Energy Flows: Towards Determinant-Free Training of Normalizing Flows

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Abstract
Normalizing flows are a popular approach for constructing probabilistic and generative models. However, maximum likelihood training of flows is challenging due to the need to calculate computationally expensive determinants of Jacobians. This paper takes steps towards addressing this challenge by introducing an approach for determinant-free training of flows inspired by two-sample testing. Central to our framework is the energy objective, a multidimensional extension of proper scoring rules that admits efficient estimators based on random projections and that outperforms a range of alternative two-sample objectives that can be derived in our framework. Crucially, the energy objective and its alternatives do not require calculating determinants and therefore support general flow architectures that are not well-suited to maximum likelihood training (e.g., densely connected networks). We empirically demonstrate that energy flows achieve competitive generative modeling performance while maintaining fast generation and posterior inference.

1 Introduction
Normalizing flows form one of the major approaches for constructing probabilistic and generative models [Rezende and Mohamed, 2015; Papamakarios et al., 2019; Kingma et al., 2016]. They feature tractable inference and maximum likelihood learning, and have applications in areas such as image generation [Kingma and Dhariwal, 2018], anomaly detection [Nalisnick et al., 2019], and density estimation [Papamakarios et al., 2017]. However, flows require calculating computationally expensive determinants of Jacobians in order to evaluate their densities; this either limits the range of architectures compatible with flows, or makes flow models with highly expressive neural architectures slow to train.

This paper takes a step towards addressing this limitation of normalizing flows by proposing an approach for determinant-free training inspired by two-sample testing and the theory of proper scoring rules. Si et al. [Si et al., 2022] recently showed that normalizing flows can be trained using objectives derived from proper scoring rules [Gneiting and Raftery, 2007] that involve only samples from the model and the data distribution (hence do not require computing densities). Although quantile flows [Si et al., 2022] are determinant-free, they are also autoregressive, and therefore inherit various limitations, such as slow sampling speed.

Here, we extend the sample-based proper scoring rule framework of Si et al. [Si et al., 2022] to models that are non-autoregressive. Central to our approach is the energy objective, a multidimensional extension of proper scoring rules that only requires model samples, and not densities. We complement this objective with efficient estimators based on random projections as well as alternative sample-based objectives that serve as strong baselines. We examine the theoretical properties of our approach, draw connections to divergence minimization, and highlight benefits over maximum likelihood training.

Our framework enables training model architectures that are more general than ones compatible with maximum likelihood learning (e.g., densely connected networks); it also enables training
Table 1: Energy Flows are invertible generative models that feature expressive architectures, exact likelihood and posterior evaluation, and their training does not require computing log-determinants, as contrasted with VAEs [Kingma and Welling, 2014], MAFs [Papamakarios et al., 2017], NAFs [Huang et al., 2018], AQFs [Si et al., 2022], GMMNets [Li et al., 2015], and CramerGANs [Bellemare et al., 2017].

| Method      | Likelihood | Posterior | Sampling     | Representation | Objective               |
|-------------|------------|-----------|--------------|----------------|-------------------------|
| VAE         | Approx.    | Approx.   | Feedforward  | Gaussian       | ELBO                    |
| MAF         | Exact      | Exact     | Autoregressive | Gaussian       | Log-Likelihood          |
| NAF         | Exact      | Exact     | N/A          | Neural         | Log-Likelihood          |
| AQF         | Exact      | Exact     | Autoregressive | Neural         | Quantile Loss           |
| GMMNet      | N/A        | N/A       | Feedforward  | Neural         | MMD                     |
| CramerGAN   | N/A        | N/A       | Feedforward  | Neural         | Discr.+Energy           |
| Energy Flow (Ours) | Exact    | Exact     | Feedforward  | Neural         | Energy Loss             |

existing architectures with a simpler determinant-free algorithm. We demonstrate the benefits of our approach through a series of generative modeling experiments. Across a number of tasks previously used to benchmark flow algorithms, our method generates samples of equal or greater quality to autoregressive models, while supporting exact posterior inference, which we demonstrate via an exploration of the models’ latent space. Table 1 compares our approach to existing methods.

Contributions. In summary, this work (1) proposes a general approach for training normalizing flows based on proper scoring rules and two-sample tests that is likelihood-free and that extends quantile flows [Si et al., 2022] to multiple dimensions. We also (2) provide specific examples of objectives within this approach, most notably the energy objective, and we derive efficient slice-based estimators that make training with these objectives possible. Finally, (3) we analyze our objectives theoretically and demonstrate their effectiveness on generation and posterior inference tasks.

2 Background

Normalizing Flow Models Generative modeling involves specifying a probabilistic model \( p(y) \in \Delta(\mathbb{R}^d) \) over a high-dimensional \( y \in \mathbb{R}^d \) [Kingma and Welling, 2014, Goodfellow et al., 2014, Ren et al., 2018a,b, Birnbaum et al., 2019]. A normalizing flow is a generative model \( p(y) \) defined via an invertible mapping \( f : \mathbb{R}^d \to \mathbb{R}^d \) between a noise variable \( z \in \mathbb{R}^d \) sampled from a prior \( z \sim p(z) \) and the target variable \( y \) [Rezende and Mohamed, 2015, Papamakarios et al., 2019]. We may obtain an analytical expression for the likelihood \( p(y) \) via the change of variables formula

\[
p(y) = \left| \frac{\partial f(z)^{-1}}{\partial z} \right| p(z), \quad \text{where } \left| \frac{\partial f(z)^{-1}}{\partial z} \right| \text{ denotes the determinant of the inverse Jacobian of } f.
\]

Computing this quantity is often expensive, hence we typically choose \( f \) to be in a class of models for which the Jacobian is tractable [Rezende and Mohamed, 2015], such as in autoregressive models [Papamakarios et al., 2017].

