TraDE: Transformers for Density Estimation

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Abstract

We present TraDE, an attention-based architecture for auto-regressive density estimation. In addition to a Maximum Likelihood loss we employ a Maximum Mean Discrepancy (MMD) two-sample loss to ensure that samples from the estimate resemble the training data. The use of attention means that the model need not retain conditional sufficient statistics during the process beyond what is needed for each covariate. TraDE performs significantly better than existing approaches such as differentiable flow based estimators on standard tabular and image-based benchmarks in terms of the log-likelihood on held out data. TraDE works well wide range of tasks that includes classification methods to ascertain the quality of generated samples, out of distribution sample detection, and handling outliers in the training data.

1. Introduction

Density estimation involves estimating a probability density \( p(x) \), given independent, identically distributed samples drawn from it. This is a versatile and important problem, as it allows one to generate synthetic data, or perform novelty and outlier detection. It is also an important subroutine in graphical models. Deep neural networks are a powerful function class and learning complex distributions with them is promising. This has resulted in a resurgence of interest in the classical problem of density estimation.

One of the more popular techniques for density estimation with deep networks is to sample from a simple reference distribution and then to learn a (sequence of) invertible transformations that allow us to adapt it to a target distribution. Flow-based methods (Durkan et al., 2019) employ this with great success. A more classical approach is to decompose \( p(x) \) in an iterative manner via conditional probabilities \( p(x_{i+1}|x_1...i) \) and fit this distribution using the data (Murphy, 2013). One may even employ implicit generative models to sample from \( p(x) \) directly, perhaps without the ability to compute the likelihood. Generative Adversarial Networks (GANs) (Goodfellow et al., 2014) reign supreme for image synthesis (Karras et al., 2017), though they do not offer a closed form probability distribution.

Implementing the above methods requires special care, e.g., the normalizing transform requires the network to be invertible with an efficiently computable Jacobian. Auto-regressive models using recurrent networks are difficult to scale to high-dimensional data due to the need to store a potentially high-dimensional conditional sufficient statistic (and due to vanishing gradients). Generative models can be difficult to train and GANs lack a closed density model. Much of current work is devoted to mitigating these issues.

Contributions. We focus on auto-regressive models.

- We show that self-attention is well-suited to auto-regressive density estimation and leads to strong empirical performance. This is in contrast to the contemporary literature (Durkan et al., 2019) which employs complex neural architectures. Our results indicate that a simple architecture with appropriate regularization is superior for density estimation. Further, TraDE can handle both continuous and discrete data distributions.
- We recognize that generative models should conform to constraints on subset marginals. A good estimator for \( p(x_1, x_2, x_3) \) should also be a good estimator for \( p(x_1, x_3) \) after marginalization. We impose this constraint as a Maximum Mean Discrepancy (MMD)-based regularizer in the training objective of TraDE.
- Current literature uses log-likelihood on held-out data as a metric. This only provides a partial view of the performance in real-world applications. We evaluate TraDE on tasks such as classification using generated samples, detecting out-of-distribution samples, and
robustness to outliers in the training data.

We provide extensive empirical evidence of the performance of TraDE on standard tabular and image-based benchmarks along with thorough ablation experiments to study the efficacy of different components of the algorithm.

2. Background and related work

Given a dataset \( \{x^1, \ldots, x^n\} \) where each sample \( x^k \in \mathbb{R}^d \) is drawn iid from some probability distribution \( p(x) \), the maximum-likelihood formulation of density estimation finds a \( \theta \)-parameterized distribution \( q_\theta(x) \) that minimizes the reverse Kullback-Leibler (KL) divergence with respect to the true distribution. That is,

\[
\hat{\theta} = \arg\min_{\theta} \text{KL} (p \| q_\theta)
\]  

(1)

Since we only have a sample from \( p \) we need to approximate the \( p \)-expectation by its empirical average via

\[
\text{KL} (p \| q_\theta) \approx \frac{1}{n} \sum_{i=1}^{n} \log q_\theta(x^i) - H(p).
\]  

(2)

The second term \( H(p) \) is the Shannon entropy of \( p \) and constant relative to \( \theta \). The candidate distribution \( q_\theta(x) \) can be parameterized in a variety of ways.

**Normalization flows** write \( x \sim q_\theta \) as a transformation of samples \( z \) from some base distribution \( p_z \) from which one can draw samples easily (Papamakarios et al., 2019). If this mapping is \( f_\theta : z \rightarrow x \), two distributions can be related using the determinant of the Jacobian as

\[
q_\theta(x) := p_z(z) \left| \frac{df_\theta}{dz} \right|^{-1}.
\]

A key property of flow-based models is that \( f_\theta \) is a diffeomorphism, i.e., it is invertible and both \( f_\theta \) and \( f_\theta^{-1} \) are differentiable. This allows gradient-based minimization of (1) which involves a term of the form \( \log |df_\theta/dz| \).

