pi_A(f) = \{ f(a) \}_{a \in A} \).

In other words, the kernel will not be evaluated directly in function space, but on the projection \( k(\pi_B(f), \pi_B(f')) \), with \( B \) being a subset of the input space given by a batch of training data points. The second consideration is to project this update back into the parameter space and evolve a set of particles there, because ultimately we are interested in representing the functions by parameterized neural networks. For this purpose, we can use the Jacobian of the \( i \)-th particle as a projector:

\[
\phi(w_i^t) = \left( \frac{\partial f_i^t}{\partial w_i^t} \right)^\top \left[ \nabla f_i^t \log p(f_i^t|D) - \mathcal{R} \left( \{ \nabla f_i^t k(\pi_B(f_i^t), \pi_B(f_j^t)) \}_{j=1}^{n} \right) \right]. \tag{5}
\]

### 2.3 Comparison to Stein variational gradient descent

Note that our update is reminiscent of SVGD [51], which in parameter space can be written as:

\[
\phi(w_i^t) = \frac{1}{n} \sum_{j=1}^{n} k(w_j^t, w_i^t) \nabla w_i^t \log p(w_i^t|D) + \frac{1}{n} \sum_{j=1}^{n} \nabla w_j^t k(w_i^t, w_j^t). \tag{6}
\]

It is important to notice that here, the gradients are averaged across all the particles using the kernel matrix. Interestingly, SVGD can be asymptotically interpreted as gradient flow of the KL divergence under a new metric induced by the Stein operator [16] [50] (see Appendix [D] for more details). Moving the inference from parameter to function space [76] leads to the update rule

\[
\phi(w_i^t) = \left( \frac{\partial f_i^t}{\partial w_i^t} \right)^\top \left( \frac{1}{n} \sum_{j=1}^{n} k(f_j^t, f_i^t) \nabla f_i^t \log p(f_i^t|D) + \nabla f_i^t k(f_i^t, f_j^t) \right). \tag{7}
\]

This way of averaging gradients using a kernel can be dangerous in high-dimensional settings, where kernel methods often suffer from the curse of dimensionality. Moreover, in Eq. (6), the posterior gradients of the particles are averaged using their similarity in weight space, which can be misleading in multi-modal posteriors. Worse yet, in Eq. (7), the gradients are averaged in function space and
are then projected back using exclusively the \(i\)-th Jacobian, which can be harmful given that it is not guaranteed that distances between functions evaluated on a subset of their input space resemble their true distance. Our proposed method, on the other hand, does not employ any averaging of the posterior gradients and thus comes closest to the true particle gradients in deep ensembles.

3 Repulsive deep ensembles are Bayesian

So far, we represented the repulsive force as a general function of the gradients of a kernel. In this section, we show how to determine the explicit form of the repulsive term, such that the resulting update rule is equivalent to the discretization of the gradient flow dynamics of the KL divergence in Wasserstein space. We begin by introducing the concepts of particle approximation and gradient flow.

3.1 Particle approximation

A particle-based approximation of a target measure depends on a set of weighted samples \(\{(x_i, w_i)\}_{i=1}^n\), for which an empirical measure can be defined as

\[
\rho(x) = \sum_{i=1}^n w_i \delta(x - x_i),
\]

where \(\delta(\cdot)\) is the Dirac delta function and the weights \(w_i\) satisfy \(w_i \in [0, 1]\) and \(\sum_{i=1}^n w_i = 1\). To approximate a target distribution \(\pi(x)\) using the empirical measure, the particles and their weights need to be selected in a principled manner that minimizes some measure of distance between \(\pi(x)\) and \(\rho(x)\) (e.g., a set of \(N\) samples with weights \(w_i = 1/N\) obtained using an MCMC method).

3.2 Gradient flow in parameter space

Given a smooth function \(J : \mathbb{R}^d \to \mathbb{R}\) in Euclidean space, we can minimize it by creating a path that follows its negative gradient starting from some initial conditions \(x_0\). The curve \(x(t)\) with starting point \(x_0\) described by that path is called gradient flow. The dynamics and evolution in time of a considered point in the space under this minimization problem can be described as the ODE

\[
\frac{dx}{dt} = -\nabla J(x). \tag{9}
\]

We can extend this concept to the space of probability distributions (Wasserstein gradient flow) \[3\]. Let us consider the space of probability measures \(\mathcal{P}_2(M)\), that is, the set of probability measures with finite second moments defined on the manifold \(M\):

\[
\mathcal{P}_2(M) = \left\{ \phi : M \to [0, \infty) \mid \int_M d\phi = 1, \int_M |x|^2 \phi(x) dx < +\infty \right\}.
\]

Taking \(\Pi(\mu, \nu)\) as the set of joint probability measures with marginals \(\mu, \nu\), we can define the Wasserstein metric on the space \(\mathcal{P}_2(M)\) as:

\[
W_2^2(\mu, \nu) = \inf_{\pi \in \Pi(\mu, \nu)} \int |x - y|^2 d\pi(x, y). \tag{10}
\]

Considering the optimization problem of a functional \(J : \mathcal{P}_2(M) \to \mathbb{R}\), such as the KL divergence between the particle approximation in Eq. \[8\] and the target posterior \(\pi(x)\),

\[
\inf_{\rho \in \mathcal{P}_2(M)} D_{KL}(\rho, \pi) = \int_M (\log \rho(x) - \log \pi(x)) \rho(x) dx,
\]

the evolution in time of the measure \(\rho\) under the equivalent of the gradient, the Wasserstein gradient flow, is described by the Liouville equation \[38\][3][64]:

\[
\frac{\partial \rho(x)}{\partial t} = \nabla \cdot \left( \rho(x) \nabla \frac{\delta}{\delta \rho} D_{KL}(\rho, \pi) \right) = \nabla \cdot \left( \rho(x) \nabla \left( \log \rho(x) - \log \pi(x) \right) \right), \tag{11}
\]

\[\text{1}\] Together with the initial condition, this is know as the Cauchy problem.