Proper Scoring Rules Consider a score or a loss \( \ell : \Delta(\mathbb{R}^d) \times \mathbb{R}^d \to \mathbb{R}_+ \) over a probabilistic forecast \( F \in \Delta(\mathbb{R}^d) \) and a sample \( y \in \mathbb{R}^d \). The loss \( \ell \) is proper if \( G \in \arg\min_F \mathbb{E}_{y \sim F} \ell(F, y) \) [Gneiting and Raftery, 2007]. A popular proper loss is the continuous ranked probability score (CRPS), defined for two cumulative distribution functions (CDFs) \( F \) and \( G \) as \( \text{CRPS}(F, G) = \int_y (F(y) - G(y))^2 \, dy \). When we only have samples from \( G \), we can generalize this score to obtain the following loss for a single sample \( y' \): \( \text{CRPS}(F, y') = \int_y (F(y) - \mathbb{I}(y - y'))^2 \, dy \), where \( \mathbb{I} \) denotes the Heaviside step function. The above CRPS can also be written as an expectation relative to the distribution \( F \):

\[
\text{CRPS}(F, y') = \frac{1}{2} \mathbb{E}_F |Y - Y'| - \mathbb{E}_F |Y - y'|,
\]

where \( Y, Y' \) are independent copies of a random variable distributed according to \( F \). Recently, [Si et al., 2022] proposed autoregressive quantile flows, which are trained using the CRPS and are determinant-free. However these flows are autoregressive; we seek to extend them to a general structure.

2
We propose training normalizing flows using objectives inspired by two-sample tests, which do not require computing densities. Specifically, a two-sample test defines a statistic \( T : \mathbb{R}^d \rightarrow \mathbb{R} \); we determine whether \( \mathcal{D}_F, \mathcal{D}_G \) originate from identical or different distributions \( F, G \) based on differences in \( T \) across \( \mathcal{D}_F, \mathcal{D}_G \). Two-sample tests motivate objectives for generative models such as generative moment matching networks (GMMNs; [Dziugaite et al., 2015, Li et al., 2015]) and generative adversarial networks (GANs; [Goodfellow et al., 2014]). Two-sample tests are also an attractive training objective for flows: because they are density-free, they do not require computing determinants.

Classical two-sample tests include Kolmogorov-Smirnov, Student’s t-test, Hotelling’s \( t^2 \)-test, and more [Massey Jr, 1951, Student, 1908, Hotelling, 1931]. More modern approaches include integral probability metrics (IPMs) [Müller, 1997], which take the form \( \max_{T \in \mathcal{T}} \mathbb{E}_{y \sim F}[T(y)] - \mathbb{E}_{y \sim G}[T(y)] \), where \( \mathcal{T} \) is a family of functions. A special case of IPMs is maximum mean discrepancy (MMD) [Gretton et al., 2008], in which \( \mathcal{T} = \{ T : \| T \|_H \leq 1 \} \) is the set of functions with bounded norm in a reproducing kernel Hilbert space (RKHS) with norm \( \| \cdot \|_H \); the CRPS objective can be shown to be a form of MMD [Gretton et al., 2008]. We use this intuition to combine proper scores and two-sample tests to create new objectives for flows.

3 Exploring Likelihood-Free Training of Normalizing Flows

In this paper, we take a step towards likelihood-free training of flows by introducing new learning objectives derived from two-sample tests and proper scoring rules [Gneiting and Raftery, 2007, Gretton et al., 2008].

3.1 Sample-Based Training of Normalizing Flows

We propose training normalizing flows using objectives inspired by two-sample tests, which do not require computing densities. This idea poses two sets of challenges: (1) most classical two-sample tests are defined in one dimension and do not have simple multivariate extensions; (2) modern two-sample tests (e.g., IPMs) extend to high dimensions, but typically require solving a costly optimization problem.

Our work nonetheless shows the existence of specific two-sample tests which motivate good learning objectives, and we use the theory of proper scoring rules to justify their validity. We describe these objectives below; in the next section, we further show how to scale them using random projections.

3.2 The Energy Objective

Recently, Si et al. [Si et al., 2022] proposed autoregressive quantile flows, which are trained using the CRPS and are Jacobian-free. We seek to extend these flows to a general structure without the limitations of autoregressivity (e.g., slow sampling). Specifically, we leverage a generalization of the sample-based form of the CRPS objective (1) to a multi-dimensional version called the energy score [Szekely, 2003, Gneiting and Raftery, 2007]:

\[
\text{CRPS}(F, y') = \frac{1}{2} \mathbb{E}_F \| Y - Y' \|_2^\beta - \mathbb{E}_F \| Y - y' \|_2^\beta,
\]

(2)

where \( \beta \in (0, 2) \), \( \| \cdot \|_2 \) denotes the Euclidean norm, and \( Y, Y' \in \mathbb{R}^d \) are independent copies of a vector-valued random variable distributed according to \( F \). Like the CRPS objective (1), the energy score can be computed from high-dimensional samples; it reduces to the CRPS when \( d = 1 \). The rightmost term \( \frac{1}{2} \mathbb{E}_F \| Y - y' \|_2^\beta \) promotes samples \( Y \) from \( F \) that are close to the data point \( y \). The leftmost term \( \frac{1}{2} \mathbb{E}_F \| Y - y' \|_2^\beta \) encourages the model to have greater variance (i.e., not concentrate all of its probability mass on \( y \)) and produce more diverse samples.

The Kernelized Energy Objective

Measuring similarity between samples via the means of kernels yields the kernelized energy loss, defined as

\[
\text{CRPS}_K(F, y') = \frac{1}{2} \mathbb{E}_F K(Y, Y') - \mathbb{E}_F K(Y, y'),
\]

(3)
The kernelized energy loss can be shown to be a proper loss Gneiting and Raftery [2007], and thus represents a valid training objective for a generative model. The flow objective consists of \(\mathbb{E}_{y \sim D}[\text{CRPS}_K(F, y')]\); this formulation also reveals the connection to two-sample tests between \(F\) and \(D\).