Good performance using normalizing flows requires that the mapping \( f_\theta \) be powerful yet invertible with a Jacobian that can be computed efficiently. There are a number of techniques in the literature to achieve this, e.g., linear mappings, planar/radial flows (Rezende & Mohamed, 2015; Tabak & Turner, 2013), Sylvester flows (Berg et al., 2018), coupling (Dinh et al., 2014) and auto-regressive models (Larochelle & Murray, 2011). One may also compose the transformations, e.g., using monotonic mappings \( f_\theta \) in each layer (Huang et al., 2018; De Cao et al., 2019).

**Auto-regressive models** have their roots in probabilistic graphical models (Koller & Friedman, 2009). These models factorize the distribution \( q_\theta \) as a product of conditional distributions \( q_\theta(x) := \prod_i q_\theta(x_i|x_{1\ldots i-1}) \).

Note that in this case the Jacobian is a lower-triangular matrix with entries \( \frac{d x_i}{d x_j} \). Moreover, the determinant is simply a product of the entries along the diagonal. Parameters of the conditionals in the product may be shared using RNNs (Oliva et al., 2018; Kingma et al., 2016).

For high-dimensional data the challenge lies in the increasingly large state space \( x_{1\ldots i-1} \) required in sampling \( x_i \). In a latent-variable autoregressive model such as an LSTM past data is stored in some representation \( h_i \) which is updated via a function \( h_{i+1} = g(h_i, x_i) \). This overcomes the problem of very high dimensional estimation, albeit at the expense of loss in fidelity. Techniques like masking the computational paths in a feed-forward network are popular to alleviate these problems further (Uria et al., 2016; Germain et al., 2015; Papamakarios et al., 2017). Choosing a good variable ordering for the factorization of \( q_\theta \) is paramount in auto-regressive models; several algorithms train ensembles over multiple orderings for good performance.

While autoregressive models are commonly applied to natural language and time series data, this setting only involves variables that are already naturally ordered (Chelba et al., 2013). In contrast, we consider continuous (and discrete) density estimation of vector valued data, e.g., tabular data, where the underlying ordering and dependencies between variables is unknown.

**Generative models** focus on drawing samples from the estimated distribution that look resemble the true distribution of data. There is a rich history of learning explicit models from variational inference (Jordan et al., 1999) that allow both drawing samples and estimating the log-likelihood or implicit models such as Generative Adversarial Networks (GANs, see Goodfellow et al. (2014)) where one may only draw samples. These have been shown to work well for natural images (Kingma & Welling, 2013) but have not obtained similar performance for tabular data. Also note some techniques somewhat less popular in deep learning, such as kernel density estimation (Silverman, 2018) and Chow-Liu trees (Chow & Liu, 1968; Choi et al., 2011).

**Remark 1 (Regularization in density estimation).** The maximum-likelihood objective in (1) does not have a regularization term that would help with outliers in the dataset. There exists a large number of classical techniques, such as maximum entropy and approximate moment matching techniques (Phillips et al., 2004; Altun & Smola, 2006) that can be used. They map to some extent to the parameter based capacity control in deep learning, such as Dropout or input permutation (or they’re implicitly determined by the choice of architecture). Instead, we use MMD to penalize differences between training data and samples from the model directly. This allows us to use powerful architectures such as the Transformer with less risk of overfitting.
3. Tools of the TraDE

Consider the 8-dimensional Markov Random Field shown above. The underlying graphical model is unknown in practice. Consider the following two orders in which to decompose the autoregressive model: \((1, 2, 3, 4, 5, 6, 7, 8)\) and \((1, 8, 2, 7, 3, 6, 4, 5)\). In the latter case the model becomes a simple sequence where e.g. \(p(x_3|x_{1,8,2,7}) = p(x_3|x_7)\) due to conditional independence in undirected graphical models. A latent variable autoregressive model only needs to preserve the most recently encountered state. While \(p(x_3|x_{1,2})\) can be be simplified further to \(p(x_3|x_2)\), however we still need to carry \(x_1\) along until the end since \(p(x_8|x_{1...7}) = p(x_8|x_{1,2})\). This is a fundamental weakness in models employing RNNs such as Oliva et al. (2018).

3.1. Vertex Ordering and Sufficient Statistics

This problem is not uncommon even sequence modeling. For instance sequence-to-sequence models handle long-range dependencies and complex state poorly. This led to the introduction of transformers (Vaswani et al., 2017). The utility of attention in the NLP literature is its effectiveness at maintaining an accurate representation of \(x_{<j}\) while predicting \(x_d\), irrespective of the distance between them.

