Approximate Inference with Amortised MCMC

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Abstract

We propose a novel approximate inference algorithm that approximates a target distribution by amortising the dynamics of a user-selected MCMC sampler. The idea is to initialise MCMC using samples from an approximation network, apply the MCMC operator to improve these samples, and finally use the samples to update the approximation network thereby improving its quality. This provides a new generic framework for approximate inference, allowing us to deploy highly complex, or implicitly defined approximation families with intractable densities, including approximations produced by warping a source of randomness through a deep neural network. Experiments consider image modelling with deep generative models as a challenging test for the method. Deep models trained using amortised MCMC are shown to generate realistic looking samples as well as producing diverse imputations for images with regions of missing pixels.

1. Introduction

Probabilistic modelling provides powerful tools for analysing and making future predictions from data. The Bayesian paradigm offers well-calibrated uncertainty estimates on unseen data, by representing the variability of model parameters given the current observations into the posterior distribution. However, Bayesian methods are typically computationally expensive, due to the computational intractability of evaluating posterior or marginal probabilities. This is especially true for complex models like neural networks, for which a Bayesian would treat all the weight matrices as random variables and integrate them out. Hence approximations have to be applied to overcome this computational intractability in order to make Bayesian methods practical for modern machine learning tasks.

Practical approaches for approximate Bayesian inference include those that are sampling-based and those which are optimisation-based. Sampling-based methods, including Markov chain Monte Carlo (MCMC) (Duane et al., 1987; Murray, 2007; Neal et al., 2011) and importance sampling methods such as sequential Monte Carlo (SMC, (Doucet et al., 2001)), approximate the posterior by drawing (approximate) samples from the posterior and use them later for inference and prediction. These approaches are non-parametric in nature, meaning that the exact posterior distribution is estimated with the empirical distribution of the simulated samples. Despite having desirable theoretical guarantees, MCMC methods are unbiased only asymptotically, and often suffer from slow convergence in practice. Furthermore, traditional MCMC is computationally prohibitive in big data settings because each likelihood evaluation requires a sweep of the whole dataset. Even worse, many learning problems require repeated applications of MCMC on many different target densities, making it highly infeasible in practice. As an example, training a (deep) generative model for image generation requires inference for the latent variable associated with each observation. Moreover, updating the generative model parameters will change the exact posterior substantially, thus requiring reinitialising the Markov chain to reflect this change.

In contrast, optimisation-based methods provide fast tools for approximate inference at large scale. These methods explicitly define an (often parametric) approximate posterior distribution, fitted to the exact posterior by optimising some objective function, and replace the exact posterior with the approximated one in inference/prediction time. An example of optimisation-based methods is variational inference (VI) (Jordan et al., 1999; Beal, 2003), which maximises the variational lower-bound in some predefined distribution family. Other examples in this regime include expectation propagation (EP) (Minka, 2001) which has been applied to large-scale industrial systems (Herbrich et al., 2006; Minka et al., 2010). Although simple and fast, these methods often require analytical solutions to the update steps, restricting the approximations to be of very simple forms and thus deteriorating the approximation quality.

Although these two types of approaches seem unrelated at first glance, recent developments in approximate inference have started to fuse both together to achieve better perfor-
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Learning Machine networks. The hyper-parameters are loaded in generative models, or weight matrices of Bayesian substantive variables/parameters that a Bayesian approach would with a prior distribution \( p \). Problem Setup

Experiments on toy data and deep generative modelling by MCMC that is initialised at the approximate posterior. deep generative models, in which inference is performed maximum likelihood estimation (MLE) method for training deploy arbitrary complex distribution families as approximations, meaning that the advantage of both worlds. The framework allows us to combine the design of approximate families that are flexible and still computationally tractable (e.g., Rezende and Mohamed, 2015; Ranganath et al., 2016b; Kingma et al., 2016); however, this requires to establish new algorithms for different posterior families on a case by case basis. Another approach, which we take in this work, is to develop more complex, universal variational approximation algorithms that do not require the density of the approximate posterior. This is highly desirable, since it allows us to separate the design of approximate families from the variational approximation engine, allowing the practitioners to focus on model design for their specific tasks.

In this paper we propose amortising MCMC to combine the advantage of both worlds. The framework allows us to deploy arbitrary complex distribution families as approximation posteriors. We further develop an approximate maximum likelihood estimation (MLE) method for training deep generative models, in which inference is performed by MCMC that is initialised at the approximate posterior. Experiments on toy data and deep generative modelling demonstrate the wide applicability of the method.

