Abstract

This work presents a new class of variational family—ergodic variational flows—that not only enables tractable i.i.d. sampling and density evaluation, but also comes with MCMC-like convergence guarantees. Ergodic variational flows consist of a mixture of repeated applications of a measure-preserving and ergodic map to an initial reference distribution. We provide mild conditions under which the variational distribution converges weakly and in total variation to the target as the number of steps in the flow increases; this convergence holds regardless of the value of variational parameters, though different parameter values may result in faster or slower convergence. We develop an implementation of the flow family using Hamiltonian dynamics combined with deterministic momentum refreshment, including a tunable step size to optimize the trade-off between simulation fidelity and computational cost. Simulated and real data experiments provide an empirical verification of the convergence theory, and demonstrate that the method provides more reliable posterior approximations than several black-box normalizing flows, as well as samples of comparable quality to those obtained from state-of-the-art MCMC methods.

1 Introduction

Bayesian statistical modelling and inference provides a principled approach to learning from data. However, for all but the simplest models, exact inference is not possible and computational approximations are required. A standard methodology for Bayesian inference is Markov chain Monte Carlo (MCMC) [Robert and Casella, 2004; Robert and Casella, 2011] Gelman et al., 2013 Ch. 11,12], which involves simulating a Markov chain whose stationary distribution is the Bayesian posterior distribution, and then treating the sequence of states as draws from the posterior. MCMC methods are supported by theory that guarantees that if one simulates the chain for long enough, Monte Carlo averages based on the sequence of states will converge to the exact posterior expectation of interest (e.g., Roberts and Rosenthal (2004)). This “exactness” property is quite compelling: regardless of how well one is able to tune the Markov chain, the method is guaranteed to eventually produce an accurate result given enough computation time. Nevertheless, it remains a challenge to assess and optimize the performance of MCMC in practice with a finite computational budget. One option is to use a Stein discrepancy (Gorham and Mackey, 2015; Liu et al., 2016; Chwialkowski et al., 2016; Gorham and Mackey, 2017; Anastasiou et al., 2021), which quantifies how well a set of MCMC samples approximates the posterior distribution. But standard Stein discrepancies are not reliable in the presence of multimodality (Wenliang and Kanagawa, 2020), are computationally expensive to estimate, and suffer from the curse of dimensionality, although recent work addresses the latter two issues to an extent (Huggins and Mackey, 2018; Gong et al., 2021). The other option is to use a traditional diagnostic, e.g., Gelman–Rubin (Gelman and Rubin, 1992; Brooks and Gelman, 1998), effective sample size (Gelman et al., 2013 p. 286), Geweke (1992), or others (Cowles and Carlin, 1996). These diagnostics detect mixing issues, but do not comprehensively quantify how well the MCMC samples approximate the posterior.

Variational inference (VI) [Jordan et al., 1999; Wainwright and Jordan, 2008; Blei et al., 2017] is an alternative to MCMC that does provide a straightforward quantification of posterior approximation error. In particular, VI involves approximating the posterior with a probability distribution—typically selected from a parametric family—that enables both i.i.d. sampling and density evaluation [Wainwright and Jordan, 2008; Rezende and Mohamed, 2015a; Ranganath et al., 2016; Papamakarios et al., 2021]. Because one can take i.i.d. draws and evaluate the density, one can estimate the Kullback-Leibler (KL) divergence [Kullback and Leibler, 1951] to the posterior up to a constant. The ability to estimate this quantity, in turn, enables scalable tuning via straightforward stochastic gradient descent algorithms [Hoffman et al., 2013; Ranganath et al., 2014], optimally
mixed approximations [Jaakkola and Jordan, 1998; Gershman et al., 2012; Zobay et al., 2014; Guo et al., 2016; Wang et al., 2016; Miller et al., 2017; Locatello et al., 2018; Wolf et al., 2019], model selection (Corduneanu and Bishop, 2001; Masa-aki, 2001; Constantinopolous et al., 2006; Ormerod et al., 2017; Chéret-Abdelatif and Alquier, 2018; Tao et al., 2018), and more. VI typically does not possess the same “exactness regardless of tuning” that MCMC does. The optimal variational distribution is not usually equal to the posterior due to the use of a limited parametric variational family; and even if it were, one could not reliably find it in general due to nonconvexity of the KL objective [Xu and Campbell, 2022]. Recent work addresses this problem by constructing variational families from parametrized Markov chains targeting the posterior. Many are related to annealed importance sampling (Salimans et al., 2015; Wolf et al., 2016; Geffner and Domke, 2021; Zhang et al., 2021; Thun et al., 2021a; Jankowiak and Phan, 2021); these methods introduce numerous auxiliary random variables and have convergence guarantees in the limit of increasing dimension of the joint distribution. Those based on normalizing flows (Neal, 2005; Caterini et al., 2018; Chen et al., 2022) avoid the increase in dimension with flow length, but typically do not have guaranteed convergence to the target. Methods involving the final-state marginal of finite simulations of standard MCMC methods do not enable tractable i.i.d. sampling and density evaluation (Zhang and Hernandez-Lobato, 2020).

In this work, we introduce a variational flow family—ergodic variational flows—that provide both MCMC-like convergence guarantees and tractable i.i.d. sampling and density evaluation (and hence ELBO estimates [Blei et al., 2017]). Ergodic variational flows are constructed by mixing over repeated application of a measure-preserving, ergodic map. Sampling using measure-preserving and ergodic maps, as well as mixed averages of pushforward distributions has appeared in past literature in various contexts (Aldous and Thomasson, 1993; Roberts and Rosenthal, 1997; Warren and Allen, 2018; Rotkoff and Vanden-Eijnden, 2019; Steeg and Galstyan, 2021; Thun et al., 2021b; Neklyudov and Welling, 2022), but our work is the first to construct a variational family and provide convergence theory. In particular, our main theoretical results (Theorems 3.1 and 3.2) provide mild conditions under which the ergodic variational distribution converges weakly and in total variation to the target as the number of flow steps increases. Since these results hold for any value of the variational parameter, we are assured that our method targets the right distribution regardless of the result of tuning—as in MCMC. But since we can take i.i.d. draws and evaluate the density, we have access to the ELBO, which enables variational parameter optimization. We present a practical instantiation of the general methodology based on Hamiltonian dynamics, with a discretization that can be tuned by maximizing the ELBO. Simulated and real data experiments verify the convergence of ergodic variational flows and showcase their performance in comparison to the No-U-Turn sampler (NUTS) (Hoffman and Gelman, 2014), standard Hamiltonian Monte Carlo (HMC) (Neal, 2011), and several black-box normalizing flows (rezende and Mohamed, 2015b; Dinh et al., 2017). Our results demonstrate a comparable output sample quality to NUTS, similar computational efficiency to HMC, and more reliable posterior approximations than standard normalizing flows.

2 Background

2.1 Variational inference with flows

Consider a set $\mathcal{X} \subseteq \mathbb{R}^d$ and a target probability distribution $\pi$ on $\mathcal{X}$ whose density with respect to the Lebesgue measure we denote $\pi(x)$ for $x \in \mathcal{X}$. In the setting of Bayesian inference, $\pi$ is the posterior distribution that we aim to approximate, and we are only able to evaluate a function $\pi(x)$ such that $\pi(x) = Z \cdot \pi(x)$ for some unknown normalization constant $Z > 0$. Throughout, we will assume all distributions have densities with respect to the Lebesgue measure on $\mathcal{X}$, and will use the same symbol to denote a distribution and its density; it will be clear from context what is meant.

Variational inference involves approximating the target distribution $\pi$ by minimizing the Kullback-Leibler (KL) divergence from $\pi$ to members of a parametric family $\{q_\lambda : \lambda \in \Lambda\}$, $\Lambda \subseteq \mathbb{R}^p$, i.e.,

$$\lambda^* = \arg\min_{\lambda \in \Lambda} D_{KL}(q_\lambda || \pi) = \arg\min_{\lambda \in \Lambda} \int q_\lambda(x) \log \frac{q_\lambda(x)}{\pi(x)} dx.$$

(1)

The two objective functions in Eq. (1) differ only by the constant $\log Z$. In order to be able to optimize $\lambda$ using standard techniques, the variational family $q_\lambda$, $\lambda \in \Lambda$ must enable both i.i.d. sampling and density evaluation. A common approach to constructing such a family is to pass draws from a simple reference distribution $q_0$ through a measurable function $T_\lambda : \mathcal{Y} \rightarrow \mathcal{X}$; $T_\lambda$ is often referred to as a flow when comprised of repeated composed functions (Tabak and Turner, 2013; rezende and Mohamed, 2015a; kobyzev et al., 2021). If $T_\lambda$ is a diffeomorphism, i.e., differentiable and has a differentiable inverse, then we can express the density of $X = T_\lambda(Y)$, $Y \sim q_0$ as

$$\forall x \in \mathcal{X}, q_\lambda(x) = \frac{q_0(T_\lambda^{-1}(x))}{J_\lambda(T_\lambda^{-1}(x))}, J_\lambda(x) = |\det \nabla_x T_\lambda(x)|.$$

(2)

In this case the optimization in Eq. (1) can be rewritten using a transformation of variables as

$$\lambda^* = \arg\min_{\lambda \in \Lambda} \int q_0(x) \log \frac{q_0(x)}{J_\lambda(x)p(T_\lambda(x))} dx.$$

(3)

One can solve the optimization problem Eq. (3) using unbiased stochastic estimates of the gradient$^7$ with respect to

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$^7$We assume throughout that differentiation and integration can be swapped wherever necessary.
\( \lambda \) based on draws from \( q_0 \) (Salimans and Knowles [2013], Kingma and Welling [2014]).

\[
\nabla_\lambda D_{KL}(q_\lambda || \pi) \approx \nabla_\lambda \log \frac{q_0(X)}{q_\lambda(X)p(T_\lambda(X))}, \ X \sim q_0.
\]

2.2 Measure-preserving and ergodic maps

Variational flows are often constructed from a flexible, general-purpose parametrized family \( \{T_\lambda : \lambda \in \Lambda\} \) that is not specialized for any particular target distribution (Pamakarios et al. [2021]); it is the job of the KL divergence minimization Eq. (5) to adapt the parameter \( \lambda \) such that \( q_\lambda \) becomes a good approximation of the target \( \pi \). However, there are certain functions—in particular, those that are both measure-preserving and ergodic for \( \pi \)—that naturally provide a means to approximate expectations of interest under \( \pi \) without the need for tuning. Intuitively, a measure-preserving map \( T \) will not change the distribution of draws from \( \pi \); if \( X \sim \pi \), then \( T(X) \sim \pi \). And an ergodic map \( T \), when applied repeatedly, will not get “stuck” in a subset of \( \mathcal{X} \) unless it has probability either 0 or 1 under \( \pi \). The precise definitions are given in Definitions 2.1 and 2.2.