A recurrent network can theoretically absorb this information into its hidden state. In fact, Long-Short-Term Memory (LSTM) (Hochreiter & Schmidhuber, 1997) units were engineered specifically to store long-range dependencies until needed. Nonetheless, storing information costs parameter space. As \(d\) and \(j\) grow in our example, the hidden state needs to store more information for a greater number of steps. The following simple lemma formalizes this.

**Lemma 2.** Denote by \(G\) the graph of an undirected graphical model over random variables \(x_1, \ldots, x_d\). Depending on the order vertices are traversed in our factorization the largest number of latent variables a recurrent autoregressive model needs to store is bounded from above and below by the minimum and the maximum number of variables with a cut edge of the graph \(G\).

**Proof.** Given a subset of known variables \(S \subseteq \{1, \ldots, d\}\) we want to estimate the conditional distribution of the variables on the complement \(C := \{1, \ldots, d\}\setminus S\). For this we need to decompose \(S\) into the Markov blanket \(M\) of \(C\) and its remainder. By definition \(M\) consists of the variables with a cut edge. Since \(p(x_C|x_S) = p(x_C|x_M)\) we are done.

The problem with long-dependencies in auto-regressive models has been noted before. For instance, recent auto-regressive models employ masking to eliminate the sequential operations of recurrent models (Papamakarios et al., 2017). There are also algorithms like Pixel RNN (Oord et al., 2016) which explicitly designs a multi-scale masking mechanism suited for natural images. Note that while there is a natural ordering of random variables in textual or image-based data, tabular data does not have any canonical ordering. An alternative is to use attention to attend only to parts of the data relevant for the conditioning. This alleviates the state space problem.

3.2. Attention

Assume that we have \(d\) query vectors which are \(d_q\)-dimensional embeddings of the input variables \(\{x_1, \ldots, x_d\}\) arranged in a matrix \(Q \in \mathbb{R}^{d \times d_q}\). Given a matrix \(K \in \mathbb{R}^{d_v \times d_q}\) of learnable “keys”, the dot product \(QK^\top\) measures how similar the encoding of a random variable \(x_i\) is to each of the columns of \(K\). An attention module computes \(\omega \left( \frac{1}{d_q} QK^\top \right) V\) where \(\omega\) is an activation function, say softmax, and \(V \in \mathbb{R}^{d \times d_v}\) consists of values. The denominator prevents the dot product from being too large in magnitude and from pushing the softmax into parts of the domain where the gradient is small. Attention amounts to taking a linear combination of the values in \(V\), a value is given more weight in this combination if the corresponding key has a large dot product with the query vector. Vaswani et al. (2017) introduced the multi-headed attention module which computes attention independently in a few different sub-spaces and then applies a linear combination on the concatenation of the outputs.

3.3. Transformer architecture

We modify the Transformer architecture of Vaswani et al. (2017) into an auto-regressive model that can be used for density estimation. The Transformer is a competitive architecture in neural sequence transduction and consists of a multi-layer encoder and decoder structure. An input sequence \((x_1, \ldots, x_d)\) is mapped to an output sequence \((z_1, \ldots, z_d)\). In our case we pick \(z_i = q_0(x_i|\{x_1, \ldots, x_{i-1}\})\). Each layer of the encoder has a multi-headed self-attention mechanism followed by a fully-connected layer. Residual connections (He et al., 2016) and layer normalization (Ba et al., 2016) are used across both the attention and fully-connected sub-layers. Note that the self-attention in the encoder already ensures the auto-regressive property for...
density estimation by preventing it from looking forward and attending to subsequent positions using a mask. The decoder in a sequence-to-sequence Transformer has a similar architecture with the difference that the multi-headed self-attention layer in the decoder takes keys and values from the output of the encoder. We will only use the self-attention-based encoder in this paper. While the Transformer predicts the target sequence using a softmax layer, we predict the conditionals \( z_i \) by parameterizing them as a mixture of multivariate Gaussians with a diagonal covariance matrix.

### 3.4. Regularization via Pseudolikelihood Loss

Density estimation is typically cast as a maximum-likelihood problem. This enforces constraints on lower-dimensional marginals only indirectly. That is, there is no direct way of ensuring that the following holds:

\[
p(x_1, x_3) = \int_{x_2} q_0(x_1) q_0(x_2|x_1) q_0(x_3|x_1, x_2) \, dx_2.
\]  

(3)

Compare this to a pseudolikelihood approach (Besag, 1977) which explicitly penalizes discrepancies on subsets of variables. We find that adding such constraints as regularizers can improve the fidelity of the estimates. In the example above this means that we want to ensure that \( p(x_1, x_3) \) is also a good model for the empirical observations (after marginalizing over \( x_2 \)).

