Learning deep kernels for exponential family densities

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Abstract
The kernel exponential family is a rich class of distributions, which can be fit efficiently and with statistical guarantees by score matching. Being required to choose a priori a simple kernel such as the Gaussian, however, limits its practical applicability. We provide a scheme for learning a kernel parameterized by a deep network, which can find complex location-dependent local features of the data geometry. This gives a very rich class of density models, capable of fitting complex structures on moderate-dimensional problems. Compared to deep density models fit via maximum likelihood, our approach provides a complementary set of strengths and tradeoffs: in empirical studies, the former can yield higher likelihoods, whereas the latter gives better estimates of the gradient of the log density, the score, which describes the distribution’s shape.

1 INTRODUCTION
Density estimation is one of the foundational problems in statistics and machine learning (Devroye and Györfi 1985; Wasserman 2006), lying at the core of both supervised and unsupervised machine learning problems. Classical techniques such as kernel density estimation, however, struggle to exploit the structure inherent to complex problems, and thus can require unreasonably large sample sizes for adequate fits. Without smoothness or regularity assumptions, the risk of density estimation based on N samples in D dimensions scales as $O(N^{-4/(4+D)})$ (Wasserman 2006, Section 6.5).

One promising approach for incorporating this necessary structure is the kernel exponential family (Cann and Smola 2006; Fukumizu 2009; Sriperumbudur et al. 2017). This model allows for any log density which is suitably smooth under a given kernel, i.e. any function in the corresponding reproducing kernel Hilbert space. Choosing a finite-dimensional kernel recovers any classical exponential family, but when the kernel is sufficiently powerful the class becomes very rich: dense in the family of continuous probability densities on compact domains in KL, TV, Hellinger, and $L^r$ distances (Sriperumbudur et al. 2017, Corollary 2). The normalization constant for this family of densities is not available in closed form, making fitting by maximum likelihood difficult, but the alternative technique of score matching (Hyvärinen 2005) allows for practical usage with theoretical convergence guarantees (Sriperumbudur et al. 2017).

The choice of kernel directly corresponds to a smoothness assumption on the model, allowing one to design a kernel corresponding to prior knowledge about the target density. Yet explicitly deciding upon a kernel to incorporate that knowledge can be complicated, and indeed previous applications of the kernel exponential family model have exclusively employed simple kernels, such as the Gaussian kernel, with a small number of parameters (e.g. the length scale) either chosen heuristically or selected via cross-validation (e.g. Sasaki et al. 2014; Strathmann et al. 2015). These kernels are typically spatially invariant, corresponding to a uniform smoothness assumption across the domain. Although such kernels are sufficient for consistency in the infinite-sample limit, the induced models can fail in practice on finite datasets, especially if the data takes differently scaled shapes in different parts of the space. Figure 1 (left) illustrates this problem when fitting a simple mixture of Gaussians. Here there are two “correct” bandwidths, one for the broad mode and one for the narrow mode. A translation-invariant kernel must pick a single one, e.g. an average between the two, and any choice will yield a poor fit on at least part of the density.

In this work, we propose to learn the kernel of an exponential family directly from data. Thus, we can achieve far more compared to simply tuning a length scale, and instead learn location-dependent kernels.

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that adapt to the underlying shape and smoothness of the target density. We will use kernels of the form
\[ k(x, y) = \kappa(\phi(x), \phi(y)), \quad (1) \]
where the deep network \( \phi \) extracts features of the input and \( \kappa \) is a simple kernel (e.g. a Gaussian) on those features. These types of kernels have seen success in supervised learning (Wilson et al. 2016, Jean et al. 2018) and critic functions for implicit generative models (Li et al. 2017, Bellemare et al. 2017, Balakrishnan et al. 2018, Arbel et al. 2018). We call the resulting model a deep kernel exponential family (DKEF).

We can train both kernel parameters (including all the weights of the deep network) and, unusually, even regularization parameters directly on the data. Normally, directly optimizing regularization parameters would lead to them always being set to 0, since their beneficial effect in preventing overfitting is by definition not seen on the training set. Here, though, we can exploit the closed-form fit of the kernel exponential family to optimize a “held-out” score (Section 3). Figure 1 (right) demonstrates the success of this model on the same mixture of Gaussians; here the learned, location-dependent kernel gives a much better fit.

We compare the results of our new model to recent general-purpose deep density estimators. These approaches fall into the categories of autoregressive models (Uria et al. 2013, Germain et al. 2015, Oord et al. 2016) and normalizing flows (Jimenez Rezende and Mohamed 2015, Dinh et al. 2017, Papamakarios et al. 2017), which learn deep networks with structures designed to compute normalized densities, and are fit via maximum likelihood. We explore the strengths and limitations of both flow and autoregressive models and deep kernel exponential families on a variety of datasets, including artificial data designed to illustrate scenarios where certain surprising problems arise, as well as benchmark UCI datasets used previously in the literature. In general, we will see that the models fit by maximum likelihood give somewhat greater likelihoods, whereas the deep kernel exponential family generally better fits the shape of the distribution. Code can be found at https://github.com/kevin-w-li/deep-kexpfam

2 BACKGROUND

Score matching Suppose we observe \( \mathcal{D} = \{x_n\}_{n=1}^N \), a set of independent samples \( x_n \in \mathbb{R}^D \) with an unknown density \( p_0(x) \). We posit a class of possible models \( \{p_\theta\} \), parameterized by \( \theta \); our goal is to use the data \( \mathcal{D} \) to select some \( \hat{\theta} \) such that \( \hat{p}_\theta \approx p_0 \). The standard approach for selecting \( \theta \) is maximum likelihood: \( \hat{\theta} = \arg \max_\theta \prod_{n=1}^N p_\theta(x_n) \).

Many interesting model classes, however, are defined as \( p_\theta(x) = \hat{p}_\theta(x)/Z_\theta \), where the normalization constant \( Z_\theta = \int_x \hat{p}_\theta(x) dx \) cannot be easily computed. In this setting, an optimization algorithm to estimate \( \theta \) by maximum likelihood requires estimating the derivative of \( Z_\theta \) for each candidate \( \theta \) considered during optimization. Moreover, the maximum likelihood solution may not even be well-defined when \( \theta \) is infinite-dimensional, and other approximations to this solution can be challenging to implement in practice (Barron and Sheu 1991, Fukumizu 2000). The intractability of maximum likelihood led Hyvärinen (2005) to propose an alternative objective, called score matching. Rather than maximizing the likelihood, one minimizes the Fisher divergence \( J(p_\theta || p_0) \):
\[ \frac{1}{2} \int p_\theta(x) \| \nabla_x \log p_\theta(x) - \nabla_x \log p_0(x) \|^2 dx. \quad (2) \]
Under mild regularity conditions, this is equal to
\[ \int_x p_\theta(x) \sum_{d=1}^D \left[ \partial^2_\| f(x)(x) + \frac{1}{2} (\partial_\| \log p_\theta(x))^2 \right] dx, \quad (3) \]
up to an additive constant depending only on \( p_0 \), which can be ignored during training. Here \( \partial^2_\| f(x) \) denotes
\[
\frac{\partial^n}{\partial x_n^m} f(x')|_{x'=x}. \]
We can estimate \( J(p_{\theta}, D) \):
\[
\frac{1}{N} \sum_{n=1}^N \sum_{d=1}^D \left[ \frac{\partial^2_d \log p_{\theta}(x_n)}{2} + \frac{1}{2} (\partial_d \log p_{\theta}(x_n))^2 \right]. \tag{4}
\]

Notably, (4) does not depend on \( Z_0 \), and so it suffices to use the unnormalized model \( \tilde{\rho}_0 \). We can thus estimate \( \theta \) by minimizing a regularized version of (4), giving an unnormalized model \( \tilde{\rho}_0 \) for \( p_0 \).

Unnormalized models \( \tilde{\rho} \) are sufficient for many tasks, including finding modes, approximating Hamiltonian Monte Carlo on targets without gradients (Strathmann et al. 2015), and learning discriminative features (Janzamin et al. 2014). If we require a normalized model, however, we can estimate the normalizing constant once, after estimating \( \theta \); this will be far more computationally efficient than estimating it at each step of a maximum likelihood optimization algorithm.