\[\text{2}\] Also referred to as continuity equation.
where $\nabla_{\theta}^2 D_{KL}(\rho, \pi) =: \nabla_{\theta_1} D_{KL}(\rho, \pi)$ is the Wasserstein gradient and the operator $\frac{\delta}{\delta \eta} : \mathcal{P}_2(\mathcal{M}) \to \mathbb{R}$ represents the functional derivative or first variation (see Appendix C for more details). In the particular case of the KL functional, we can recover the Fokker-Planck equation,

$$\frac{d \rho}{dt} = \nabla \cdot \left( \rho \nabla \log \rho - \rho \nabla \pi(x) \right) + \nabla^2 \rho(\cdot),$$

that admits as unique stationary distribution the posterior $\pi(x)$. The deterministic particle dynamics ODE [2] related to Eq. (11), namely mean-field Wasserstein dynamics, is then given by:

$$\frac{dx}{dt} = -\nabla \left( \log \rho(x) - \log \pi(x) \right). \quad (12)$$

Considering a discretization of Eq. (12) for a particle system $\{x\}^n_{i=1}$ and small stepsize $\epsilon_t$, we can rewrite Eq. (12) as:

$$x^{t+1}_i = x^t_i + \epsilon_t \left( \nabla \log \pi(x^t_i) - \nabla \log \rho(x^t_i) \right). \quad (13)$$

Unfortunately, we do not have access to the analytical form of the gradient $\nabla \log \rho$, so an approximation is needed. At this point, it is crucial to observe the similarity between the discretization of the Wasserstein gradient flow in Eq. (13) and the repulsive update in Eq. (3) to notice how, if the kernelized repulsion is an approximation of the gradient of the empirical particle measure, the update rule minimizes the KL divergence between the particle measure and the target posterior. Different sample-based approximations of the gradient that use a kernel function have been recently studied. The simplest one is given by the kernel density estimation (KDE) (details in Appendix E):

$$\hat{\rho}(x) = \frac{1}{n} \sum_{i=1}^n k(x, x^t_i),$$

where $k(\cdot, \cdot) : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ and the gradient of its log density is given by [70]:

$$\nabla \log \rho(x^t_i) \approx \sum_{i=1}^n \nabla x^t_i k(x^t_i, x^t_j) \sum_{j=1}^n k(x^t_i, x^t_j). \quad (14)$$

Using this approximation in Eq. (13) we obtain:

$$x^{t+1}_i = x^t_i + \epsilon_t \left( \nabla \log \pi(x^t_i) - \sum_{j=1}^n \nabla x^t_i k(x^t_i, x^t_j) \sum_{j=1}^n k(x^t_i, x^t_j) \right), \quad (15)$$

where, if we substitute the posterior for $\pi$, we obtain an expression for the repulsive force in Eq. (3). This shows that if the repulsive term in Eq. (3) is the normalized sum of the gradients $R = \left( \sum_{j=1}^n k(w_i^t, w_j^t) \right)^{-1} \sum_{j=1}^n \nabla w_i^t k(w_i^t, w_j^t)$, we do not only encourage diversity of the ensemble members and thus avoid collapse, but surprisingly—in the asymptotic limit of $n \to \infty$, where the KDE approximation is exact [66]—also converge to the true Bayesian posterior!

Nevertheless, approximating the gradient of the empirical measure with the KDE can lead to suboptimal performance, as already studied by Li and Turner [46]. They instead introduced a new Stein gradient estimator (SGE) that offers better performance, while maintaining the same computational cost. Even more recently, Shi et al. [69] introduced a spectral method for gradient estimation (SSGE), that also allows for a simple estimation on out-of-sample points. These two estimators can be used in Eq. (13), to formulate the following update rules with two alternative repulsive forces. The one using the Stein estimator, that we will call SGE-WGD, is:

$$x^{t+1}_i = x^t_i + \epsilon_t \left( \nabla \log \pi(x^t_i) + \sum_{j=1}^n (K + \eta I)^{-1} \sum_{k=1}^n \nabla x^t_k k(x^t_k, x^t_j) \right), \quad (16)$$

where $K$ is the kernel Gram matrix, $\eta$ a small constant, and $I$ the identity matrix. We can notice an important difference between KDE and SGE, in that the former is only considering the interaction of the $i$-th particle being updated with all the others, while the latter is simultaneously considering also the interactions between the remaining particles. The spectral method, that we will call SSGE-WGD, leads to the following update rule:

$$x^{t+1}_i = x^t_i + \epsilon_t \left( \nabla \log \pi(x^t_i) + \sum_{j=1}^n \frac{1}{\sqrt{\lambda_j}} \sum_{m=1}^n \sum_{k=1}^n u_{jk} \nabla x_m k(x^t_m, x^t_k) \cdot \sum_{l=1}^n u_{jl} k(x^t_l, x^t_j) \right), \quad (17)$$

where $\lambda_j$ is the $j$-th eigenvalue of the kernel matrix and $u_{jk}$ is the $k$-th component of the $j$-th eigenvector. Computationally, both SSGE and SGE have a cost of $O(M^3 + M^2d)$, with $M$ being the number of points and $d$ their dimensionality. SSGE has an additional cost for predictions of $O(M(d + J))$, where $J$ is the number of eigenvalues.
3.3 Gradient flow in function space