In practice, let \( S = \{i_1, \ldots, i_{|S|}\} \) be a set of indices with each \( i_k \in \{1, \ldots, d\} \). Let \( x_S \) denote the distribution with all variables \( x_i \) with \( i \notin S \) marginalized out. We can again use a KL-divergence penalty of the form \( KL(p(x_S) \mid \mid q_0(x_S)) \) to achieve the constraint (3). This however involves marginalizing over all variables \( \{x_i : i < \max(S), i \notin S\} \) to evaluate \( q_0(x_S) \), the integral in (3) needs to be computed at each mini-batch update. Alternatively we can impose a very similar constraint directly using samples.

### 3.5. Maximum Mean Discrepancy (MMD)

An alternative to maximum likelihood estimation, and in some cases a dual to it (Altun & Smola, 2006), is to perform nonparametric moment matching. In this paper we combine both a log-likelihood loss and a two-sample test based loss to ensure that the model has high fidelity.

We can test whether two distributions \( p \) and \( q \) supported on a space \( \mathcal{X} \) are different using samples drawn from each of them by finding a smooth function that is large on samples drawn from \( p \) and small on samples drawn from \( q \). This leads to so-called Integral Probability Metrics (IPM) Dudley (2018, Lemma 9.3.2): if \( x \sim p \) and \( y \sim q \), then \( p = q \) if and only if \( \mathbb{E}_x [f(x)] = \mathbb{E}_y [f(y)] \) for all bounded continuous functions \( f \) on \( \mathcal{X} \). We can exploit this result computationally by restricting the test functions to some class \( f \in \mathcal{F} \) and finding the worst test function. This leads to the maximum mean discrepancy (MMD) metric defined below (Fortet & Mourier, 1953; Müller, 1997; Gretton et al., 2012; Sriperumbudur et al., 2016). MMD can be used in GANs (Li et al., 2017) as an alternative adversarial loss.

**Definition 3.** For a class \( \mathcal{F} \) of functions \( f : \mathcal{X} \rightarrow \mathbb{R} \), the maximum mean discrepancy between distributions \( p, q \) is

\[
\text{MMD}[^\mathcal{F}, p, q] = \sup_{f \in \mathcal{F}} \left( \mathbb{E}_{x \sim p} [f(x)] - \mathbb{E}_{y \sim q} [f(y)] \right). 
\]

(4)

**Computing MMD with kernels.** We can pick the function class \( \mathcal{F} \) to be the unit ball in a universal Reproducing Kernel Hilbert Space (RKHS) Gretton et al. (2012)) with kernel \( k \). There one may embed \( p \) using the so-called mean embedding \( \mu_p \in \mathcal{F} \) which has the property that \( \mathbb{E}_{x \sim p} [\varphi] = \langle \varphi, \mu_p \rangle_\mathcal{F} \). The MMD is then a metric and is given by \( \text{MMD}[^\mathcal{F}, p, q] = ||\mu_p - \mu_q||_\mathcal{F} \) given by

\[
\text{MMD}[^\mathcal{F}, k, p, q] = \mathbb{E}_{x,x' \sim p} [k(x, x')] - 2 \mathbb{E}_{x \sim p, y \sim q} [k(x, y)] + \mathbb{E}_{y,y' \sim q} [k(y, y')]. 
\]

(5)

As Steinwart (2001) showed, Gaussian and Laplace kernels are universal. Further, we can obtain an empirical estimate of the MMD above using samples (Gretton et al., 2012).

**Remark 4 (Kernel design for TraDE).** In principle, any universal kernel \( k \) will suffice to ensure that two distributions are close. In practice, though, it is important to ensure that not only \( p(x) \) but also its marginals \( p_S(x_S) \) as restricted on subsets of variables \( S \subseteq \{1, \ldots, d\} \) are suitably matched. We can either pick a pre-specified number of them, say \( \{1, \ldots, i\} \) for all \( 1 \leq i \leq d \) or alternatively we can design a kernel that does this automatically. For Gaussian RBF kernels this holds for

\[
k(x, x') = \prod_{i=1}^d \left( \exp(-\sigma(x_i - x'_i)^2) + c \right)
\]

(6)

\[
= \sum_{S \subseteq \{1, \ldots, d\}} \exp(-\sigma||x_S - x'_S||^2)e^{d-|S|}
\]

(7)

for \( c \geq 0 \). That is, a polynomial expansion will contain all products of terms and thus all subsets. At each mini-batch update we sample from the entire joint distribution of the auto-regressive model and calculate the MMD term in (5). Since MMD is a metric, imposing this constraint implies all the other subset marginal constraints.