Asymptotically, score matching is consistent in the well-specified setting (Hyvärinen 2005, Theorem 2). Lyu (2009) connected it to maximum likelihood, arguing score matching finds a fit which is robust to infinitesimal amounts of noise.

**Kernel exponential families** We next describe the kernel exponential family (Cam and Smola 2006; Sriperumbudur et al. 2017). This is a class of densities whose negative *energy* (LeCun et al. 2006) is of the form \( \log \tilde{\rho}(x) = f(x) + \log q_0(x) \), where \( q_0 \) is some fixed function and \( f \) is any function satisfying a certain smoothness constraint. Specifically, \( f \) should belong to the reproducing kernel Hilbert space \( \mathcal{H} \), with kernel \( k \). The reproducing property \( f(x) = \langle f, k(x, \cdot) \rangle_{\mathcal{H}} \) shows that this class generalizes exponential families to have a natural parameter \( f \) and sufficient statistic \( k(x, \cdot) \):
\[
\hat{p}_f(x) = \exp (f(x)) q_0(x) = \exp (\langle f, k(x, \cdot) \rangle_{\mathcal{H}}) q_0(x).
\]

Using a simple finite-dimensional \( \mathcal{H} \), we can recover any standard exponential family, e.g., normal, gamma, or Poisson; if \( \mathcal{H} \) is infinite-dimensional and sufficiently rich, then this family can approximate any continuous distribution with tails like \( q_0 \) arbitrarily well (Sriperumbudur et al. 2017, Example 1 and Corollary 2).

These models do not in general have a closed-form normalizer, making fitting by maximum likelihood challenging. For some choices of \( f \) and \( q_0 \), \( \hat{p}_f \) may not even be normalizable, but choosing \( q_0 \) to be Gaussian and most kernels of the form (1) guarantees a normalizer will exist (Proposition 2 in Appendix A).

Sriperumbudur et al. (2017) proved good statistical properties for choosing \( f \in \mathcal{H} \) by minimizing a regularized form of (4), \( f = \arg \min_{f \in \mathcal{H}} J(\hat{p}_f, D) + \lambda \|f\|_2^2 \), but their algorithm has an impractical computational cost of \( \mathcal{O}(N^3D^3) \). This can be alleviated with the Nyström-type “lite” approximation (Strathmann et al. 2015; Sutherland et al. 2018): select \( M \) inducing points \( z_m \in \mathbb{R}^D \), and find \( f \in \mathcal{H} \) of the form
\[
f_{\alpha, z}^k(x) = \sum_{m=1}^M \alpha_m k(x, z_m), \quad \hat{p}_{\alpha, z}^k = \hat{p}_{f_{\alpha, z}}^k. \tag{5}
\]

As the span of \( \{k(z, \cdot)\}_{z \in \mathbb{R}^D} \) is dense in \( \mathcal{H} \), this is a natural approximation, similar to classical RBF networks (Broomhead and Lowe 1988). The “lite” model often yields excellent empirical results at much lower computational cost than the full estimator. We can regularize (4) in several ways and still find a closed-form solution for \( \alpha \). In this work, our loss \( J(f_{\alpha, z}, \lambda, D) \) will be
\[
J(\hat{p}_{\alpha, z}, D) + \frac{\lambda_2}{2} \|\alpha\|^2 + \frac{\lambda_C}{2N} \sum_{n=1}^N \sum_{d=1}^D [\partial^2_d \log \hat{p}_{\alpha, z}(x_n)]^2.
\]

Sutherland et al. (2018) used a small \( \lambda_\alpha \) for numerical stability but primarily regularized with \( \lambda_H \|f_{\alpha, z}\|_2^2 \). As we change \( k \), however, \( \|f\|_H \) changes meaning, and we found empirically that this regularizer tends to perform poorly. The \( \lambda_C \) term was recommended by Kingma and LeCun (2010), encouraging the learned energy function to be smooth without much extra computation. Given \( k, z, \) and \( \lambda \), Proposition 3 (Appendix B) shows we can find the optimal \( \alpha \) by solving an \( M \times M \) linear system in \( \mathcal{O}(M^2ND+M^3) \) time: the \( \alpha \) which minimizes \( J(f_{\alpha, z}, \lambda, D) \) is
\[
\alpha(\lambda, k, z, D) = - (G + \lambda_\alpha I + \lambda_C U)^{-1} b \tag{6}
\]
\[
G_{m,m'} = \frac{1}{N} \sum_{n=1}^N \sum_{d=1}^D \partial_d k(x_n, z_m) \partial_d k(x_n, z_{m'})
\]
\[
U_{m,m'} = \frac{1}{N} \sum_{n=1}^N \sum_{d=1}^D \partial^2_d k(x_n, z_m) \partial^2_d k(x_n, z_{m'})
\]
\[
b_{m} = \frac{1}{N} \sum_{n=1}^N \sum_{d=1}^D \partial_d k(x_n, z_m) + \partial_d \log q_0(x_n) \partial_d k(x_n, z_m)
\]
\[
+ \lambda_C \partial^2_d \log q_0(x_n) \partial^2_d k(x_n, z_m).
\]

Previous attempts at deep score matching Kingma and LeCun (2010) used score matching to train a network to output an energy. Given software limitations at the time, they used only a single layer. This approach can also essentially be viewed in the kernel exponential family framework: let \( \phi_w : \mathbb{R}^D \to \mathbb{R} \) and use the kernel \( k_w(x, y) = \phi_w(x) \phi_w(y) \). Then the function \( f_{\alpha, z}^k(x) \) from (5) is
\[
\sum_{m=1}^M \alpha_m \phi_w(z_m) \phi_w(x) = \left[ \sum_{m=1}^M \alpha_m \phi_w(z_m) \right] \phi_w(x),
\]
where the scalar in brackets is fit analytically.

Saremi et al. (2018) recently also attempted parameterizing the energy as a deep network, using an approximation called Parzen score matching. Unfortunately, this approximation requires a global constant bandwidth to define the Parzen window size for the loss function, fit to the dataset before learning the model. This likely is only sensible on datasets for which simple fixed-bandwidth kernel density is appropriate; on more complex datasets, the loss may be poorly motivated.

It also evidently leads to substantial over-smoothing, as is visible in their results. As they did not provide code for their method, we do not compare to it empirically.

3 FITTING DEEP KERNELS

All previous applications of score matching in the kernel exponential family of which we are aware (e.g. Sriperumbudur et al. 2017; Strathmann et al. 2015; Sun et al. 2015; Sutherland et al. 2018) have used kernels of the form \( k(x, y) = \exp(-\frac{1}{2\sigma^2}\|x - y\|^2) + r(x^Ty + c)^2 \), with kernel parameters and regularization weights either fixed a priori or selected via cross-validation. This simple form allows the various kernel derivatives required in \(|\nabla_m \alpha| \) to be easily computed by hand, and the small number of parameters makes grid search adequate for model selection. But, as discussed in Section 4, these simple kernels are insufficient for complex datasets. Thus we wish to use a richer class of kernels \( \{k_w\} \), with a large number of parameters \( w \) – in particular, kernels defined by a neural network. This prohibits model selection via simple grid search.

One could attempt to directly minimize \( \tilde{J}(\tilde{f}_{\alpha, z}^w; \lambda, D) \) jointly in the kernel parameters \( w \), the model parameters \( \alpha \), and perhaps the inducing points \( z \). Consider, however, the case where we simply use a Gaussian kernel and \( \{z_m\} = D \). Then we can achieve arbitrarily small values of (6) by taking \( \sigma \to 0 \), thus overfitting to the training set \( D \).

We can avoid this problem – and additionally find the best values for the regularization weights \( \lambda \) – by splitting our training procedure. First, we find a good kernel and regularization via stochastic gradient descent; then, fixing those parameters, we find the final \( \alpha \) for the model via (6). To do SGD for \( w, \lambda \), and possibly \( z \), we sample two disjoint sets \( D_t, D_v \subset D \). We then take a gradient step to minimize the score matching loss (4) evaluated on \( D_v \), using the model with the current values of \( w, \lambda, z \), and the optimal \( \alpha \) on \( D_t \) viewed as a function of those parameters. That is, we take a step following \( \nabla_x \phi_w \cdot \dot{J}(\tilde{f}_{\alpha, z}^w; \lambda, D_t, D_v) \). To do this, the closed-form expression (6) for \( \alpha \) is essential. Because we used small minibatches in this procedure, for the final fit we use the whole dataset: first, we freeze \( w \) and \( z \) and find the optimal \( \lambda \) for the whole training data, then finally fit \( \alpha \) with the new \( \lambda \). This process is summarized in Algorithm 1.