To theoretically justify the update rule introduced in function space in Eq. (5), we can rewrite the Liouville equation for the gradient flow in Eq. (11) in function space as

$$\frac{\partial \rho(f)}{\partial t} = \nabla \cdot \left( \rho(f) \nabla \delta D_{KL}(\rho, \pi) \right)$$

$$= \nabla \cdot \left( \rho(f) \nabla \left( \log \rho(f) - \log \pi(f) \right) \right).$$  (18)

Following this update, the mean field functional dynamics are

$$\frac{df}{dt} = -\nabla \left( \log \rho(f) - \log \pi(f) \right).$$  (19)

Using the same KDE approximation as above, we can obtain a discretized evolution in function space and with it an explicit form for the repulsive force in Eq. (4) as

$$f_{i+1}^t = f_i^t + \epsilon_t \left( \nabla_f \log \pi(f_i^t) - \frac{\sum_{j=1}^n \nabla_f k(f_i^t, f_j^t)}{\sum_{j=1}^n k(f_i^t, f_j^t)} \right).$$  (20)

The update rules using the SGE and SSGE approximations follow as for the parametric case. It is important to notice that this update rule requires the function space prior gradient: \( \nabla_f \log p(f_j|x, y) = \nabla_f \log p(y|x, f_j) + \nabla_f \log p(f_j) \). If one wants to use an implicit prior defined in weight space, an additional estimator is needed due to its analytical intractability. We again adopted the SSGE, introduced by Shi et al. [69], which was already used for a similar purpose in Sun et al. [71]. It is also interesting to note that the update rule in Eq. (20) readily allows for the use of alternative priors that have an analytical form, such as Gaussian processes. This is an important feature of our method that allows for an explicit encoding of function space properties that can be useful for example in achieving better out of distribution detection capabilities [14].

3.4 The choice of the kernel

A repulsive effect can always be created in the ensemble by means of the gradient of any kernel function that is measuring the similarity between two members. Nevertheless, it is important to keep in mind that to ensure the asymptotic convergence to the Bayesian posterior, the repulsive component must be a consistent estimator of the gradient in Eq. (13), as shown in Section 3. Therefore, some important constraints over the kernel choice are needed. In particular, the SGE and SSGE need a kernel function belonging to the Stein class (see Shi et al. [69] for more details). On the other hand, for the KDE, any symmetric probability density function can be used. On this subject, the work of Aggarwal et al. [1] has shown how the Manhattan distance metric (L1 norm) might be preferable over the Euclidean distance metric (L2 norm) for high-dimensional settings. We performed some additional experiments using the L1 norm (Laplace kernel) for the KDE but we could not observe any substantial difference compared to using the L2 norm. Further investigations regarding this hypothesis are left for future research.
4 Experiments

In this section, we compare the different proposed WGD methods with deep ensembles and SVGD on synthetic sampling, regression, and classification tasks and real-world image classification tasks. We use an RBF kernel (except where otherwise specified) with the popular median heuristic [51] to choose the kernel bandwidth. In our experiments, an adaptive bandwidth leads to better performance than fixing and tuning a single constant value for the entire evolution of the particles. We also quantitatively assess the uncertainty estimation of the methods in terms of calibration and OOD detection. In our experiments, we report the test accuracy, negative log-likelihood (NLL), and the expected calibration error (ECE) [58]. To assert the robustness on out-of-distribution (OOD) data, we report the ratio between predictive entropy on OOD and test data points ($H_o/H_t$), and the OOD detection area under the ROC curve AUROC(H) [47]. Moreover, to assess the diversity of the ensemble generated by the different methods in function space, we measure the functional diversity using the model disagreement (MD) (details in Appendix B). In particular, we report the ratio between the average model disagreement on the OOD and test data points ($MD_o/MD_t$) and additionally the OOD detection AUROC(MD) computed using this measure instead of the entropy.

Sampling from synthetic distributions As a sanity check, we first assessed the ability of our different approximations for Wasserstein gradient descent (using KDE, SGE, and SSGE) to sample from a two-dimensional Gaussian distribution (Figure 2). We see that our SGE-WGD, SSGE-WGD and the SVGD fit the target almost perfectly. We also tested the different methods in a more complex two-dimensional Funnel distribution [59] and present the results in Figure F.1 in the Appendix. There, SGE-WGD and SVGD also perform best.

BNN 1D regression We then assessed the different methods in fitting a BNN posterior on a synthetically generated one-dimensional regression task. The results are reported in Figure 1 consisting of the mean prediction and ±1, 2, 3 standard deviations of the predictive distribution. We can see that all methods performing inference in the weight space (DE, w-SVGD, WGD) are unable to capture the epistemic uncertainty between the two clusters of training data points. Conversely, the functional methods (f-SVGD, fWGD) are perfectly able to infer the diversity of the hypotheses in this region due to the lack of training evidence. They thereby achieve a predictive posterior that very closely resembles the one obtained with the gold-standard HMC sampling.