### 3.6. TraDE

We combine two objectives: the log-likelihood objective ensures consistency of the estimate. Overall, entropic objective functions have proven to work well in many applications beyond density estimation. Second we add a two-sample loss that is capable of detecting obvious discrepancies. The
MMD loss is quite effective here. Note that in theory, MMD with a universal kernel would be equally consistent. In practice, a combination of both objectives yields superior results. We arrive at the TraDE objective

$$-rac{1}{n} \sum_{i=1}^{n} \log q_{\phi}(x_i) + \lambda \text{MMD}^2[k, p, q_{\phi}].$$  \hspace{1cm} (8)

The hyper-parameter $\lambda \geq 0$ controls the strength of the MMD term.

The first term in (8) is the reverse KL-divergence between the true distribution $p$ and the candidate $q_{\phi}$. This encourages $q_{\phi}$ to put probability mass in regions where $p$ may not have samples. As we have discussed before, this is a maximum-likelihood objective and does not have any regularization. The second term in (8) forces $q_{\phi}$ to be close to $p$ as measured by a kernel $k$.

This objective is minimized using mini-batch gradient-based updates. The gradient of the log-likelihood term can be computed using standard back-propagation. For the MMD term some more care is needed.

**Remark 5 (Gradient of the TraDE objective).** Evaluating the gradient of the MMD term involves differentiating the samples from $q_{\phi}$ with respect to the parameters $\theta$. If the model predicts a multi-variate Gaussian distribution for each conditional, this is easily done using the reparametrization trick (Kingma & Welling, 2013). For experiments on discrete data (binarized MNIST) in Section 4.3, we calculate the gradient using the Gumbel softmax trick (Maddison et al., 2016). The objective of TraDE is thus general enough to handle both continuous and discrete data distributions.

### 3.7. RNN embeddings as inputs to the Transformer

A key issue in transformers is that they require a position encoding. For instance, for textual embeddings one uses Fourier features to delineate the position of tokens relative to each other Vaswani et al. (2017). Unfortunately, no canonical order exists for tabular data. One option would be to learn the embeddings per coordinate as an auxiliary set of features. This requires significant amounts of capacity, given the dimensionality of the inputs required for the transformer. An alternative is to use a simple RNN as an initial embedding layer for position and values. We employ Gated Recurrent Units (GRU) to deal with long-range dependencies (Cho et al., 2014). This allows us to learn both an initial mapping and the positions in one step. Our experiments show that this leads to superior accuracy. Note that this parallels recent findings from language modeling where Wang et al. (2019) also used an initial RNN embedding to generate inputs to the transformer.

**Computational complexity.** Incorporating a recurrent layer at the input does not slow down TraDE at inference time; the complexity of drawing samples is still $\mathcal{O}(d)$; the complexity of training is marginally higher due to recurrence in the input layer, however the strong performance of the recurrent embedding makes up for this.

### 4. Experiments

To gain insight into how TraDE works we evaluate it on a number of toy datasets in Section 4.2 and when sampling MNIST digits in Section 4.4. This is followed by results on benchmark datasets (Section 4.3) commonly used to evaluate flow-based density estimators. We then present three different ways to evaluate the performance of density estimation on downstream tasks (Section 4.5) along with some ablation studies (Section 4.6). This section shows that TraDE not only achieves superior log-likelihoods but it is also well-suited to numerous downstream tasks, including novelty detection and data synthesis. These problems are of independent relevance and the subject of future research. Details for all the experiments in this section, including hyper-parameters are provided in the Appendix.

#### 4.1. Protocol

We follow the setup of Papamakarios et al. (2017)\(^1\) to ensure the same training/validation/test dataset splits in our evaluation. In particular, the preprocessing (ignoring some variables and data whitening) of all the datasets is kept the same as that of Papamakarios et al. (2017). The datasets named POWER, GAS (Vergara et al., 2012), HEPMASS, MINIBOONE and BSDS300 (Martin et al., 2001) were taken from the UCI machine learning repository\(^2\) (Dua & Graff, 2017).

The MNIST dataset (LeCun et al., 1990) is used to evaluate TraDE on high-dimensional image-based data; we follow the variational inference literature, e.g., Oord et al. (2016), and use the binarized version of MNIST. The datasets for anomaly detection tasks, namely Pendigits, ForestCover and Satimage-2 are from the Outlier Detection DataSets (OODS) library\(^3\) (Rayana, 2016). We normalized the OODS data by subtracting the per-feature mean and dividing by the standard deviation.

**Remark 6 (Log-likelihood in density estimation).** Note that the solution of (1) and (8) is a variational approximation to $p(x)$ and in general $q_{\phi}(x)$ need not be close to $p(x)$. Contemporary literature often compares density estimation algorithms in terms of their predictive log-likelihood $\log q_{\phi}(x)$ on held-out test data. While this has the nice property of

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\(^1\)https://github.com/gpapamak/maf
\(^2\)https://archive.ics.uci.edu/ml
\(^3\)http://odds.cs.stonybrook.edu
being a single scalar number, a high value of log-likelihood is not necessarily a good indicator of the performance of the model on downstream tasks (Theis et al., 2015).