Computing kernel derivatives Solving for \( \alpha \) and computing the loss (4) require matrices of kernel second derivatives, but current deep learning-oriented automatic differentiation systems are not optimized for evaluating many similar higher-order derivatives at once. We therefore implemented backpropagation to compute \( G, U, \) and \( b \) of (4) as TensorFlow operations (Abadi et al. 2015), and used TensorFlow’s automatic differentiation only to optimize \( w, z, \) and \( \lambda \). Backpropagation to find these second derivatives is quite expensive, particularly as the model grows; this limits the size of kernels that our model can use.

Kernel architecture Our kernel \( k_w(x, y) \) will be

\[
\sum_{r=1}^{R} \rho_r \exp\left(-\frac{1}{2\sigma_r^2}\|\phi_w(x) - \phi_w(y)\|^2\right).
\]

This is a mixture of \( R \) Gaussian kernels with length scales \( \sigma_r \), taking in features of the data extracted by a neural network \( \phi_w(\cdot) \). Combining \( R \) such kernels makes it easier to account for both short-range and long-range dependencies. We constrain \( \rho_r \geq 0 \) to ensure a valid kernel, and \( \sum_{r=1}^{R} \rho_r = 1 \) for simplicity.

The neural networks \( \phi_w \) are made up of \( L \) fully connected layers. For \( L > 1 \), we found that adding a

Algorithm 1: Full training procedure

`input`: Dataset \( D \); initial inducing points \( z \), kernel parameters \( w \), regularization \( \lambda = (\lambda_r, \lambda_C) \)

1. Split \( D \) into \( D_t \) and \( D_v \);
2. Optimize \( w, \lambda, \) and maybe \( z \);
3. while \( J(\hat{f}_{\alpha, z}^w(\lambda, k_w, x, D_t, D_v)); D_v) \) still improving do
4. Sample disjoint data subsets \( D_t, D_v \subset D \);
5. \( f() = \sum_{m=1}^{M} \alpha_m (\lambda, k_w, z, D_t) k_w(z_m, \cdot) \), with (6); \( \hat{J} = \frac{1}{|D_v|} \sum_{m=1}^{D_v} \sum_{d=1}^{D} \left[ \partial_d^2 f(x_n) + \frac{1}{2} (\partial_d f(x_n))^2 \right] \);
6. Take SGD steps in \( J \) for \( w, \lambda, \) and maybe \( z \);
7. end
8. Optimize \( \lambda \) for fitting on larger batches:
9. while \( J(\hat{p}_{\alpha, z}^w(\lambda, k_w, x, D_t, D_v)); D_v) \) still improving do
10. \( f() = \sum_{m=1}^{M} \alpha_m (\lambda, k_w, z, D_t) k_w(\cdot, z_m) \), with (6); \( \hat{J} = \frac{1}{|D_v|} \sum_{m=1}^{D_v} \sum_{d=1}^{D} \left[ \partial_d^2 f(x_n) + \frac{1}{2} (\partial_d f(x_n))^2 \right] \);
11. Take SGD steps in \( J \) for \( \lambda \) only;
12. end
13. Finalize \( \alpha \) on \( D_t \);
14. Find \( \alpha = \alpha(\lambda, k_w, z, D_t) \);
15. return: \( \log \hat{p}(\cdot) = \sum_{m=1}^{M} \alpha_m k_w(\cdot, z_m) + \log q_0(\cdot) \);
skip connection from data directly to the top layer speeds up learning. We use a softplus nonlinearity, \(\log(1 + \exp(x))\), to ensure that the model is twice-differentiable and \(f\) is well-defined.\(^1\)

### 3.1 Behavior on Mixtures

One interesting limitation of score matching is the following: suppose that \(p_0\) is composed of two disconnected components, \(p_0(x) = \pi p_1(x) + (1-\pi)p_2(x)\) for \(\pi \in (0, 1)\) and \(p_1, p_2\) having disjoint, separated support. Then \(\nabla \log p_0(x)\) will be \(\nabla \log p_1(x)\) in the support of \(p_1\), and \(\nabla \log p_2(x)\) in the support of \(p_2\): notably, \(\pi\) does not appear in the loss function at all, and so the score matching loss \(f\) is ambivalent among any weighting of the two components.

If all modes are connected by regions of positive density, then the log density gradient in between components will determine their relative weight, and indeed score matching is then consistent (Hyvärinen 2005 Theorem 2). But when \(p_0\) is nearly zero between two dense components, so that there are no or few samples in between, score matching will generally have insufficient evidence to weight nearly-separate components.

**Proposition 4** (Appendix C) studies the behavior of the kernel exponential family in this case. Given two components that are completely separated according to \(k\), the kernel exponential family fits them as if it would fit on each separately, except that the effective \(\lambda_\alpha\) is scaled: smaller components are regularized more.

Appendix C.1 studies a simplified case where the kernel length scale \(\sigma\) is far wider than the component; then the density ratio between components, which should be \(\frac{\pi}{\sigma^D}\), is approximately \(\exp\left(\frac{D}{2\sigma^D} (\pi - \frac{1}{2})\right)\). Depending on the value of \(\frac{D}{2\sigma^D}\), this ratio will often either be quite extreme, or nearly 1. It is unclear, however, how well this result generalizes to other settings.

A heuristic workaround to this issue when disjoint components are suspected is as follows: simply run a clustering algorithm to identify disjoint components, separately fit a model to each cluster, then weight each model according to its sample count. When the modes are fully disjoint, this clustering is straightforward, but it may be an issue in high-dimensional cases when samples are sparse but not fully separated.

\(^1\)One might expect a piecewise-linear nonlinearity to simplify \(f\) by making the second-derivative term almost surely zero. In fact, it becomes a Dirac delta, so \(f\) depends on the true density \(p_0\) where the kink is achieved.

### 3.2 Model Evaluation

In addition to qualitatively evaluating fits, we will evaluate our models with three quantitative criteria. The first is the finite-set Stein discrepancy (FSSD; Jitkrittum et al. 2017), a measure of model fit which does not depend on the normalizer \(Z_\theta\). It examines the fit of the model at \(J\) test locations \(V = \{v_b\}_{b=1}^B\) by

\[
\frac{1}{B} \sum_{b=1}^B \| \mathbb{E}_{x \sim p_0} [k(x, v_b)] \nabla_x \log p(x) + \nabla_x k(x, v_b) \|^2_2.
\]

With randomly selected \(V\) and some mild assumptions, it is zero if and only if \(p = p_0\). We use a Gaussian kernel with bandwidth equal to the median distance between test points,\(^2\) and choose \(V\) by adding small Gaussian noise to data points. Jitkrittum et al. (2018) construct a hypothesis test to test which of \(p\) and \(p'\) is closer to \(p_0\) in the FSSD. We will report a score – the \(p\) value of this test – which is near 0 when model \(p\) is better, near 1 when model \(p'\) is better, and around \(\frac{1}{2}\) when the two models are equivalent. We emphasize that we are using this as a model comparison score on an interpretable scale, but not following a hypothesis testing framework. Another similar performance measure is the kernel Stein discrepancy (KSD) (Chwialkowski et al. 2016), where the model’s goodness-of-fit is evaluated at all test data points rather than at random test locations. We omit the results as they are essentially identical to that of the FSSD, even across a wide range of kernel bandwidths.

As all our models are twice-differentiable, we also compare the score-matching loss \(f\) on held-out test data. A lower score-matching loss implies a smaller Fisher divergence between model and data distributions.