BNN 2D classification Next, we investigated the predictive performance and quality of uncertainty estimation of the methods in a two-dimensional synthetic classification setting. The results are displayed in Figure 3. We can clearly observe that the weight-space methods are overconfident and do not capture the uncertainty well. Moreover, all the functions seems to collapse to the optimal classifier. These methods thus only account for uncertainty close to the decision boundaries and to the origin.
Table 1: **BNN image classification. AUROC(H)** is the AUROC computed using the entropy whereas AUROC(MD) is computed using the model disagreement. \( H_o / H_t \) is the ratio of the entropies on OOD and test sets respectively and \( MD_o / MD_t \) is the ratio for model disagreement. We see that the best accuracy is achieved by our WGD methods, while our fWGD methods yield the best OOD detection and functional diversity. All our proposed methods improve over standard deep ensembles in terms of accuracy and diversity, highlighting the effect of our repulsion.

| Method          | AUROC(H) | AUROC(MD) | Accuracy | \( H_o / H_t \) | \( MD_o / MD_t \) | ECE   | NLL |
|-----------------|----------|-----------|----------|-----------------|-------------------|-------|-----|
| Deep ensemble   | 0.843 ± 0.004 | 0.736 ± 0.005 | 85.552 ± 0.076 | 2.244 ± 0.006  | 1.667 ± 0.008 | 0.049 ± 0.001 | 0.277 ± 0.001 |
| SVGD [51]       | 0.825 ± 0.001 | 0.710 ± 0.002 | 85.142 ± 0.017 | 2.106 ± 0.003  | 1.567 ± 0.004 | 0.052 ± 0.001 | 0.287 ± 0.001 |
| f-SVGD [76]     | 0.783 ± 0.001 | 0.712 ± 0.001 | 84.510 ± 0.031 | 1.968 ± 0.004  | 1.624 ± 0.003 | 0.049 ± 0.001 | 0.292 ± 0.001 |
| hyper-DE [80]   | 0.789 ± 0.001 | 0.743 ± 0.001 | 84.743 ± 0.011 | 1.951 ± 0.010  | 1.690 ± 0.015 | 0.046 ± 0.001 | 0.288 ± 0.001 |
| kde-WGD (ours)  | 0.838 ± 0.001 | 0.735 ± 0.004 | 85.904 ± 0.030 | 2.205 ± 0.003  | 1.661 ± 0.008 | 0.051 ± 0.001 | 0.276 ± 0.001 |
| sge-WGD (ours)  | 0.832 ± 0.003 | 0.731 ± 0.005 | 85.638 ± 0.038 | 2.182 ± 0.015  | 1.655 ± 0.001 | 0.049 ± 0.001 | 0.276 ± 0.001 |
| kde-fWGD (ours) | 0.791 ± 0.002 | 0.758 ± 0.002 | 84.888 ± 0.030 | 1.970 ± 0.004  | 1.749 ± 0.005 | 0.044 ± 0.001 | 0.282 ± 0.001 |
| sge-fWGD (ours) | 0.795 ± 0.001 | 0.754 ± 0.002 | 84.766 ± 0.060 | 1.894 ± 0.003  | 1.729 ± 0.002 | 0.047 ± 0.001 | 0.288 ± 0.001 |
| ssge-fWGD (ours)| 0.792 ± 0.002 | 0.752 ± 0.002 | 84.762 ± 0.034 | 1.970 ± 0.006  | 1.723 ± 0.005 | 0.046 ± 0.001 | 0.286 ± 0.001 |

**FashionMNIST classification** Moving on to real-world data, we used an image classification setting using the FashionMNIST dataset [33] for training and the MNIST dataset [43] as an out-of-distribution (OOD) task. The results are reported in Table 1 (top). We can see that all our methods improve upon standard deep ensembles and SVGD, highlighting the effectiveness of our proposed repulsion terms when training neural network ensembles. In particular, the sge-WGD offers the best accuracy, whereas the methods in function space all offer a better OOD detection. This is probably due to the fact that these methods achieve a higher entropy ratio and functional diversity measured via the model disagreement when compared to their weight-space counterparts. Interestingly, they also reach the lowest NLL values. We can also notice how the model disagreement (MD) not only serves its purpose as a metric for the functional heterogeneity of the ensemble but also allows for a better OOD detection in comparison to the entropy. To the best of our knowledge, this insight has not been described before, although it has been used in continual learning [31]. Interestingly, using this metric, the hyper-deep ensemble [80] shows OOD detection performance comparable with our repulsive ensemble in function space.

**CIFAR classification** Finally, we use a ResNet32 architecture [29] on CIFAR-10 [41] with the SVHN dataset [61] as OOD data. The results are reported in Table 1 (bottom). We can see that in this case, the weight-space methods achieve better performance in accuracy and OOD detection using the entropy than the ones in function space. Nevertheless, all our repulsive ensembles improve functional diversity, accuracy, and OOD detection when compared to standard SVGD, whereas the standard deep ensemble achieves the best OOD detection using the entropy.

5 **Related Work**

The theoretical and empirical properties of SVGD have been well studied [40, 48, 13] and it can also be seen as a Wasserstein gradient flow of the KL divergence in the Stein geometry [16, 50].
(see Appendix D for more details). Interestingly, a gradient flow interpretation is also possible for (stochastic gradient) MCMC-type algorithms [48], which can be unified under a general particle inference framework [10]. Moreover, our Wasserstein gradient descent using the SGE approximation can also be derived using an alternative formulation as a gradient flow with smoothed test functions [48]. A projected version of WGD has been studied in Wang et al. [75], which could also be readily applied in our framework. Besides particle methods, Bayesian neural networks [54, 59] have gained popularity recently [22, 19, 36], using modern MCMC [59, 79, 22, 24, 21] and variational inference techniques [5, 12, 17, 34]. On the other hand, ensemble methods have also been extensively studied [42, 18, 82, 23, 80, 32, 85, 78]. Moreover, repulsive interactions between the members have also been studied in Wabartha et al. [74]. Moreover, providing Bayesian interpretations for deep ensembles has been previously attempted through the lenses of stationary SGD distributions [56, 8], ensembles of linear models [57], additional random functions [62, 12, 27], approximate inference [82], Stein variational inference [15], and marginal likelihood lower bounds [53], and ensembles have also been shown to provide good approximations to the true BNN posterior in some settings [36]. Furthermore, variational inference in function space has recently gained attention [71] and the limitations of the KL divergence have been studied in Burt et al. [7].