2. Problem Setup

We start by defining a probabilistic model \( p(x|z, \theta) \) along with a prior distribution \( p_0(z) \). Here \( z \) denotes the latent variables/parameters that a Bayesian approach would integrate out, e.g. latent representation variables of deep generative models, or weight matrices of Bayesian neural networks. The hyper-parameters are loaded in \( \theta \) which will be learned by (approximate) maximum likelihood estimation (MLE), requiring the computation of marginal likelihood \( p(x|\theta) \). Also given the observation \( x \), inference requires computing the expectation of some function \( F(z) \) in interest, under the exact posterior \( p(z|x, \theta) = \frac{1}{p(x|\theta)p_0(z)p(x|z, \theta)}. \) Through out this paper we assume the log-likelihood terms are tractable, but even so the exact posterior and model evidence can be tractably evaluated point-wise, i.e. having prohibitive computational costs to evaluate, and hence require approximations in most cases.

The core idea of approximate inference is to fit an approximate posterior distribution \( q(z|x) \) in a “tractable” distribution family \( Q \) to the exact posterior \( p(z|x, \theta) \), such that \( \mathbb{E}_{p(z|x, \theta)}[F(z)] \) can be well approximated by \( \mathbb{E}_{p(z|x, \theta)}[F(z)] \approx \mathbb{E}_{q(z|x)}[F(z)]. \) (1)

The RHS expression of (1) is the approximate predictive likelihood in Bayesian neural network context, when the function \( F \) is \( F(z) = p(x^*|z, \theta) \) for unseen data \( x^* \). Historically, approximate distributions of simple form, such as mean-field approximation and factorised Gaussians (Jordan et al., 1999), have been proposed in order to obtain analytical solutions of the approximated expectation. This often requires the probabilistic model to comprise conjugate exponential families (Hoffman et al., 2013), which excludes a wide range of powerful models including models that warp variables through neural networks. Instead, modern approximate inference introduces Monte Carlo (MC) estimation techniques to approximate the predictive likelihood (Paisley et al., 2012; Ranganath et al., 2014), in which at inference time, samples are drawn from the approximate posterior and the required quantity is estimated by \( \mathbb{E}_{q(z|x)}[F(z)] \approx \frac{1}{K} \sum_{k=1}^{K} F(z^k), \quad z^k \sim q(z|x). \) (2)

MC estimation enables both a wider class of generative models to be amendable to VI (the requirement is that the log-joint can be computed point-wise), and a wider class of distributions to be deployed as the approximate posterior, and the only requirement is that sampling from \( q \) can be done efficiently. We refer these type of flexible \( q \) distributions as wild approximations (to distinguish from the black-box variational inference (Ranganath et al., 2014)). It is generally believed that such a flexible family of approximate distributions can return very accurate results if they are fitted to the exact posterior.

Unfortunately, except a few very recent attempts (Ranganath et al., 2016a; Wang and Liu, 2016; Mescheder et al., 2017), most approximate inference algorithms impose a further constraint: given a configuration of \( z \), the density \( q(z|x) \) must be computable in a fast way. More precisely, these optimisation-based methods require evaluating the \( q \) density for every single update. In other words, the “tractability” requirements of the distribution family \( Q \) in most existing MC-based variational methods are (i) fast sampling and (ii) fast density evaluation. But observing that MC inference in prediction time only requires (i), it
raises an outstanding research question: can we design efficient approximate inference algorithms to train flexible approximate posterior distributions without access to an explicit density function?

In the rest of the paper we try to answer the above question by proposing an MCMC amortisation algorithm. Before the presentation of the new algorithm, we provide several examples of the wild approximations. We use $\phi$ to denote the parameters for $q$, and in this paper we consider gradient-based optimisation methods for learning $\phi$. We will explicitly write $q(z|x) = q_\phi(z|x)$ when necessary.

**Example 1.** (Deterministic transform) Sampling $z \sim q(z|x)$ is defined by first sampling some random noise $\epsilon \sim p(\epsilon)$, then transforming it with a deterministic mapping $z = f(\epsilon, x)$, which might be defined by a (deep) neural network. These distributions are also called variational programs in (Ranganath et al., 2016a), or implicit models in the generative model context (Mohamed and Lakshminarayanan, 2016). An important note here is that $f$ might not be invertible, which differs from the invertible transform techniques discussed in (Rezende and Mohamed, 2015; Kingma et al., 2016).

**Example 2.** (Truncated Markov chain) Here the samples $z \sim q(z|x)$ are defined by finite-step transitions of a Markov chain. Examples include Gibbs sampling in contrastive divergence (Hinton, 2002), or finite-step simulation of an SG-MCMC algorithm such as SGLD (Welling and Teh, 2011). It has been shown in (Maclaurin et al., 2016; Mandt et al., 2016) that the trajectory of SGD can be viewed as a variational approximation to the exact posterior. In these examples the variational parameters are the parameters of the transition kernel, e.g. step-sizes and/or preconditioning matrices. Related work includes Salimans et al. (2015) which integrates MCMC into VI objective. These methods are more expensive as they require evaluations of $\nabla_z \log p(x, z|\theta)$, but they can be much cheaper than sampling from the exact posterior.