We also compare test log-likelihoods, using importance sampling estimates of the normalizing constant \(Z_\theta\):

\[
\tilde{Z}_\theta = \frac{1}{U} \sum_{u=1}^U r_u \text{ where } r_u := \tilde{p}_0(y_u) / q_0(y_u), \quad y_u \sim q_0,
\]

so \(E \tilde{Z}_\theta = \int \tilde{p}_0(y) q_0(y) \, dy = Z_\theta\). Our log-likelihood estimator is \(\log \tilde{p}_\theta(x) = \log \tilde{p}_0(x) - \log \tilde{Z}_\theta\). This estimator is consistent, but Jensen’s inequality tells us that \(\mathbb{E} \log \tilde{p}_\theta(x) > \log \tilde{p}_0(x)\), and our evaluation will be over-optimistic. Misleadingly, the variance of \(\log \tilde{Z}_\theta\) can be relatively small when the bias is still quite large; we observed this in our experiments. We can, however, bound the amount of bias:

**Proposition 1.** Suppose that \(a, s \in \mathbb{R}\) are such that \(\Pr(r_u \geq a) = 1\) and \(\Pr(r_u \leq s) \leq \rho < \frac{1}{2}\). Define \(t := (s + a)/2\), \(\psi(q, Z_\theta) := \log \frac{Z_\theta}{q} + \frac{q}{Z_\theta} - 1\), and let

\(^2\)This reasonable choice avoids tuning any parameters.

We do not optimize the kernel or the test locations to avoid a situation in which model \(p\) is deemed better than \(p'\) in some respects but \(p'\) better than \(p\) in others; instead, we use a simple default mode of comparison.
\[ P := \max (\psi(a, Z_\theta), \psi(t, Z_\theta)). \quad \text{Then} \]
\[
\log Z_\theta - \mathbb{E} \log \hat{Z}_\theta \leq \frac{\psi(t, Z_\theta) \operatorname{Var}[r_t]}{(Z_\theta - t)^2} + P (4(1 - \rho))^{\mathbb{V}}.
\]

(Proof in Appendix D) We estimate the bound using the procedure described in Appendix D. This yields an estimate of an upper bound which is itself biased upwards (Proposition 6), so it is likely (but not guaranteed) that the estimate overstates the amount of bias.

## 4 EXPERIMENTAL RESULTS

In our experiments, we compare to several alternative methods. The first group are all fit by maximum likelihood, and broadly fall into (at least) one of two categories: \textit{autoregressive models} decompose \( p(x_1, \ldots, x_D) = \prod_{d=1}^{D} p(x_d|x_{<d}) \) and learn a parametric density model for each of these conditionals. \textit{Normalizing flows} instead apply a series of invertible transformations to some simple initial density, say standard normal, and then compute the density of the overall model via the Jacobian of the transformation. We use implementations of the following several models in these categories by Papamakarios et al. (2017):

- **MADE** (Germain et al. 2015) masks the connections of an autoencoder to fit an autoregressive form. We used two hidden layers, and each conditional a Gaussian. **MADE-MOG** is the same but with each conditional a mixture of 10 Gaussians.

- **Real NVP** (Dinh et al. 2017) is a normalizing flow; we use a general-purpose form for non-image datasets.

- **MAF** (Papamakarios et al. 2017). A combination of a normalizing flow and MADE, where the base density is modeled by MADE, with 5 autoregressive layers. **MAF-MOG** instead models the base density by MADE-MOG with 10 components.

For the models above, we used 30 neurons in each layer for experiments on synthetic data, and 100 neurons for benchmark datasets.

- **KCEF** (Arbel and Gretton 2018). Inspired by autoregressive models, the density is modeled by a cascade of kernel conditional exponential family distributions, fit by score matching with Gaussian kernels.

- **DKEF**. On synthetic datasets, we consider four variants of our model with one kernel component, \( R = 1 \), parameterized by a three-layer network. KEF-G refers to the model using a Gaussian kernel with a learned bandwidth. DKEF-G-15 has a Gaussian kernel on top of a network with 15 neurons in each layer. DKEF-G-50 is the same with 50 neurons per layer. To investigate whether the top Gaussian kernel helps performance, we also train DKEF-L-50, whose kernel is \( k_\theta(x, y) = \phi_w(x) \cdot \phi_w(y) \) with 50 neurons in each layer. To compare with the architecture of Kingma and LeCun (2010), DKEF-L-50-1 has the same architecture as DKEF-L-50 except that we add an extra layer with a single neuron, and use \( M = 1 \). On benchmark datasets, we use DKEF-G-30 with three kernel components, \( R = 3 \).

All exponential family models use \( q_0 = \mathcal{N}(0, 4I) \); benchmark datasets were whitened so that this is reasonably broad.

### 4.1 Behavior on Synthetic Datasets

We first demonstrate the behavior of the models on several 2-D synthetic datasets: Funnel, Banana, Ring, Square, Cosine, Mixture of Gaussians (MoG) and Mixture of Rings (MoR). Together, they cover a range of geometric complexities and multimodality.

We visualize the fit of various methods by showing the log density function in Figure 2. For each model fit on each distribution, we report the normalized log likelihood (left) and Fisher divergence (right). We first discuss the unimodal distributions. Among the kernel exponential families, DKEF-G outperformed previous versions where ordinary Gaussian kernels were used for either joint (KEF-G) or autoregressive (KCEF) modeling. However, when the Gaussian kernel is replaced with linear kernel (DKEF-L-50), the fit was worse even if the neural network was made much larger. DKEF-G-50 does not substantially improve over DKEF-G-15; we omit it for space. We can gain additional insights into the model by looking at the shape of the learned kernel, shown by the colored lines; the kernels do indeed adapt to the local geometry.

DKEF-L-50 and DKEF-L-50-1 show good performance when the target density has simple geometries, but failed otherwise. It seems, then, that a Gaussian kernel with inducing points provides much stronger representational features than a using linear kernel and/or a single inducing point. A large enough network \( \phi_w \) would likely be able to perform the task well, but the second derivatives in the score matching loss limit our ability to use very large networks. A similar phenomenon was observed by Bińkowski et al. (2018) in the context of GAN critics, where combining some analytical RKHS optimization with deep networks allowed much smaller networks to work well.

As expected, models fit by score matching generally have smaller Fisher divergences than likelihood-based methods. For Funnel and Banana, the true densities
Figure 2: Log densities learned by different models. Our model is DKEF-G-15 at the bottom row. Columns are different toy datasets. The rightmost columns shows a mixture of each model (except KCEF) on the same clustering of MoR. We subtracted the maximum from each log density, and clipped the minimum value at $-9$. Above each panel are shown the average log-likelihoods (left) and Fisher divergence (right) on held-out data points. Bold indicates the best fit. For DKEF-G models, faint colored lines correspond to contours at 0.9 of the kernel evaluated at different locations. Seemingly-empty panels for DKEF-L-50 and DKEF-L-50-1 had regions with very high density values far away from the data.
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Figure 3: Results on the real datasets; bars show means, points show each of 15 individual runs, excluding invalid or outlying values. (1st row) The estimate of the squared FSSD, a measure of model goodness of fit based on derivatives of the log density; lower is better. (2nd row) The $p$-value of a test that each model is no better than DKEF in terms of the FSSD; values near 0 indicate that DKEF fits the data significantly better than the other model. (3nd row) Value of the loss $\ell$; lower is better. (4th row) Log-likelihoods; higher is better. DKEF estimates are based on $10^{10}$ samples for $\hat{Z}_\theta$, with vertical lines showing the bias bound from Proposition 1. Except on MiniBoone and some runs of Parkinsons, the bias bound is too small to be easily visible.

are simple transformations of Gaussians, and the normalizing flows models perform relatively well. But on Ring, Square, and Cosine, the shape of the learned distribution by likelihood-based methods exhibits noticeable artifacts, especially at the boundaries. These artifacts, particularly the "breaks" in Ring, may be caused by a normalizing flow’s need to be invertible and smooth. By contrast, the shape learned by DKEF-G-15 is much cleaner.

On multimodal distributions with disjoint components, likelihood-based and score matching-based methods show interesting failure modes. The likelihood-based models often connect separated modes with a "bridge", even for MADE-MOG and MAF-MOG which use explicit mixtures. On the other hand, DKEF is able to find the shapes of the components, but the weighting between modes is unstable. As suggested in Section 3.1, we also fit mixtures of all models (except KCEF) on a partition of MoR found by spectral clustering (Shi and Malik 2000).

Another challenge we observed in our experiments is that the estimator of the objective function, $\hat{J}$, tends to be more noisy as the model fit improves. This happens particularly on datasets where there are "sharp" features, such as Square, where the model's curvature becomes extreme at some points. This can give rise to higher variance in the gradients of the parameters, and more difficulty in optimization.