6 Conclusion

We have presented a simple and principled way to improve upon standard deep ensemble methods. To this end, we have shown that the introduction of a kernelized repulsion between members of the ensemble not only improves the accuracy of the predictions but—even more importantly—can be seen as Wasserstein gradient descent on the KL divergence, thus transforming the MAP inference of deep ensembles into proper Bayesian inference. Moreover, we have shown that incorporating functional repulsion between ensemble members can improve the quality of the estimated uncertainties on simple synthetic examples and OOD detection on real-world data and can approach the true Bayesian posterior more closely.

In future work, it will be interesting to study the impact of the Jacobian in the fWGD update and its implications on the Liouville equation in more detail, also compared to other neural network Jacobian methods, such as neural tangent kernels [37] and generalized Gauss-Newton approximations [35]. Moreover, it would be interesting to derive explicit convergence bounds for our proposed method and compare them to the existing bounds for SVGD [40].

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Supplementary Material: Repulsive Deep Ensembles are Bayesian

A Non-identifiable neural networks

Deep neural networks are parametric models able to learn complex non-linear functions from few training instances and thus can be deployed to solve many tasks. Their overparameterized architecture, characterized by a number of parameters far larger than that of training data points, enables them to retain entire datasets even with random labels \[84\]. Even more, this overparameterized regime makes neural network approximations of a given function not unique in the sense that multiple configurations of weights might lead to the same function. Indeed, the output of a feed forward neural network given some fixed input remains unchanged under a set of transformations. For instance, certain weight permutations and sign flips in MLPs leave the output unchanged \[9\]. The invariance of predictions and therefore of parameterized functions under a given weight transformation translates to invariance of the likelihood function. This effect is commonly denoted as non-identifiability of neural networks \[68\]. More in detail, let \( g : (x, w) \mapsto f(x; w) \) be the map that maps a data point \( x \in \mathcal{X} \) and a weight vector \( w \in \mathbb{R}^d \) to the corresponding neural network output and denote \( f_i := f(x; w_i) \) the output with a certain configuration of weights \( w_i \). Then for any non-identifiable pair \( \{w_i, w_j\} \subseteq \mathbb{R}^d \) and \( f_i, f_j \in \mathcal{F} \) their respective functions:

\[
    f_i = f_j \implies p(w_i | \mathcal{D}) = p(w_j | \mathcal{D}) \implies w_i = w_j.
\]

Strictly speaking, the map \( g : \mathcal{X} \times \mathcal{W} \to \mathcal{F} \) is not injective (many to one). Denoting by \( T \) the class of transformations under which a neural network is non-identifiable in the weights space, it is always possible to identify a cone \( K \subseteq \mathbb{R}^d \) such that for any parameter configuration \( w \) there exist a point \( \eta \in K \) and a transformation \( \tau \in T \) for which it holds that \( \tau(\eta) = w \). This means that every parameter configuration has an equivalent on the subset given by the cone \[30\]. Modern neural networks containing convolutional and max-pooling layers have even more symmetries than MLPs \[4\]. Given that in practice we cannot constraint the support of the posterior distribution to be the cone of identifiable parameter configurations and given that the likelihood model is also invariant under those transformations that do not change the function, the posterior landscape includes multiple equally likely modes that despite their different positions represent the same function. It is important to notice that this is always true for the likelihood but not for the posterior. Indeed, for the modes to be equally likely, the prior should also be invariant under those transformations, condition that is in general not true. Nevertheless, the fact that there are multiple modes of the posterior parametrizing for the same function remains true but they might be arbitrarily re-scaled by the prior\[1\]. As we will see in the following, this redundancy of the posterior is problematic when we want to obtain samples from it. Moreover it is interesting to notice how this issue disappears when the Bayesian inference is considered in the space of functions instead of weights. In this case, indeed, every optimal function has a unique mode in the landscape of the posterior and redundancy is not present:

\[
    f_i \neq f_j \implies p(f_i | \mathcal{D}) \neq p(f_j | \mathcal{D}).
\]

In spite of that, performing inference over distributions of functions is prohibitive in practice due to the infinite dimensionality of the space in consideration. Only in very limited cases like the one of Gaussian Process, Bayesian inference is exact. Interestingly Neural network model in the limit of infinite width are Gaussian processes with a particular choice of the kernel determined by the architecture \[44\ [81\ [60\]. In this limit Bayesian inference over functions can be performed analytically.