**Example 3.** (Stochastic regularisation techniques (SRT)) SRT for deep neural network training, e.g. dropout (Srivastava et al., 2014) and related variants (Wan et al., 2013; Singh et al., 2016), have been re-interpreted as a variational inference network for posterior weights $z = \{W\}$ (Gal and Ghahramani, 2016; Gal, 2016). The variational parameters $\phi = \{M\}$ are the weight matrices of a Bayesian neural network without SRT. The output is computed as $h = \sigma(\epsilon \odot x)M$, with $\sigma(\cdot)$ the activation function and $\epsilon$ some randomness. This is equivalent to setting $W = \text{diag}(\epsilon)M$, making SRT a special case of example 1. Fast evaluation of $q(z|x)$ during training is intractable as different noise values $\epsilon$ are sampled for different inputs in a mini-batch. This means multiple sets of weights are processed if we were to evaluate the density, which has prohibitive costs especially when the network is wide and deep.

### 3. Amortised MCMC

We propose an amortised MCMC method based on the idea of training an inference network that learns to “distil” from an MCMC dynamics. From a bird’s eye view, our method deploys a student-teacher, or actor-critic framework that iterates the following steps:

1. The “$q$ network” (student) generates initial samples which are shown to an MCMC teacher.
2. The MCMC sampler (teacher) takes the samples and runs MCMC transitions to improve the samples.
3. The “$q$ network” takes feedbacks from the teacher and adjust itself in order to generate the improved samples next time.

One might expect that the “$q$ network”, if flexible enough, would sample from the true target distribution at equilibrium, when the MCMC teacher can no longer further improve the quality of the student’s samples. We now give a more detailed account of the framework.

#### 3.1. MCMC Basics

We first discuss some MCMC basics upon which the derivation is based. An MCMC algorithm is typically specified by its transition kernel $K(\cdot|\cdot)$ in which the state at time-step $t$ is drawn conditioned on the previous state:

$$z_t|z_{t-1} \sim K(z_t|z_{t-1}), \quad t = 1, 2, ...$$

For $t = 0$ we call $z_0$ the initial state which is sampled from some initial distribution. We say $p$ is a stationary distribution of the kernel $K$ if for any configuration of $z$,

$$p(z) = \int p(z')K(z|z')dz'.$$

The proposed algorithm is established on the following assumptions:

(A1) The exact posterior $p(z|x)$ is the unique stationary distribution of $K$.

(A2) The distribution of the Markov chain converges to its stationary distribution when $T \rightarrow +\infty$.

#### 3.2. Learning to Distil MCMC

Now we present *amortised MCMC* which trains an inference network $q(z|x)$ to draw sample from the target posterior $p(z|x)$. Assume $K(z_t|z_{t-1})$ is a Markov transition kernel satisfying (A1)-(A2). Given an initial state $z_0 \sim q(z|x)$ drawn from the current inference network, we denote by $z_T$ the state we obtained by running the Markov
chain for $T$ steps. The distribution of $z_T$ is

$$q_T(z_T|x) = \int \prod_{t=1}^{T} K(z_t|z_{t-1}) q(z_0|x) dz_{0:T-1}$$

$$= \int K_T(z_T|z_0) q(z_0|x) dz_0$$

(5)

By the convergence of the Markov chain, $z_T$ and $q_T(z_T|x)$ should form a better approximation to the exact posterior. This motivates us to update the $q$ distribution to be $q_T(z_T|x)$ and repeat this process until convergence. If the approximating family $Q$ is flexible enough and contains the exact posterior, then at the fixed point, the $q(z|x)$ must be the stationary distribution of the transition kernel $K(z_t|z_{t-1})$, and hence should equal the exact posterior by the uniqueness assumption (A1).

In practice, we may not perform the update exactly, because $q_T$ is implicitly parametrised by the approximate posterior $q$. Instead, we take a projection-based approach and update $q$ by minimizing a divergence/discrepancy $D[\cdot||\cdot]$ to $q_T$:

$$q \leftarrow \arg\min_{q' \in Q} D[q_T||q'].$$  

(6)

where $Q$ is a parametric distribution family with parameters $\phi$. This projection update is further approximated by a gradient descent step

$$\phi \leftarrow \phi - \eta (\nabla_\phi q, \nabla_{q'} D[q_T||q']|_{q' = q}).$$

(7)

At convergence the gradient term in (7) is zero, hence $q$ converges to the exact posterior, with the assumption that $\nabla_\phi q \neq 0$ whenever $\nabla_{q'} D[q_T||q']|_{q' = q} \neq 0$. In practice this is often not true and local minima exist, however this problem also applies to other approximate inference methods with parametric $q$ distributions such as the VAE (Kingma and Welling, 2014; Rezende et al., 2014).

In summary, our method requires three main ingredients:

1. an architecture for the $q$ distribution (student);
2. an MCMC sampler with kernel $K(z_t|z_{t-1})$ (teacher);
3. a divergence $D[\cdot||\cdot]$ and update rule for $q$ (feedback).