4.2 Results on Benchmark Datasets

Following recent work on density estimation (Uria et al. 2013; Arbel and Gretton 2018; Papamakarios et al. 2017; Germain et al. 2015), we trained DKEF and the likelihood-based models on five UCI datasets (Dheeru and Karra Taniskidou 2017); in particular, we used RedWine, WhiteWine, Parkinson, HepMass, and MiniBoone. We did not run KCEF due to its computational expense. For details of the experiments, including data preprocessing and model parameters, see Appendix E.2. All performances were measured on held-out test sets.

Figure 3 shows results. In gradient matching as measured by the FSSD, DKEF tends to have the best values. Test set sizes are too small to yield a confident $p$-value on the Wine datasets, but the model comparison test confidently favors DKEF on datasets with large-enough test sets. The FSSD results agree with KSD, which is omitted. In the score matching loss

---

\[ \ell \]

The implementation of Papamakarios et al. (2017)
DKEF is the best on Wine datasets and most runs on Parkinson, but worse on Hepmass and Mini-Boone. FSSD is a somewhat more “global” measure of shape, and is perhaps more weighted towards the bulk of the distribution rather than the tails. In likelihoods, DKEF is comparable to other methods except MADE on Wines but worse on the other, larger, datasets. Note that we trained DKEF while adding Gaussian noise with standard deviation 0.05 to the (whitened) dataset; training without noise improves the score matching loss but harms likelihood, while producing similar results for FSSD.

5 DISCUSSION

Learning deep kernels helps make the kernel exponential family practical for large, complex datasets of moderate dimension. We can exploit the closed-form fit of the $\alpha$ vector to optimize kernel and even regularization parameters using a “held-out” loss, finding smoothness assumptions that fit the data rather than arbitrarily choosing them a priori.

Computational expense makes score matching with deep kernels difficult to scale to models with large kernel networks, limiting the dimensionality of possible targets. Combining with the kernel conditional exponential family might help alleviate that problem by splitting the model up into several separate but marginally complex components. The kernel exponential family, and score matching in general, also struggles to correctly balance datasets with nearly-disjoint components, but it seems to generally learn density shapes better than maximum likelihood-based deep approaches.

Acknowledgments

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A DKEFs can be normalized

**Proposition 2.** Consider the kernel \( k(x, y) = \kappa(\phi(x), \phi(y)) \), where \( \kappa \) is a kernel such that \( \kappa(a, a) \leq L_\kappa \|a\|^2 + C_\kappa \) and \( \phi \) a function such that \( \|\phi(x)\| \leq L_\phi \|x\| + C_\phi \). Let \( q_0(x) \) be the density of a multivariate Gaussian distribution with mean \( \mu \) and covariance \( \Sigma \), with \( \Sigma \) strictly positive definite. Then, for any function \( f \) in the RKHS \( \mathcal{H} \) corresponding to \( k \),

\[
\int \exp(f(x)) q_0(x) \, dx < \infty.
\]

**Proof.** First, we have that \( f(x) = \langle f, k(x, \cdot) \rangle_\mathcal{H} \leq \|f\|_\mathcal{H} \sqrt{k(x, x)} \), and

\[
k(x, x) = \kappa(\phi(x), \phi(x)) \leq L_\kappa \|\phi(x)\|^2 + C_\kappa \leq L_\kappa (L_\phi \|x\|^2 + C_\phi) + C_\kappa.
\]

Combining these two yields

\[
f(x) \leq \|f\|_\mathcal{H} \sqrt{L_\kappa L_\phi \|x\|^2 + L_\kappa C_\phi + C_\kappa} \leq \|f\|_\mathcal{H} \sqrt{L_\kappa L_\phi} \|x\| + \|f\|_\mathcal{H} \sqrt{L_\kappa C_\phi + C_\kappa}.
\]

Letting \( C_1 := \|f\|_\mathcal{H} \sqrt{L_\kappa L_\phi} \) and \( C_0 := \|f\|_\mathcal{H} \sqrt{L_\kappa C_\phi + C_\kappa} \), we thus have, letting \( V \) be such that \( \Sigma = V V^T \),

\[
\int \exp(f(x)) q_0(x) \, dx \leq \mathbb{E}_{z \sim q_0} [\exp(C_0 + C_1 \|x\|)]
\]

\[
= \exp(C_0) \mathbb{E}_{z \sim N(0, I)} [\exp(C_1 \|V z + \mu\|)]
\]

\[
\leq \exp(C_0) \exp(C_1 \|\mu\|) \mathbb{E}_{z \sim N(0, I)} [\exp(C_1 \|V z\|)]
\]

\[
= \exp(C_0) \exp(C_1 \|\mu\|) M_{\|z\|} (C_1 \|V\|_2).
\]

Here \( M_{\|z\|} \), the moment-generating function of \( \|z\| \sim \chi(D) \), is finite for any input. \( \square \)

The condition on \( \phi \) holds for any \( \phi \) given by a deep network with Lipschitz activation functions. The condition on \( \kappa \) also holds for a linear kernel (where \( L_\kappa = 1, C_\kappa = 0 \)), any shift-invariant kernel (\( L_\kappa = 0, C_\kappa = \kappa(0,0) \)), or mixtures thereof. If \( \kappa \) is bounded, the integral is finite for any function \( \phi \).

The given proof would not hold for a quadratic \( \kappa \), which has been used previously in the literature; indeed, it is clearly possible for such an \( f \) to be unnormalizable.

B Finding the optimal \( \alpha \)

We will show a slightly more general result than we need, also allowing for an \( \|f\|^2_\mathcal{H} \) penalty. This result is related to Lemma 4 of Sutherland et al. (2018), but is more elementary and specialized to our particular needs while also allowing for more types of regularizers.

**Proposition 3.** Consider the loss

\[
\hat{J}(f^k_{\alpha,z}, \lambda, D) = \hat{J}(p^k_{\alpha,z}, D) + \frac{1}{2} \left[ \lambda_\alpha \|\alpha\|^2 + \lambda_\mathcal{H} \|f^k_{\alpha,z}\|^2_\mathcal{H} + \lambda_C \frac{1}{N} \sum_{n=1}^N \sum_{d=1}^D \left[ \partial_d^2 \log \hat{p}^k_{\alpha,z}(x_n) \right]^2 \right]
\]

where

\[
\hat{J}(p^k_{\alpha,z}, D) = \frac{1}{N} \sum_{n=1}^N \sum_{d=1}^D \left[ \partial_d^2 \log \hat{p}^k_{\alpha,z}(x_n) + \frac{1}{2} \left( \partial_d \log \hat{p}^k_{\alpha,z}(x_n) \right)^2 \right].
\]
For fixed $k$, $z$, and $\lambda$, as long as $\lambda_\alpha > 0$ then the optimal $\alpha$ is

$$
\alpha(\lambda, k, z, D) = \arg \min_{\alpha} \hat{J}(f^k_{\alpha, z}, \lambda, D) = -(G + \lambda_\alpha I + \lambda_H K + \lambda_C U)^{-1} b
$$

$$
G_{m, m'} = \frac{1}{N} \sum_{n=1}^{N} \sum_{d=1}^{D} \partial_d k(x_n, z_m) \partial_d k(x_n, z_{m'})
$$

$$
U_{m, m'} = \frac{1}{N} \sum_{n=1}^{N} \sum_{d=1}^{D} \partial_d^2 k(x_n, z_m) \partial_d^2 k(x_n, z_{m'})
$$

$$
K_{m, m'} = k(z_m, z_{m'})
$$

$$
\alpha = \frac{1}{N} \sum_{n=1}^{N} \sum_{d=1}^{D} \partial_d k(x_n, z_m) + \partial_d \log q_0(x_n) \partial_d k(x_n, z_m) + \lambda_C \partial_d^2 \log q_0(x_n) \partial_d^2 k(x_n, z_m).
$$