### 3.3 Gaussian Two-Sample Baselines

We use the following classical objectives as baselines for our work and to illustrate examples of alternative methods that can be derived from our two-sample-based approach; both tests make a Gaussian modeling assumption.

**Hotelling’s Two-Sample Test** Being closely related to Student’s t-test, it uses the following statistic:

\[
H_2(D_F, D_G) = (m_F - m_G)^T S^{-1}(m_F - m_G),
\]

where \(m_F = \frac{1}{m} \sum_{y^{(i)} \in D_F} y^{(i)}, m_G = \frac{1}{m} \sum_{y^{(i)} \in D_G} y^{(i)}\) are the sample means, and the matrices \(S_F = \frac{1}{m-1} \sum_{y^{(i)} \in D_F}(y^{(i)} - m_F)(y^{(i)} - m_F)^T, S_G = \frac{1}{m-1} \sum_{y^{(i)} \in D_G}(y^{(i)} - m_G)(y^{(i)} - m)^T\) are sample covariances, while \(S = (S_F + S_G)/2\) is their average. This objective encourages the two samples to have similar means.

**Fréchet Distance** This is another Gaussian-based distance that we use as an objective:

\[
R(D_F, D_G) = ||m_F - m_G||_2^2 + \text{tr}(S_F + S_G - 2(S_F + S_G)^{1/2}),
\]

where we are using the same notation as above. This objective is encouraging the model to produce data with similar means and variances. It is derived from the Fréchet distance between two Gaussians.

### 3.4 Theoretical Properties

**Divergence Minimization** When the variable \(y \in \mathbb{R}\) is one-dimensional, the objective \(\text{CRPS}_F, G\) is precisely equivalent to the Crámer divergence \(\ell^2_2(F, G) = \int_{-\infty}^{\infty} (F(y) - G(y))^2 dy\) between distributions \(F, G\). The square root of this objective, denoted \(\ell_2\), is a proper distance function. Szekely [Szekely, 2003] showed that the one-dimensional version of the energy loss (2) is precisely equivalent to \(\ell^2_2\). Its kernelized version can be shown to also represent a valid divergence between distributions [Gneiting and Raftery, 2007].

The connection to divergence minimization lends additional support to using (2), (3) as principled objectives for training normalizing flow models. More specifically, if \(G\) is the data distribution, minimizing (2), (3) over a space of models will produce a model \(F\) that is close to \(G\).

**Unbiased Gradient Estimation** Our learning procedures for optimizing (2), (3) will rely on stochastic gradient descent; thus, we need to be able to form estimators of the gradients of our objectives. Formally, we need to have the property that given a sequence \(Y_K\) of \(K\) samples \(y_1, y_2, \ldots, y_K\) from \(G\), the gradient of the empirical distribution over these samples yields an unbiased estimate of the gradient of the expected loss:

\[
\nabla_\theta \mathbb{E}_{Y_K} \ell(F_\theta, \hat{G}_K) = \nabla_\theta \ell(F_\theta, G)
\]

where \(\ell\) is one of our objective functions, \(\hat{G}_K\) is the empirical distribution over \(Y_K\) and \(F_\theta\) is a model with parameters \(\theta\) that we are optimizing. The above fact follows directly from the fact that both the energy and the CRPS objectives are proper scoring rules [Bellemare et al., 2017].

**Why Energy Objectives?** Consider the set of objectives \(\ell^p_F(G, y) = \int_{-\infty}^{\infty} (F(y) - G(y)^p) dy\) for \(p \geq 1\) over \(y \in \mathbb{R}\); these are also known as Wasserstein \(p\)-metrics. The energy objective corresponds to \(\ell^2_2\), and it is the only \(\ell^p_F\) objective to support unbiased gradients [Bellemare et al., 2017]. In high dimensions, IPMs are general-purpose two-sample tests; popular IPMs include the Kantorovich metric [Kantorovich and Rubinstein, 1958], Fortet-Mourier metric [Fortet and Mourier, 1953], the Lipschitz (or Dudley) metric [Dudley, 1966], and the total variation distance. In general, IPMs are defined in terms of a potentially costly optimization problem; out of the aforementioned IPMs, only
the energy objective has a known analytical (optimization-free) solution, and it also features a faster statistical convergence rate [Sriperumbudur et al., 2009].

Overall, we summarize the above facts as part of the following formal result.

**Theorem 1.** The energy objectives (2) and (3) are consistent estimators for the data distribution and feature unbiased gradients as in Equation 6).

This follows from properties of proper scoring rules and MMD; see the Appendix for a full proof.

4 Scaling Sample-Based Flow Objectives Using Random Projections

The framework of IPMs provides a wide range of high-dimensional sample-based objectives [Müller, 1997]. However, most of these objectives involve costly optimization problems, with the energy loss being a rare exception. At the same time, there exist many popular one-dimensional two-sample tests that have appealing statistical and computational properties and can yield training objectives.

We propose further improving our objective via random projections, specifically slicing, which projects data into one dimension [Kolouri et al., 2019, Nguyen et al., 2020, Song et al., 2019]. Formally, we define a sampling probability \( p(v) \) over one-dimensional vectors \( v \in \mathbb{R}^d \). We define a sliced version of a one-dimensional loss function \( F(x, y) : \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R} \) as

\[
F_p(x, y) = \mathbb{E}_{v \sim p(v)} \left[ F(v^\top x, v^\top y) \right].
\]

(7)

We approximate the expectation with a number of Monte-Carlo samples. This approach increases the number of sample-based objectives that can be used to train flows and improves the scalability of multi-variate objectives. We give examples below.

4.1 Sliced Energy Objectives

The sliced energy objective applies Equation 1 to the projected data. In practice, we find that the number of slices needed for good performance is far lower than the dimensionality of the data, resulting in a favorable computational profile. Furthermore, we can formally prove that the resulting objective has appealing statistical properties.