The log-likelihood is rather insufficient to ascertain the real-world performance, e.g. in terms of verissimilitude of the data generated. For instance, since the variational family used in different algorithms is different, the generated samples may differ greatly (and thus the log-likelihoods are not comparable). This is a major motivation for us to develop complementary evaluation methodologies in Section 4.5. However, we also report log-likelihood results to be consistent with published literature.

4.2. Toy-datasets

We first train on two-dimensional data to visualize the model. These datasets were taken from the code provided by Nash & Durkan (2019). As Fig. 2 shows, TraDE learns an accurate estimate of the true distribution. The spiral and the checkerboard patterns evaluate the algorithm on multi-modal data while the dot-board pattern shows that TraDE can be precise in how it puts its probability mass on the domain. The bottom three pictures of Shannon, Einstein and Turing demonstrate that TraDE can handle complex correlations in the input variables. We computed the value of the model log-likelihood on a fine grid across the entire domain to get these figures.

4.3. Benchmark datasets with tabular data

We show the results of fitting density estimators on benchmark datasets in Table 1. There is a wide diversity in the algorithms in density estimation and we make an effort to provide a complete comparison of known results irrespective of the specific methodology. Some methods like Neural Spline Flows (NSF) by Durkan et al. (2019) are quite complex to implement; others like Masked Autoregressive Flows (MAF) Papamakarios et al. (2017) use ensembles to estimate the density; some others like Autoregressive Energy Machines (AEM) of Nash & Durkan (2019) average the log-likelihood over a large number of importance samples. As the table shows, TraDE obtains significant performance improvements over all these methods in terms of the log-likelihood. This performance is persistent across all datasets, except MINIBOONE where TraDE is competitive although not the best. The improvement is drastic for the POWER, HEPMASS and BSDS300 datasets.

4.4. Sampling MNIST images

Next, we evaluate TraDE on the MNIST dataset in terms of the log-likelihood on test data. As Table 2 shows TraDE obtains high log-likelihood even compared to sophisticated models such as Pixel-RNN (Oord et al., 2016). This is a difficult dataset for density estimation because of the high dimensionality. We also show the quality of the samples generated by the model in Fig. 3.

4.5. Evaluating density estimators

1. Checking the quality of samples. We designed two experiment to check the quality of samples draw from the
Table 1. Average test log-likelihood in nats (higher is better) for benchmark datasets. Entries marked with * evaluate standard deviation across 3 independent runs of the algorithm; all others are mean ± standard error. TraDE achieves significantly better log-likelihood than other algorithms on all datasets except MINIBOONE. This is in spite of the fact that some methods, e.g., MAF train an ensemble.

| Dataset | POWER | GAS | HEPMASS | MINIBOONE | BSDS300 |
|---------|-------|-----|---------|-----------|--------|
| REAL NVP | 0.17 ± 0.01 | 8.33 ± 0.14 | -18.71 ± 0.02 | -13.84 ± 0.52 | 153.28 ± 1.78 |
| MADE MoG | 0.4 ± 0.01 | 8.47 ± 0.02 | -15.15 ± 0.02 | -12.27 ± 0.47 | 153.71 ± 0.28 |
| MAF MoG | 0.3 ± 0.01 | 9.59 ± 0.02 | -17.39 ± 0.02 | -11.68 ± 0.44 | 156.36 ± 0.28 |
| FFJORD | 0.46 | 8.59 | -14.92 | -10.43 | 157.4 |
| NAF | 0.62 ± 0.01* | 11.96 ± 0.33* | -15.09 ± 0.4* | -8.86 ± 0.15* | 157.43 ± 0.3* |
| TAN | 0.6 ± 0.01 | 12.06 ± 0.02 | -13.78 ± 0.02 | -11.01 ± 0.48 | 159.8 ± 0.07 |
| BNAF | 0.61 ± 0.01* | 12.06 ± 0.09* | -14.71 ± 0.38* | -8.95 ± 0.07* | 157.36 ± 0.03* |
| NSF | 0.66 ± 0.01* | 13.09 ± 0.02* | -14.01 ± 0.03* | -9.22 ± 0.48* | 157.31 ± 0.28* |
| AEM | 0.70 ± 0.01 | 13.03 ± 0.01 | -12.85 ± 0.01 | -10.17 ± 0.26 | 158.71 ± 0.14 |
| **TRADE (ours)** | **0.73 ± 0.00** | **13.27 ± 0.01** | **-12.01 ± 0.03** | **-9.49 ± 0.13** | **160.01 ± 0.02** |

Regression. First, we create a regression task where a random variable, say \( x_d \) is regressed using data from the others \( x_{-d} = (x_1, \ldots, x_{d-1}) \). The procedure is as follows: we use the training set of the HEPMASS dataset (\( d = 21 \)) to fit the density estimator; create a synthetic dataset with both inputs \( x_{-d} \) and targets \( x_d \) sampled from the model. Two boosted decision forest-based regressors are fitted, one on the real data and another on this synthetic data. Both these regressors are tested on real test data from the HEPMASS dataset. If the model synthesizes good samples, one would expect that the test performance of the regressor fitted on synthetic data would be comparable to the regressor fitted on real data.