**Proof.** We will show that the loss is quadratic in $\alpha$. Note that

$$
\frac{1}{N} \sum_{n=1}^{N} \sum_{d=1}^{D} \partial_d^2 \log p^{k}_{\alpha, z}(x_n) = \frac{1}{N} \sum_{n=1}^{N} \sum_{d=1}^{D} \left[ \sum_{m=1}^{M} \alpha_m \partial_d^2 k(x_n, z_m) + \partial_d^2 \log q_0(x_n) \right]
$$

$$
= \alpha^T \left[ \frac{1}{N} \sum_{n=1}^{N} \sum_{d=1}^{D} \partial_d^2 k(x_n, z_m) \right] + \text{const}
$$

$$
\frac{1}{N} \sum_{n=1}^{N} \sum_{d=1}^{D} \frac{1}{2} (\partial_d \log p^{k}_{\alpha, z}(x_n))^2 = \frac{1}{N} \sum_{n=1}^{N} \sum_{d=1}^{D} \frac{1}{2} \left( \sum_{m, m'=1}^{M} \alpha_m \alpha_{m'} \partial_d k(x_n, z_m) \partial_d k(x_n, z_{m'}) + 2 \sum_{m=1}^{M} \alpha_m \partial_d \log q_0(x_n) \partial_d k(x_n, z_m) + (\partial_d \log q_0(x_n))^2 \right)
$$

$$
= \frac{1}{2} \alpha^T GU + \alpha^T \left[ \frac{1}{N} \sum_{n=1}^{N} \sum_{d=1}^{D} \partial_d \log q_0(x_n) \partial_d k(x_n, z_m) \right] + \text{const}
$$

The $\lambda_C$ term is of the same form, but with second derivatives:

$$
\frac{1}{2N} \sum_{n=1}^{N} \sum_{d=1}^{D} (\partial_d^2 \log p^{k}_{\alpha, z}(x_n))^2 = \frac{1}{2} \alpha^T GU + \alpha^T \left[ \frac{1}{N} \sum_{n=1}^{N} \sum_{d=1}^{D} \partial_d^2 \log q_0(x_n) \partial_d^2 k(x_n, z_m) \right] + \text{const}
$$

We also have as usual

$$
\frac{1}{2} \| f^{k}_{\alpha} \|^2_H = \frac{1}{2} \sum_{m=1}^{M} \sum_{m'=1}^{M} \alpha_m \langle k(z_m, \cdot), k(z_{m'}, \cdot) \rangle_H \alpha_{m'} = \frac{1}{2} \alpha^T K \alpha.
$$

Thus the overall optimization problem is

$$
\alpha(\lambda, k, z, D) = \arg \min_{\alpha} \hat{J}(f^k_{\alpha, z}, \lambda, D)
$$

$$
= \arg \min_{\alpha} \frac{1}{2} \alpha^T (G + \lambda_\alpha I + \lambda_H K + \lambda_C U) \alpha + \alpha^T b.
$$

Because $\lambda_\alpha > 0$ and $G$, $K$, $U$ are all positive semidefinite, the matrix in parentheses is strictly positive definite, and the claimed result follows directly from standard vector calculus.

**C Behavior on mixtures**

**Proposition 4.** Let $D = \bigcup_{i=1}^{I} D_i$, where $D_i \subset X_i$, $|D_i| = \pi_i N$, $\sum_{i=1}^{I} \pi_i = 1$. Also suppose that the inducing points are partitioned as $Z = \{Z_1; \ldots; Z_I\}$, with $Z_i \subset X_i$. Further let the kernel $k$ be such that $k(x_1, x_2) = 0$. 


when \( x_1 \in \mathcal{X}_i, x_2 \in \mathcal{X}_j \) for \( i \neq j \), with its first and second derivatives also zero. Then the kernel exponential family solution of Proposition 3 is

\[
\alpha(\lambda, k, z, D) = \left[ \alpha \left( \left( \frac{\lambda_\alpha}{\pi_1}, \frac{\lambda_\mu}{\pi_1}, \lambda_C \right), k, Z_1, D_1 \right) \right. \\
\vdots \\
\left. \alpha \left( \left( \frac{\lambda_\alpha}{\pi_1}, \frac{\lambda_\mu}{\pi_1}, \lambda_C \right), k, Z_I, D_I \right) \right]
\]

**Proof.** Let \( G_i, b_i \) be the \( G, b \) of Proposition 3 when using only \( Z_i \) and \( D_i \). Then, because the kernel values and derivatives are zero across components, if \( m \) and \( m' \) are from separate components then

\[
G_{m,m'} = \frac{1}{N} \sum_{n=1}^N \sum_{d=1}^D \partial_d k(x_n, z_m) \partial_d k(x_n, z_{m'}) = 0,
\]

as at least one of the kernel derivatives will be zero for each term of the sum. When \( m \) and \( m' \) are from the same component, the total will be the same except that \( N \) is bigger, giving

\[
G = \begin{pmatrix}
\pi_1 G_1 & 0 & \cdots & 0 \\
0 & \pi_2 G_2 & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & \pi_I G_I
\end{pmatrix}.
\]

\( U \) is of the same form and factorizes in the same way. \( K \) does not scale:

\[
K = \begin{bmatrix}
K_1 & \cdots & 0 \\
\vdots & \ddots & \vdots \\
0 & \cdots & K_I
\end{bmatrix}
\]

Recall that \( b \) is given as

\[
b_m = \frac{1}{N} \sum_{n=1}^N \sum_{d=1}^D \partial_d^2 k(x_n, z_m) + \partial_d \log q_0(x_n) \partial_d k(x_n, z_m) + \lambda_C \partial_d^2 \log q_0(x_n) \partial_d^2 k(x_n, z_m).
\]

Each term in the sum for which \( x_n \) is in a different component than \( z_m \) will be zero, giving \( b = (\pi_1 b_1, \ldots, \pi_I b_I) \). Thus \( \alpha(\lambda, k, z, D) \) becomes

\[
\alpha = -\left( G + \lambda_\alpha I + \lambda_H K + \lambda_C U \right)^{-1} b = \\
\begin{pmatrix}
\pi_1 G_1 + \lambda_\alpha I + \lambda_H K_1 + \lambda_C \pi_1 U_1 & \cdots & 0 \\
\vdots & \ddots & \vdots \\
0 & \cdots & \pi_I G_I + \lambda_\alpha I + \lambda_H K_I + \lambda_C \pi_I U_I
\end{pmatrix}^{-1}
\begin{pmatrix}
\pi_1 b_1 \\
\vdots \\
\pi_I b_I
\end{pmatrix}
\]

\[
= \begin{pmatrix}
-\left( G_1 + \frac{\lambda_\alpha}{\pi_1} I + \frac{\lambda_\mu}{\pi_1} K_1 + \lambda_C U_1 \right)^{-1} b_1 \\
\vdots \\
-\left( G_I + \frac{\lambda_\alpha}{\pi_I} I + \frac{\lambda_\mu}{\pi_I} K_I + \lambda_C U_I \right)^{-1} b_I
\end{pmatrix}.
\]

Thus the fits for the components are essentially added together, except that each component uses a different \( \lambda_\alpha \) and \( \lambda_H \); smaller components are regularized more. \( \lambda_C \), interestingly, is unscaled.

It is difficult in general to tell how two components will be weighted relative to one another; the problem is essentially equivalent to computing the overall normalizing constant of a fit. However, we can gain some insight by considering the case of a Gaussian component where the kernel is also Gaussian with a much wider bandwidth. This simplest possible case is analyzed in Appendix C.1.
C.1 Small Gaussian components with a large Gaussian kernel

