Gradient Estimators for Implicit Models

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Abstract

Implicit models, which allow for the generation of samples but not for point-wise evaluation of probabilities, are omnipresent in real world problems tackled by machine learning and a hot topic of current research. Some examples include data simulators that are widely used in engineering and scientific research, generative adversarial networks (GANs) for image synthesis, and hot-off-the-press approximate inference techniques relying on implicit distributions. The majority of existing approaches to learning implicit models rely on approximating the intractable distribution or optimisation objective for gradient-based optimisation, which is liable to produce inaccurate updates and thus poor models. This paper alleviates the need for such approximations by proposing the Stein gradient estimator, which directly estimates the score function of the implicitly defined distribution. The efficacy of the proposed estimator is empirically demonstrated by examples that include meta-learning for approximate inference, and entropy regularised GANs that provide improved sample diversities.

1 Introduction

Modelling is fundamental to the success of technological innovations for artificial intelligence. A powerful model learns a useful representation of the observations for a specified prediction task, and generalises to unknown instances that follow similar generative mechanics. A well established area of machine learning research focuses on developing prescribed probabilistic models [8], where learning is based on evaluating the probability of observations under the model. Implicit probabilistic models, on the other hand, are defined by a stochastic procedure that allows for direct generation of samples, but not for the evaluation of model probabilities. These are omnipresent in scientific and engineering research involving data analysis, for instance ecology, climate science and geography, where simulators are used to fit real-world observations to produce forecasting results. Within the machine learning community there is a recent interest in a specific type of implicit models, generative adversarial networks (GANs) [10], which has been shown to be one of the most successful approaches to image and text generation [29, 49, 2, 5]. Very recently, implicit distributions have also been considered as approximate posterior distributions for Bayesian inference, e.g. see [22, 47, 19, 17, 26, 13, 20, 43]. These examples demonstrate the superior flexibility of implicit models, which provide highly expressive means of modelling complex data structures.

Whilst prescribed probabilistic models can be learned by standard (approximate) maximum likelihood or Bayesian inference, implicit probabilistic models require substantially more severe approximations due to the intractability of the model distribution. Many existing approaches first approximate the model distribution or optimisation objective function and then use those approximations to learn the associated parameters. However, for any finite number of data points there exists an infinite number of functions, with arbitrarily diverse gradients, that can approximate perfectly the objective function, and thus optimising such approximations can lead to unstable training and poor results. Recent research on GANs, where the issue is highly prevalent, suggest that restricting the representational power of the discriminator is effective in stabilising training (e.g. see [21]). However, such restrictions
often introduce undesirable biases, responsible for problems such as mode collapse in the context of
GANs, and the underestimation of uncertainty in variational inference methods [44].

In this paper we explore approximating the score function as an alternative method for training
implicit models. An accurate approximation of the score function then allows the application of many
well-studied algorithms, such as maximum likelihood, maximum entropy estimation, variational
inference and gradient-based MCMC, to implicit models. Concretely, our contributions include:

- the Stein gradient estimator, a novel generalisation of the score matching estimator [14],
  with both parametric and non-parametric versions;
- a comparison of the proposed estimator with the score matching and the KDE plug-in
  estimators on performing gradient-free MCMC, meta-learning of approximate posterior
  samplers for Bayesian neural networks, and entropy based regularisation of GANs.

2 Learning implicit probabilistic models

Given a dataset \( \mathcal{D} \) containing i.i.d. samples we would like to learn a probabilistic model \( p(x) \) for the
underlying data distribution \( p_D(x) \). In the case of implicit models, \( p(x) \) is defined by a generative
process. For example, to generate images, one might define a generative model \( p(x) \) that consists of
sampling randomly a latent variable \( z \sim p_0(z) \) and then defining \( x = f_\theta(z) \). Here \( f \) is a function
parametrised by \( \theta \), usually a deep neural network or a simulator. We assume \( f \) to be differentiable
w.r.t. \( \theta \). An extension to this scenario is presented by conditional implicit models, where the addition
of a supervision signal \( y \), such as an image label, allows us to define a conditional distribution
\( p(x|y) \) implicitly by the transformation \( x = f_\theta(z, y) \). A related methodology, wild variational
inference [22] [19] assumes a tractable joint density \( p(x, z) \) but uses implicit proposal distributions
to approximate an intractable exact posterior \( p(z|x) \). Here the approximate posterior \( q(z|x) \) can
likewise be represented by a deep neural network, but also by a truncated Markov chain, such as that
given by Langevin dynamics with learnable step-size.

Though providing extreme flexibility and expressive power, the intractability of density evaluation
also brings serious optimisation issues for implicit models. This is because many learning algorithms,
e.g. maximum likelihood estimation (MLE), rely on minimising a distance/divergence/discrepancy
measure \( D[p||p_D] \), which often requires evaluating the model density (c.f. [30] [22]). Thus good
approximations to the optimisation procedure are the key to learning implicit models that can describe
complex data structures. In the context of GANs, the Jensen-Shannon divergence is approximated by
a variational lower-bound represented by a discriminator [3] [10]. Related work for wild variational
inference [19] [26] [13] [43] uses a GAN-based technique to construct a density ratio estimator for
\( q/p_0 \) [41] [42] [45] [27] and then approximate the KL-divergence term in the variational lower-bound:

\[
\mathcal{L}_{VI}(q) = E_q [\log p(x|z)] - KL[q(z|x)||p_0(z)].
\]

In addition, [19] and [26] exploit the additive structure of the KL-divergence and suggest discriminating
between \( q \) and an auxiliary distribution that is close to \( q \), making the density ratio estimation
more accurate. Nevertheless all these algorithms involve a minimax optimisation, and the current
practice of gradient-based optimisation is notorious for unstable training.