B Quantify functional diversity

As illustrated in Section \[2\], in the Bayesian context, predictions are made by doing a Monte-Carlo estimation of the BMA. Functional diversity, and so the diversity in the hypotheses taken in consideration when performing the estimation, determines the epistemic uncertainty and the confidence over the predictions. Importantly, the epistemic uncertainty allows for the quantification

\footnote{Note that for the fully factorized Gaussian prior commonly adopted, the invariance under permutations is true}
of the likelihood of a test point to belong to the same distribution from which the training data points were sampled \[65]. Following this, the uncertainty can be used for the problem of Out-of-distribution (OOD) detection \[11] that is often linked to the ability of a model to "know what it doesn’t know". A common way used in the literature to quantify the uncertainty is the Entropy \[\mathcal{H}\] of the predictive distribution:

\[
\mathcal{H}\{p(y' | x', D)\} = - \sum_y p(y' | x', D) \log p(y' | x', D).
\] (21)

Nevertheless, it has been argued in recent works \[55\] that this is not a good measure of uncertainty because it does not allow for a disentanglement of epistemic and aleatoric uncertainty. Intuitively, we would like the predictive distribution of an OOD point to be uniform over the different classes. However, using the entropy and so the average prediction in the BMA, we are not able to distinguish between the case in which all the hypotheses disagree very confidently due to the epistemic uncertainty or are equally not confident due to the aleatoric uncertainty. To overcome this limitation, we can use a direct measure of the model disagreement computed as:

\[
\mathcal{M}D^2(y'; x', D) = \int_w [p(y' | x', w) - p(y' | x', D)]^2 p(w | D) dw.
\] (22)

It is easy to see how the quantity in Eq. (22), measuring the deviation from the average prediction is zero when all models agree on the prediction. The latter can be the case of a training point where all hypotheses are confident or a noisy point where all models “don’t know” the class and are equally uncertain. On the other side the model disagreement will be greater the zero the more the model disagrees on a prediction representing like this the epistemic uncertainty. To obtain a scalar quantity out of Eq. (22) we can consider the expectation over the output space of \( y \):

\[
\mathcal{M}D^2(x') = \mathbb{E}_y \left[ \int_w [p(y' | x', w) - p(y' | x', D)]^2 p(w | D) dw \right].
\] (23)

### C Functional derivative of the KL divergence

In this section, we show the derivation of the functional derivative for the KL divergence functional. We start with some preliminary definitions.

Given a manifold \( \mathcal{M} \) embedded in \( \mathbb{R}^d \), let \( F[\rho] \) be a functional, i.e. a mapping from a normed linear space of function (Banach space) \( \mathcal{F} = \{ \rho(x) : x \in \mathcal{M}\} \) to the field of real numbers \( F : \mathcal{F} \rightarrow \mathbb{R} \). The functional derivative \( \delta F[\rho]/\delta \rho(x) \) represents the variation of value of the functional if the function \( \rho(x) \) is changed.

**Definition 2 (Functional derivative).** Given a manifold \( \mathcal{M} \) and a functional \( F : \mathcal{F} \rightarrow \mathbb{R} \) with respect to \( \rho \) is defined as:

\[
\int \frac{\delta F}{\delta \rho(x)} \phi(x) dx = \lim_{\epsilon \rightarrow 0} \frac{F[\rho(x) + \epsilon \phi(x)] - F[\rho(x)]}{\epsilon} = \frac{d}{d\epsilon} F[\rho(x) + \epsilon \phi(x)] \big|_{\epsilon=0}
\] (24)

for every smooth \( \phi \).

**Definition 3 (KL divergence).** Given \( \rho \) and \( \pi \) two probability densities on \( \mathcal{M} \), the KL-divergence is defined as:

\[
D_{KL}(\rho, \pi) = \int_{\mathcal{M}} (\log \rho(x) - \log \pi(x)) \rho(x) \ dx.
\] (25)

**Proposition 1.** The functional derivative of the KL divergence in Eq. \[25\] is:

\[
\frac{\delta D_{KL}}{\delta \rho(x)} = \log \frac{\rho(x)}{\pi(x)} + 1
\] (26)

\footnote{The continuous case is analogous using the differential entropy}
We see that the metric tensor of the manifold acts like a perturbation of the gradient. Secondly, we can rewrite the integrals in the previous equation as:

\[
\int \frac{\partial D_{KL}}{\partial \phi(x)} \, d\phi(x) = \frac{d}{d\epsilon} D_{KL}(\rho + \epsilon \phi, \pi) \bigg|_{\epsilon = 0}
\]

\[
= \int \frac{d}{d\epsilon} \left[ (\rho(x) + \epsilon \phi(x)) \log \frac{(\rho(x) + \epsilon \phi(x))}{\pi(x)} \right] \bigg|_{\epsilon = 0} \, dx
\]

\[
= \int \left[ \phi(x) \log \frac{(\rho(x) + \epsilon \phi(x))}{\pi(x)} + \frac{d(\rho(x) + \epsilon \phi(x))}{d\epsilon} \right] \bigg|_{\epsilon = 0} \, dx
\]

\[
= \int \left[ \log \frac{\rho(x)}{\pi(x)} + 1 \right] \phi(x) \, dx
\]

\[\square\]

## D SVGD as Wasserstein gradient flow

To understand the connection between the Wasserstein gradient flow and the SVGD method, we first need to introduce the concept of gradient flow on a manifold. Let’s consider a Riemannian manifold \(\mathcal{M}\) equipped with the metric tensor \(G(x)\) defined for all \(x \in \mathcal{M}\). Here, \(G(x) : T_x \mathcal{M} \times T_y \mathcal{M} \rightarrow \mathbb{R}\) defines a smoothly varying local inner product on the tangent space at each point of the manifold \(x\). For manifolds over \(\mathbb{R}^d\), the metric tensor is a positive definite matrix that defines local distances for infinitesimal displacements \(d(x, x + dx) = \sqrt{dx \cdot G(x) dx}\). Considering a functional \(J : \mathcal{M} \rightarrow \mathbb{R}\), the evolution in Eq. (9) and so the gradient flow, becomes:

\[
\frac{dx}{dt} = -G(x)^{-1} \nabla J(x).
\]