Consider, for the sake of our study of mixture fits, one of the simplest possible situations for a kernel exponential family: \( p_0 = \mathcal{N}(0, I) \), with a kernel \( k(x, y) = \exp \left( -\frac{1}{\sigma^2} \|x - y\|^2 \right) \) for \( \sigma \gg \sqrt{D} \), so that \( k(x, y) \approx 1 \) for all \( x, y \) sampled from \( p_0 \). Let \( q_0 \) be approximately uniform, \( q_0 = \mathcal{N}(0, q I) \) for \( q \gg \sigma^2 \), so that \( \nabla \log q_0(x) = \frac{q - 1}{\sigma^2} x \approx 0 \). Also assume that \( N \to \infty \), but \( M \) is fixed. Then we have

\[
G_{m,m'} = \frac{1}{N} \sum_{n=1}^{N} \sum_{d=1}^{D} \frac{\partial_d k(x_n, z_m) \partial_d k(x_n, z_{m'})}{\sigma^2} \\
= \frac{1}{N} \sum_{n=1}^{N} \sum_{d=1}^{D} \left( \frac{z_{m,d} - x_d}{\sigma^2} k(x_n, z_m) \right) \left( \frac{z_{m',d} - x_d}{\sigma^2} k(x_n, z_{m'}) \right) \\
\approx \sigma^{-4} E_{x \sim p_0} \left( (z_m - x)^T (z_{m'} - x) \right) \\
= \sigma^{-4} (z_m z_{m'} + D) \\
G \approx \frac{1}{\sigma^4} ZZ^T + \frac{D}{\sigma^4} I \\
b_m = \frac{1}{N} \sum_{n=1}^{N} \sum_{d=1}^{D} \partial_d^2 k(x_n, z_m) + \partial_d \log q_0(x_n) \partial_d k(x_n, z_m) \\
\approx E_{x \sim p_0} \left[ \sum_{d=1}^{D} \partial_d^2 k(x_n, z_m) \right] \\
= E_{x \sim p_0} \left[ \sum_{d=1}^{D} \left( \frac{(x_d - z_{m,d})^2}{\sigma^4} - \frac{1}{\sigma^2} \right) k(x, z_m) \right] \\
\approx E_{x \sim p_0} \left[ \frac{\|x_d - z_m\|^2}{\sigma^4} - \frac{D}{\sigma^2} \right] \\
b \approx \frac{1}{\sigma^4} \text{diag}(ZZ^T) - \frac{D(\sigma^2 - 1)}{\sigma^4} \mathbf{1}.
\]

Because \( k(z, x) \approx k(z', x) \) for any \( z, z' \) near the data in this setup, it’s sufficient to just consider a single \( z = 0 \). In that case,

\[
\alpha = -(G + \lambda I)^{-1} b \\
\approx - \left( \frac{1}{\sigma^4} ZZ^T + \left( \frac{D}{\sigma^4} + \lambda \right) I \right)^{-1} \left( \frac{1}{\sigma^4} \text{diag}(ZZ^T) - \frac{D(\sigma^2 - 1)}{\sigma^4} \mathbf{1} \right) \\
= - \left( \frac{D}{\sigma^4} + \lambda \right)^{-1} \left( - \frac{D(\sigma^2 - 1)}{\sigma^4} \mathbf{1} \right) \\
= \frac{1}{D \sigma^{-4} + \lambda} \frac{D(\sigma^2 - 1)}{\sigma^4} \mathbf{1} \\
= \frac{\sigma^2 - 1}{1 + \lambda \sigma^4 / D} \mathbf{1}
\]

and so

\[
f_\alpha(0) \approx \frac{\sigma^2 - 1}{1 + \lambda \sigma^4 / D}.
\]

Thus, if we attempt to fit the mixture \( \pi \mathcal{N}(0, I) + (1 - \pi) \mathcal{N}(r, I) \) with \( q^2 \gg \|r\|^2 \gg \sigma^2 \gg D \), we are approxi-
mately in the regime of Proposition 4 and so the ratio between the two components in the fit is
\[
\exp(f(0) - f(r)) \approx \exp\left(\frac{\sigma^2 - 1}{1 + \frac{\lambda \sigma^4}{D}} - \frac{\sigma^2 - 1}{1 + \frac{\lambda \sigma^4}{(1-\pi)D}}\right)
\]
\[
= \exp\left(\lambda \sigma^4 (\sigma^2 - 1) \left(1 + \frac{\lambda \sigma^4}{D} + \frac{\lambda \sigma^4}{(1-\pi)D} + \frac{\lambda^2 \sigma^8}{D^2}\right)\right)
\]
\[
= \exp\left(\frac{1}{2} \lambda \sigma^4 (\sigma^2 - 1) \left(\frac{\pi - \frac{1}{2}}{D(1-\pi) + \lambda \sigma^4 + \lambda^2 \sigma^8}\right)\right).
\]
If \( \pi = \frac{1}{2} \), the density ratio is correctly 1. If we further assume that \( \lambda \gg D/\sigma^4 \), so that the denominator is dominated by the last term, then the ratio becomes approximately
\[
\exp(f(0) - f(r)) \approx \exp\left(\frac{D}{2\sigma^2 \lambda} \left(\pi - \frac{1}{2}\right)\right).
\]
Thus, depending on the size of \( D/(2\sigma^2 \lambda) \ll \sigma^2/2 \), the ratio will usually either remain too close to \( \frac{1}{2} \) or become too extreme as \( \pi \) changes; only in a very narrow parameter range is it approximately correct.

D Upper bound on normalizer bias

Recall the importance sampling setup of Section 3.2.
\[
\hat{Z}_\theta = \frac{1}{U} \sum_{u=1}^{U} r_u \text{ where } y_u \sim q_0, r_u := \frac{\hat{\rho}_\theta(y_u)}{q_0(y_u)} \text{ so } \mathbb{E} \hat{Z}_\theta = \frac{\hat{\rho}_\theta(y_u)}{q_0(y_u)} q_0(y_u) = Z_\theta.
\]

**Proposition 1.** Suppose that \( a, s \in \mathbb{R} \) are such that \( \Pr(r_u \geq a) = 1 \) and \( \Pr(r_u \leq s) \leq \rho < \frac{1}{2} \). Define \( t := (s + a)/2, \psi(q, Z_\theta) := \log \frac{Z_\theta}{q} + \frac{\rho}{2} - 1 \), and let \( P := \max(\psi(a, Z_\theta), \psi(t, Z_\theta)) \). Then
\[
\log Z_\theta - \mathbb{E} \log \hat{Z}_\theta \leq \frac{\psi(t, Z_\theta)}{(Z_\theta - t)^2} \frac{\text{Var}[r_u]}{U} + P \left(4\rho(1-\rho)\right)^{\frac{U}{2}}.
\]

**Proof.** Inspired by the technique of Liao and Berg (2018), we will decompose the bias as follows. (We will suppress the subscript \( \theta \) for brevity.)

First note that the following form of a Taylor expansion holds identically:
\[
\varphi(x) = \varphi(Z) + \varphi'(Z)(x - Z) + h(x, Z)(x - Z)^2
\]
\[
h(x, Z) := \frac{\varphi(x) - \varphi(Z) - \varphi'(Z)(x - Z)}{(x - Z)^2}.
\]

We can thus write the bias as the following, where \( \varphi(x) = -\log(x) \), \( P \) is the distribution of \( \hat{Z} \), and \( t \geq a \):
\[
\mathbb{E}[\varphi(\hat{Z})] - \varphi(\mathbb{E} \hat{Z}) = \int_a^\infty (\varphi(x) - \varphi(Z)) \, dP(x)
\]
\[
= \int_a^\infty (\varphi'(Z)(x - Z) + h(x, Z)(x - Z)^2) \, dP(x)
\]
\[
= \varphi'(Z) \left( \int_a^\infty x \, dP(x) - Z \right) + \int_a^\infty h(x, Z)(x - Z)^2 \, dP(x)
\]
\[
= \int_a^t h(x, Z)(x - Z)^2 \, dP(x) + \int_t^\infty h(x, Z)(x - Z)^2 \, dP(x)
\]
\[
\leq \left[ \sup_{a \leq x \leq t} h(x, Z)(x - Z)^2 \right] \int_a^t dP(x) + \left[ \sup_{x \geq t} h(x, Z) \right] \int_t^\infty (x - Z)^2 dP(x)
\]
\[
\leq \left[ \sup_{a \leq x \leq t} h(x, Z)(x - Z)^2 \right] \Pr(\hat{Z} \leq t) + \left[ \sup_{x \geq t} h(x, Z) \right] \text{Var}[\hat{Z}].
\]
We can evaluate \( \lim \) is convex in \( x \) and thus its supremum is max \((\log \frac{Z}{a} + \frac{a}{2} - 1, \log \frac{Z}{r} + \frac{r}{2} - 1)\), with the term at \( a \) being necessarily larger as long as \( t < Z \).

Picking \( t = (s + a)/2 \) gives the desired bound on \( \Pr(Z \leq t) \) via Lemma 5.