Table 3 shows the results of this experiment. Observe that the classifier trained on data synthetized by TraDE performs very similarly to the one trained on the original data. The MSE of a RNN-based auto-regressive density estimator, which is higher, is provided for comparison.

Classification. Next we train a boosted decision-forest-based classifier to differentiate between real data and synthetic data. The idea is similar to a two-sample test (Lopez-Paz & Oquab, 2016) in the discriminator of a GAN: if the samples generated by the auto-regressive model are good, the discriminator should have an accuracy of 50%. As Table 4 shows the samples generated by TraDE is much closer to the real data than those generated by the RNN model.

Table 3. Mean squared error of regression on HEPMASS.

|           | Real data | Synthetic data (TRADE) | Synthetic data (RNN) |
|-----------|-----------|------------------------|----------------------|
| Mean      | 0.773     | 0.780                  | 0.803                |

Table 4. Accuracy of the discriminator trained to classify real data from synthesized data on HEPMASS. These numbers are the average accuracy of multiple experiments, each of which uses a different subset of columns \( x_1, (x_1, x_2), \ldots, (x_1, \ldots, x_d) \) as feature for the discriminator.

|           | Synthetic data (TRADE) | Synthetic data (RNN) |
|-----------|------------------------|----------------------|
| Accuracy  | 51 ± 1 %               | 55 ± 4 %             |

2. Out-of-distribution detection. This is a classical application of density estimation techniques where we seek to discover unlikely samples in a given dataset. We follow the setup of Oliva et al. (2018): we call a sample out-of-distribution if the likelihood of the sample under the model \( q_θ(x) \leq t \) for a chosen threshold \( t \geq 0 \). We compute the average precision of detecting out-of-distribution samples by sweeping across different values of \( t \). The results are shown in Table 5. Observe that TraDE obtains extremely good performance, of more than 0.95 average precision, on the three datasets.

3. Outliers in the training data. It is important in view of the maximum-likelihood objective that a density estimator...
Table 5. Average precision for out-of-distribution detection
The numbers for NADE, NICE and TAN were (precisely) eyeballed from the plots of Oliva et al. (2018).

|        | NADE | NICE | TAN | TraDE |
|--------|------|------|-----|-------|
| Pendigits | 0.91 | 0.92 | 0.97 | 0.98  |
| ForestCover | 0.87 | 0.80 | 0.94 | 0.95  |
| Satellite-2 | 0.98 | 0.975 | 0.98 | 1.0   |

be robust to outliers in the training data. Methods such as NSF (Durkan et al., 2019) or MAF (Papamakarios et al., 2017) indirectly handle this using permutations of the input data or masking within hidden layers. Note that these operations are not explicitly designed to be robust to noisy data. We next study how TraDE deals with this scenario; this experiment therefore compares the MMD regularization against the above techniques. To that end, we add noise to 10% of the entries in the training data; we then fit both TraDE and NSF on this noisy data; both are evaluated on clean test data. As Table 6 shows, the degradation of both TraDE and NSF is about the same; the former obtains a higher log-likelihood as noted in Table 1. We attribute this to the effectiveness of the MMD regularizer in (8).

Table 6. Average test log-likelihood in nats for HEPMASS dataset with and without additive noise in the training data.

|         | Clean Data | Noisy Data |
|---------|------------|------------|
| NSF     | -14.51     | -14.98     |
| TraDE   | -11.98     | -12.43     |

4.6. Ablation Experiments

To understand the effect of the design decisions in TraDE we disable (or replace) them one at a time. In particular, we aim to understand the effect of recurrent networks for auto-regressive models, using only multi-headed self-attention in the Transformer without the position encoding, the TraDE model without the MMD regularizer which uses a GRU for embedding the input, and the full TraDE algorithm.