We see that the metric tensor of the manifold acts like a perturbation of the gradient. Secondly, we need to reformulate the update equation in [6] in continuous time, as the following ODE:

\[
\frac{dx_i}{dt} = \frac{1}{n} \sum_{j=1}^{n} \left[ k(x_j, x_i) \nabla x_j \log p(x_j) + \nabla x_j k(x_j, x_i) \right]
\]

that in the mean field limit \(n \rightarrow \infty\) becomes:

\[
\frac{dx}{dt} = \int \left[ k(x', x) \nabla_x' \log \pi(x') + \nabla_x' k(x', x) \right] \rho(x') \, dx'
\]

\[
= \int k(x', x) \nabla_x' \log \pi(x') \rho(x') \, dx' + \int \nabla_x k(x', x) \rho(x') \, dx'.
\]

Due to the boundary condition of a Kernel in the Stein class (see Liu et al. [52] for more details), without loss of generality, we can rewrite the integrals in the previous equation as:

\[
\frac{dx}{dt} = \int k(x', x) \nabla_x' \log \pi(x') \rho(x') \, dx' + \int \nabla_x k(x', x) \rho(x') \, dx' \bigg|_{||x'|| \rightarrow \infty}
\]

\[= 0\]

and notice how the second and the third terms are the result of an integration by parts:

\[
\frac{dx}{dt} = \int k(x', x) \nabla_x' \log \pi(x') \rho(x') \, dx' - \int k(x', x) \nabla_x' \rho(x') \, dx'
\]

\[
= \int k(x', x) \nabla_x' \log \pi(x') \rho(x') \, dx' - \int k(x', x) \nabla_x' \log \rho(x') \rho(x') \, dx'
\]

\[
= \int k(x', x) \nabla_x' [ \log \pi(x') - \log \rho(x')] \rho(x') \, dx'
\]

\[
= \mathbb{E}_{x' \sim \rho} [k(x', x) \nabla_x (\log \pi(x') - \log \rho(x'))]
\]

which is exactly the functional derivative of the KL divergence in [11] approximated in the RKHS of the kernel [16, 50]. Following this, the Liouville equation of the SVGD dynamics in the mean field
\[
\frac{\partial \rho(x)}{\partial t} = -\nabla \cdot \left( \rho(x) \int k(x', x) \nabla_{x'} \left[ \log \pi(x') - \log \rho(x') \right] \rho(x') dx' \right) 
\]

(32)

Defining the linear operator \( (K_\rho \phi)(x) := \mathbb{E}_{x' \sim \rho}[k(x', x) \phi(x')] \) the ODE in Eq. (31) becomes:

\[
\frac{dx}{dt} = K_\rho \nabla x' \left( \log \pi(x') - \log \rho(x') \right). 
\]

(33)

And the Liouville equation describing the evolution of the empirical measure of the particles:

\[
\frac{\partial \rho}{\partial t} = \nabla \cdot \left( \rho(x) K_\rho \nabla x' \delta D_{KL}(\rho, \pi) \right). 
\]

(34)

Notice how the only solution of the previous equation is \( \rho = \pi \). If we now compare Eq. (34) and Eq. (11) we can see how they only differ for the application of the operator \( K_\rho \); moreover the operator seems to act like a perturbation of the gradient and defines a local geometry in the same way the Riemannian metric tensor \( G(x) \) is doing in 28. The intuition suggest then that the SVGD can be reinterpreted as a gradient flow in the Wasserstein space under a particular Stein geometry [16] induced on the manifold by the kernel and where \( K_\rho \) is the metric.

## E Kernel density estimation

Kernel Density Estimation (KDE) is a nonparametric density estimation technique [66]. When an RBF kernel is used, it can be thought as a smoothed version of the empirical data distribution. Given some training datapoints \( D = \{x_1, ..., x_n\} \) with \( x_i \sim p(x) \) and \( x \in \mathbb{R}^D \) their empirical distribution \( q_0(x) \) is a mixture of \( n \) Dirac deltas centered at each training data:

\[
q_0(x) = \frac{1}{N} \sum_{i=1}^{N} \delta(x - x_i). 
\]

(35)

We can now smooth the latter by replacing each delta with an RBF kernel:

\[
k_\epsilon(x, x_i) = \frac{1}{h} \exp \left( -\frac{||x - x_i||^2}{h} \right) 
\]

(36)

where \( h > 0 \). The kernel density estimator is then defined as:

\[
q_h(x) = \frac{1}{N} \sum_{i=1}^{N} k_h(x, x_i) 
\]

(37)

In the limit of \( h \to 0 \) and \( N \to \infty \) the kernel density estimator is unbiased: it is equal to the true density. Indeed \( k_{h \to 0}(x, x_i) \to \delta(x - x_i) \) and so \( q_{h \to 0}(x) \to q_0(x) \) and:

\[
\lim_{N \to \infty} q_0(x) = \lim_{N \to \infty} \frac{1}{N} \sum_{i=1}^{N} \delta(x - x_i) 
= \mathbb{E}_{p(x')} \left[ \delta(x - x') \right] 
= \int_{\mathbb{R}^D} \delta(x - x') p(x') dx' = p(x) 
\]

(38)
Figure F.1: Neal’s funnel. The SGE-WGD and SVGD again fit the distribution best.

F Additional experiments

In this section, we report the additional results for the different methods when sampling from the Funnel distribution \( p(x, y) = \mathcal{N}(y | \mu = 0, \sigma = 3) \mathcal{N}(x | 0, \exp(y/2)) \), the results are reported in Figure F.1.