The stabilisation of GAN training is itself a recent trend of related research (e.g. [33] [2]). However, as
the gradient-based optimisation only interacts with gradients, there is no need to use a discriminator
if an accurate approximation to the intractable gradients could be obtained. For example, notice that
the variational lower-bound can be rewritten as

\[
\mathcal{L}_{VI}(q) = E_q [\log p(x|z)] + H[q_\phi(z|x)],
\]

the gradient of the variational parameters \( \phi \) can be computed by a sum of the path gradient of the first
term (i.e. \( E_\epsilon [\nabla_f \log q(f(\epsilon, x)|x)\nabla_\phi f(\epsilon, x)] \)) and the gradient of the entropy term \( \nabla_\phi H[q(z|x)] \). Expanding the latter, we have

\[
\nabla_\phi H[q(z|x)] = E_\epsilon [\nabla_f \log q(f(\epsilon, x)|x)^T \nabla_\phi f(\epsilon, x)] + E_\epsilon [\nabla_\phi \log q_\phi(z|x)],
\]

in which the second term on the RHS is zero [32]. As we typically assume the tractability of \( \nabla_\phi f \), an
accurate approximation to \( \nabla_\phi f \) would remove the requirement of discriminators, speed-up
the learning and obtain potentially a better model. Many gradient approximation techniques exist
[39] [9] [50] [7], and in particular, we will review score matching methods [14] in more detail in the
next section, and motivate the main contribution of the paper.
3 Gradient approximation with the Stein gradient estimator

In this section we propose the Stein gradient estimator as a novel generalisation of the score matching gradient estimator. Before presenting it we first set-up the notations. Column vectors and matrices are boldfaced. The random variable under consideration is \( x \in \mathcal{X} \) with \( \mathcal{X} = \mathbb{R}^{d \times 1} \) if not specifically mentioned. To avoid misleading notation we use the distribution \( q(x) \) to derive the gradient approximations for general cases. As Monte Carlo methods are heavily used for implicit models, in the rest of the paper we mainly consider approximating the gradient \( \hat{q}(x^k) := \nabla_{x^k} \log q(x^k) \) for \( x^k \sim q(x), k = 1, ..., K \). We use \( x_j^i \) to denote the \( j \)th element of the \( i \)th sample \( x^i \). We also denote the matrix form of the collected gradients as \( G := (\nabla_{x^1} \log q(x^1), \cdots, \nabla_{x^K} \log q(x^K))^T \in \mathbb{R}^{K \times d} \), and its approximation \( \hat{G} := (\hat{g}(x^1), \cdots, \hat{g}(x^K))^T \) with \( \hat{g}(x^k) = \nabla_{x^k} \log \hat{q}(x^k) \) for some \( \hat{q}(x) \).

3.1 KDE gradient estimator: plug-in estimator with kernel density estimation

A naive approach for gradient approximation would first estimate the intractable density \( \hat{q}(x) \approx q(x) \) (up to a constant), then approximate the exact gradient by \( \nabla_x \log \hat{q}(x) \approx \nabla_x \log q(x) \). One may favour complex density approximation schemes for better accuracy, but here we focus on “quick and dirty” approximations as the gradient approximation is repeatedly required for the optimisation procedure. Specifically we consider kernel density estimation (KDE) with the reproducing kernel \( \mathcal{K}(x, \cdot) \) of an RKHS \( \mathcal{H} \), i.e. \( \hat{q}(x) = \frac{1}{K} \sum_{k=1}^{K} \mathcal{K}(x, x^k) \times C \). Simple derivations \([36]\) reveal the KDE gradient estimator as

\[
G_{ij}^{\text{KDE}} = \sum_{k=1}^{K} \frac{\nabla_{x^k} \mathcal{K}(x^i, x^k)}{\sum_{k=1}^{K} \mathcal{K}(x^i, x^k)}. \tag{4}
\]

3.2 Score matching gradient estimator

The KDE estimator performs indirect approximation of the gradient via density estimation, which can be inaccurate. An alternative approach directly approximates the gradient \( \nabla_x \log q(x) \) by minimising the expected \( l_2 \) error \( F(\hat{g}) := \mathbb{E}_q [||\hat{g}(x) - \nabla_x \log q(x)||_2^2] \) w.r.t. the approximation \( \hat{g}(x) = (\hat{g}_1(x), \cdots, \hat{g}_d(x))^T \). It has been shown in \([14]\) that the objective can be reformulated as

\[
F(\hat{g}) = \mathbb{E}_q [||\hat{g}(x)||_2^2 + 2 \langle \nabla, \hat{g}(x) \rangle] + C, \quad \langle \nabla, \hat{g}(x) \rangle = \sum_{j=1}^{d} \nabla_{x_j} \hat{g}_j(x). \tag{5}
\]

The key insight here is the usage of integration by parts: after expanding the \( l_2 \) loss objective, the cross term can be rewritten as \( \mathbb{E}_q [\langle \hat{g}(x)^T \nabla_x \log q(x) \rangle] = -\mathbb{E}_q [\langle \nabla, \hat{g}(x) \rangle] \), if assuming the boundary condition: \( q(x) \hat{g}(x) \bigg|_{\partial \mathcal{X}} = 0 \), or \( \lim_{x \to \infty} q(x) \hat{g}(x) = 0 \) if \( \mathcal{X} = \mathbb{R}^d \). This condition holds for many distributions, e.g. those with Gaussian-like tails. The optimum of \( (5) \) is referred as the score matching estimator. \([34]\) and \([40]\) derived a parametric solution by first approximating the log density up to a constant with the RBF kernel \( \mathcal{K}(x, x^r) := \exp \left[ -\frac{1}{\alpha^2} ||x - x^r||_2^2 \right] \) (i.e. \( \log \hat{q}(x) := \sum_{k=1}^{K} \alpha_k \mathcal{K}(x, x^k) + C \)), then minimising \( (5) \) to obtain the coefficients \( \alpha_k \). A slightly different approach \([35]\) proposes an estimator for \( \nabla_x q(x) \), by minimising the \( l_2 \) error \( \int (\hat{g}_j(x) - \nabla_{x_j} q(x))^2 dx \) and removing explicit calculations of \( \nabla_x q(x) \) in an analogous way as to derive \( (5) \).