**Theorem 2.** The sliced versions of the energy objectives (2) and (3) are consistent estimators for the data distribution and feature unbiased gradients.

Intuitively, the first proposition is true because the CRPS objective is a special case of the MMD. At the same time, for each \( v \) the objective remains a proper score; a weighted combination of proper scores is also a proper score, hence the second part holds. See the Appendix for a full proof.

Recall also that in one dimension, the energy loss reduces to the CRPS, which is equivalent to the Wasserstein-2 distance. Wasserstein distances have more favorable convergence properties [Arjovsky et al., 2017] than maximum likelihood training, which lends more support to our choice of objective.

4.2 Sliced Two-Sample Baselines

Slicing also allows us to use univariate two-sample tests as objectives. We give examples below.

**Kolmogorov-Smirnov** One of the most popular ways of comparing the similarity between two distributions is via the quantity

\[
\text{KS}(F, G) = \sup_y |F(y) - G(y)|,
\]

(8)

the maximum distance between two CDFs \( F \) and \( G \). Empirical CDFs can be used for samples. While this test corresponds to an IPM, it does not have a widely accepted extension to higher dimensions.

**Hotelling’s Univariate Objective** The sliced version of Hotelling’s objective corresponds to using Hotelling’s \( t^2 \) univariate test (which is just the squared version of Student’s \( t \)-test) as an objective.

\[
H_u(D_F, D_G) = \frac{(m_F - m_G)^2}{s^2},
\]

(9)
where \( m_F, m_D, \) and \( s^2 \) are respectively the sample mean of \( D_F \), the sample mean of \( D_G \), and the combined sample variance, defined as in the multivariate version. Note that this formula is much less computationally expensive than the multi-dimensional one, which requires performing a matrix inversion (in worst-case \( O(d^3) \) time), while the sliced version takes only \( O(d) \) time.

**Fréchet Univariate Objective**  Similarly, the sliced version of the Fréchet objective is written as:

\[
R_u(D_F, D_G) = (m_F - m_G)^2 + (s^2_F - s^2_G)^2,
\]

which encourages the sample means \( m_F, m_G \) and the sample variances \( s_F, s_G \) to be the same. Again, this \( O(d) \) formula is less computationally expensive than in higher-dimensions, where it requires performing multiple matrix multiplications and a matrix square root (\( O(d^3) \)).

5 **Architectures for Energy Flows**

Next, we introduce energy flows, a class of models trained with our proposed Jacobian-free objectives. An energy flow is defined by an invertible mapping between \( z \) and \( y \) and is trained using the energy loss. As a result, energy flows improve over classical flow models by, among other things, supporting flexible architectures and by simultaneously providing fast training and sampling. We describe several flow architectures that are compatible with our objective below.

**Dense Invertible Layers**  The simplest architecture we consider consists of a sequence of small \( \mathbb{R}^d \rightarrow \mathbb{R}^d \) dense layers with invertible non-linearities (such as \text{tanh} or leaky ReLUs). We enforce the invertibility of the dense layers by adding a scaled identity component \( \sigma I_d \) for small \( \sigma > 0 \); other options for inducing invertibility include positivity constraints on the weights [Huang et al., 2018]. Although the \text{tanh} non-linearities are invertible, numerical values close to \( \{-1, 1\} \) tend to introduce numerical instability during inversion; we address this issue by via activity regularization [Chollet et al., 2015]. With these two architectural choices, we were able to compute both \( z \rightarrow y \) and \( y \rightarrow z \) mappings analytically and in a numerically stable way for modestly sized \( d \)'s; we provide experiments below.

**Invertible Residual Networks**  Recently, residual networks with spectral normalization have been proposed as a flexible invertible architecture [Behrmann et al., 2019]. Although one of the two directions of the flow is not computable analytically, it may be approximated using a fixed-point iteration algorithm. Invertible residual networks are typically trained using maximum likelihood; computing the determinant of the Jacobian of each layer requires a sophisticated approximation based on Taylor series expansion. Interestingly, when training these flows using maximum likelihood, the "fast" direction needs to be \( y \rightarrow z \) in order to enable fast training, but generation becomes non-analytic; when training using an energy objective, the \( z \rightarrow y \) direction is fast both for training and generation.

**Rectangular Flow Architectures**  Recently, several authors explored rectangular flows, in which the dimensionality of \( y \) and \( z \) is not equal [Nielsen et al., 2020, Cunningham and Fiterau, 2021, Caterini et al., 2021]. Training with maximum likelihood involves sophisticated extensions to the change of variables formula; however, these models can be trained without modification using an energy loss as long as one can sample from them efficiently. At the same time, we may retain their pseudo-invertibility to perform posterior inference.

6 **Experiments**

We demonstrate the benefits of our approach through a series of generative modeling experiments. Across a number of tasks previously used to benchmark flow algorithms, our method generates samples of equal or greater quality to more slower autoregressive models. Unlike other types of feed-forward methods [Kingma and Welling, 2014, Dziugaite et al., 2015], our architectures support exact posterior inference, which we demonstrate via an exploration of the latent space of our models.
6.1 Setup

We evaluate our framework on a range of UCI datasets [Dua and Graff, 2017] as well as datasets of handwritten digits (Pedregosa et al. [2011], Deng [2012]). We leverage the following classes of models and performance metrics.

Classical Normalizing Flows

We benchmark our models using normalizing flows trained using maximum likelihood and that use two types of architectures: autoregressive and non-autoregressive. Our autoregressive models are based on baselines from earlier work [Papamakarios et al., 2017, Si et al., 2022] and include Neural Autoregressive Quantile Flows (NAQF), and Masked Autoregressive Flows (MAF-LL). These models assume a parameterization \( p(y|z) = \prod_{j=1}^{d} p(y_j|y_{<j}, z_j) \), where each \( p(y_j|y_{<j}) \) is a probability conditioned on the previous variables and \( z_j \). In MAFs, the \( p(y_j|y_{<j}) \) are Gaussian; in NAQFs they are parameterized by a flexible quantile flow [Si et al., 2022]. At each step, the parameters defining \( p(y_j|y_{<j}, z_j) \) are given by a neural network. In our UCI experiments, this consists of a single LSTM layer with hidden dimensions equal to the dimension of the data followed by a fully-connected linear layer. In our image experiments, we used a variant of the PixelCNN architecture.