Lemma 1 of Liao and Berg [2018] shows that since \( \varphi'(x) = -1/x \) is concave, \( h(x, Z) \) is decreasing in \( x \). Thus \( \sup_{x \geq t} h(x, Z) = h(t, Z) \), giving the claim. \( \Box \)

**Lemma 5.** Let \( a \) and \( s \) be such that \( \Pr(r_u \geq a) = 1 \) and \( \Pr(r_u \leq s) \leq \rho < \frac{1}{2} \), with \( a < s \). Then

\[
\Pr\left( \frac{1}{U} \sum_{i=1}^{U} r_u \leq \frac{s + a}{2} \right) \leq (4\rho(1 - \rho))^\frac{U}{2}.
\]

**Proof.** Let \( K \) denote the number of samples of \( r_u \) which are smaller than \( s \), so that \( U - K \) samples are at least \( s \). Then we have

\[
\Pr\left( \frac{1}{U} \sum_{i=1}^{U} r_u \leq \frac{s + a}{2} \right) \leq \Pr\left( \frac{K}{U} a + \frac{U - K}{U} s \leq \frac{s + a}{2} \right)
= \Pr\left( K(a - s) \leq U \frac{a - s}{2} \right)
= \Pr\left( K \geq \frac{U}{2} \right).
\]

\( K \) is distributed binomially with probability of success at most \( \rho < \frac{1}{2} \), so applying Theorem 1 of Arratia and Gordon [1989] yields

\[
\Pr\left( \frac{1}{U} \sum_{i=1}^{U} r_u \leq \frac{s + a}{2} \right) \leq \exp\left( -U \left[ \frac{1}{2} \log \frac{1}{2\rho} + \frac{1}{2} \log \frac{1}{2(1 - \rho)} \right] \right)
= \exp\left( \frac{U}{2} \log (4\rho(1 - \rho)) \right)
= (4\rho(1 - \rho))^\frac{U}{2}.
\]

**Proposition 6.** The function \( \chi_t(x) := (\log \frac{x}{2} + \frac{1}{2} - 1) / (x - t)^2 \) is strictly convex for all \( x > 0 \). Thus we have that \( \mathbb{E} \chi_t(Z) \geq \chi_t(\mathbb{E}Z) = \chi_t(Z) \), with equality only if \( \Pr(Z = Z) = 1 \).

**Proof.** We can compute that

\[
\chi''_t(x) = \frac{2r^3 - 9r^2 + 18\frac{x}{2} - 11 - 6 \log \frac{x}{2}}{(x - t)^4}.
\]

Let \( r := t/x \), so \( x \in [t, \infty) \) corresponds to \( r \in (0, 1] \), and \( x \in (0, t] \) corresponds to \( r \in [1, \infty) \). Then

\[
\chi''_t \left( \frac{t}{r} \right) = \frac{2r^3 - 9r^2 + 18r - 11 - 6 \log r}{t^4 \left( \frac{1}{r} - 1 \right)^4}.
\]

We can evaluate \( \lim_{r \to 1} \chi''(t/r) = \frac{3}{2\pi^2} > 0 \). For \( r \neq 1 \), \( \chi''_t > 0 \) if and only if \( f(r) > 0 \), where

\[
f(r) := 2r^3 - 9r^2 + 18r - 11 - 6 \log r.
\]

Clearly \( \lim_{r \to 0} f(r) = \infty \) and \( f(1) = 0 \). But notice that

\[
f'(r) = 6r^2 - 18r + 18 - \frac{6(r - 1)^3}{r},
\]

so that \( f(r) \) is strictly decreasing on \((0, 1)\), and strictly increasing on \((1, \infty)\). Thus \( f(r) > 0 \) for all \( r \in (0, 1) \cup (1, \infty) \), and \( \chi''_t(x) > 0 \) for all \( x > 0 \). The claim follows by Jensen’s inequality. \( \Box \)
D.1 Estimator of bias bound

For a kernel such as (7) bounded in \([0, 1]\), \(a := \exp\left(\sum_{m=1}^{M} \min(\alpha_m, 0)\right)\) is a uniform lower bound on \(r_u\).

For large \(U\), essentially any \(\rho < \frac{1}{2}\) will make the second term practically zero, so we select \(s\) as the 40th percentile of an initial sample of \(r_u\), and confirm a high-probability (0.999) Hoeffding upper bound \(\rho\) on \(\Pr(r_u \leq s)\) with another sample. We use \(10^7\) samples for each of these.

We estimate \(\text{Var}[r_u]\) on a separate sample with the usual unbiased estimator, using \(10^9\) samples for most cases but \(10^{10}\) for MiniBoone.

To finally estimate the bound, we estimate \(Z_\theta\) on yet another independent sample, again usually of size \(10^9\) but \(10^{10}\) for MiniBoone.

Crucially, the function \(\psi(t, x)/(x−t)^2\) is convex (Proposition 6); because the variance is unbiased, our estimate of the bias bound is itself biased upwards. As Proposition 1’s bound is also not tight, our estimate thus likely overstates the actual amount of bias.

E Additional experimental details

E.1 Toy datasets

For each toy distribution, we sample 10 000 random points from the distribution, 1 000 of which are used for testing; of the rest, 90\% (8 100) are used for training, and 10\% (900) are used for validation. Training was early stopped when validation cost does not improve for 200 minibatches. The current implementation of KCEF does not include a Nyström approximation, and trains via full-batch L-BFGS-B, so we down-sampled the training data to 1000 points. We used the Adam optimizer (Kingma and Ba 2015) for all other models. For MADE, RealNVP, and MAF, we used minibatches of size 200 and the learning rate was \(10^{-3}\) For KEF-G and DKEF, we used 200 inducing points, used \(|\mathcal{D}_t| = |\mathcal{D}_v| = 100\), and learning rate \(10^{-3}\). The same parameters are used for each component for mixture models trained on MoR.

E.2 Benchmark datasets

Pre-processing RedWine and WhiteWine are quantized, and thus problematic for score matching; we added to each dimension uniform noise with support equal to the median distances between two adjacent values. For HepMass and MiniBoone, we removed ill-conditioned dimensions as did Papamakarios et al. (2017). For all datasets except HepMass, 10\% of the entire data was used as testing, and 10\% of the remaining was used for validation with an upper limit of 1 000 due to time cost of validation at each iteration. For HepMass, we used the same splitting as done in Papamakarios et al. (2017) and with the same upper limit on validation set. The data is then whitened before fitting and the whitening matrix was computed on at most 10 000 data points.

Likelihood-based models We set MADE, MADE-MOG, each autoregressive layer of MAF and each scaling and shifting layers of real NVP to have two hidden layers of 100 neurons. For real NVP, MAF and MAF-MOG, five autoregressive layers were used; MAF-MOG and MADE-MOG has a mixture of 10 Gaussians for each conditional distribution. Learning rate was \(10^{-3}\) The size of a minibatch is 200.

Deep kernel exponential family We set the DKEF model to have three kernels \((R = 3)\), each a Gaussian on features of a 3-layer network with 30 neurons in each layer. There was also a skip-layer connection from data directly to the last layer which accelerated learning. Length scales \(\sigma_r\) were initialized to 1.0, 3.3 and 10.0. Each \(\lambda\) was initialized to 0.01. The weights of the network were initialized from a Gaussian distribution with standard deviation equal to \(1/\sqrt{30}\). We also optimized the inducing points \(z_m\) which were initialized with random draws from training data. The number of inducing points \(M = 300\), and \(|\mathcal{D}_t| = |\mathcal{D}_v| = 100\). The learning rate was \(10^{-2}\).

FSSD tests were conducted using 100 points \(v_b\) selected at random from the test set, with added normal noise of standard deviation 0.2, using code provided by the authors.

We estimated \(\log Z_\theta\) with \(10^{10}\) samples proposed from \(q_0\), as in Section 3.2 and estimated the bias as in
We added independent $\mathcal{N}(0, 0.05^2)$ noise to the data in training. This is similar to the regularization applied by (Kingma and LeCun 2010; Saremi et al. 2018), except that the noise is added directly to the data instead of the model.

For all models, we stopped training when the objective (4 or log likelihood) did not improve for 200 minibatches. We also set a time budget of 3 hours on each model; this was fully spent by MAF, MOG-MAF and Real NVP on HepMass. We found that MOG-MADE had unstable runs on some datasets. Out of 15 runs on each dataset, 7 on WhiteWine and 7 on MiniBoone produced invalid log likelihoods, 1 run on WhiteWine yielded likelihood of $-4.2 \times 10^{37}$, 3 on Parkinsons yielded $\leq -25$, 4 on MiniBoone yielded $\leq -10^4$. 1 run of DKEF on HepMass yielded $-42.5$. These results were discarded in Figure 3 log likelihood panels.