As a side note, score matching can also be used to learn the parameters of an unnormalised density. In this case the target distribution \( q \) would be the data distribution and \( \hat{q} \) is often a Boltzmann distribution with intractable partition function. As a parameter estimation technique, score matching is also related to contrastive divergence \([12]\), pseudo likelihood estimation \([15]\), and denoising auto-encoders \([46]\). Generalisations of score matching methods are also presented in \([24]\) \([25]\).

3.3 Stein gradient estimator: inverting Stein’s identity

Recall the derivation of the score matching objective \( (5) \) that uses integration by parts and the boundary condition. Using the same idea Stein’s identity \([37]\) can also be derived. Can we directly exploit Stein’s identity to obtain an estimator of the gradients? In this section we investigate the multivariate version of Stein’s identity \([39]\) to derive a new gradient estimator that we call the Stein
gradient estimator. Let $h : \mathbb{R}^{d \times 1} \rightarrow \mathbb{R}^{d \times 1}$ be a differentiable multivariate test function satisfying the boundary condition, which maps $x$ to a column vector $h(x) = [h_1(x), h_2(x), \ldots, h_d(x)]^T$. Now we introduce the multivariate Stein’s identity \cite{38}

$$E_q[h(x) \nabla_x \log q(x)^T + \nabla_x h(x)] = 0,$$

in which the gradient matrix term $\nabla_x h(x) = (\nabla_x h_1(x), \ldots, \nabla_x h_d(x))^T \in \mathbb{R}^{d \times d}$. We further approximate the above with Monte Carlo (MC):

$$\frac{1}{K} \sum_{k=1}^{K} -h(x^k) \nabla_{x^k} \log q(x^k)^T + \text{err} = \frac{1}{K} \sum_{k=1}^{K} \nabla_{x^k} h(x^k), \quad x^k \sim q(x^k),$$

with $\text{err} \in \mathbb{R}^{d \times d}$ the random error due to MC approximation, which has mean 0 and vanishes as $K \rightarrow +\infty$. Now by temporarily denoting $H = (h(x^1), \ldots, h(x^K)) \in \mathbb{R}^{d \times K}$, $\nabla_x h = \frac{1}{K} \sum_{k=1}^{K} \nabla_{x^k} h(x^k) \in \mathbb{R}^{d \times d}$, equation (7) can be rewritten as $-\frac{1}{K} H G + \text{err} = \nabla_x h$. Thus we consider a ridge regression method (i.e. adding an $l_2$ regulariser) to estimate $G$:

$$G_V^{\text{Stein}} := \arg \min_{G \in \mathbb{R}^{K \times d}} \|\nabla_x h + \frac{1}{K} H G\|^2_F + \frac{\eta}{2K^2} \|G\|^2_F,$$

with $\| \cdot \|_F$ the Frobenius norm of a matrix and $\eta \geq 0$. Simple calculation shows that

$$G_V^{\text{Stein}} = -(K + \eta I)^{-1} \langle \nabla, K \rangle,$$

where $K := H^T H$, $K_{ij} = K(x^i, x^j) := h(x^i)^T h(x^j)$, and $\langle \nabla, K \rangle := K H^T \nabla_x h$, $\langle \nabla, K \rangle_{ij} = \sum_{k=1}^{K} \nabla_{x^k} K(x^i, x^j)$. One can show that the RBF kernel satisfies Stein’s identity \cite{23}. In this case $h(x) = K(x, \cdot), d' = +\infty$ and by the reproducing kernel property, $h(x)^T h(x') = \langle K(x, \cdot), K(x', \cdot) \rangle_H = K(x, x')$. Interestingly for translation invariant kernels $K(x, x') = K(x-x')$ the KDE gradient estimator \cite{4} can be rewritten as $G^{\text{KDE}} = -\text{diag}(K) K^{-1} \langle \nabla, K \rangle$. Thus in this case the Stein gradient estimator can be viewed as a "smoothed" version of the KDE gradient estimator.

### 3.4 Stein gradient estimator minimises the kernelised Stein discrepancy

So far we have presented the Stein gradient estimator and compared it to the KDE estimator. In this section we derive the Stein gradient estimator again but from a divergence/discrepancy minimisation perspective. Stein’s method also provides a tool for checking if two distributions are identical. If the test function set $\mathcal{H}$ is sufficiently rich, then one can define a Stein discrepancy measure by

$$S(q, \hat{q}) := \sup_{h \in \mathcal{H}} E_q \left[ \nabla_x \log \hat{q}(x)^T h(x) + \langle \nabla, h, \rangle \right],$$