Our non-autoregressive models consist of variational auto-encoders (VAEs) trained using the evidence lower bound (ELBO) on the maximum likelihood and based on a fully-connected architecture (see below for details). In order to understand the benefits of our objective, we fit a VAE model with the same invertible architecture for the generator as the one used by our energy flow models; we refer to the resulting method as a dense invertible flow trained using maximum log-likelihood (DIF-LL).

Energy Flow Models

We constructed flow models using dense invertible layers, referring the resulting model as a Dense Invertible Flow trained with an energy loss (DIF-E). The DIF-E model consists of three feedforward invertible layers and Leaky ReLU activation functions, and is trained using the kernelized energy loss 3 with a mixture of RBF kernels with bandwidth in \{2, 5, 10, 20, 40, 80\}. We also use the energy score to train non-invertible rectangular flows trained with the energy loss (REF-E). In particular, rectangular flows are parametrized by layers of size \([d/8, d/4, d/2, d]\) as compared to DIF-E which requires all layers to be of size \(d\) for invertibility.

We also compared DIF-E to autoregressive models trained with a Jacobian-free objective. Specifically, we trained our autoregressive MAF models with the quantile loss [Si et al., 2022] in addition to the NAQF models. We denote these as MAF-QL and AQF-QL respectively.

Metrics

We evaluate the models in terms of log-likelihood (when available and appropriate) and using variants of the CRPS metric. For VAE-type models trained using the ELBO, we report the ELBO as a lower bound on the log-likelihood. We use two CRPS-style metrics which have the following structure: the first is a sample-based version as in Equation 2. The second, marked as univariate CRPS (U-CRPS), is the sum of one-dimensional CRPS measured for each output dimension and estimates the quality of marginal distributions [Si et al., 2022]. Both versions of the CRPS use the \(\ell_1\) norm.

In our image datasets, we are also interested in estimating in a quantitative way the quality of the generated samples and their similarity to the data distribution. In order to do that, we define a metric called the D-loss. The D-Loss is measured by the accuracy of a discriminative model to determine whether an image is generated. Details can be found in the appendix.

6.2 Understanding the Sample-Based Objectives

We start with experiments that analyze the properties of the sliced energy objectives and compare them to the baseline two-sample objectives on the UCI and image datasets.

Energy Objective vs. Two-Sample Baselines

We claim that the energy objective is a particularly favorable training criterion for flows; we empirically establish this fact by comparing it against the other two-sample objectives, which we see as strong baselines. We train an invertible flow model on the Miniboone UCI dataset. The model consists of 4 layers of size 43 (to match Miniboone dimension) and each objective is trained for 200 epochs with a learning rate of 1e-3. Complexity is
Table 2: Objective Results and Complexity.

| Metrics  | KS | 1D Hotelling | Hotelling | 1D-FD | FD | 1D-Energy | Energy |
|----------|----|--------------|-----------|-------|----|-----------|--------|
| CRPS     | 1.53 | 0.57 | 0.717 | 0.558 | 0.559 | 0.545 | 0.548 |
| Complexity | n log b | n | d³ | n | d³ | bd | bn |

Table 4: Model performance on UCI datasets as measured by CRPS.

| Dataset     | n    | d    | MAF-LL | MAF-QL | AQF-QL | DIF-E | DIF-E Proj |
|-------------|------|------|--------|--------|--------|-------|------------|
| BSDS 300   | 1050000 | 63 | .044   | .036   | .033   | .039  | .040 |
| Miniboone  | 32840  | 43  | .567   | .561   | .525   | .524  | .545 |
| Gas        | 946859 | 8   | .645   | .565   | .513   | .548  | .551 |
| Power      | 1844352 | 6  | .542   | .506   | .502   | .451  | .454 |
| Hepmass    | 350136 | 21  | .617   | .614   | .523   | .589  | .587 |

written where b denotes the batch size, d denotes the dataset dimension, and n denotes the number of projections made.

Flows trained using the energy objective achieve the best performance in Table 2, outperforming the strong baselines; we focus on the energy objective in subsequent in-depth experiments.

**Improvements in Scalability Form Slicing**

Next, we seek to understand the scalability improvements from slicing. We train a projection based model on MNIST using projected energy loss for 200 epochs with learning rate 1e-3. The model consists of 4 dense layers of size 784 with leaky relu activation functions for the first three layers and a sigmoid activation function for the last. When we calculate the loss, we take n projections into a single dimension, which we denote in table 3 as n for the projection parameters. We see in Table 3 that sliced objectives perform comparably to non-sliced objectives with a fraction of the dimension, while having improved computational complexity.

Table 3: Slicing on MNIST.

| n    | 400 | 200 | 100 | 50 |
|------|-----|-----|-----|----|
| U-CRPS | 0.088 | 0.088 | 0.088 | 0.091 |
| CRPS  | 0.191 | 0.191 | 0.192 | 0.195 |

**6.3 UCI Experiments**

Non-autoregressive energy flows can capture joint dependencies without the slow generation process of autoregressive models. We implemented energy flows on five UCI datasets used previously as benchmarks by [Papamakarios et al., 2017] and [Si et al., 2022], which are: BSDS 300, Miniboone, Gas, Power and Hepmass. The size of the datasets are noted in Table 4. We used an LSTM architecture for all autoregressive models. All models were trained with a batch size of 200 and learning rate of 1e-3 using the Adam optimizer for 200 epochs for the smaller datasets (Miniboone, Hepmass) and 20 epochs for the larger ones (Gas, Power, BSDS 300).