By selecting these components tailored to a specific approximate inference task, the method provides a highly generic framework, applicable to both continuous and discrete distribution cases, and as we shall see later, extendible to wild approximations without a tractable density.

3.3. The Choice of Divergence Measure

The choice of the divergence/discrepancy measure $D[\cdot||\cdot]$ and ways to estimate it plays a crucial role in our framework, and it should be carefully selected to ensure both strong discrimination power and computational tractability with respect to the parametric family of $q$ that we use. We first discuss a simple choice based on KL divergence, and then discuss adversarially estimated divergences that we find works efficiently in wild approximation settings.

**KL Divergence** We first discuss a simple choice based on the inclusive KL-divergence

$$D_{KL}[q_T||q] = E_{q_T} \left[ \log \frac{q_T(z|x)}{q(z|x)} \right],$$

and using the projection-based method it only requires an MC estimate of $-E_{q_T} [ \log q(z|x) ]$. This gives a simple algorithm that hybrids MCMC and variational inference, and appears to be new to our knowledge. Similar algorithms include the so called cross entropy method (De Boer et al., 2005) which replaces $q_T$ with an importance weighted distribution, and methods for tuning proposal distributions for SMC (Cornebise, 2009; Gu et al., 2015).

**Adversarially Estimated Divergences** Unfortunately, the inclusive KL divergence requires the $q$ density to be computable, and therefore it cannot be used directly for wild approximation. In the wild approximation settings, we assume that we have access to both $q$ and $q_T$ only through samples $\{z^i_0\} \sim q(z|x)$ and $\{z^i_T\} \sim q_T(z|x)$, and we need to estimate the divergence based on the two samples.

In order to do this, we borrow the idea of generative adversarial networks (GAN) (Goodfellow et al., 2014) to construct a sample-based estimator of the selected divergence. As an example, consider using the Jensen-Shannon divergence as the objective:

$$D_{JS}[q_T||q] = \frac{1}{2} D_{KL}[q_T||\tilde{q}] + \frac{1}{2} D_{KL}[q||\tilde{q}]$$

(8)

with $\tilde{q} = \frac{1}{2} q + \frac{1}{2} q_T$. Since none of the three distributions have tractable density, a discriminator $d_\psi(z|x)$ is trained to compute a stochastic lower-bound to the divergence

$$D_{adv}[\{z_T^k\}||\{z_0^k\}] = \frac{1}{K} \sum_{k=1}^{K} \log (d_\psi(z_T^k|x))$$

$$+ \frac{1}{K} \sum_{k=1}^{K} \log (1 - \sigma(d_\psi(z_0^k|x))),$$

(9)

with $\sigma(\cdot)$ the sigmoid function and $z_0^k, z_T^k$ samples from $q$ and $q_T$, respectively. Recent work (Nowozin et al., 2016) extends adversarial training to $f$-divergences where the two KL-divergences are special cases in that rich family. In such case $D_{adv}$ also corresponds to the variational lower-bound to the selected $f$-divergence and the discriminator can also be defined accordingly. Furthermore, density ratio estimation literature (Nguyen et al., 2010; Sugiyama et al.,
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(2009; 2012) suggests that the discriminator $d_\phi$ in (9) can be used as an estimator of $\log \frac{q_\theta}{q}$, meaning that the objective function for $q$ could be decoupled from that for the discriminator (Mohamed and Lakshminarayanan, 2016).

4. Approximate MLE with Amortised MCMC

Learning latent variable models has become an important research topic with increasing interest. These models are optimised using approximate maximum likelihood (MLE), with the latent variables being inferred during training. In short, current practices of approximate MLE often maximise the variational lower-bound:

$$\max_\theta \mathbb{E}_q [\log p(x|z; \theta)] - D_{KL}[q(z|x)||p_0(z)] = \log p(x|\theta) - D_{KL}[q(z|x)||p(z|x, \theta)].$$ (10)

As a by-product of the proposed amortisation framework, we discuss approximate MLE with MCMC samples in the generative modelling context. First notice that, by the second law of thermodynamics (Cover and Thomas, 1991) $D_{KL}[q||p] \geq D_{KL}[q_T||p]$ if $p$ is the stationary distribution of the Markov chain. Hence given a variational approximation $q$, the following objective

$$\log p(x|\theta) - D_{KL}[q_T(z|x)||p(z|x, \theta)]$$ (11)

forms a tighter lower-bound to the marginal likelihood. Moreover, optimising (11) w.r.t. $\theta$ only requires computing

$$\mathbb{E}_{q_T}[\log p(x|z, \theta)] \approx \frac{1}{K} \sum_k \log p(x|z^k, \theta)$$

with samples $z^k \sim q_T$ from the Markov chain initialised at $q$, hence density evaluation of $q_T$ is not needed. This is especially desirable at the early stage of learning, as the $q$ distribution is still far away from the exact posterior.