see \cite{11} for an example derivation. When $\mathcal{H}$ is defined as a unit ball in an RKHS induced by a kernel $K(x, \cdot), \cite{23}$ and \cite{6} showed that the supremum in (10) can be analytically obtained as (with $\mathbb{K}_{x'x}$ shorthand for $K(x, x')$): $S^2(q, \hat{q}) = E_{x, x' \sim q} \left[ (\hat{g}(x) - g(x))^T \mathbb{K}_{x'x} (\hat{g}(x') - g(x')) \right]$, which is also named kernelised Stein discrepancy (KSD). For universal kernels satisfying the boundary condition, KSD is indeed a discrepancy measure: $S^2(q, \hat{q}) = 0 \Leftrightarrow q = \hat{q}$ \cite{8}. Furthermore, if the kernel is twice differentiable, then using the same technique as to derive \cite{5} one can compute KSD by

$$S^2(q, \hat{q}) = E_{x, x' \sim q} \left[ \hat{g}(x)^T \mathbb{K}_{x'x} \hat{g}(x') + \hat{g}(x)^T \nabla_x \mathbb{K}_{x'x} \hat{g}(x') + \nabla_x \mathbb{K}_{x'x} \hat{g}(x') + \text{Tr}(\nabla_x \mathbb{K}_{x'x} \hat{g}(x')) \right].$$

In practice KSD is estimated with samples $\{x^k\}_{k=1}^{K} \sim q$, and simple derivations show that the $\text{V}$-statistic of KSD can be reformulated as $S^2_V(q, \hat{q}) = \frac{1}{K} \text{Tr}(\hat{G}^T K \hat{G} + 2 \hat{G}^T (\nabla, K)) + C$. Thus the $l_2$ error in \cite{6} is equivalent to the $\text{V}$-statistic of KSD if $h(x) = K(x, \cdot)$, and we have the following: \textbf{Theorem 1.} $G_V^{\text{Stein}}$ is the solution of the following KSD $\text{V}$-statistic minimisation problem

$$G_V^{\text{Stein}} = \arg \min_{G \in \mathbb{R}^{K \times d}} S^2_V(q, \hat{q}) + \frac{\eta}{2K^2} \|G\|^2_F.$$

The score matching objective $\mathcal{F}(q, \hat{q}) = E_q \left[ \|\nabla_x \log \hat{q}(x) - \nabla_x \log q(x)\|^2 \right]$ is also called Fisher divergence \cite{16} which is a special case of KSD by selecting $K(x, x') = \delta_{x=x'}$. Thus the Stein gradient estimator can be viewed as a generalisation of the score matching estimator. Importantly
the proposed estimator is non-parametric in that it directly optimises over functions evaluated at locations \( \{ x_k \}_{k=1}^K \), which removes the approximation error due to the use of restricted family of parametric approximations. Conversely, it is difficult to perform direct estimation by minimising the Fisher divergence as it involves computing second-order gradient terms.

Though providing more accurate approximations, the non-parametric estimator has no predictive power. The corresponding \( \hat{q} \) for the non-parametric estimator is not unique, thus it cannot approximate the gradient evaluated at unseen data. For tasks that require predicting gradient functions at future observations, one can also minimise KSD using parametric approximations as described in Section 3.2. In the appendix we show that, with the RBF kernel used for both KSD and the parametric approximation \( \log \hat{q}(x) := k_{ aux } (x, x^k) + C \), and temporarily defining the “gram matrix” \( X_{ij} = (x^i)^T x^j \), the optimal solution for minimising KSD V-statistic is

\[
\begin{align*}
\Lambda &= X \odot (KKK) + K(K \odot X)K - ((KK) \odot X)K - K((KK) \odot X), \\
b &= (K \text{diag}(X)K + (KK) \odot X - K((KK) \odot X) - (K \odot X)K)1.
\end{align*}
\]

One can also minimise the U-statistic of KSD to obtain gradient approximations, in which we provide a derivation of corresponding optimal solutions in the appendix. In experiments we use V-statistic solutions and leave comparisons between these methods to future work.

4 Applications

We present some case studies that apply the gradient estimators for implicit models. Detailed settings (architecture, learning rate, etc.) are presented in the appendix. Implementation will be released at https://github.com/FirstAuthor/SteinEstimator upon acceptance.

4.1 Synthetic example: Hamiltonian flow with approximate gradients

We first consider a simple synthetic example to demonstrate the accuracy of the proposed gradient estimator. More precisely we consider the kernel induced Hamiltonian flow (not an exact sampler) on a 2-dimensional banana-shaped object: \( x \sim B(x; b = 0.03, v = 100) \Leftrightarrow x_1 \sim N(x_1; 0, v), x_2 = \epsilon + b(x_2^2 - v), \epsilon \sim N(\epsilon; 0, 1) \). The approximate Hamiltonian flow is constructed using the same operator as in Hamiltonian Monte Carlo (HMC), except that the exact score function \( \nabla_x \log \mathcal{B}(x) \) is replaced by the approximate gradients. We still use the exact target density to compute the rejection step as we mainly focus on testing the accuracy of the gradient estimators. The parametric Stein gradient estimator is tested here, since once fitted it is much faster to compute compared to the non-parametric version. We fit the gradient estimators on \( K = 1,000 \) training datapoints from the target density. The bandwidth of the RBF kernel is computed by the median heuristic and scaled up by 4. All three methods are simulated for \( T = 1,000 \) iterations, share the same initial locations that are constructed by target distribution samples plus Gaussian noises of standard deviation 4, and the results are averaged over 200 parallel chains.