**Results.** As shown in Table 4, energy flows perform comparably to the neural AQF-QL baseline. Both methods are trained using variants of the CRPS and obtain top performance across the five datasets. However, the DIF-E model is non-autoregressive, hence provides advantage in terms of sampling speed. Our experiments thus illustrates that non-autoregressive models can match the performance of autoregressive models trained with log-likelihood or versions of the CRPS objective.

**6.4 Image Generation on Digits**

Next, we test our methods on a standard generative modeling task: digit generation [Pedregosa et al., 2011]. We use a PixelCNN architecture for the autoregressive models, which we denote PixelMAF-LL, PixelMAF-QL, and PixelAQF-QL. The PixelCNN has receptive field 15 which maps

Table 5: Digits Generation Experiments

| Method      | U-CRPS | CRPS | NLL | D-Loss |
|-------------|--------|------|-----|--------|
| PixelMAF-LL | 0.136  | 0.206| -102.2 | 0.974 |
| PixelMAF-QL | 0.131  | 0.204| 90   | 0.883 |
| PixelAQF-QL | 0.127  | 0.199| n/a  | **0.681** |
| DIF-LL (VAE)| 0.138  | 0.207| ≤ 23.8 | 0.941 |
| REF-E       | 0.127  | 0.201| n/a  | 0.823 |
| DIF-E       | 0.126  | **0.197** | n/a | 0.807 |
| DIF-E-Proto | 0.127  | 0.199| n/a  | 0.815 |
Results. The proposed energy flow model performs comparably on the U-CRPS and CRPS metrics to the AQF model, although the latter is more discriminable (has a better D-loss). On the other hand the samples generated by the DIF-EE outperforms those of any of the other autoregressive architectures, as well as the samples from non-autoregressive DIF-LL model, which is trained with maximum log likelihood.

Inversion and Interpolation. A key feature of the DIF-E model is exact posterior inference (despite not being trained with log-likelihood). To demonstrate this, we create intermediate representations between pairs of digits through which we can smoothly interpolate (Figure 1). By taking the inverse of the decoder model by inverting the activation functions and weight matrices, we are able to create an encoder similar to that of the VAE. Like the VAE, the energy flow can generate interpolated samples, with the added advantage of exact posterior inference.

6.5 MNIST

For this set of experiments, we once again trained autoregressive models with the PixelCNN architecture. Each model was trained for 300 epochs with a learning rate of 1e-3, and has hidden layer size 784. In addition, we trained a rectangular flow model using the ELBO approximation of the log-likelihood (REF-LL), which results in a model equivalent to a VAE. We computed the same metrics as we did for the experiments on the digits dataset for all methods.

Results. From the samples in Figure 2, the results generated from the MAF-QL seems to be much more visually accurate than MAF-LL, which is trained on a LL-based loss, even though they have the same architecture. However, both of these models still suffer from an autoregressive architecture for image generation, in comparison to the single prediction models with the DIF-LL and Energy Flow models. In addition, though the DIF-LL performed similarly on the CRPS metrics in Table 6, discriminating between real and fake digits with

| Method       | U-CRPS | CRPS  | NLL   | D-Loss |
|--------------|--------|-------|-------|--------|
| PixelMAF-LL  | .128   | .279  | -6011 | 1.00   |
| PixelMAF-QL  | .099   | .215  | -5888 | .983   |
| PixelAQF-QL  | .119   | .228  | n/a   | .986   |
| REF-LL (VAE) | .090   | .189  | ≤ 125 | .903   |
| DIF-LL (VAE) | .089   | .190  | ≤ 105 | .855   |
| REF-E        | .085   | .187  | n/a   | .778   |
| DIF-E        | .084   | .186  | n/a   | .701   |
| DIF-E-Proj   | .088   | .191  | n/a   | .819   |
an SVM was more difficult than with other models, which generated images generated that were much more toned down and blurred.

7 Previous Work, Discussion, and Conclusion

Normalizing Flows  Our work extends the framework of flows [Papamakarios et al., 2017, 2019] to use a novel learning objectives. Most existing flows feature autoregressive architectures where each dimension leverages integration-based transformers [Wehenkel and Louppe, 2021], spline approximations [Müller et al., 2019, Durkan et al., 2019, Dolatabadi et al., 2020], piece-wise separable models, and others. Recently, there has been interest in non-autoregressive architectures [Behrmann et al., 2019] and rectangular flows [Caterini et al., 2021], trained with maximum likelihood. [Si et al., 2022] proposed auto-regressive quantile flows, which generalize implicit quantile networks Dabney et al. [2018] and are invertible flows trained using proper scores.

Comparison to Other Models  We provide a complete comparison to other models in Table 1. Our approach contrasts against VAE style models [Kingma and Welling, 2014] by providing exact inference and likelihood evaluation. Unlike MAFs [Papamakarios et al., 2017], our models are non-autoregressive and do not make any Gaussianity assumptions and instead use a fully neural parameterization of the output probabilities, which contributes to improved performance and modeling flexibility. Approaches like AQF [Si et al., 2022] and NAF [Huang et al., 2018] also provide neural approximators, but they are autoregressive. Closely related feedforward models include GMMNets [Li et al., 2015, Dziugaite et al., 2015] and CramerGANs [Bellemare et al., 2017], but they do not offer likelihood evaluation and posterior inference. Our framework is closely related to Maximum Mean Discrepancy (MMD) [Gretton et al., 2008] and its generalizations (Li et al. [2015], Dziugaite et al. [2015]). However, unlike models optimizing MMD [Li et al., 2015, Dziugaite et al., 2015], ours provide latent variable inference and exact density evaluation using the change of variables formula.