**Definition 2.1** (Measure-preserving map (Eisner et al. [2015], pp. 73, 105)). A measurable function \( T : \mathcal{X} \to \mathcal{X} \) is measure-preserving for \( \pi \) if \( \pi(T^{-1}(A)) = \pi(A) \) for each measurable set \( A \subseteq \mathcal{X} \).

**Definition 2.2** (Ergodic map (Eisner et al. [2015], pp. 73, 105)). A measurable function \( T : \mathcal{X} \to \mathcal{X} \) is ergodic for \( \pi \) if for all measurable sets \( A \subseteq \mathcal{X} \), \( T(A) = A \) implies that \( \pi(A) \in \{0, 1\} \).

If a map \( T \) satisfies both Definitions 2.1 and 2.2, then long-run averages resulting from repeated applications of \( T \) will converge to expectations under \( \pi \), as shown by Theorem 2.3.

**Theorem 2.3** (Ergodic Theorem [Birkhoff [1931], Eisner et al. [2015] p. 212]). Suppose \( T : \mathcal{X} \to \mathcal{X} \) is measure-preserving and ergodic for \( \pi \), and \( f \in L^1(\pi) \). Then

\[
\lim_{N \to \infty} \frac{1}{N} \sum_{n=0}^{N-1} f(T^n x) = \int f d\pi \quad \pi\text{-a.e.} \ x \in \mathcal{X}.
\]

Fig. 1a provides an example illustration of this result when \( \pi \) is the uniform distribution \( \text{Unif}[0, 1] \), \( T : [0, 1] \to [0, 1] \) is the shift map \( T(x) = x + \lambda \mod 1 \) for some \( \lambda \in \mathbb{R} \), and \( x \) is initialized to 0.5. In particular, for any irrational \( \lambda \in \mathbb{R} \) (here \( \pi/16 \)), the shift map is both measure-preserving and ergodic for \( \pi \). As the number of applications increases, the collection of iterates \( (T^n x)_{n=1}^{\infty} \) forms a discrete approximation to \( \text{Unif}[0, 1] \). On the other hand, for a rational \( \lambda \in \mathbb{R} \) (here \( 1/4 \)), the shift map is measure-preserving but not ergodic. In this case the iterates are trapped in the finite set \( \{0, 0.25, 0.5, 0.75, 1\} \) and do not approximate \( \text{Unif}[0, 1] \).

3 Ergodic variational flows

In this section, we develop a parametrized family of ergodic variational flows that enable tractable i.i.d. sampling and density evaluation, and that converge to the target distribution both weakly and in total variation in the limit of increasingly many flow steps (Theorems 3.1 and 3.2) regardless of parameter tuning effort. Thus, ergodic variational flows provide the same compelling convergence result as MCMC, but with the added benefit of i.i.d. sampling and density evaluation, and hence unbiased ELBO estimates.

3.1 Variational family

Define a reference distribution \( q_0 \) on \( \mathcal{X} \) for which i.i.d. sampling and density evaluation is tractable, and a collection of measurable functions \( T_\lambda : \mathcal{X} \to \mathcal{X} \) parametrized by \( \lambda \in \Lambda \) such that for each parameter value \( \lambda \), the map \( T_\lambda \) is measure-preserving and ergodic for \( \pi \). Then the ergodic variational flow family generated by \( q_0 \) and \( T_\lambda \) is the collection of distributions

\[
q_{\lambda,N} = \frac{1}{N} \sum_{n=0}^{N-1} T^n q_0 \quad \text{for} \quad \lambda \in \Lambda, \ N \in \mathbb{N},
\]

where \( T^n q_0 \) denotes the pushforward of the distribution \( q_0 \) under \( n \) repeated applications of \( T_\lambda \). Fig. 1b displays a simple example of this family where \( q_0 \) is a mixture of beta distributions \( q_0 = 0.6 \cdot \text{Beta}(2, 6) + 0.4 \cdot \text{Beta}(6, 1) \).

Figure 1: The effect of the shift map \( T(x) = x + \lambda \mod 1 \) for shift \( \lambda \in \mathbb{R} \). Note that \( T \) is measure-preserving for \( \pi = \text{Unif}[0, 1] \). Green denotes irrational \( \lambda = \pi/16 \), blue denotes rational \( \lambda = 1/4 \), and the red line shows the uniform density. (A): Starting from \( x = 0.5 \), repeated application of an irrational shift map eventually creates a discrete probability measure that converges weakly to \( \text{Unif}[0, 1] \); the rational shift map is periodic and so does not exhibit this behaviour. (B): Starting from a mixture of beta distributions, averaging over repeated applications of the shift map does converge to \( \text{Unif}[0, 1] \) in total variation when \( \lambda \) is irrational.
3.2 Convergence guarantees

In this section, we show that for all \( \lambda \in \Lambda \), the distribution \( q_{\lambda,N} \) converges to \( \pi \) as \( N \to \infty \) (proofs may be found in Appendix [A]). Thus, regardless of the ability to tune the parameter \( \lambda \), we are guaranteed that \( q_{\lambda,N} \) can approximately approximate \( \pi \) given enough computational effort (i.e., large enough \( N \)). In particular, we demonstrate this convergence in three senses: weak, setwise, and in total variation. Recall that a sequence of probability distributions \( q_n \) converges weakly to \( \pi \) if for all bounded, continuous \( f : \mathcal{X} \to \mathbb{R} \), \( \lim_{n \to \infty} \int f(x)q_n(dx) = \int f(x)\pi(dx) \), and converges setwise to \( \pi \) if for all measurable \( A \subseteq \mathcal{X} \), \( \lim_{n \to \infty} q_n(A) = \pi(A) \).

**Theorem 3.1.** Suppose \( q_0 \ll \pi \) and \( T_\lambda \) is measure-preserving and ergodic for \( \pi \). Then \( q_{\lambda,N} \) converges both setwise and weakly to \( \pi \) as \( N \to \infty \).

We obtain a stronger result—convergence in total variation—when we can express the density of \( q_{\lambda,N} \) using the transformation of variables formula Eq. (2). Recall that a sequence of distributions \( q_n \) converges in total variation to \( \pi \) if \( D_{TV}(q_n,\pi) = \sup_A |q_n(A) - \pi(A)| \to 0 \) as \( n \to \infty \).

**Theorem 3.2.** Suppose \( q_0 \ll \pi \), \( T_\lambda \) is a diffeomorphism, and \( T_{\lambda} \) is measure-preserving and ergodic for \( \pi \). Then \( q_{\lambda,N} \) converges in total variation to \( \pi \) as \( N \to \infty \).

This result is asymptotic in nature, which suffices for our purposes to guarantee that the family can well-approximate the target \( \pi \) in the large-\( N \) limit; in practice we use the ELBO (see Section 3.4) to tune \( \lambda \) and \( N \). Although similar nonasymptotic results exist for the ergodic average law of Markov chains [Roberts and Rosenthal 1997], the required technical conditions (minorization and drift conditions) do not apply to our deterministic setting. It is also worth noting that while Theorem 3.2 pertains to the total variation distance, the KL divergence is more relevant in the context of variational inference. However, a small total variation distance implies a small KL divergence in many practical scenarios, e.g., when the density ratio \( q(x)/\pi(x) \) is bounded (Proposition A.3 [Verdú 2014, Theorem 7]).

**Algorithm 1** Sample \( q_{\lambda,N} \): Take a draw from \( q_{\lambda,N} \)

**Require:** reference distribution \( q_0 \), flow map \( T_\lambda \), number of steps \( N \)

\[
\begin{align*}
K & \leftarrow \text{Sample(Uniform(0, 1, ..., N - 1))} \\
x_0 & \leftarrow \text{Sample}(q_0) \\
T_\lambda^K(x_0) & \leftarrow \end{align*}
\]

**Algorithm 2** \( \log q_{\lambda,N}(x) \): Evaluate the log-density of \( q_{\lambda,N} \)

**Require:** location \( x \), reference distribution \( q_0 \), flow map \( T_\lambda \), Jacobian \( J_\lambda \), number of steps \( N \)

\[
\begin{align*}
L & \leftarrow 0 \\
w_0 & \leftarrow \log q_0(x) \\
& \text{for } n = 1, \ldots, N - 1 \text{ do} \\
& \quad x \leftarrow T_\lambda^n(x) \\
& \quad L \leftarrow L + \log J_\lambda(x) \\
& \quad w_n \leftarrow \log q_0(x) - L \\
& \text{end for} \\
& \text{return } \log \text{SumExp}(w_0, \ldots, w_{N-1}) - \log N
\end{align*}
\]

**Algorithm 3** \( \text{EstELBO}(\lambda, N) \): Obtain an unbiased estimate of the ELBO for \( q_{\lambda,N} \)

**Require:** reference \( q_0 \), unnormalized target \( p \), flow map \( T_\lambda \), Jacobian \( J_\lambda \), number of flow steps \( N \)

\[
\begin{align*}
x_0 & \leftarrow \text{Sample}(q_0) \\
J_0 & \leftarrow J_\lambda(x_0) \\
& \text{for } n = 1, \ldots, N - 1 \text{ do} \\
& \quad x_n \leftarrow T_\lambda(x_{n-1}) \\
& \quad J_n \leftarrow J_\lambda(x_n) \\
& \quad x_{n+1} \leftarrow T_\lambda^{-1}(x_{n+1}) \\
& \quad J_{n+1} \leftarrow J_\lambda(x_{n+1}) \\
& \text{end for} \\
J & \leftarrow \prod_{j=1}^{N-1} J_{n+1} \\
& \text{for } n = 1, \ldots, N - 1 \text{ do} \\
& \quad q_n \leftarrow \frac{1}{N} q_0(x_{n-1})/J \\
& \quad z_n \leftarrow \log \left( \frac{z_{n+1} - q_n}{J_{n+1} + \frac{1}{N} q_0(x_n)} \right) \\
& \text{if } n < N - 1 \text{ then} \\
& \quad J \leftarrow J \cdot J_{n+1}/J_{n+1} \\
& \text{end if} \\
& \text{return } \log \text{SumExp}(w_0, \ldots, w_{N-1}) - \log z_n
\end{align*}
\]

3.3 Density evaluation and sampling

If \( T_\lambda : \mathcal{X} \to \mathcal{X} \) is a diffeomorphism with Jacobian \( J_\lambda \), we can express the density of \( q_{\lambda,N} \) by using a transformation of variables formula on each component in the mixture:

\[
q_{\lambda,N}(x) = \frac{1}{N} \sum_{n=0}^{N-1} \frac{q_0(T_{\lambda}^{-n}x)}{\prod_{j=1}^{n} J_\lambda(T_{\lambda}^{-j}x)}.
\]

This density can be computed efficiently using \( N - 1 \) evaluations of \( T_{\lambda}^{-1} \) and \( J_\lambda \) each (Algorithm 2). For sampling, we can obtain an independent draw \( X \sim q_{\lambda,N} \) by treating
We refer to this estimate as the trajectory-averaged estimate of \( f(x)q_{\lambda,N}(dx) \).