We visualise the samples and some MCMC statistics in Figure 1. Both the score matching and Stein gradient estimators return similar sets of samples, with reasonably high acceptance rate and autocorrelation/KSD metrics close to HMC. Interestingly the Stein approach slightly over-estimates the probability density at the extremities of the distribution. On the other hand, the visualised trajectory of the particle (in yellow) for the Stein approach is more HMC-like. These results indicate that the two methods have different advantages: the score matching estimator generalises better at locations that are further away from the training points (cyan crossed dots), while the Stein gradient estimator provides more accurate approximations at proximal locations. We conjecture these different properties might due to the usage of different kernels for KSD (delta function versus RBF). Investigations on the effect of kernel selection to Hamiltonian dynamics could be useful in the future.

4.2 Meta-learning of approximate posterior samplers for Bayesian neural networks

One of the recent focuses on meta-learning has been on learning optimisers for training deep neural networks, e.g. see [1]. Could analogous goals be achieved for approximate inference? In this section we take the attempt to learning an approximate posterior sampler for Bayesian neural networks that generalises to unseen datasets and architectures. More specifically, we consider a binary classification task: \( p(y = 1|x, \theta) = \text{sigmoid} (\text{NN}_\theta (x)), p_0(\theta) = N(\theta; 0, I) \). After observing the training
We use ionosphere as the validation set to tune \( \zeta \). We briefly describe the test protocol. We take from the UCI repository \([21]\) six binary classification datasets (australian, breast, crabs, ionosphere, pima, sonar), train an approximate sampler on crabs with a small neural network that has one 20-unit hidden layer with ReLU activation, and generalise to the remaining datasets with a bigger network that has 50 hidden units and uses sigmoid activation.

The remaining 4 datasets are further split into 40\% training and 60\% test subsets, where the training subset is used for simulating samples from the approximate sampler, and the test subset is used to evaluate the sampler’s performance.

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The coordinates of the noise standard deviation \( \sigma_{\phi}(\theta_t, \nabla_t) \) and the moving direction \( \Delta \phi(\theta_t, \nabla_t) \) are parametrised by a coordinate-wise neural network. If properly trained, this neural network will learn the best combination of the current location and gradient information, and produce approximate posterior samples efficiently on different probabilistic modelling tasks. Here we propose using the variational inference objective \([2]\) computed on the samples \( \{ \theta^k_t \} \) to learn the variational parameters \( \phi \). Since in this case the gradient of the log joint distribution can be computed analytically, we only approximate the gradient of the entropy term \( \mathbb{H}[q] \) as in \([3]\), with the exact score function replaced by the presented gradient estimators. We report the results using the non-parametric Stein gradient estimator as we found it works better than the parametric version. The RBF kernel is applied for gradient estimation, with the bandwidth computed using the median heuristic.

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Figure \( \[2\] \) presents the (negative) test log-likelihood (LL), classification error, and an estimate of the KSD U-statistic \( S^2_U(p(\theta|D), q(\theta)) \) (with data sub-sampling) over 5 splits of each test datasets. Note that by the time of submission we failed to obtain desirable results with the score matching estimator thus we omit the corresponding results here. Besides the gradient estimators we also compare with two baselines: an approximate posterior sampler trained by maximum a posteriori (MAP), and stochastic gradient Langevin dynamics (SGLD) \([48]\) evaluated on the test datasets directly. Overall the Stein approach performs a little better than SGLD, whereas the KDE method is slightly worse. The MAP model under-performs for test log-likelihood and KSD metrics, presumably because the noise variance \( \sigma \) has been turned off by optimisation thus having learned an optimiser instead. Future work should investigate the usage of advanced recurrent neural networks such as an LSTM, which is expected to return better performance.

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We empirically investigate the entropy regularisation idea on BEGAN using (continuous) MNIST, and where the rest of the optimisation objectives remains as in (14). This procedure would maintain we use the very recently proposed boundary equilibrium GAN (BEGAN) [5] as a running example. 

\[
\text{J} = \lambda \left( \log p(x) - \log \int p(z) \, dz \right) + \phi
\]

The main idea behind BEGAN is that, as the reconstruction loss \( \text{J} (\cdot) \) is approximately Gaussian distributed, with \( \gamma = 1 \) the discriminator loss \( \mathcal{J}_{\text{dis}} \) is (approximately) proportional to the Wasserstein distance between loss distributions induced by the data distribution \( p_{\text{data}} (x) \) and the generator \( p(x) \). In practice it is beneficial to maintain the equilibrium \( \gamma \mathbb{E}_{p_{\text{data}}} [\mathcal{J} (x)] = \mathbb{E}_{p} [\mathcal{J} (x)] \) through the optimisation procedure described in (14) that is motivated by proportional control theory. This approach effectively stabilises training, however it suffers from catastrophic mode collapsing problem (see the left most panel in Figure 3). To address this issue, we simply subtract an entropy term from the generator’s loss function, i.e. with \( K \) samples \( z^{1}, \ldots, z^{K} \sim p_{0}(z) \),

\[
\mathcal{J}_{\text{gen}} (\theta; \varphi) = \frac{1}{K} \sum_{k=1}^{K} \mathcal{J} (f_{\theta} (z^{k})) + \alpha \frac{1}{K} \sum_{k=1}^{K} \log p (f_{\theta} (z^{k})),
\]

where the rest of the optimisation objectives remains as in (14). This procedure would maintain the equilibrium \( \gamma \mathbb{E}_{p_{\text{data}}} [\mathcal{J} (x)] = \mathbb{E}_{p} [\mathcal{J} (x)] - \alpha \mathbb{H} [p] \). We approximate the gradient \( \nabla_{\theta} \mathbb{H} [p] \) using the estimators presented above. For the purpose of updating the control rate \( \beta_{t}\) two strategies are considered to approximate the contribution of the entropy term. The first proposal considers a plug-in estimate of the entropy term with a KDE estimate of \( p(x) \), which is consistent with the KDE estimator but not necessary with the other two (as they use kernels when representing \( \log p(x) \) or \( \nabla_{x} \log p(x) \)). The second one uses a proxy of the entropy loss \( -\mathbb{H} [p] \approx \frac{1}{K} \sum_{k=1}^{K} \nabla_{x^{k}} \log p (x^{k})^T x^{k} \) with generated samples \( \{x^{k}\} \) and \( \nabla_{x^{k}} \log p (x^{k}) \) approximated by the gradient estimator in use.