Conclusion  Despite the emergence of proper-scoring based models which aim to capture the uncertainty within a model, they have thus far been autoregressive in nature, making them slow to sample. We proposed Energy Flows, a non-autoregressive architecture using the energy loss from [Gneiting and Raftery, 2007], allowing it to retain the benefits of proper scoring rules while being able to sample faster from a joint distribution. From our different generative experiments, this joint model remains competitive with autoregressive models. Concurrently, using an invertible flow architecture allows us to take advantage of several of its properties such as exact posterior inference. We see our work as a first step towards designing Jacobian-free normalizing flows via the introduction of novel learning objectives.
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A Appendix

A.1 D-Loss

The D-Loss is derived from an ensemble of SVM discriminators (with RBF kernels having a bandwidth parameter \( \gamma \) of 0.0001, 0.001, 0.01, 0.1, 1, 10, 100, 1000, and 10000) used to differentiate the real data versus the sampled data from the model. More details are included in the appendix. The D-Loss for a single discriminator model \( D : \mathbb{R}^n \rightarrow \{0, 1\} \) is measured as the accuracy achieved by the best SVM, which is gotten through a 80:20 train-validation split on the 300 real and 300 fake images: \( \text{D-Loss} = \max_\gamma \text{D-Loss}_\gamma \).

A.2 Theorem Proofs

Multi-Variate Objectives  In this section, we make the assumption that the kernels \( K \) used to define our objectives are measurable and bounded by \( \kappa \). Under these conditions, when using a kernelized objective with kernel \( K \), each distribution \( F \) can be represented by a mean embedding \( \mu_F \) in the reproducing kernel Hilbert space (RKHS) induced by \( K \) [Gretton et al., 2008]. We also assume that there exists a unique mapping between \( \mu_F \) and \( F \) for every \( F \) in the class of model distributions \( \mathcal{F} \). Note that this can be satisfied for any Borel probability measure if the kernel \( K \) is chosen to be universal or characteristic [Gretton et al., 2008]. Alternatively, we may satisfy this claim by choosing \( F \) to be a restricted set of distributions for which the above claim is true.

**Theorem.** The energy objectives (2) and (3) are consistent estimators for the data distribution and feature unbiased gradients as in Equation 6.

**Proof.** First, we seek to establish the consistency of the minimize of our objectives as an estimator of the data distribution. Our argument uses the fact that the (kernelized) energy score is closely connected to the maximum mean discrepancy (MMD; [Gretton et al., 2008]). Observe that

\[
\begin{align*}
\mathbb{E}_{y' \sim \mathcal{P}} \text{CRPS}_K(F, y') &= \frac{1}{2} \mathbb{E}_F K(\mathbf{Y}, \mathbf{Y}') - \mathbb{E}_{F, \mathcal{D}} K(\mathbf{Y}, \mathbf{Y}') \\
&= \left( \frac{1}{2} \mathbb{E}_F K(\mathbf{Y}, \mathbf{Y}') - \mathbb{E}_{F, \mathcal{D}} K(\mathbf{Y}, \mathbf{Y}') \right) + \frac{1}{2} \mathbb{E}_{y', y'' \sim \mathcal{D}} K(y, y') \\
&= -\frac{1}{2} \text{MMD}_K^2(F, \mathcal{D}) + \text{const};
\end{align*}
\]

hence, by maximizing the CRPS over a set of possible models \( F \), we are minimizing a monotonic transformation of the MMD. Since (2) is a special case of (3) with the distance kernel [Sejdinovic et al., 2013], the above claim also holds for the non-kernelized energy objective (2).

We would like to establish that minimizing objectives (2) and (3) over a data distribution \( \mathcal{D}_n \) of \( n \) samples from the true data distribution \( \mathcal{P} \) yields a model \( F_n \) that is similar to what we would obtain if we searched for the best \( F \) using the full data distribution \( \mathcal{P} \); in other words:

\[
\mathbb{E}[L(F_n, \mathcal{P})] \leq \inf_{F \in \mathcal{F}} L(F, \mathcal{P}) + o(n),
\]

where \( L(F, \mathcal{P}) \) is a metric or pseudo-metric\(^1\) that we will instantiate shortly, \( \mathcal{F} \) is the hypothesis class for the model \( F \), \( F_n \) is the empirical risk minimization solution (from our method) over a dataset \( \mathcal{D}_n \), and the additive \( o(n) \) term decays to zero as we increase \( n \). Note that if the model is well-specified (i.e., \( \mathcal{P} \in \mathcal{F} \)), we have \( \mathbb{E}[L(F_n, \mathcal{P})] = o(n) \), and we have a consistent estimator.

\(^1\)A metric \( d(x, y) \) satisfies four properties: symmetry, triangle inequality, \( d(x, x) = 0 \) and \( d(x, y) = 0 \iff x = y \). A pseudo-metric satisfies only the first three properties. The MMD objective is a metric if its kernel is characteristic or universal (or more generally if there is a one-to-one mapping between \( \mu_F \) and \( F \); otherwise, it is a pseudo-metric.)
To establish this fact, we will derive a version of the above identity for a modified version of the MMD and under the assumption of this section; we will also argue that the kernelized energy estimate satisfies that identity.

First, let $L(F, P) = \text{MMD}(F, P)$. By the properties of MMD and kernels, we know that $\text{MMD}(F, P) = ||\mu_F - \mu_P||_{\mathcal{H}}$, and MMD is a pseudo-metric. Note that we have by the triangle inequality

$$L(F_n, P) \leq L(F_n, D_n) + L(D_n, P),$$

where we overload notation and use $D_n$ to also denote the empirical distribution. Note that because our objective is a monotonic transformation ($\frac{1}{2} \text{MMD}^2 + \text{const}$) of the MMD, the $F_n$ minimizes the MMD within $F$. Thus we can write for any $F \in F$

$$L(F_n, P) \leq L(F, D_n) + L(D_n, P) \leq L(F, P) + 2L(D_n, P)$$

where we have used once more the triangle inequality in the last line. Taking expectations on both sides and using the fact that $F \in F$ was arbitrary, we find that

$$\mathbb{E}L(F_n, P) \leq \inf_{F \in F} L(F, P) + 2\mathbb{E}L(D_n, P) \leq \inf_{F \in F} L(F, P) + 2\sqrt{\mathbb{E}L(D_n, P)^2}.$$