We refer to this estimate as the trajectory-averaged estimate of \( f \). The trajectory-averaged estimate of \( f \) is preferred over the naïve estimate based on a single draw \( f(X) \), \( X \sim q_{\lambda,N} \), as its cost is of the same order \( (N-1) \) applications of \( T_\lambda \) but it typically has a significantly lower variance; see Proposition A.1.

### 3.4 ELBO estimation

We can minimize the KL divergence from \( q_{\lambda,N} \) to \( \pi \) by maximizing the ELBO \( \mathbb{E}[\log p(x)q_{\lambda,N}(x)] \), given by

\[
\text{ELBO}(\lambda, N) = \frac{1}{N} \sum_{n=0}^{N-1} \log p(T^n \lambda X_0) q_{\lambda,N}(T^n \lambda X_0). \tag{4}
\]

The naïve method to compute this estimate—sampling \( X_0 \) and then computing the log density ratio for each term—requires \( O(N^2) \) computation because each evaluation of \( q_{\lambda,N}(x) \) is \( O(N) \). Algorithm 3 provides an efficient way of computing \( \text{ELBO}(\lambda, N) \) in \( O(N) \) operations, which is on par with taking a single draw from \( q_{\lambda,N} \) or evaluating \( q_{\lambda,N}(x) \) once. The key insight in Algorithm 3 is that we can evaluate the collection of values \( \{q_{\lambda,N}(X_0), q_{\lambda,N}(T_\lambda X_0), \ldots, q_{\lambda,N}(T_{(N-1)} \lambda X_0)\} \) incrementally, starting from \( q_{\lambda,N}(X_0) \) and iteratively computing each \( q_{\lambda,N}(T^n \lambda X_0) \) for increasing \( n \) in constant time. Note that Algorithm 3 still requires \( O(N) \) memory; Algorithm 5 in Appendix B provides an \( O(N) \) time, \( O(1) \) memory implementation of Eq. (4).

### 3.5 Numerical stability

Density evaluation (Algorithm 2) and ELBO estimation (Algorithm 3) both involve repeated applications of \( T_\lambda \) and \( T^{-1}_\lambda \). This poses no issue in theory, but in a computer—where floating point computations are used—it is critical to code the map \( T_\lambda \) and its inverse \( T^{-1}_\lambda \) in a numerically precise way such that the composition of \( (T^n_\lambda) \circ (T^{-K}_\lambda) \) is the identity map for large \( K \in \mathbb{N} \). In practice, we check the limits of stability of our flow implementation by taking draws from \( q_0 \) and evaluating \( T^K \lambda \) followed by \( T^{-K}_\lambda \) (and vice versa) for increasing \( K \) until we cannot reliably invert the flow. See Fig. 7 in the appendix for an example usage of this diagnostic. Note that for sample generation specifically (Algorithm 1), numerical stability is not a concern as it only requires forward evaluation of the map \( T_\lambda \).

### 4 Hamiltonian ergodic variational flows

In this section, we provide an implementation of an ergodic variational flow based on Hamiltonian dynamics. The construction is inspired by Hamiltonian Monte Carlo (HMC) \cite{Neal:2011,Neal:1996}, in which each iteration involves simulating Hamiltonian dynamics followed by a stochastic momentum refreshment; our method replaces the stochastic refreshment with a deterministic transformation. In particular, consider the augmented target density on \( \mathcal{X} \times \mathbb{R}^d \times [0, 1] \),

\[
\tilde{\pi}(x, \rho, u) = \pi(x) m(\rho) \mathbb{I}[0 \leq u \leq 1], \quad m(\rho) = \prod_{i=1}^d r(\rho_i),
\]

with auxiliary variables \( \rho \in \mathbb{R}^d, u \in [0, 1] \), and some almost-everywhere differentiable univariate probability density \( r : \mathbb{R} \to \mathbb{R}_+ \). The \( x \)-marginal distribution of \( \tilde{\pi} \) is the original target distribution \( \pi \); therefore if we are able to obtain i.i.d. draws from \( \tilde{\pi} \), we can obtain i.i.d. draws from \( \pi \) by simply discarding the \( \rho \) and \( u \) components. We construct \( T_\lambda \) by composing the following three steps in sequence:

1. **Hamiltonian dynamics** We first apply

   \[
   (x', \rho') \leftarrow H_L(x, \rho),
   \]

   where \( H_L : \mathcal{X} \times \mathbb{R}^d \to \mathcal{X} \times \mathbb{R}^d \) is the map of Hamiltonian dynamics with position \( x \) and momentum \( \rho \) simulated for a time interval of length \( L \in \mathbb{R}_+ \).

   \[
   \frac{d\rho}{dt} = \nabla \log \pi(x) \quad \frac{dx}{dt} = -\nabla \log m(\rho). \tag{5}
   \]

   One can show that this preserves density (and hence is measure preserving) and it is also unit Jacobian \cite{Neal:2011}.

2. **Pseudotime shift** Second, we apply a constant shift to the pseudotime variable \( u \),

   \[
   u' \leftarrow u + \xi \mod 1,
   \]

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where $\xi \in \mathbb{R}$ is a fixed irrational number (say, $\xi = \pi/16$). As this is a constant shift, it is unit Jacobian and density-preserving (and hence measure-preserving). The $u$ component will act as a notion of “time” of the flow, and ensures that the refreshment of $\rho$ in step (3) below will take a different form even if $x$ visits the same location again.

(3) Momentum refreshment  Finally, we refresh the momentum variables via

$$\forall i = 1, \ldots, d, \quad \rho_i^t \leftarrow R^{-1}(R\rho_i^t + z(x^t, u^t) \mod 1),$$

where $R$ is the cumulative distribution function (CDF) of density $r$, and $z : \mathcal{X} \times [0, 1] \to \mathbb{R}$ is a differentiable “pseudorandom” function, e.g., $z(x_i, u) = \sin(ax_i + u)$ for some large value of $a \in \mathbb{R}$; this generalizes the map from Neal (2012); Murray and Elliott (2012) to enable the shift to depend on the state $x$ and pseudotime $u$. In essence, this step (3) is an attempt to replicate the independent resampling of $\rho \sim m$ from HMC using only deterministic maps. This map is measure-preserving as it involves mapping the momentum to a Unif$[0, 1]$ random variable via the CDF, shifting by an amount that only depends on $x$, $u$, and then mapping back using the inverse CDF. The Jacobian is the joint momentum density ratio $m(\rho')/m(\rho^t)$.

Composition of (1-3) The composition of these three steps forms a measure-preserving map $T_\lambda$ for the augmented target $\hat{\pi}$. Note that the variational parameter $\lambda$ can include any parameter in these steps that maintains the measure-preserving nature of $T_\lambda$. For example, $\lambda = (L, \xi)$, where $L \in \mathbb{R}_+$ is the simulation length in step 1 and $\xi \in \mathbb{R}$ is the shift parameter in step 2.

Practical implementation In practice, we cannot simulate the dynamics in step (1) perfectly. Instead, we approximate the dynamics in Eq. [5] by running $L$ steps of the leapfrog method, where each leapfrog map $\hat{H}_L : \mathbb{R}^{2d} \to \mathbb{R}^{2d}$ involves interleaving three discrete transformations with step size $\epsilon > 0$,

$$\hat{\rho}_{k+1} = \rho_k + \epsilon \nabla \log \pi(x_k),$$

$$x_{k+1} = x_k - \epsilon \nabla \log m(\hat{\rho}_{k+1})$$

$$\rho_{k+1} = \hat{\rho}_{k+1} + \frac{\epsilon}{2} \nabla \log \pi(x_{k+1}).$$

Denote the map $T_{\hat{\lambda}_\epsilon}$ to be the composition of the three steps with Hamiltonian dynamics replaced by the leapfrog integrator; Algorithm 8 provides the pseudocode in Appendix C. Note that this map does not maintain invariance of $\hat{\pi}$ due to the discretized steps. To address this, we could make $T_{\hat{\lambda}_\epsilon}$ arbitrarily close to measure-preserving by making $\epsilon$ quite small; but rather than that, we can simply tune $\epsilon$ as a variational parameter in addition to $\lambda$ by maximizing the ELBO. Indeed, in our experiments, we find that the optimal step size $\epsilon$ is not vanishingly small, but instead trades off simulation fidelity and computational efficiency.

In our experiments we tune the number of leapfrog steps $\lambda = L$ and the step size $\epsilon$ by maximizing the ELBO. We also tune the number of refreshments $N$ to achieve a desirable computation-quality tradeoff by visually inspecting the convergence of the ELBO.