Now we turn to the algorithmic design for optimising $q$ as the initial proposal. A naïve approach would maximise the variational lower-bound (10) w.r.t. $\phi$ if the density is tractable. These white-box proposals could also be learned with amortised MCMC, if the inclusive KL divergence is selected. In the case where the approximate posterior is wild, we train another discriminator $d_\phi$ to estimate the selected divergence, and propagate learning signals back through the samples from $q$.

We present the full method in Algorithm 1. Note here the update step for the discriminator and the $q$ distribution could be executed for more iterations in order to achieve better approximations to the current posterior. This strategy turns the algorithm into a stochastic EM procedure with MCMC methods approximating the E-step (Celeux and Diebolt, 1985; Celeux et al., 1995). Two-sample based techniques, such as kernel maximum mean discrepancy (MMD) (Gretton et al., 2012), can also be applied as the discrepancy measure in step 3, and clearly this avoids the usage of a discriminator and unstable adversarial learning. However computing an accurate empirical estimate $\hat{D}[q_T||q]$ of MMD requires many samples from both distributions, and the number of samples required grows with the dimensionality of the latent variable $z$. Furthermore, in general we need to simulate $2K$ parallel Markov chains to remove the correlation between samples of $z_T$ and $z_0$, which brings in prohibitive cost for tasks like training deep generative models. We continue discussing this correlation issue in the appendix, and in the experiments we only consider $z^k_T$ generated by a Markov chain started at $z^k_0$.

Algorithm 1 Amortised MCMC with adversarially estimated divergences (one update iteration)

1: sample $z^0_1, \ldots, z^0_K \sim q_\phi(z|x)$
2: simulate $z^1_T \sim K_T(\cdot|x)$ starting from $z^0_1$.
3: compute $D_{ab}(\{z^1_T\}, \{z^1_T\})$ using discriminator $\psi$.
4: update $\phi$ and $\psi$ by 1-step gradient ascent.
5: if learning $\theta$: compute 1-step gradient ascent with $\nabla_\theta \frac{1}{K} \sum_{k=1}^K \log p(x|z^k_T, \theta)$

We also briefly discuss the effect of the Markov chain length $T$ on the approximation quality, in the context of using adversarially estimated divergences. In theory, even when selecting $T = 1$, minimising $D[q_T||q]$ would return the exact approximation if $q$ is sufficiently flexible to capture the exact posterior. However in practice using small $T$ introduces strong correlations between $z$ and $z_T$, hence the discriminator could be easily fooled, and the learning signal provided by the estimated divergence will be too weak, especially for a flexible $q$ distribution to learn the posterior landscape (e.g. those produced using neural networks with stochastic inputs). Though this could potentially be avoided by using uncorrelated $z$ and $z_T$, but again it is computationally too expensive for the tasks we consider.

5. Related Work

Since Goodfellow et al. (2014), generative adversarial networks (GAN) have attracted large attention from both academia and industry. We should distinguish the problem scope of our work with that of GAN: amortised MCMC aims to match an (implicitly defined) $q$ to the posterior distribution $p$, while GAN aims to match a $q$ with an observed sample, which we leverage as an inner loop for the divergence minimisation. Hence our framework could also benefit from the recent advances in this area (Nowozin et al., 2016; Mohamed and Lakshminarayanan, 2016).
The amortisation framework is in similar spirit to (Snelson and Ghahramani, 2005; Korattikara et al., 2015) in that both approaches “distill” an MCMC sampler with a parametric model. Unlike the proposed framework, Snelson and Ghahramani (2005) and Korattikara et al. (2015) used a student model to approximate the predictive likelihood, and that student model is not used to initialise the MCMC transitions. We believe that initialising MCMC with the student model is important in amortising dynamics, as the teacher can “monitor” the student’s progress and provide learning signals tailored to the student’s need. Moreover, since the initialisation is improved after each student update, the quality of the teacher’s samples also improves. Another related, but different approach (Rasmussen, 2003) considered speeding-up Hybrid Monte Carlo by approximating the transition kernel using a Gaussian process model. Amortised MCMC could also benefit from this line of research if the MCMC samples are too expensive to simulate.

Perhaps the most related approaches to our framework (in the sense of using q of very flexible form) are operator variational inference (OPVI, Ranganath et al. (2016a)), Stein-GAN (Wang and Liu, 2016), and adversarial variational Bayes (AVB, Mescheder et al. (2017)). These works assumed the q distribution to be represented by a neural network warping the input noise (example 1). OPVI minimises Stein discrepancy (Stein, 1972) between the exact and approximate posterior, where the optimal test function is determined by optimising a discriminator. Though theoretically appealing, this method seems still impractical for large scale problems. SteinGAN can be viewed as a special case of our framework, which specifically uses a deterministic Stein variational gradient dynamic (Liu and Wang, 2016) and an l2-norm as the divergence measure. AVB estimates the KL-divergence term D_{KL}(q||p_{0}) in the variational lower-bound (10) with GAN and density ratio estimation methods, making it closely related to the adversarial autoencoder (Makhzani et al., 2015). However we conjecture that the main learning signal of AVB comes from the “reconstruction error” term \( E_{q}[\log p(x|z, \theta)] \), and the regularisation power strongly depends on the adversarial estimation of D_{KL}(q||p_{0}), which presumably is very weak as the discriminator is non-optimal in almost all cases.