Table 7. Average test log-likelihood in nats (higher is better) on benchmark datasets for four algorithms: an RNN for standard auto-regressive density estimation, a Transformer with multi-head attention without positional encoding, TraDE with $\lambda = 0$ in (8) and the full TraDE algorithm.

|          | POWER | GAS | HEPMASS | MINIBOONE | BSDS300 |
|----------|-------|-----|---------|-----------|--------|
| RNN      | 0.51  | 6.26 | -15.87  | -13.13    | 157.29 |
| Transformer | 0.71  | 12.95 | -15.80  | -22.29    | 134.71 |
| TraDE w/o MMD | 0.72  | 13.26 | -12.22  | -9.44     | 159.97 |
| TraDE    | 0.73  | 13.27 | -12.01  | -9.49     | 160.01 |

As Table 7 shows, the performance of an RNN as an auto-regressive model is quite poor for all datasets. Using a Transformer network (without position encoding) improves this log-likelihood by a lot but this does not work for all datasets. The biggest improvement is obtained upon adding a GRU-based embedding to the Transformer. The MMD loss improves the log-likelihood by a large amount for HEPMASS and a small amount for POWER, the effect for other datasets is marginal. The other algorithms in this table use the same hyper-parameters (architecture and training) as those of TraDE.

Table 8 compares the performance of the GRU-based input encoding against a Transformer with position encoding. Compare the first row of this table with the second row of Table 7: the performance of the Transformer with position encoding is significantly better than the one without it. This suggests that incorporating the information about the position is critical for auto-regressive models (also see Section 3). A recurrent network to incorporate the position information obtains significant performance boost as seen in the second row of Table 8.

Table 8. Log-likelihood in nats of using position encoding versus a recurrent network for input embedding.

|         | HEPMASS | MINIBOONE | BSDS300 |
|---------|---------|-----------|--------|
| Transformer w/ position encoding | -13.89  | -12.28    | 147.94 |
| TraDE w/o MMD | -12.22  | -9.44     | 159.97 |

5. Discussion

We demonstrated that self-attention in the Transformer architecture is naturally amenable to building auto-regressive models and is well-suited for density estimation problems. Our second key finding is a new regularized objective for density estimation that uses MMD explicitly. Note that this is reminiscent to maximum entropy models where one aims to find a distribution matching moments between empirical averages and the expectations generated by the model. In the parlance of MaxEnt models we are effectively combining dual constraints (via log-likelihood) and primal ones (via MMD) to ensure a good fit. This is appropriate since the models we use are not optimal within their function class (local minima, entropy maximization, etc.). Hence it is advantageous to enforce desirable constraints directly.

This is relevant since deep learning based density estimation approaches typically do not use explicit regularization in the objective; there may be some implicit regularization via dropout, weight-decay or mini-batch-based training while training the neural network. This is particularly important due to the popularity of high-capacity deep neural networks that are prone to overfitting.
The third contribution of our paper is to offer a suite of additional experiments on downstream tasks such as classification, detecting out of distribution samples and training with noisy data; these tasks help evaluate density estimation on real-world scenarios in contrast to simply comparing the log-likelihood on held-out data.

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A. Hyper-parameters for benchmark datasets

All models are trained for 1000 epochs with the Adam optimizer. The MMD kernel is a mixture of up to 5 Gaussians for all datasets, i.e., \( k(x, y) = \sum_{i=1}^{5} k_i(x, y) \) where each \( k_i(x, y) = e^{-\|x-y\|^2/\sigma_i^2} \) of bandwidths \( \sigma_i \in \{1, 2, 4, 8, 16\} \).

|                | POWER | GAS  | HEPMASS | MINIBOONE | BSDS300 | MNIST |
|----------------|-------|------|---------|-----------|---------|-------|
| MMD coefficient \( \lambda \) | 0.2   | 0.1  | 0.1     | 0.4       | 1.2     | 0.1   |
| Gaussian mixture components | 150   | 100  | 100     | 20        | 100     | 1     |
| Number of layers | 5     | 8    | 6       | 8         | 5       | 6     |
| Multi-head attention head | 8     | 16   | 8       | 8         | 2       | 4     |
| Gradient clipping norm | 5     | 5    | 5       | 5         | 5       | 5     |
| Hidden neurons | 512   | 400  | 128     | 64        | 128     | 256   |
| Dropout | 0.1   | 0.1  | 0.1     | 0.2       | 0.3     | 0.1   |
| Learning rate | 3E-4  | 3E-4 | 5E-4    | 5E-4      | 5E-4    | 5E-4  |
| Mini-batch size | 512   | 512  | 512     | 64        | 512     | 16    |
| Weight decay | 1E-6  | 1E-6 | 1E-6    | 0         | 1E-6    | 1E-6  |
| Gumbel softmax temperature | n/a   | n/a  | n/a     | n/a       | n/a     | 1.5   |

B. Sampling MNIST images

To further investigate the quality samples generated by our model, we show more samples in Fig. 4.

Figure 4. Samples from TraDE fitted on binary MNIST.