5 Experiments

In this section, we demonstrate the performance of our method (ErgFlow) on 7 synthetic and 7 real data targets, which include a range of challenging features such as heavy tails, high dimensions, multimodality, and weak identifiability. We compare the posterior approximation quality against several black-box normalizing flow methods (NF): PlanarFlow, RadialFlow, and RealNVP with various architectural settings (Papamakarios et al. 2021). To make the methods comparable via the ELBO, we train all NFs on the same joint space as ErgFlow. We also compare the marginal sample quality of ErgFlow against 5,000 samples from NUTS and NFs. Finally, we compare sampling time with all competitors, and effective sample size (ESS) per second with HMC. For all experiments, we use the standard Laplace distribution as the momentum distribution; although Gaussians are more commonly used in HMC, we find that the Laplace was more numerically stable to work with (see Fig. 7 in Appendix E). More experimental details may be found in Appendix C. All experiments were conducted on a machine with an AMD Ryzen 9 3900X and 32GB of RAM.
5.1 Qualitative assessment

We begin with a qualitative examination of the i.i.d. samples and the approximated targets produced by ErgFlow initialized at $q_0 = N(0, 1)$ for three one-dimensional synthetic distributions: a Gaussian, a mixture of Gaussians, and the standard Cauchy. We excluded the pseudotime variable $u$ here in order to visualize the full joint density of $(x, \rho)$ in 2 dimensions. More details can be found in Appendix E.1. Figs. 2a to 2c show histograms of 10,000 i.i.d. $x$-marginal samples generated by ErgFlow for each of the three targets, all of which nearly perfectly match the true target marginals. Figs. 2d to 2g also show that log $q_{0,N}$ is generally a good approximation of the log joint target density.

We then present similar visualizations on four more challenging synthetic target distributions: the banana (Haario et al., 2001), Neal’s funnel (Neal, 2003), a cross-shaped Gaussian mixture, and a warped Gaussian. All four examples have a 2-dimensional state $x \in \mathbb{R}^2$, and hence $(x, \rho, u) \in \mathbb{R}^5$. In each example we set the initial distribution $q_0$ to be the mean-field Gaussian approximation. More details can be found in Appendix E.2. Figs. 2d to 2g shows the scatter plots consisting of 1,000 i.i.d. $x$-marginal samples drawn from ErgFlow, as well as the approximated ErgFlow log density and exact log density sliced as a function of $x \in \mathbb{R}^2$ for a single value of $(\rho, u)$ chosen randomly via $(\rho, u) \sim \text{Lap}(0, 1) \times \text{Unif}[0, 1]$ (which is required for visualization, as $(x, \rho, u) \in \mathbb{R}^5$). We see that, qualitatively, both the samples and approximated densities from ErgFlow closely match the target. Finally, Fig. 8 in Appendix E.2 provides a more comprehensive set of sample histograms (showing the $x$-, $\rho$-, and $u$-marginals). These visualizations confirm our theory that ErgFlow exhibits MCMC-like convergence.

5.2 Posterior approximation quality

Next, we provide a quantitative copmarison of ErgFlow, NPs, and NUTS on 7 real data experiments outlined in Appendix E.4. We tune each NP method under various settings (Tables 1 and 2 and Appendix E.4.5), and present the best one for each example. ELBOs of ErgFlow are estimated with Algorithm 3, averaging over 1,000 independent trajectories. ELBOs of NPs are based on 2,000 samples. To obtain an assessment for the target marginal distribution itself (not the augmented target), we also compare methods using the kernel Stein discrepancy (KSD) with an inverse quadratic (IMQ) kernel (Gorham and Mackey, 2017). Both NUTS and NPs use 5,000 samples for KSD estimation, while ErgFlow is based on 2,000 i.i.d. draws (Algorithm 1). For KSD comparisons, all variational methods are tuned by maximizing the ELBO (Figs. 3 and 14).

Augmented target distribution Fig. 3 displays the ELBO comparison. First, Fig. 3a shows how different step sizes $\epsilon$ and number of refreshments $N$ affects approximation quality. Overly large step sizes typically result in errors due to the use of discretized Hamiltonian dynamics, while overly small step sizes result in a flow that makes slow progress towards the target. ErgFlow with a tuned step size generally shows a comparable joint ELBO value to the best NP method, yielding a competitive target approximation. Similar comparisons and assessment of the effect of step size for the synthetic examples are presented in Figs. 6, 9, and 13. Note that in three examples (Figs. 3a, 3d and 3g), the tuned RealNVP ELBO exceeds ErgFlow by a small amount; but this required expensive architecture search and parameter tuning, and as we will describe next, ErgFlow is actually more reliable in terms of target marginal sample quality and density estimation.

Original target distribution The second row of Fig. 3 displays a comparison of KSD for the target distribution itself (instead of the augmented target). In particular, ErgFlow produces comparable sample quality to that from NUTS—an exact MCMC method—and clearly outperforms all of the NP competitors. The scatter plots of samples in Fig. 16 confirm the improvement in sample quality of ErgFlow over variational competitors. Further, Fig. 4 shows the (sliced) densities on two difficult real data examples: Bayesian student-t regression (with a heavy-tailed posterior), and a high-dimensional sparse regression (parameter dimension is 84). This result demonstrates that the densities provided by ErgFlow more closely match those of the original target distribution than those of the best NP. Notice that ErgFlow accurately captures the skew and heavy tails of the exact target, while the NP density fails to do so and contains many spurious modes.

5.3 Ease of tuning

In order to tune ErgFlow, we simply run a 1-dimensional parameter sweep for the step size $\epsilon$, and use a visual inspection of the ELBO to set an appropriate number of flow steps $N$. In contrast, tuning an NP requires optimizing its architecture, number of layers, and its (typically many) parameters. Not only is this time consuming—in our experiments, tuning took 10 minutes to roughly 1 hour (Fig. 5)—but the optimization can also behave in unintuitive ways. For example, performance can be heavily dependent on the number of flow layers, and adding more layers does not necessarily improve quality. Fig. 13, Tables 1 and 2, and Appendix E.4.5 show that using more layers does not necessarily help, and slows tuning considerably. In the case of RealNVP specifically, tuning can be unstable, especially for more complex models. The optimizer often returns NaN values for flow parameters during training (see Table 1). This instability has been noted in earlier work (Dinh et al., 2017, Sec. 3.7).
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Figure 3: ELBO and KSD comparison for real data examples. Fig. 3a displays the effect of step size for the linear regression problem: $\epsilon_1 = 0.0001, \epsilon_2 = 0.001$ and tuned $\epsilon = 0.0005$; see Fig. 14 for step sizes for all other experiments. Lines indicate the median, and error regions indicate 25th to 75th percentile from 5 runs. Fig. 3b does not include ELBOs of PlanarFlow as values are significantly worse than all other methods and are hard to visualize (see its ELBOs in Fig. 14a).

Figure 4: Sliced log conditional densities on student-t regression (Fig. 4a) and high-dimensional sparse regression (Fig. 4b). We visualize the log conditional density of the first coordinate by fixing other coordinates to value 0. The NF methods are chosen to be the best performing ones from Figs. 3e and 3g. Since we only know the log posterior density up to an unknown normalizing constant, we shift all log densities to have maximal value 0 for visualization.

Figure 5: Timing results (100 trials), showing sampling time (first row) and ESS per second (second row).

5.4 Time efficiency

Finally, Fig. 5 presents timing results for two of the real data experiments (additional comparisons in Figs. 11 and 15). In this figure, we use EF iid to refer to i.i.d. sampling from ErgFlow, and EF single to refer to collecting all intermediate states on a single trajectory. This result shows that the per sample time of EF single is similar to NUTS and HMC, as one would expect. EF iid is the slowest because each sample is generated by passing through the entire flow. The NF generates the fastest draws, but recall that this comes at the cost of significant initial tuning time; in the time it takes NF to generate its first sample, ErgFlow single has generated millions of samples in Fig. 5. See Appendix E.3.1 for a detailed discussion of this trade-off.

Figs. 5 and 15 further show the computational efficiency in terms of ESS per second on real data examples, which reflects the autocorrelation between drawn samples. In practice, a dependent sample sequence with lower ESS usually has a lower estimation power. Results show that ErgFlow produce comparable ESS per second to HMC. EF single behaves similarly to HMC as expected since the pseudo-momentum refreshment we proposed (steps (2-3) of Section 4) resembles the momentum resample step of HMC. The ESS efficiency of EF iid depends on the trade-off between a slower sampling time and i.i.d. nature of drawn samples. In these real data examples, EF iid typically produces a high ESS per second; but in the synthetic examples (Fig. 11b), EF iid is similar to the others.

6 Conclusion

This work presented ergodic variational flows, a new variational family that provides tractable i.i.d. sampling, density evaluation, and MCMC-like convergence guarantees. Experiments demonstrate a comparable sample quality to NUTS and more reliable posterior approximations than standard normalizing flows. A main limitation of our methodology is numerical stability; reversing the flow for long trajectories can be unstable in practice. Future work includes developing more stable momentum refreshment schemes and extensions via involutive MCMC (Neklyudov et al., 2020; Spanbauer et al., 2020; Neklyudov and Welling, 2022).
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A Proofs

Proposition A.1. Suppose $X \sim q_{\lambda,N}$, $X_0 \sim q_0$, and $f \in L^2(q_{\lambda,N})$. Then $E[f(X)] = E \left[ \frac{1}{N} \sum_{n=0}^{N-1} f(T^n X_0) \right]$ and $Var[f(X)] \geq Var \left[ \frac{1}{N} \sum_{n=0}^{N-1} f(T^n X_0) \right]$.