6. Experiments

We evaluate amortised MCMC with both toy and real-world examples. For simplicity we refer the proposed framework as AMC.

6.1. Mixture of Gaussians

We first consider fitting a Gaussian mixture \( p(z) = \frac{1}{2}N(z; -3, 1) + \frac{1}{2}N(z; 3, 1) \) with the variational program proposed by (Ranganath et al., 2016a) as the following:

\[ \epsilon_1, \epsilon_2, \epsilon_3 \sim N(0, 1), z = \mathbb{1}_{\epsilon_1 \geq 0} \text{ReLU}(w_1 \epsilon_1 + b_1) - \mathbb{1}_{\epsilon_3 < 0} \text{ReLU}(w_2 \epsilon_2 + b_2). \]

We further tested a small multilayer perceptron (MLP) model of size \([3, 20, 20, 1]\) which warps the same Gaussian noise input as the variational program to the samples. The Jensen-Shannon divergence is adversarially estimated with an MLP of the same architecture. The MCMC sampler used is Langevin dynamics with rejection (Roberts and Rosenthal, 1998), and in training 10 parallel Markov chains are used. The fitted approximations are visualised in Figure 1(a) (variational program in red and MLP in blue; best viewed in colour). Both models cover both modes, however the variational program performs better in terms of estimating the variance of each Gaussian component. This indicates that intelligent design of the q network can achieve better performance with much fewer number of parameters.

We empirically investigate the effect of chain length \( T \) on the approximation quality using the MLP approximation. Time steps \( T = 1, 5, 10 \) with step-sizes \( \eta = 0.1, 0.02, 0.01 \) are tested (each repeating 10 times), where by making \( T \eta = 1.0 \) a constant, the particles approximately move equal distances during MCMC transitions. Results are depicted in Figure 1(b), where the measure in use is the Kernel Stein Discrepancy (KSD, Liu et al. (2016)) whose computation does not require a tractable q density. With small chain length the student quickly learns the posterior shape, but running more MCMC transitions results in better approximation accuracy. A potential way to balance the time-accuracy trade-off is to initially use short Markov chains for AMC, but to lengthen them as AMC converges. This strategy has been widely applied to contrastive-divergence like methods (Hinton, 2002; Salakhutdinov and Murray, 2008). We leave the exploration of this idea to future work.

6.2. Deep Generative Models

We next consider training deep generative models on the dynamically binarised MNIST dataset, containing 60,000 training datapoints and 10,000 test images (Burda et al., 2016). For benchmark a convolutional VAE with dim(z) =
32 latent variables is tested. The Gaussian encoder consists of a convolutional network with $5 \times 5$ filters, stride 2 and $[16, 32, 32]$ feature maps, followed by a fully connected network of size $[500, 32 \times 2]$. The generative model has a symmetric architecture but with stride convolution replaced by deconvolution layers. This generative model architecture is fixed for all the tests. We also test AMC with inclusive KL divergence on Gaussian encoders, and compare to the naïve approach which trains the encoder by maximising variational lower-bound (MCMC-VI).

We construct two non-Gaussian encoders for tests of AVB and AMC. Both encoders start from a CNN with $3 \times 3$ filters, stride 2 and $[32, 64, 128, 256]$ feature maps, followed by a reshaping operation. Then the first model (CNN-G) splits the output vector of the CNN into $[h(x), \mu(x), \log \sigma(x)]$, samples a Gaussian noise variable of 32 dimensions $\epsilon \sim \mathcal{N}(\epsilon; \mu(x), \text{diag}([\sigma^2(x)]))$, and feeds $[h(x), \epsilon]$ to an MLP which has hidden layer sizes $[500, 500, 32]$. The second encoder (CNN-B) simply applies multiplicative Bernoulli noise with dropout rate 0.5 to the CNN output vector, and uses the same MLP architecture as CNN-G. A discriminator is trained for AVB and AMC methods, with a CNN (of the same architecture as the encoder) acting on the input image $x$ only, and a MLP of $[32+1024, 500, 500, 1]$ layers. All networks use leaky ReLU activation functions with slope parameter 0.2, except for the output of the deconvolution network which uses sigmoid activation. Batch normalisation is applied to non-Gaussian encoders and the discriminator. The Adam optimiser (Kingma and Ba, 2015) is used with learning rates tuned on the last 5000 training images. Rejection steps are not used in the Langevin dynamics as we found this slows down the learning.