We empirically investigate the entropy regularisation idea on BEGAN using (continuous) MNIST, and in this case the non-parametric V-statistic Stein gradient estimator is in use. We use a convolutional generative network and a convolutional auto-encoder and select \( \gamma \in \{0.3, 0.5, 0.7\} \), \( \alpha \in [0, 1] \) and \( \lambda = 0.001 \). The Epanechnikov kernel \( K(x, x') := \frac{1}{d} \sum_{j=1}^{d} (1 - (x_{j} - x'_{j})^2) \) is used as the pixel values lie in a unit interval (see appendix for the expression of the score matching estimator), and to
ensure the boundary condition we clip the pixel values into range $[1e^{-8}, 1 - 1e^{-8}]$. The generated images are visualised in Figure 3. BEGAN without the entropy regularisation fails to generate diverse samples even when trained with learning rate decay. The other three images clearly demonstrate the benefit of the entropy regularisation technique, with the Stein approach obtaining the highest diversity without compromising visual quality.

We further consider four metrics to assess the trained models quantitatively. First 500 samples are generated for each trained model, then we compute their nearest neighbours in the training set using $l_1$ distance, and obtain a probability vector $p$ by averaging over these neighbour images’ label vectors. In Figure 4, we depict the entropy of $p$ (top left), averaged $l_1$ distances to the nearest neighbour (top right), and the difference between the largest and smallest elements in $p$ (bottom right). The error bars are obtained by 5 independent runs. These results demonstrate that the Stein approach performs significantly better than the other two, in that it learns a better generative model not only faster but also in a more stable way. Interestingly the KDE approach achieves the lowest average $l_1$ distance to nearest neighbours, possibly because it tends to memorise training examples. We next train a fully connected network \( \pi(y|x) \) on MNIST that achieves 98.16% text accuracy, and compute on the generated images an empirical estimate of the inception score \( E_p(x) [\text{KL}[\pi(y|x)||\pi(y)]] \) with \( \pi(y) = E_{p(x)}[\pi(y|x)] \) (bottom left panel). High inception score indicates that the generate images tend to be both realistic looking and diverse, and again the Stein approach out-performs the others in this metric by a large margin.

5 Conclusions and future work

We have presented the Stein gradient estimator as a novel generalisation to the score matching gradient estimator. With a focus on learning implicit models, we have empirically demonstrated the efficacy of the proposed estimator by showing state-of-the-art results on three canonical learning tasks: approximating gradient-free MCMC, meta-learning for approximate posterior samplers, and unsupervised learning for image generation. Future work will expand the understanding of gradient estimators in both theoretical and practical sides. Theoretical development will compare both the V-statistic and U-statistic Stein gradient estimators and formalise consistency proofs. Practical work will improve the sample efficiency of kernel estimators in high dimensions and develop fast yet accurate approximations to the matrix inversion part. Finally follow-up work will study the generalisation of the Stein gradient estimator to non-kernel settings and discrete distributions.
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A Score matching estimator: derivations

In this section we provide analytical solutions for the score matching estimator, more specifically, the linear coefficient \( a = (a_1, ..., a_K) \) for the case of the Epanechnikov kernel.

A.1 The RBF kernel case

The derivations for the RBF kernel case is referred to [20], and for completeness we include the final solutions here. Assume the parametric approximation is defined as \( \log \hat{q}(x) = \sum_{k=1}^{K} a_k \mathcal{K}(x, x^k) + C \), where the RBF kernel uses bandwidth parameter \( \sigma \). Then the optimal solution of the coefficients \( \mathbf{a}^{\text{score}} = (\Sigma + \eta I)^{-1} \mathbf{v} \), with

\[
\mathbf{v} = \sum_{i=1}^{d} \left[ \sigma^2 \mathbf{K}1 - \left( \mathbf{K}(x_i \odot x_i) + \text{diag}(x_i) \mathbf{K}1 - 2\text{diag}(x_i) \mathbf{K}x_i \right) \right],
\]

\[
\Sigma = \sum_{i=1}^{d} \left[ \text{diag}(x_i) \mathbf{K} - \mathbf{K} \text{diag}(x_i) \right] \left[ \mathbf{K} \text{diag}(x_i) - \text{diag}(x_i) \mathbf{K} \right],
\]

\[
x_i = (x_{i1}, x_{i2}, ..., x_{iK})^T \in \mathbb{R}^{K \times 1}.
\]

A.2 The Epanechnikov kernel case

Epanechnikov kernel is defined as \( \mathcal{K}(x, x') = \frac{1}{2} \sum_{i=1}^{d} \left( 1 - (x_i - x_i')^2 \right) \), where the first and second order gradients w.r.t. \( x_i \) is

\[
\nabla_{x_i} \mathcal{K}(x, x') = \frac{d}{d} x_i - x_i, \quad \nabla_{x_i} \nabla_{x_i} \mathcal{K}(x, x') = -\frac{2}{d}.
\]