Proof of Proposition A.1. By the change of variable formula, we can express $E[f(X)]$ as follows:

$$E[f(X)] = \frac{1}{N} \sum_{n=0}^{N-1} q_n(x) f(T^n x) dx = \frac{1}{N} \sum_{n=0}^{N-1} E[f(T^n X_0)] = E \left[ \frac{1}{N} \sum_{n=0}^{N-1} f(T^n X_0) \right]. \quad (6)$$

Then, to compare the variance, it is sufficient to show $E[f^2(X)] \geq E \left[ \left( \frac{1}{N} \sum_{n=0}^{N-1} f(T^n X_0) \right)^2 \right]$. Notice that by Jensen’s inequality, we have

$$E \left[ \left( \frac{1}{N} \sum_{n=0}^{N-1} f(T^n X_0) \right)^2 \right] \leq E \left[ \frac{1}{N} \sum_{n=0}^{N-1} f^2(T^n X_0) \right] = E[f^2(X)].$$

The last equality is by the same application of change of variable formula as Eq. (6). \qed

Proof of Theorem 3.1. Since setwise convergence implies weak convergence, we will focus on proving setwise convergence. We have that $q_{\lambda,N}$ converges setwise to $\pi$ if and only if for all measurable bounded $f : \mathcal{X} \to \mathbb{R}$,

$$E[f(X_N)] \to E[f(X)], \quad X_N \sim q_{\lambda,N}, \quad X \sim \pi.$$

The proof proceeds by directly analyzing $E[f(X_N)]$:

$$E[f(X_N)] = \int f(x) q_{\lambda,N}(dx) = \frac{1}{N} \sum_{n=0}^{N-1} \int f(x) (T^n x q_0)(dx) = \frac{1}{N} \sum_{n=0}^{N-1} \int f(T^n x) q_0(dx) = \int \frac{1}{N} \sum_{n=0}^{N-1} f(T^n x) q_0(dx).$$

Since $q_0 \ll \pi$, by the Radon-Nikodym theorem, there exists a density of $q_0$ with respect to $\pi$, so

$$E[f(X_N)] = \int \frac{1}{N} \sum_{n=0}^{N-1} f(T^n x) \frac{dq_0}{d\pi}(x) \pi(dx).$$

By the pointwise ergodic theorem (Theorem 2.3), $f_N(x) = \frac{1}{N} \sum_{n=0}^{N-1} f(T^n x)$ converges pointwise $\pi$-a.e. to $\int f d\pi$; and because $f$ is bounded, $f_N$ is uniformly bounded for all $N \in \mathbb{N}$. Hence by the Lebesgue dominated convergence theorem,

$$\lim_{N \to \infty} E[f(X_N)] = \lim_{N \to \infty} \int \frac{1}{N} \sum_{n=0}^{N-1} f(T^n x) \frac{dq_0}{d\pi}(x) \pi(dx) = \left( \int f d\pi \right) \cdot 1 = E[f(X)].$$

\qed

Theorem A.2 (Mean ergodic theorem in Banach spaces [Yosida, 1938; Kakutani, 1938; Riesz, 1938; Eisner et al., 2015] Theorem 8.5). Let $T$ be a bounded linear operator on a Banach space $E$, define the operator

$$A_N = \frac{1}{N} \sum_{n=0}^{N-1} T^n,$$
and let
\[ \text{fix}(T) = \{ v \in E : Tv = v \} = \ker(I - T). \]

Suppose that \( \sup_{N \in \mathbb{N}} \| A_N \| < \infty \) and that \( \frac{1}{N} T^N v \to 0 \) for all \( v \in E \). Then the subspace
\[ V = \{ v \in E : \lim_{N \to \infty} A_N v \text{ exists} \} \]
is closed, \( T \)-invariant, and decomposes into a direct sum of closed subspaces
\[ V = \text{fix}(T) \oplus \text{range}(I - T). \]
The operator \( T|_V \) on \( V \) is mean ergodic. Furthermore, the operator
\[ A : V \to \text{fix}(T) \quad A v = \lim_{N \to \infty} A_N v \]
is a bounded projection with kernel \( \ker(A) = \text{range}(I - T) \) and \( AT = A = TA. \)

**Proof of Theorem 3.2.** Denote \( \mu \) to be the Lebesgue measure on \( \mathbb{R}^d \), and consider the Banach space \( L^1(\mu) \) and linear operator \( T \) on \( L^1(\mu) \) defined by
\[ Tf = \frac{f(T^{-1}(x))}{J(T^{-1}(x))}, \]
where \( J(x) \) is the Jacobian determinant of \( T(x) \). We suppress \( \lambda \) subscripts for brevity, and note the slight abuse of notation involving the same symbol for \( T : \mathcal{X} \to \mathcal{X} \) the associated operator. By a simple change of variables,
\[ \|Tf\|_1 = \int |Tf(x)| \mu(dx) = \int |f(x)| \mu(dx) = \|f\|_1, \]
and so \( T \) is bounded with \( \|T\| = 1 \). Hence \( \frac{1}{N} T^N f \to 0 \) for all \( f \in L^1(\mu) \), and if we define the operator
\[ \forall N \in \mathbb{N}, \quad A_N = \frac{1}{N} \sum_{n=0}^{N-1} T^n, \]
we have that \( \sup_{N \in \mathbb{N}} \| A_N \| \leq 1 \). Therefore by the mean ergodic theorem in Banach spaces [Yosida 1938, Kakutani 1938, Riesz 1938, Eisner et al. 2015, Theorem 8.5], we have that
\[ A : E \to \text{fix}(T) \quad Af = \lim_{N \to \infty} A_N f \]
where \( E = \{ f \in L^1(\mu) : \lim_{N \to \infty} A_N f \text{ exists} \} \). [Eisner et al. 2015, Theorem 8.20] guarantees that \( E = L^1(\mu) \) as long as the weak limit of \( A_N f \) exists for each \( f \in L^1(\mu) \). Note that since \( \mu \) is \( \sigma \)-finite, the dual space of \( L^1(\mu) \) is the set of linear functionals
\[ f \mapsto \int f(x) \phi(x) \mu(dx), \quad \phi \in L^\infty(\mu). \]
So therefore we have that \( E = L^1(\mu) \) if for each \( f \in L^1(\mu) \), there exists a \( g \in L^1(\mu) \) such that
\[ \forall \phi \in L^\infty(\mu), \quad \int (A_N f)(x) \phi(x) \mu(dx) \to \int g(x) \phi(x) \mu(dx). \]
The same technique using a transformation of variables and the pointwise ergodic theorem from the proof of Theorem 3.1 provides the desired weak convergence. Therefore we have \( L^1 \) convergence to \( \text{fix}(T) \) and hence total variation convergence to an element of \( \text{fix}(T) \). Since \( q_0 \ll \pi \), Theorem 3.1 guarantees weak convergence to \( \pi \); and since we know \( A_N f \to \text{fix}(T) \) and \( \pi \in \text{fix}(T) \), we have that \( D_{TV}(q_0, \pi) \to 0 \).

**Proposition A.3 (Verdú 2014, Theorem 7).** Suppose \( q, \pi \) are two probability distributions on \( \mathcal{X} \) such that \( q \ll \pi \) and both have a density with respect to a common base measure. If
\[ \alpha = \sup_{x \in \mathcal{X}} \frac{q(x)}{\pi(x)} < \infty, \]
then
\[ D_{TV}(q, \pi) \geq \frac{\alpha - 1}{2\alpha \log \alpha} D_{KL}(q||\pi). \]
Proof. We provide a proof for completeness. The KL divergence is
\[ D_{KL}(q||\pi) = \int q(x) \log \frac{q(x)}{\pi(x)} dx = \int \pi(x) \frac{q(x)}{\pi(x)} \log \frac{q(x)}{\pi(x)} dx. \]

Note that \( \alpha \geq 1 \) by definition, and that \( \forall y \in [0, \alpha], \quad \frac{\alpha \log \alpha}{\alpha - 1} |y - 1| \geq y \log y. \)

Therefore
\[ D_{KL}(q||\pi) \leq \frac{\alpha \log \alpha}{\alpha - 1} \int \pi(x) \left| \frac{q(x)}{\pi(x)} - 1 \right| dx = \frac{2 \alpha \log \alpha}{\alpha - 1} \int |q(x) - \pi(x)| dx = \frac{2 \alpha \log \alpha}{\alpha - 1} D_{TV}(q, \pi). \]

\[ \square \]

B Memory efficient ELBO estimation

Algorithm 4 DensityTriple(\( x \)): Evaluate \( T_{\lambda}^{-N+1}(x), q_{\lambda,N}(x), \) and \( \prod_{j=1}^{N-1} J_{\lambda}(T_{\lambda}^{-j}x) \) with \( O(N) \)-time, \( O(1) \)-memory.

Require: location \( x \), reference distribution \( q_0 \), flow map \( T_{\lambda} \), Jacobian \( J_{\lambda} \), number of steps \( N \)

\[
\begin{align*}
L &\leftarrow 0 \\
w &\leftarrow q_0(x) \\
&\text{for } n = 1, \ldots, N - 1 \text{ do} \\
&\quad x \leftarrow T_{\lambda}^{-1}(x) \\
&\quad L \leftarrow L + \log J_{\lambda}(x) \\
&\quad w \leftarrow \text{LogSumExp}(w, \log q_0(x) - L) \\
&\text{end for} \\
&\quad w \leftarrow w - \log N \\
&\text{return } x, \exp(w), \exp(L)
\end{align*}
\]

Algorithm 5 EstELBO(\( \lambda, N \)): Estimate the ELBO for \( q_{\lambda,N} \) in \( O(N) \)-time, \( O(1) \)-memory.

Require: reference \( q_0 \), unnormalized target \( p \), flow map \( T_{\lambda} \), Jacobian \( J_{\lambda} \), number of flow steps \( N \)

\[
\begin{align*}
x &\leftarrow \text{Sample}(q_0) \\
x', z, J &\leftarrow \text{DensityTriple}(x) \\
f &\leftarrow \log p(x) \\
g &\leftarrow \log z \\
&\text{for } n = 1, \ldots, N - 1 \text{ do} \\
&\quad \hat{q} \leftarrow \frac{1}{N} q_0(x')/J \\
&\quad J_{n-1} \leftarrow J_{\lambda}(x) \\
&\quad z \leftarrow (z - \hat{q})/J_{n-1} \\
&\quad x \leftarrow T_{\lambda}(x) \\
&\quad z \leftarrow z + \frac{1}{N} q_0(x) \\
&\quad f \leftarrow f + \log p(x) \\
&\quad g \leftarrow g + \log z \\
&\quad \text{if } n < N - 1 \text{ then} \\
&\quad\quad J \leftarrow J \cdot J_{n-1}/J_{\lambda}(x') \\
&\quad\text{end if} \\
&\quad x' \leftarrow T_{\lambda}(x') \\
&\text{end for} \\
&\text{ELBO}(\lambda, N) \leftarrow \frac{1}{N} (f - g) \\
&\text{return } \text{ELBO}(\lambda, N)
\end{align*}
\]
C Hamiltonian flow pseudocode

Algorithm 6 Compute $T_{\lambda,\epsilon}$ and its Jacobian $J_{\lambda,\epsilon}$ for Hamiltonian flow with leapfrog integrator