To establish our claim, we need to bound the last term. Let $x_i$ denote the i.i.d. samples from $D_n$, let $\phi$ denote the embedding induced by the kernel $K$ in its RKHS $\mathcal{H}$, and note that we have

$$\mathbb{E}L(D_n, P)^2 = \mathbb{E}||\frac{1}{n} \sum_{i=1}^{n} \phi(x_i) - \mathbb{E}\phi(x)||_{\mathcal{H}}$$

$$= \text{Var}(\frac{1}{n} \sum_{i=1}^{n} \phi(x_i))$$

$$= \frac{1}{n} \text{Var}(\phi(x_1))$$

$$\leq \frac{2}{n} \mathbb{E}||\phi(x_1)||_{\mathcal{H}}$$

$$\leq \frac{2\kappa}{n}$$

Thus, our main claim follows with

$$\mathbb{E}L(F_n, P) \leq \inf_{F \in F} L(F, P) + 2\sqrt{\frac{2\kappa}{n}}.$$

Thus the estimated model $F_n$ satisfies the above inequality and if the data distribution $P \in F$, our consistency claim holds.

We can establish that the gradients are unbiased by leveraging properties of proper scoring rules. Recall from the background section that a loss $L : \Delta(\mathbb{R}^d) \times \mathbb{R}^d \to \mathbb{R}$ is strictly proper [Gneiting and Raftery, 2007] if $G = \arg\min_F \mathbb{E}_{y \sim G} L(F, y)$. In the context of the CRPS objective $L$, we have by definition of a proper loss

$$L(F, G) = \mathbb{E}_{y' \sim G} \text{CRPS}_K(F, y') = \mathbb{E}_{y' \sim G} \text{CRPS}_K(F, G_{y'})$$

where $G_{y'}$ is the empirical distribution derived from $y'$.

Let $P$ denote the true data distribution, $D_n$ a dataset of size $n$ drawn from $P$, and $G_n$ the resulting empirical distribution. Then we have:

$$\nabla_\theta \mathbb{E}_{D_n \sim P} L(F_\theta, G_n)) = \nabla_\theta \mathbb{E}_{D_n \sim P} \mathbb{E}_{y' \sim D_n} L(F_\theta, y')$$

$$= \nabla_\theta \mathbb{E}_{y' \sim P} L(F_\theta, y')$$

$$= \nabla_\theta L(F_\theta, P),$$

which is equivalent to the statement in (6) that we wanted to prove. □
Alternative Approaches to Showing Consistency  The fact that consistency holds also follows from properties of the MMD for general classes \( \mathcal{F} \); for example as shown in Dziugaite et al. [Dziugaite et al., 2015] (Theorem 1),
\[
\mathbb{E}[\text{MMD}^2(F_n, \mathcal{P})] \leq \inf_{F \in \mathcal{F}} \text{MMD}^2(F, \mathcal{P}) + o(n),
\]
if \( \mathcal{F} \) satisfies a fat-shattering condition. The desired consistency claim with \( L(F, G) \) being our kernelized energy objective \( \text{CRPS}_K \) then follows directly from our earlier derivation by applying an affine transformation on each side of the above equation.

Alternative Approaches to Showing that Gradients are Unbiased  Note that a special case of the unbiased gradient property for the non-kernelized objective (1) has been established using techniques discussed in Bellemare et al. [Bellemare et al., 2017] (Proposition 3). This result also follows from our aforementioned connection to the MMD and Lemma 6 in Gretton et al. (2012) [Gretton et al., 2008].

Sliced Objectives

**Theorem.** The sliced versions of the energy objectives (2) and (3) are consistent estimators for the data distribution and feature unbiased gradients.

**Proof.** We establish the first part of the claim by observing that the sliced version of the energy objective
\[
\text{CRPS}(F, y') = \mathbb{E}_{w \sim p(w)} \left[ \frac{1}{2} \mathbb{E}_F K(w^\top Y, w^\top Y') - \mathbb{E}_F K(w^\top Y, w^\top y') \right],
\]
where \( K \) is a kernel in 1D, is an affine transformation of squared MMD. Then the first part of the claim follows by the argument in Theorem 1. To see this, first, define the function \( K_w : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R} \) as
\[
K_w(x, y) = K(w^\top x, w^\top y),
\]
where \( K \) is the kernel used as part of the sliced energy objective. It is easy to see that \( K_w(x, y) \) is a kernel. Consider any dataset \( S = \{x_i\}_{i=1}^k \); then the matrix \( M \) defined as \( M_{ij} = K_w(x_i, x_j) \) will be semi-definite because the corresponding matrix \( M' \) defined as \( M'_{ij} = K(w^\top x_i, w^\top x_j) \) is also positive definite, because it is the kernel matrix for the set \( S = \{w^\top x_i\}_{i=1}^k \). Hence, by Mercer’s theorem \( K_w \) is a kernel.

Next, define the function \( \bar{K} : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R} \) as
\[
\bar{K}(x, y) = \mathbb{E}_{w \sim p(w)} K_w(x, y).
\]
This is also a kernel, because it is a sum of kernels. Next, note that
\[
\text{CRPS}(F, y') = \mathbb{E}_{w \sim p(w)} \left[ \frac{1}{2} \mathbb{E}_F K(w^\top Y, w^\top Y') - \mathbb{E}_F K(w^\top Y, w^\top y') \right] = \frac{1}{2} \mathbb{E}_F \bar{K}(Y, Y') - \mathbb{E}_{F \sim \mathcal{P}} \bar{K}(Y, y'),
\]
which is an instance of the kernelized energy objective that uses a modified kernel. Note that this is both a proper score and a rescaled version of the squared MMD with a modified kernel. The two claims of this theorem follow directly from Theorem 1.

\[\square\]