Thus the score matching objective with \( \log \hat{q}(x) = \sum_{k=1}^{K} a_k \mathcal{K}(x, x^k) + C \) is reduced to

\[
\mathcal{F}(\mathbf{a}) = \frac{1}{K} \sum_{j=1}^{K} \left[ \frac{1}{d^2} \sum_{k=1}^{K} a_k \left( \frac{2}{d} (x_i - x_i')^2 \right) - \frac{2}{d} \sum_{k=1}^{K} a_k \frac{2}{d} \right]
\]

\[
= \frac{1}{K} \frac{1}{d^2} \sum_{j=1}^{K} \left[ \sum_{k=1}^{K} \sum_{k'=1}^{K} a_k a_{k'} (x_i - x_i') (x_i - x_i')^T \right]
\]

\[
:= 4 (\mathbf{a}^T \Sigma \mathbf{a} - \mathbf{a}^T \mathbf{1}),
\]

with the matrix elements

\[
\Sigma_{kk'} = \frac{1}{d^2} \left[ (x_i)^T x_i' + \frac{1}{K} \sum_{j=1}^{K} \left[ (x_i) (x_i')^T - ((x_i + x_i')^T \mathbf{x}_j) \right] \right].
\]

Define the “gram matrix” \( \mathbf{X}_{ij} = (\mathbf{x}_i)^T \mathbf{x}_j \), we write the matrix form of \( \Sigma \) as

\[
\Sigma = \frac{1}{d^2} \left[ \mathbf{X} + \frac{1}{K} (\text{Tr}(\mathbf{X}) - 2 \mathbf{X} 1^T) \right].
\]

Thus with an \( l_2 \) regulariser, the fitted coefficients are

\[
\mathbf{a}^{\text{score}} = \frac{d^2}{2} \left[ \mathbf{X} + \frac{1}{K} (\text{Tr}(\mathbf{X}) - 2 \mathbf{X} 1^T) + \eta I \right]^{-1}.
\]

B Stein gradient estimator: derivations

B.1 Direct minimisation of KSD V-statistic and U-statistic

The V-statistic of KSD is the following: given samples \( x^k \sim q, k = 1, ..., K \) and recall \( \mathbf{K}_{jl} = \mathcal{K}(x^j, x^l) \)

\[
S_{V}^2(q, \hat{q}) = \frac{1}{K^2} \sum_{j=1}^{K} \sum_{l=1}^{K} \left[ \hat{g}(x^j)^T \mathbf{K}_{jl} \hat{g}(x^l) + \hat{g}(x^j)^T \nabla_{x^j} \mathbf{K}_{jl} + \nabla_{x^j} \mathbf{K}_{jl} \hat{g}(x^j) + \text{Tr}(\nabla_{x^j} \mathbf{K}_{jl}) \right].
\]

The last term \( \nabla_{x^j} \mathbf{K}_{jl} \) will be ignored as it does not depend on the approximation \( \hat{g} \). Using matrix notations defined in the main text, readers can verify that the V-statistic can be computed as

\[
S_{V}^2(q, \hat{q}) = \frac{1}{K^2} \text{Tr}(\mathbf{K} \mathbf{G}^T \mathbf{G}) + 2 (\nabla \cdot \mathbf{K}) + C.
\]
Using the cyclic invariance of matrix trace leads to the desired result in the main text. The U-statistic of KSD removes terms indexed by $j = l$ in (17), in which the matrix form is

$$S_U^2(q, \hat{q}) = \frac{1}{K(K - 1)} \text{Tr}((K - \text{diag}(K)) \hat{G} G^T + 2((\nabla, K) - \nabla \text{diag}(K)) \hat{G}^T) + C. \quad (19)$$

with the $j$th row of $\nabla \text{diag}(K)$ defined as $\nabla_{x_j} K(x', x')$. For most translation invariant kernels this extra term $\nabla \text{diag}(K) = 0$, thus the optimal solution of $G$ by minimising KSD U-statistic is

$$G^\text{Stein}_U = -(K - \text{diag}(K) + \eta I)^{-1} \langle \nabla, K \rangle. \quad (20)$$

**B.2 Parametric Stein gradient estimator with the RBF kernel**

We define a parametric approximation in a similar way as for the score matching estimator:

$$\log \hat{q}(x) := \sum_{k=1}^{K} a_k K(x, x^k) + C, \quad K(x, x') = \exp \left[ -\frac{1}{2\sigma^2} ||x - x'||^2 \right]. \quad (21)$$

Now we show the optimal solution of $a = (a_1, ..., a_K)^T$ by minimising (17). To simplify derivations we assume the approximation and KSD use the same kernel. First note that the gradient of the RBF kernel is

$$\nabla_x K(x, x') = \frac{1}{\sigma^2} K(x, x')(x' - x). \quad (22)$$

Substituting (22) into (17):

$$S_V^2(q, \hat{q}) = C + \mathbf{\Phi} + 2\mathbf{\Phi},$$

$$\mathbf{\Phi} = \frac{1}{K^2} \sum_{k=1}^{K} \sum_{k'=1}^{K} \sum_{j=1}^{K} \sum_{l=1}^{K} a_k a_{k'} K_{k,j} K_{l,j} K_{k',l} \frac{1}{\sigma^2} (x^k - x')^T (x^{k'} - x'),$$

$$\mathbf{\Phi} = \frac{1}{K^2} \sum_{k=1}^{K} \sum_{k'=1}^{K} \sum_{j=1}^{K} \sum_{l=1}^{K} a_k a_{k'} K_{k,j} K_{l,j} \frac{1}{\sigma^2} (x^k - x')^T (x^{j} - x^l). \quad (24)$$