Require: initial state $x \in \mathcal{X}$, $\rho \in \mathbb{R}^d$, $u \in [0, 1]$, step size $\epsilon$, shift $\xi \in \mathbb{R}$, pseudorandom shift $z(\cdot, \cdot)$

\begin{align*}
x_0, \rho_0 & \leftarrow x, \rho \\
\text{for } \ell = 1, \ldots, L & \text{ do} \\
& x_{\ell}, \rho_{\ell} \leftarrow H_{\ell}(x_{\ell-1}, \rho_{\ell-1}) \\
\text{end for} \\
& x', \rho' \leftarrow x_L, \rho_L \\
u' & \leftarrow u + \xi \mod 1 \\
\text{for } i = 1, \ldots, d & \text{ do} \\
& \rho''_i \leftarrow R^{-1}(R(\rho'_i) + z(x'_i, u') \mod 1) \\
\text{end for} \\
J & \leftarrow m(\rho')/m(\rho'') \\
\text{return } (x', \rho'', u'), J
\end{align*}

D Extensions

Tunable reference So far we have assumed that the reference distribution $q_0$ for the flow is fixed. Given that $q_0$ is often quite far from the target $\pi$, this forces the variational flow to spend some of its steps just moving the bulk of the mass to $\pi$. But this can be accomplished much easier with, say, a simple linear transformation that efficiently allows large global moves in mass. For example, if $q_0 = \mathcal{N}(0, I)$, we can include a map $M_0$

$$q_{\lambda,N} = \frac{1}{N} \sum_{n=0}^{N-1} T^n_\lambda M_0 q_0,$$

where $M_0(x) = \theta_1 x + \theta_2$, where $\theta_1 \in \mathbb{R}^{d \times d}$ and $\theta_2 \in \mathbb{R}^d$. Note that it is possible to optimize the reference and flow jointly, or to optimize the reference distribution by itself first and then use that fixed reference in the flow optimization.

Automated burn-in A common practice in MCMC is to throw away a first fraction of the states in the sequence to ensure that the starting sample is in a high probability region of the target distribution, thus reducing the bias from initialization (“burn-in”). Usually one needs a diagnostic to check when burn-in is completed. In the case of ErgFlow, we can monitor the burn-in phase in a principled way by evaluating the ELBO. Once the flow is trained, the variational distribution with $M$ burn-in samples is simply

$$q_{\lambda,M,N} = \frac{1}{N - M} \sum_{n=M}^{N-1} T^n_\lambda q_0,$$

We can easily optimize this by estimating the ELBOs for $M = 1, \ldots, N$.

Mixed flows One can build multiple flows starting from multiple different initial reference distributions; when the posterior is multimodal, it may be the case that some of these flows converge to different modes but do not mix across modes. In this scenario, it can be helpful to mix several flows, i.e., build an approximation of the form

$$q_{\lambda,N}^k = \sum_{k=1}^{K} w_k(q_{\lambda,N})_k, \quad \sum_{k=1}^{K} w_k = 1.$$

Because each component flow provides access to i.i.d. samples and density evaluation, ErgFlow provides the ability to optimize the weights by maximizing the ELBO (i.e., minimizing the KL divergence).

E Additional experimental details

In this section, we provide details for each experiment presented in the main text, as well as additional results regarding numerical stability and a high-dimensional synthetic experiment. Aside from the univariate synthetic example, all examples include a pseudotime shift step with $\xi = \pi/16$, and a momentum refreshment with $z(x, u) = 0.5 \sin(2x + u) + 0.5$. For the kernel Stein discrepancy, we use a IMQ kernel $k(x, y) = (c^2 + \|x - y\|^2_2)^\beta$ with $\beta = -0.5, c = 1$, the same setting as in [Gorham and Mackey, 2017]. For all experiments, unless otherwise stated, NUTS uses 20,000 steps for adaptation, targeting at an average acceptance ratio 0.7, and generates 5,000 samples for KSD estimation. The KSD for ErgFlow is estimated using 2,000 samples. As for NUTS, we use the Julia package
The three target distributions tested in this experiment were AdvancedHMC.jl (Xu et al., 2020) with all default settings. The ESS is computed using the R package mcmcse, which is based on batch mean estimation. We implement all NFs using the Julia package Bijectors.jl (Fjelde et al., 2020). The flow layers of PlanarFlow and RadialFlow, as well as the coupling layers of RealNVP are implemented in Bijectors.jl. The affine coupling functions of RealNVP—a scaling function and shifting function—are both parameterized using fully connected neural networks of three layers, of which the activation function is LeakyReLU and number of hidden units is by default the same dimension as the target distribution, unless otherwise stated.

### E.1 Univariate synthetic examples

The three target distributions tested in this experiment were

- normal: $\mathcal{N}(2, 2^2)$,
- synthetic Gaussian mixture: $0.5\mathcal{N}(-3, 1.5^2) + 0.3\mathcal{N}(0, 0.8^2) + 0.2\mathcal{N}(3, 0.8^2)$, and
- Cauchy: Cauchy(0, 1).

For all three examples, we use a momentum refreshment without introducing the pseudotime variable; this enables us to plot the full joint density of $(x, \rho) \in \mathbb{R}^2$:

$$\rho'' \leftarrow R_{\text{lap}}^{-1}(R_{\text{lap}}(\rho') + (\sin(2x') + 1)/2 \mod 1).$$

For the three examples, we used the leapfrog stepsize $\epsilon = 0.05$ and run $L = 50$ leapfrogs between each refreshment. For both the Gaussian and Gaussian mixture targets, we use 100 refreshments. In the case of the Cauchy, we used 1,000 refreshments.

### E.2 Multivariate synthetic examples

The three target distributions tested in this experiment were

- the banana distribution (Haario et al., 2001):
  $$y = \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} \sim \mathcal{N} \left( 0, \begin{bmatrix} 100 & 0 \\ 0 & 1 \end{bmatrix} \right), \quad x = \begin{bmatrix} y_1 \\ y_2 + b y_1^2 - 100 b \end{bmatrix}, \quad b = 0.1;$$

- Neals’ funnel (Neal, 2003):
  $$x_1 \sim \mathcal{N}(0, \sigma^2), \quad x_2 \mid x_1 \sim \mathcal{N} \left( 0, \exp \left( \frac{x_1}{2} \right) \right), \quad \sigma^2 = 36;$$

- a cross-shaped distribution: in particular, a Gaussian mixture of the form
  $$x \sim \frac{1}{4} \mathcal{N} \left( 2 \right) + \frac{1}{4} \mathcal{N} \left( \begin{bmatrix} -2 \\ 0 \end{bmatrix} \right) + \frac{1}{4} \mathcal{N} \left( \begin{bmatrix} 0 \\ 1 \end{bmatrix} \right) + \frac{1}{4} \mathcal{N} \left( \begin{bmatrix} 0 \\ 0.15^2 \end{bmatrix} \right);$$

- and a warped Gaussian distribution
  $$y = \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} \sim \mathcal{N} \left( 0, \begin{bmatrix} 0.15^2 \\ 0.12^2 \end{bmatrix} \right), \quad x = \begin{bmatrix} \|y\|_2 \cos \left( \text{atan2} \left( y_2, y_1 \right) \right) - \frac{1}{2} \|y\|_2 \\ \|y\|_2 \sin \left( \text{atan2} \left( y_2, y_1 \right) \right) - \frac{1}{2} \|y\|_2 \end{bmatrix},$$

where $\text{atan2}(y, x)$ is the angle, in radians, between the positive $x$ axis and the ray to the point $(x, y)$.

For each target distribution we used a flow with 1,000 refreshments; between each refreshment we used 50 leapfrog steps for the banana distribution, 60 for the cross distribution, and 80 for the funnel and warped Gaussian. Note that in all four examples, we individually tuned the step size $\epsilon$ by maximizing the estimated ELBO, as shown in Fig. 6a. Fig. 6b also demonstrates how the ELBO varies versus the number of refreshments $N$. For small step sizes $\epsilon$, the discretized Hamiltonian dynamics approximates the continuous dynamics, and the ELBO generally increases with $N$ indicating convergence to the target. For larger step sizes $\epsilon$, the ELBO increases to a peak and then decreases, indicating that the discretized dynamics do not exactly target the desired distribution.

Fig. 7 shows why we opted to use a Laplace momentum distribution as opposed to a Gaussian momentum. In particular, the numerical error of composing $T^K_\Lambda \circ T_\Lambda^{-K}$ and $T_\Lambda^{-K} \circ T^K_\Lambda$ (denoted as “Bwd” and “Fwd” in the legend, respectively) indicate that the flow using the Laplace momentum is more reliably invertible for larger numbers of refreshments than the flow with a Gaussian momentum. This is largely due to the fact that the normal has very light tails; for example, for large momentum values in the right tail, the CDF is $\approx 1$, which gets rounded to exactly 1 in floating point representation. Note that our implementation of the CDF and inverse CDF was fairly naive; more stable computation could be achieved with more care taken to prevent rounding.

Finally, Fig. 8 provides a more comprehensive set of sample histograms for these experiments, showing the $x$, $\rho$, and $u$-marginals. It is clear that ErgFlow generates samples for each variable reliably from the target marginal.
**Figure 6:** Tuning for the four multivariate synthetic examples, and KSD comparison to NUTS of the tuned ErgFlow.

**Figure 7:** Stability of composing $T_{\lambda}^{-K} \circ T_{\lambda}^{K}$ ($Fwd$) and $T_{\lambda}^{K} \circ T_{\lambda}^{-K}$ ($Bwd$) for the four multivariate experiments with flows constructed using Gaussian ($Gauss$) and Laplace ($Lap$) momentum distributions. The vertical axis shows the 2-norm error of reconstructing $(x, \rho, u)$ sampled from $q_0$; the horizontal axis shows increasing numbers of refreshments $K$. The lines indicate the median, and error regions indicate 25th to 75th percentile for 100 independent samples.

**E.3 Higher-dimensional synthetic experiment**

We also tested two higher dimensional Neal’s funnel target distributions of $x \in \mathbb{R}^d$ where $d = 5, 20$. In particular, we used the target distribution

$$x_1 \sim \mathcal{N}(0, \sigma^2), \quad \text{and} \quad \forall i \in \{2, \ldots, d\}, x_i \mid x_1 \overset{i.i.d.}{\sim} \mathcal{N}(0, \exp(x_1^2)),$$

with $\sigma^2 = 36$. We use 80 leapfrogs between refreshments and $\epsilon = 0.0009$ when $d = 5$, and 100 leapfrogs between refreshments and $\epsilon = 0.001$ when $d = 20$ (Figs. 9a and 9c shows the ELBO comparison used to tune the step size $\epsilon$). Figs. 9b and 9d confirm via the KSD that the method performs as well as NUTS in higher-dimensional cases.