6.2.1. Missing data imputation

First we consider missing data imputation with pixels missing from contiguous sections of the image, i.e. not at random. In this case we remove the pixels in the lower half of the input image, making the imputation task an underdetermined inverse problem. We follow (Rezende et al., 2014) using an approximate Gibbs sampling procedure for imputation. With observed and missing pixels denoted as $x_o$ and $x_m$, the approximate sampling procedure iteratively applies the following transition steps:

1. sample $z \sim q(z|x_o, x_m)$ given the imputation $x_m$;
2. sample $x^* \sim p(x^*|z, \theta)$ and set $x_m \leftarrow x_m^*$.

In other words, the encoder $q(z|x)$ is used to approximately generate samples from the exact posterior. As ambiguity exists, the exact conditional distribution $p(x_m|x_o, \theta)$ is expected to be multi-modal here.

We visualise the imputed images in Figure 2, where starting from the third column the remaining ones show samples for every 2 Gibbs steps. More imputation results are shown in the appendix. Clearly the approximate Gibbs sampling for the benchmark VAE is trapped in local modes due to the uni-modal approximation $q$ to the exact posterior. On the other hand, models trained with AMC return diverse imputations that vary quickly, as an example, CNN-B returns imputed images for digit “9” with answers 2, 0, 9, 3 and 8. To quantify this diversity, we simulate the approximate Gibbs sampling for $T = 100$ steps on the first 100 test datapoints (10 images for each digit class), find the nearest neighbour in $l_1$-norm of these imputed images in the training dataset, and then compute the entropy on the label distribution over these training images. The entropy values and the average $l_1$-distance to the nearest neighbours are presented in Table 1. These metrics indicate that AMC trained models generate more diverse imputations compared to VAE, yet these imputed images are about the same distance from the training data.

6.2.2. Test log-likelihood results

Next we report the test log-likelihood results in Table 2. Here we follow (Burda et al., 2016) to compute the test log-likelihood with 5000 importance samples, and for the

![Figure 2. Imputation results from benchmark VAE and non-Gaussian encoders (trained with AMC, $T = 50$ and $\eta = 0.02$).](image)

| Dataset | VAE | CNN-G | CNN-B |
|---------|-----|-------|-------|
| Entropy | $0.411 \pm 0.0389$ | $0.701 \pm 0.0476$ | $0.933 \pm 0.0491$ |
| $l_1$-norm | $0.061 \pm 0.0002$ | $0.059 \pm 0.0001$ | $0.064 \pm 0.0002$ |

Table 1. Label entropy on nearest neighbours. The $l_1$ distance is divided by the number of pixels $\text{dim}(x) = 784$ in the image.
Table 2. Average Test log-likelihood (LL/nats).

| Encoder | Method | LL     | ESS   |
|---------|--------|--------|-------|
| Gaussian| VAE    | -81.31 | 104.11|
|         | MCMC-VI, $T = 5$, $\eta = 0.2$ | -84.38 | 65.64 |
|         | AMC, $T = 5$, $\eta = 0.2$    | -96.04 | 68.94 |
| CNN-G   | AMC, $T = 5$, $\eta = 0.2$    | -90.84 | 31.60 |
|         | AMC, $T = 50$, $\eta = 0.02$  | -83.30 | 6.84  |
|         | AVB    | -94.97 | 11.30 |
| CNN-B   | AMC, $T = 5$, $\eta = 0.2$    | -90.75 | 34.17 |
|         | AMC, $T = 50$, $\eta = 0.02$  | -83.62 | 8.88  |
|         | AVB    | -89.47 | 8.98  |

Figure 3. Samples from the approximate posterior $q$ (in green), the teacher’s distribution $q_T$ (in blue), and a 1-sigma contour plot of the Gaussian evaluator (red dash lines). Model in test is with the setting CNN-B + AMC, $T = 50$ and $\eta = 0.02$.

Figure 4. Samples from the trained generative models. Non-Gaussian encoders are trained with AMC, $T = 50$ and $\eta = 0.02$.

non-Gaussian encoders we train another Gaussian encoder with VI as the proposal distribution. VAE remains the best method by this metric, and the best AMC model is about 2nats behind. However we doubt if importance sampling is appropriate for evaluating models trained using wild approximations, especially for those trained by AMC. The approximate MLE using the variational lower-bound biases the generative network towards the model whose exact posterior is close to the inference network $q$ (Turner and Sahani, 2011). As the MCMC-guided approximate MLE trains the generative model with $q_T$ (which could be highly non-Gaussian), the VI-fitted Gaussian proposal, employed in the IWAE, can under-estimates the true test log-likelihood by a significant amount.

To quickly verify this we also compute an empirical estimate of the effective sample size (ESS), where these values are significantly smaller than that of the benchmark VAE for models trained with non-Gaussian encoders. We further visualise in Figure 3 the samples from the learned encoder $q$ conditioned on a test image, the teacher’s sample distribution $q_T$, and the trained Gaussian distribution for importance sampling (only the first dimensions are shown). We find that $q_T$ is non-Gaussian and has a long tail that is not axis aligned. This means a mean-field Gaussian distribution is a bad proposal in this case and this explains small effective sample size we got. As the stochastic IWAE lower-bound improves as the number of (effective) samples increases, this suggests that the values reported here may significantly under-estimate the true test log-likelihood. Future work should evaluate the test log-likelihood results with robust estimation methods, e.g. bidirectional Monte Carlo (Grosse et al., 2015; Wu et al., 2017).