We first consider summing the $j$, $l$ indices in $\mathbf{\Phi}$. Recall the “gram matrix” $X_{ij} = (x^T)^T x^l$, the inner product term in $\mathbf{\Phi}$ can be expressed as $X_{k,k'} + X_{j,l} - X_{k,l} - X_{j,k'}$. Thus the summation over $j$, $l$ can be re-written as

$$\Lambda := \sum_{j=1}^{K} \sum_{k=1}^{K} K_{k,j} K_{l,j} (X_{k,k'} + X_{j,l} - X_{k,l} - X_{j,k'}).$$

And thus $\mathbf{\Phi} = \frac{1}{\sigma^2} a^T \Lambda a$. Similarly the summation over $j$, $l$ in $\mathbf{\Phi}$ can be simplified into

$$-b := \sum_{j=1}^{K} \sum_{l=1}^{K} K_{j,j} (X_{kj} + X_{jl} - X_{kl} - X_{jj})$$

$$= - (K_{\text{diag}}(X) K + (K K) \circ X - K(K \circ X) - (K \circ X) K) 1,$$

which leads to $\mathbf{\Phi} = -\frac{1}{\sigma^2} a^T b$. Thus minimising $S_V^2(q, \hat{q})$ plus an $l_2$ regulariser returns the Stein estimator $a^\text{Stein}_V$ in the main text.

Similarly we can derive the solution for KSD U-statistic minimisation. The U statistic can also be represented in quadratic form $S_U^2(q, \hat{q}) = C + \mathbf{\Phi} + 2\mathbf{\Phi}$, with $\mathbf{\Phi} = \mathbf{\Phi}$ and

$$\mathbf{\Phi} = \mathbf{\Phi} - \frac{1}{K^2} \sum_{k=1}^{K} \sum_{k'=1}^{K} \sum_{j=1}^{K} \sum_{l=1}^{K} a_k a_{k'} K_{k,j} K_{l,j} \frac{1}{\sigma^2} (X_{k,k'} + X_{j,l} - X_{k,l} - X_{j,k'}).$$

Summing over the $j$ indices for the second term, we have

$$\sum_{j=1}^{K} K_{k,j} K_{k,j} (X_{k,k'} + X_{j,l} - X_{k,l} - X_{j,k'})$$

$$= X \circ (K_{\text{diag}}(K) K) + K_{\text{diag}}(K \circ X) K - (K_{\text{diag}}(K) \circ X) K - K((\text{diag}(K) K) \circ X).$$

Working through the analogous derivations reveals that $a^\text{Stein}_U = (\hat{\Lambda} + \eta I)^{-1} b$, with

$$\hat{\Lambda} = X \circ (K(K - \text{diag}(K)) K) + K((\text{diag}(K) K) - \text{diag}(K \circ X)) K - ((K(K - \text{diag}(K))) \circ X) K - K(((K - \text{diag}(K)) K) \circ X).$$
C Experimental settings

We describe the detailed experimental set-up in this section. All experiments use Adam optimiser [18] with standard parameter settings.

C.1 Approximate posterior sampler experiments

We use a one hidden layer neural network with 20 hidden units to compute the noise variance and the moving direction of the next update. In a nutshell it takes the ith coordinate of the current position and the gradient \( \theta_t(i), \nabla_t(i) \) as the inputs, and output the corresponding coordinate of the moving direction \( \Delta \phi(\theta_t, \nabla_t)(i) \) and the noise variance \( \sigma_\phi(\theta_t, \nabla_t)(i) \). Softplus non-linearity is used for the hidden layer and to compute the noise variance we apply ReLU activation to ensure non-negativity. The step-size \( \zeta \) is selected as 1e-5 which is tuned on the KDE approach. For SGLD step-size 1e-5 also returns overall good results.

The training process is the following. We simulate the approximate sampler for 100 transitions and sum over the variational lower-bounds computed on the samples of every step. Truncated back-propagation is used every 10 transition steps to avoid vanishing gradients. These simulated samples are stored to initialise the Markov chain for the next iteration, and for every 50 iterations we restart the simulation by randomly sampling the locations from the prior. Early stopping is applied using the validation dataset, and the learning rate is set to 0.001.

C.2 BEGAN experiments

We construct a deconvolutional net for the generator and a convolutional auto-encoder for the discriminator. The convolutional encoder consists of 3 convolutional layers with filter width 3, stride 2, and number of feature maps [32, 64, 64]. These convolutional layers are followed by two fully connected layers with [512, 64] units. The decoder and the generative net have a symmetric architecture but with stride convolutions replaced by deconvolutions. ReLU activation function is used for all layers except the last layer of the generator, which uses sigmoid non-linearity. The reconstruction loss in use is the squared \( l_2 \) norm \( || \cdot ||^2_2 \). The randomness \( p_0(z) \) is selected as uniform distribution in [-1, 1] as suggested in the original paper [5]. Learning rate is initialised at 0.0002 and decayed by 0.9 every 10 epochs, which is tuned on the KDE model. The selected \( \gamma \) and \( \alpha \) values are: for KDE estimator approach \( \gamma = 0.3, \alpha \gamma = 0.05 \), for score matching estimator approach \( \gamma = 0.3, \alpha \gamma = 0.1 \), and for Stein approach \( \gamma = 0.5 \) and \( \alpha \gamma = 0.3 \). The presented results use the KDE plug-in estimator for the entropy estimates (used to tune \( \beta \)) for the KDE and score matching approaches. Initial experiments found that for the Stein approach, using the KDE entropy estimator works slightly worse than the proxy loss, thus we report results using the proxy loss. An advantage of using the proxy loss is that it directly relates to the approximate gradient. Furthermore we empirically observe that the performance of the Stein approach is much more robust to the selection of \( \gamma \) and \( \alpha \) when compared to the other two methods.