**E.3.1 Additional experiments for synthetic examples**

In this section, we provide additional comparisons on sample quality and sampling efficiency of ErgFlow, using all four synthetic examples in Appendix E.2 against NUTS, HMC, and a generic normalizing flow method—planar flow (NF) (Rezende and Mohamed, 2015b). For this set of experiments, all of the settings for ErgFlow are the same as outlined in Appendix E.2. HMC uses the same leapfrog step size and number of leapfrogs steps (between refreshments) as ErgFlow. For NF, 5 Planar layers (Rezende and Mohamed, 2015b) that contain 40 parameters to be optimized (4 translation parameters and 4 scaling parameters per layer) are used unless otherwise stated. We train NF using ADAM until convergence (100,000 iterations except where otherwise noted) with the initial step size set...
Figure 8: Scatter plots and histograms for the \( x \), \( \rho \), and \( u \)-marginals in the four synthetic experiments.

Figure 9: ELBO versus step size (9a, 9c) and KSD comparison with NUTS (9b, 9d) for the 5- and 20-dimensional Neal’s funnel examples.
Figure 10: Performance of NF for the four multivariate synthetic examples.

(a): Sampling time comparison to NF, NUTS, and HMC (100 trials).

(b): Per second ESS comparison to NUTS and HMC (100 trials).

Figure 11: Time results for four multivariate synthetic examples: from left to right, each column corresponds to Banana, Neal’s funnel, Cross, and warped Gaussian respectively.

Figure 12: Streaming mean and standard deviation (SD) estimation (50,000 samples) for four 2-dimensional synthetic distributions. For each distribution, the two plots on the top row correspond to the two marginal means, and the two plots on the bottom row correspond to the two marginal SDs. Each plot shows the evolution of coordinate-wise mean/SD estimates, using samples from ErgFlow single (green), NUTS (blue), HMC (red), and NF (purple); black dashed line indicates the true target mean/SD, which is estimated using 50,000 samples from the actual synthetic target distribution. The lines indicate the median, and error regions indicate 25th to 75th percentile from 10 runs.
We consider two Bayesian linear regression problems, with both a standard normal prior and a heavy tail prior using two sets of real data. We drop observations with missing values, and using Principle component analysis for feature dimension reduction, we selected 50 MLDatasets $y_i$.

All settings for ErgFlow when we increase the number of layers to 500,000 to ensure the convergence of flows with increased numbers of layers. As demonstrated in the second and third column of Fig. 13, examining its performance as we increase the number of planar layers (5, 10, 20, 50). All settings for NF are identical to the above, except that we increase the optimization iteration to 500,000 to ensure the convergence of flows with increased numbers of layers. As demonstrated in the second and third column of Fig. 13, both training time and sampling time scale with the number of layers roughly linearly. Although a trained NF is still generally faster in sample generation (see also Fig. 11), for these synthetic examples with 4-dimensional joint target distributions, training time can take up to 30 minutes. More importantly, the corresponding target approximations of NF are still not as good as those of ErgFlow in all four examples, even when we increase the number of layers to 50, which corresponds to optimizing 400 parameters from the flow. One may also notice from Fig. 13 that a more complex normalizing flow does not necessarily lead to better performance. This is essentially because the (usually non-convex) KL optimization problem of standard NF becomes more complex to solve as the flow becomes more flexible. As a result, even though theoretically, NF becomes more expressive with more layers, there is no guarantee on how well it approximates the target distribution. In contrast, ErgFlow is optimization-free and is asymptotically exact—with a proper choice of hyper-parameter, more computation typically leads to better performance (Fig. 16). With the 30 minutes training time of NF, ErgFlow iid can generate 18,000 i.i.d. samples and ErgFlow single can generate over 10 million i.i.d. samples, both of which are more than sufficient for most estimations under these target distributions.

E.4 Real data examples

All settings for ErgFlow, NUTS and HMC are identical to those in synthetic examples. All NFs are trained using ADAM for 200,000 iterations with initial step size set to 0.001.

E.4.1 Bayesian linear regression

We consider two Bayesian linear regression problems, with both a standard normal prior and a heavy tail prior using two sets of real data. The two statistical models take the following form:

$$\log \sigma^2_{i.i.d.} \sim \mathcal{N}(0, 1), \quad y_j | \beta, \sigma^2_{i.d} \sim \mathcal{N}(x_j^T \beta, \sigma^2)$$

Normal: $\beta_{i.i.d} \sim \mathcal{N}(0, 1)$, Cauchy: $\beta_{i.i.d} \sim \text{Cauchy}(0, 1)$

where $y_j$ is the response and $x_j \in \mathbb{R}^p$ is the feature vector for data point $j$. For linear regression problem with a normal prior, we use the Boston housing prices dataset [Harrison Jr. and Rubinfeld, 1978]. Dataset available in the MLDatasets Julia package at [https://github.com/JuliaML/MLDatasets.jl](https://github.com/JuliaML/MLDatasets.jl) containing $J = 506$ suburbs/towns in the Boston area; the goal is to use suburb information to predict the median house price. We standardize all features and responses. For linear regression with a heavy-tail prior, we use the communities and crime dataset [com] containing 122 attributes that potentially connect to crime; the goal is to predict per-capita violent crimes using the information of the community, such as the median family income, per capita number of police officers, and etc. For the data preprocessing, we drop observations with missing values, and using Principle component analysis for feature dimension reduction; we selected 50...
principle components with leading eigenvalues. The posterior dimensions of the two linear regression inference problems are 15 and 52, respectively.

Figure 13: Additional NF results with number of planar layers (5, 10, 20, 50). First column shows the ELBO value. Each ELBO is estimated using 2000 i.i.d. samples from trained flow. The second and third columns correspond to the training time and per-sample time (100 trials) of NF given increasing planar layers.
E.4.2 Bayesian generalized linear regression

We then consider two Bayesian generalized linear regression problems—a hierarchical logistic regression and a poisson regression:

**Logis. Reg.:** \( \alpha \sim \text{Gam}(1, 0.01), \beta \mid \alpha \sim N(0, \alpha^{-1} I), \)
\[ y_j \mid \beta \text{ indep Bern} \left( \frac{1}{1 + e^{-x_j^T \beta}} \right), \]

**Poiss. Reg.:** \( \beta \sim N(0, I), \)
\[ y_j \mid \beta \text{ indep Poiss} \left( \log \left( 1 + e^{-x_j^T \beta} \right) \right), \]

For logistic regression, we use a bank marketing dataset (Moro et al., 2014) downsampled to \( J = 400 \) data points. Original dataset is available at [https://archive.ics.uci.edu/ml/datasets/bank+marketing](https://archive.ics.uci.edu/ml/datasets/bank+marketing) the goal is to use client information to predict whether they subscribe to a term deposit. We include 8 features from the bank marketing dataset (Moro et al., 2014): client age, marital status, balance, housing loan status, duration of last contact, number of contacts during campaign, number of days since last contact, and number of contacts before the current campaign. For each of the binary variables (marital status and housing loan status), all unknown entries are removed. All features of the dataset are also standardized. Hence the posterior dimension of the logistic regression problem is 9 and the overall \((x, \rho, u)\) state dimension of the logistic regression inference problems are 19.

For Poisson regression problem, we use an airport delays dataset with 15 features and \( J = 500 \) data points (subsampled), resulting a 16-dimensional posterior distribution. The airport delays dataset was constructed using flight delay data from [http://stat-computing.org/dataexpo/2009/the-data.html](http://stat-computing.org/dataexpo/2009/the-data.html) and historical weather information from [https://www.wunderground.com/history/](https://www.wunderground.com/history/) relating daily weather information to the number of flights leaving an airport with a delay of more than 15 minutes. All features are standardized as well.

E.4.3 Bayesian Student-t regression

We also consider a Bayesian Student-t regression problem, of which the posterior distribution is heavy-tail. The Student-t regression model is as follows:

\[ y_i \mid X_i, \beta \sim T_5(X_i^T \beta, \sigma^2), \quad \beta \text{ i.i.d. Cauchy}(0, 1). \]

In this example, we use the creatinine dataset (Liu and Rubin, 1995), containing a clinical trial on 34 male patients with 3 covariates. Original dataset is available in [https://github.com/faosorios/heavy/blob/master/data/creatinine.rda](https://github.com/faosorios/heavy/blob/master/data/creatinine.rda) The 3 covariates consist of body weight in kg(WT), serum creatinine concentration (SC), and age in years. The goal is to predict the endogenous creatinine clearance (CR) using these covariates. We apply the data transformation recommended by Liu and Rubin (1995) by transferring response into \( \log(CR) \), and transferring covariates into \( \log(WT), \log(SC), \log(140 - \text{age}) \).

E.4.4 Bayesian sparse regression

Finally, we compare the methods on the Bayesian sparse regression problem applied to two datasets: a prostate cancer dataset containing 9 covariates and 97 observations, and a superconductivity dataset (Hamidieh, 2018), containing 83 features and 100 observations (subsampled). The prostate cancer dataset is available at [https://hastie.su.domains/ElemStatLearn/datasets/prostate.data](https://hastie.su.domains/ElemStatLearn/datasets/prostate.data) The superconductivity dataset is available at [https://archive.ics.uci.edu/ml/datasets/superconductivty+data](https://archive.ics.uci.edu/ml/datasets/superconductivty+data) The model is as follows:

\[ \log \sigma^2 \text{ i.i.d. } N(0, 1), \beta \text{ i.i.d. } \frac{1}{2} N(0, \tau_1^2) + \frac{1}{2} N(0, \tau_2^2), \]
\[ y_j \mid \beta, \sigma^2 \text{ indep } N \left( x_j^T \beta, \sigma^2 \right), \]

For both two datasets, we set \( \tau_1 = 0.1, \tau_2 = 10 \). The resulting posterior dimension for both datasets are 10 and 84 respectively. When data information is weak, the posterior distribution in this model typically contains multiple modes (Xu and Campbell, 2022). We standardize the covariates during the preprocessing procedure for both datasets.