Although test log-likelihood is an important measures of model quality, Theis et al. (2016) has shown that this metric is often largely orthogonal to one that tests visual fidelity when the data is high dimensional. We visualise the generated images in Figure 4, and we see that AMC trained models produce samples of similar quality to VAE samples.

7. Conclusion and Future Work

We have proposed an MCMC amortisation algorithm which deploys a student-teacher framework to learn the approximate posterior. By using adversarially estimated divergences, the algorithm allows approximations of arbitrary form to be learned. Application to training deep generative networks returned models that could generate high quality images, and the learned approximation captured multi-modality in generation. Future work should cover both theoretical and practical directions. Convergence of the amortisation algorithm will be studied. Flexible approximations will be designed to capture multi-modality. Efficient MCMC samplers should be applied to speed-up the fitting process. Practical algorithms for approximating discrete distributions will be further developed.
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A. Approximate MLE with MCMC: Mathematical Details

In main text we stated that $D_{KL}[q||p] \geq D_{KL}[q_T||p]$ if $q$ is the stationary distribution of the kernel $K$. This is a direct result of the following lemma, and we provide a proof from (Cover and Thomas, 1991) for completeness.

**Lemma 1.** (Cover and Thomas, 1991) Let $q$ and $r$ be two distributions for $z_0$. Let $q_t$ and $r_t$ be the corresponded distributions of state $z_t$ at time $t$, induced by the transition kernel $K$. Then $D_{KL}[q_t||r_t] \geq D_{KL}[q_t+1||r_t+1]$ for all $t \geq 0$.

**Proof.**

$$D_{KL}[q_t||r_t] = \mathbb{E}_{q_t} \left[ \log \frac{q_t(z_t)}{r_t(z_t)} \right] = \mathbb{E}_{q_t} (z_t) \mathbb{K}(z_{t+1}|z_t) \left[ \log \frac{q_t(z_t)\mathbb{K}(z_{t+1}|z_t)}{r_t(z_t)\mathbb{K}(z_{t+1}|z_t)} \right]$$

$$= \mathbb{E}_{q_{t+1}(z_{t+1})q_t+1(z_t|z_{t+1})} \left[ \log \frac{q_t(z_t)\mathbb{K}(z_{t+1}|z_t)}{r_t(z_t)\mathbb{K}(z_{t+1}|z_t)} \right]$$

$$= D_{KL}[q_{t+1}||r_{t+1}] + \mathbb{E}_{q_{t+1}} D_{KL}[q_{t+1}(z_t|z_{t+1})||r_{t+1}(z_t|z_{t+1})].$$

B. Uncorrelated versus Correlated Simulations

In our algorithm, we generate $\{z_k^k\}$ by simulating Markov transition for $T$ steps starting from $\{z_k^0\} \sim q$, and use these two samples $\{z_k^0\}$ and $\{z_k^T\}$ to estimate the divergence $D[q_T||q]$. However, note that $\{z_k^0\}$ and $\{z_k^T\}$ is corrected, and this may introduce bias in the divergence estimation. A way to eliminate this correction is to simulate another $\{z_k^0\}$ independently and use it to replace the original sample. In practice, we find that the correlated/uncorrelated samples exhibit different behaviour during training. We consider the extreme case $K = 1$ and small $T$ as an example. Using correlated samples would cause the teacher and the student’s samples remaining in the same mode with high probability and thus easily confuse the discriminator and the student (generator) improves fast. On the other hand, if $z_T$ is simulated from a Markov chain independent with $z_0$, then these samples might be far away from each other (especially when $q$ is forced to be multimodal), hence the discriminator can easily get saturated, providing no learning signal to the student. The above problem could potentially be solved using advanced techniques, e.g. Wasserstein GAN (Arjovsky et al., 2017) which proposed minimising (an adversarial estimate of) Wasserstein-1 distance. In that case the gradient of $q$ won’t saturate even when the two sets of samples are separated. But minimising Wasserstein distance would fit the $q$ distribution to the posterior in an “optimal transport” way, which presumably prefers moving the $q$ samples to their nearest modes in the exact posterior.

C. More Visualisation Results
Figure 5. Samples of $q$ (in green), $q_T$ (in blue), and the 1-sigma contour plot for Gaussian evaluator (red dashed lines). Model tested is the CNN-B encoder, trained with AMC, $T = 50$, $\eta = 0.02$. 
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Figure 6. Missing data imputation results. Removing the lower half pixels.
Figure 7. Missing data imputation results. Removing the upper half pixels.
Figure 8. Missing data imputation results. Removing the right half pixels.
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Figure 9. Missing data imputation results. Removing the left half pixels.