G Implementation details

In this section, we report details on our implementation in the experiments we performed. The code is partially based on von Oswald et al. [73] and can be found at [https://github.com/ratschlab/repulsive_ensembles](https://github.com/ratschlab/repulsive_ensembles). All the experiments were performed on the ETH Leonhard scientific compute cluster with NVIDIA GTX 1080 Ti and took roughly 150 GPU hours.

G.1 Sampling from synthetic distributions

**Single Gaussian:** we created a two-dimensional Gaussian distribution with mean \( \mu = (-0.6871, 0.8010) \) and covariance \( \Sigma = \begin{pmatrix} 1.130 & 0.826 \\ 0.826 & 3.389 \end{pmatrix} \). We used a normal initialization with zero mean and standard deviation \( \sigma^2 = 3 \). We sampled 100 initial particles and optimized them for 5000 iterations using Adam with a fixed learning rate of 0.1. The kernel bandwidth was estimated using the median heuristic for all methods. For the SSGE we used all the eigenvalues. The random seed was fixed to 42.

**Funnel:** the target distribution followed the density \( p(x, y) = \mathcal{N}(y | \mu = 0, \sigma = 3) \mathcal{N}(x | 0, \exp(y/2)) \). We used a normal initialization with zero mean and standard deviation \( \sigma^2 = 3 \). We sampled 500 initial particles and optimized them for 2000 iterations using Adam with a fixed learning rate of 0.1. The kernel bandwidth was fixed to 0.5 for all methods. For the SSGE we used all the eigenvalues. The random seed was fixed to 42.

G.2 1D regression

We generated the training data by sampling 45 points from \( x_i \sim \text{Uniform}(1.5, 2.5) \) and 45 from \( x_i \sim \text{Uniform}(4.5, 6.0) \). The output \( y_i \) for a given \( x_i \) is then modeled following \( y_i = x_i \sin(x_i) + \epsilon_i \) with \( \epsilon_i \sim \mathcal{N}(0, 0.25) \). We use a standard Gaussian likelihood and standard normal prior \( \mathcal{N}(0, I) \). The model is a feed-forward neural network with 2 hidden layers and 50 hidden units with ReLU activation function. We use 50 particles initialized with random samples from the prior and optimize them using Adam [39] with 15000 gradient steps, a learning rate of 0.01 and batchsize 64. The kernel
bandwidth is estimated using the median heuristic. We tested the models on 100 uniformly distributed points in the interval \([0, 7]\). The random seed was fixed to 42.

G.3 2D classification

We generate 200 training data points sampled from a mixture of 5 Gaussians with means equidistant on a ring of radius 5 and unitary covariance. The model is a feed-forward neural network with 2 hidden layers and 50 hidden units with ReLU activation function. We use a softmax likelihood and standard normal prior \(\mathcal{N}(0, I)\). We use 100 particles initialized with random samples from the prior and optimize them using Adam \([39]\) with 10,000 gradient steps, a learning rate of 0.001 and batchsize 64. The kernel bandwidth is estimated using the median heuristic. The random seed was fixed to 42.

G.4 Classification on FashionMNIST

On this dataset, we use a feed-forward neural network with 3 hidden layers and 100 hidden units with ReLU activation function. We use a softmax likelihood and standard normal prior \(\mathcal{N}(0, I)\). We use 50 particles initialized with random samples from the prior and optimize them using Adam \([39]\) for 50000 steps, a learning rate was 0.001 for sge-WGD,kde-WG,ssge-WGD and 0.0025 for kde-fWGD,ssge-fWGD,sge-fWGD, Deep ensemble, fSVGD, SVGD, and batchsize was 256. The kernel bandwidth is estimated using the median heuristic for all different methods. The learning rates were searched over the following values \((1e^{-4}, 5e^{-4}, 1e^{-3}, 5e^{-3}, 25e^{-4})\) we tested for 50000 and 30000 total number of iterations, 50 and 100 particles and batchsize 256 and 128. For the hyper-deep ensemble, we implemented it on the L2 parameter by first running a random search to select a set of 5 top values in the range \([1e^{-3}, 1e3]\), which we subsequently used to create an ensemble with the same number of members as the other methods. All results in Table 1 are averaged over the following random seeds \((38, 39, 40, 41, 42)\).

G.5 Classification on CIFAR-10

On this dataset, we used a residual network (ResNet32) with ReLU activation function. We use a softmax likelihood and standard normal prior \(\mathcal{N}(0, 0.1I)\). We use 20 particles initialized using He initialization \([28]\) and optimize them using Adam \([39]\) for 50000 steps, a learning rate was 0.00025 for sge-fWGD,kde-fWGD,ssge-fWGD,fSVGD and 0.0005 for kde-WGD,ssge-WGD,sge-fWGD, Deep ensemble and SVGD, and batchsize was 128. The kernel bandwidth is estimated using the median heuristic for all different methods. The learning rates were searched over the following values \((1e^{-4}, 5e^{-4}, 1e^{-3}, 5e^{-3}, 25e^{-4}, 5e^{-5})\) we tested for 50000 and 30000 total number of iterations, 20 and 10 particles. For the hyper-deep ensemble, we implemented it on the L2 parameter by first running a random search to select a set of 5 top values in the range \([1e^{-3}, 1e3]\), which we subsequently used to create an ensemble with the same number of members as the other methods. All results in Table 1 are averaged over the following random seeds \((38, 39, 40, 41, 42)\).