E.4.5 Additional experiments for real data examples
Table 1: Comparison of ELBO between ErgFlow and RealNVP with different number of layers on real data example. Each setting of RealNVP is run in 5 trials. ELBOs of ErgFlow are estimated using 1000 independent trajectories and ELBOs of RealNVP are estimated using 2000 independent samples.

| STEPSIZE   | #LEAPFROG | #REFRESHMENT | ELBO       | #SAMPLE |
|------------|-----------|--------------|------------|---------|
| Lin Reg    | 0.0005    | 30           | 2000       | -429.98 | 1000    |
| Lin Reg Heavy | 0.000025  | 50           | 2500       | 117.1   | 1000    |
| Log Reg    | 0.002     | 50           | 1500       | -250.5  | 1000    |
| Poiss Reg  | 0.0001    | 50           | 2000       | 82576.9 | 1000    |
| Student t Reg | 0.0008   | 80           | 2000       | -145.41 | 1000    |
| Sparse Reg | 0.001     | 30           | 600        | -125.9  | 1000    |
| Sparse Reg High Dim | 0.0012 | 50           | 2000       | -538.36 | 2000    |

| #LAYER | #HIDDEN | MEDIAN       | IQR          | #NAN |
|--------|---------|--------------|--------------|------|
| Lin Reg | 5       | -429.43      | (-429.56, -429.42) | 0    |
| Lin Reg | 10      | -429.41      | (-429.43, -429.36) | 1    |
| Lin Reg Heavy | 5       | 116.47       | (116.34, 116.49)    | 0    |
| Lin Reg Heavy | 8       | 116.65       | (116.56, 116.73)    | 3    |
| Lin Reg Heavy | 10      | 116.26       | (116.11,116.41)     | 3    |
| Log Reg  | 5       | -250.76      | (-250.76, -250.75)  | 3    |
| Log Reg  | 8       | -250.65      | (-250.75, -250.64)  | 2    |

| #LAYER | #HIDDEN | MEDIAN       | IQR          | #NAN |
|--------|---------|--------------|--------------|------|
| Poiss Reg | 3       | 82576.87     | (82575.57, 82577.53) | 1    |
| Poiss Reg | 5       | 82580.77     | (82580.13, 82583.72) | 2    |
| Poiss Reg | 8       | N/A          | N/A          | 5    |
| Student t Reg | 5       | -145.52      | (-145.53, -145.51) | 0    |
| Student t Reg | 10      | -145.52      | (-145.52, -145.49) | 0    |

| #LAYER | #HIDDEN | MEDIAN       | IQR          | #NAN |
|--------|---------|--------------|--------------|------|
| Sparse Reg | 5       | -126.33      | (-126.36, -126.32) | 0    |
| Sparse Reg | 8       | -126.35      | (-126.36, -126.33) | 1    |
| Sparse Reg High Dim | 5       | -531.75      | (-533.41, -522.60) | 0    |
| Sparse Reg High Dim | 8       | N/A          | N/A          | 5    |
Table 2: Comparison of ELBO between ErgFlow and PlanarFlow with different number of layers on real data example. Each setting of PlanarFlow is run in 5 trials. ELBOs of ErgFlow are estimated using 1000 independent trajectories and ELBOs of PlanarFlow are estimated using 2000 independent samples.

### ErgFlow

| STEPSIZE | #LEAPFROG | #REFRESHMENT | ELBO   | #SAMPLE |
|----------|-----------|--------------|--------|---------|
| Lin Reg  | 0.0005    | 30           | 2000   | -429.98 | 1000 |
| Lin Reg Heavy | 2.5E-05 | 50           | 2500   | 117.1   | 1000 |
| Log Reg  | 0.002     | 50           | 1500   | -250.5  | 1000 |
| Poiss Reg| 0.0001    | 50           | 2000   | 82576.9 | 1000 |
| Student t Reg | 0.0008 | 80           | 2000   | -145.41 | 1000 |
| Sparse Reg| 0.0012   | 30           | 600    | -125.9  | 1000 |
| Sparse Reg High Dim | 0.0012 | 50           | 2000   | -538.36 | 2000 |

### PlanarFlow

| #LAYER | MEDIAN    | IQR       | #NAN |
|--------|-----------|-----------|------|
| Lin Reg| -434.73   | (-435.01, -434.65) | 0    |
| Lin Reg| -438.79   | (-439.25, -436.77) | 0    |
| Lin Reg| -442.4384675 | (-444.64, -440.93) | 0    |
| Lin Reg Heavy | 79.65   | (-75.92, 99.10) | 0    |
| Lin Reg Heavy | 23.13   | (21.29, 100.10) | 0    |
| Log Reg | -879.1909019 | (-1641.19, -392.80) | 0    |
| Log Reg | -251.71   | (-251.85, -251.41) | 0    |
| Log Reg | -251.8    | (-252.03, -251.80) | 0    |

### PlanarFlow

| #LAYER | MEDIAN    | IQR       | #NAN |
|--------|-----------|-----------|------|
| Poiss Reg| 82569.58  | (82569.33, 82569.68) | 0    |
| Poiss Reg| 82568.49  | (82568.12, 82569.57) | 0    |
| Poiss Reg| 82566.40441 | (82552.57, 82568.05) | 2    |
| Student t Reg | -145.69  | (-145.71, -145.64) | 0    |
| Student t Reg | -145.72  | (-145.73, -145.69) | 0    |
| Student t Reg | -145.7579931 | (-145.77, -145.72) | 0    |

### PlanarFlow

| #LAYER | MEDIAN    | IQR       | #NAN |
|--------|-----------|-----------|------|
| Sparse Reg| -127.58   | (-127.60, -127.42) | 0    |
| Sparse Reg| -127.75   | (-127.87, -127.68) | 0    |
| Sparse Reg| -127.6677415 | (-128.48, -127.65) | 0    |
| Sparse Reg High Dim | -571.97  | (-572.09, -565.10) | 0    |
| Sparse Reg High Dim | -571.7   | (-573.22, -565.55) | 0    |
| Sparse Reg High Dim | -577.1338885 | (-580.30, -569.39) | 0    |
Table 3: Comparison of ELBO between **ErgFlow** and **RadialFlow** with different number of layers on real data example. Each setting of **RadialFlow** is run in 5 trials. ELBOs of **ErgFlow** are estimated using 1000 independent trajectories and ELBOs of **RadialFlow** are estimated using 2000 independent samples.

### ErgFlow

| STEPSIZE | #LEAPFROG | #REFRESHMENT | ELBO     | #SAMPLE |
|----------|-----------|--------------|----------|---------|
| Lin Reg  | 0.0005    | 30           | 2000     | -429.98 | 1000    |
| Lin Reg Heavy | 2.50E-05 | 50           | 2500     | 117.1   | 1000    |
| Log Reg  | 0.002     | 50           | 1500     | -250.5  | 1000    |
| Poiss Reg | 0.0001   | 50           | 2000     | 82576.9 | 1000    |
| Student t Reg | 0.0008  | 80           | 2000     | -145.41 | 1000    |
| Sparse Reg | 0.001    | 30           | 600      | -125.9  | 1000    |
| Sparse Reg High Dim | 0.0012 | 50           | 2000     | -538.36 | 2000    |

### RadialFlow

| #LAYER | MEDIAN | IQR | #NAN |
|---------|--------|-----|------|
| Lin Reg | -434.14 | (-434.36, -434.12) | 0 |
| Lin Reg | -434.12 | (-434.19, -434.12) | 0 |
| Lin Reg | -433.82 | (-433.73, -433.73) | 0 |
| Lin Reg Heavy | 111.99 | (111.91, 112.01) | 0 |
| Lin Reg Heavy | 111.99 | (111.89, 112.00) | 0 |
| Lin Reg Heavy | 111.7  | (111.61, 111.71) | 0 |
| Log Reg  | -251.33 | (-251.31, -251.31) | 0 |
| Log Reg  | -251.17 | (-251.06, -251.06) | 0 |
| Log Reg  | -250.96 | (-250.95, -250.95) | 0 |

### RadialFlow

| #LAYER | MEDIAN | IQR   | #NAN |
|---------|--------|-------|------|
| Poiss Reg | 82570.5 | (82570.19, 82570.57) | 0 |
| Poiss Reg | 82571.02 | (82570.76, 82571.05) | 0 |
| Poiss Reg | 82571.08 | (82570.90, 82571.12) | 0 |
| Student t Reg | -145.61 | (-145.61, -145.61) | 0 |
| Student t Reg | -145.59 | (-145.59, -145.59) | 0 |
| Student t Reg | -145.58 | (-145.57, -145.57) | 0 |

### RadialFlow

| #LAYER | MEDIAN | IQR   | #NAN |
|---------|--------|-------|------|
| Sparse Reg | -127.28 | (-127.37, -127.27) | 0 |
| Sparse Reg | -127   | (-126.88, -127.03) | 0 |
| Sparse Reg | -126.68 | (-126.61, -126.69) | 0 |
| Sparse Reg High Dim | -548.05 | (-547.98, -548.54) | 0 |
| Sparse Reg High Dim | -547.2 | (-547.16, -547.74) | 0 |
| Sparse Reg High Dim | -547.03 | (-546.76, -547.78) | 0 |
Figure 14: ELBO comparison against NFs for real examples (except for linear regression, which is displayed in Fig. 3a. Each NF method is tuned under various settings, and only the best one is present for each example. Each figure also shows the effect of step sizes on ErgFlow; overly large or small step sizes influence the performance of ErgFlow negatively. Lines indicate the median, and error regions indicate 25\textsuperscript{th} to 75\textsuperscript{th} percentile from 5 runs.
Figure 15: Time results (sampling time comparison to NF, NUTS, and HMC, and per second ESS comparison to HMC; each repeated 100 trials) for two linear regression problems (Figs. 15a and 15b), two generalized linear regression problems (Figs. 15c and 15d), and one sparse regression problem (Fig. 15e).
Figure 16: Sample quality visualization of 2,000 i.i.d. samples draw from each of ErgFlow (green scatters) and NF (orange scatters) on 4 real data examples: linear regression, linear regression with heavy tail prior, poisson regression, and high-dimensional sparse regression. Pairwise kernel density estimation (KDE) is based on 20,000 NUTS samples, which is initialized with the Gaussian mean of the mean-field Gaussian approximation to posterior distribution, uses 20,000 steps for adaptation (targeting at an average acceptance rate 0.7). NF is chosen to be the same one as compared in Figs. 5 and 15.