Noise Contrastive Meta-Learning for Conditional Density Estimation using Kernel Mean Embeddings

Jean-François Ton  
University of Oxford  
ton@stats.ox.ac.uk

Lucian Chan  
University of Oxford  
leung.chan@stats.ox.ac.uk

Yee Whye Teh  
University of Oxford  
te@stats.ox.ac.uk

Dino Sejdinovic  
University of Oxford  
dino.sejdinovic@stats.ox.ac.uk

Abstract

Current meta-learning approaches focus on learning functional representations of relationships between variables, i.e. on estimating conditional expectations in regression. In many applications, however, we are faced with conditional distributions which cannot be meaningfully summarized using expectation only (due to e.g. multimodality). Hence, we consider the problem of conditional density estimation in the meta-learning setting. We introduce a novel technique for meta-learning which combines neural representation and noise-contrastive estimation with the established literature of conditional mean embeddings into reproducing kernel Hilbert spaces. The method is validated on synthetic and real-world problems, demonstrating the utility of sharing learned representations across multiple conditional density estimation tasks.

1 Introduction

The estimation of conditional densities $p(y|x)$ based on paired samples $\{(x_i, y_i)\}_{i=1}^n$ is a general and ubiquitous task when modelling relationships between random objects $x$ and $y$. While the problem of regression focuses on estimating the conditional expectations $E[y|x]$ of responses $y$ given the features $x$, many scenarios require a more expressive representation of the relationship between $x$ and $y$. In particular, the distribution of $y$ given $x$ may exhibit multimodality or heteroscedasticity, thus requiring a flexible nonparametric model of the full conditional density. Estimating conditional densities becomes even more challenging when the sample size is small, especially when $x$ and $y$ are multivariate. Hence, we approach this problem from a meta-learning perspective, where we are faced with a number of conditional density estimation tasks, allowing us to transfer information between them via a shared learned representation of both the responses $y$ and the features $x$.

Our contribution can be viewed as a development which parallels that of neural processes [Garnelo et al., 2018b] and conditional neural processes [Garnelo et al., 2018a] in the context of regression and functional relationships, but is applicable to a much broader set of relationships between random objects, i.e. those where the response $y$ cannot be meaningfully represented using a single function $f(x)$ of the features $x$. To that end, we will make use of the framework of conditional mean embeddings (CME) of distributions into reproducing kernel Hilbert spaces (RKHSs) [Song et al., 2013, Muandet et al., 2017].

Let us consider a simple illustrative example of one such relationship where there is no functional relationship between $x$ and $y$ in the data space. Assume that we are given a dataset $D = \{(x_i, y_i)\}_{i=1}^n$ sampled uniformly from an annulus $r^2 \leq x^2 + y^2 \leq R^2$. Any regression model would fail to capture...
We first introduce some notation that we use throughout this paper. We denote the observed dataset \( \Phi \) which represent relationships between dihedral angles in molecular structures, as well as on the NYC taxi data used in Trippe and Turner [2018] to model the conditional densities of dropoff locations properties, namely on Ramachandran plots from computational chemistry [Gražulis et al., 2011], and are infinite-dimensional. However, such kernels can often be too simplistic for specific tasks (e.g. a simple Gaussian kernel is known to be characteristic). Moreover, even though they give a unique representation of a probability distribution and can be a useful tool to represent conditional distributions of (similar) conditional density estimation tasks simultaneously. While CME estimation for fixed feature maps \( \phi \) require a much more expressive feature mapping \( \phi \) and \( \phi \) by adopting the meta-learning framework, i.e. by considering a number of (similar) conditional density estimation tasks simultaneously. While CME estimation for fixed feature maps is well understood [Song et al., 2013, Muandet et al., 2017], we are here concerned with the challenge of linking our CME estimates back to the conditional density estimation (CDE) task, while simultaneously learning the feature maps defining CME. To address this challenge, we propose to use a technique based on noise contrastive estimation (NCE) [Gutmann and Hyvärinen, 2012], treating CMEs as dataset features in the binary classifier discriminating between the true and artificially generated samples of \( (x_i, y_i) \) pairs.

The proposed method is validated on synthetic and real-world data demonstrating multimodal properties, namely on Ramachandran plots from computational chemistry [Gražulis et al., 2011], which represent relationships between dihedral angles in molecular structures, as well as on the NYC taxi data used in Trippe and Turner [2018] to model the conditional densities of dropoff locations given the taxi tips.

2 Background

We first introduce some notation that we use throughout this paper. We denote the observed dataset by \( D = \{ (x_j, y_j) \}_{j=1}^n \), with \( x_j \in \mathcal{X} \) and \( y_j \in \mathcal{Y} \). We also define the learned RKHS/feature maps of inputs \( X \) and responses \( Y \) as \( \mathcal{H}_X / \phi_x \) and \( \mathcal{H}_Y / \phi_y \) respectively.

2.1 Conditional Mean Embeddings (CME)

Kernel mean embeddings of distributions provide a powerful framework for representing and manipulating probability distributions [Song et al., 2013, Muandet et al., 2017]. Formally, given sets \( \mathcal{X} \) and \( \mathcal{Y} \), with a distribution \( P \) over the random variables \( (X,Y) \) taking values in \( \mathcal{X} \times \mathcal{Y} \), the conditional mean embedding (CME) of the conditional distribution of \( Y \mid X = x \), assumed to have density \( p(y \mid x) \), is defined as:

\[
\mu_{Y \mid X = x} := \mathbb{E}_{Y \mid X = x} [\phi_y(Y)] = \int_{\mathcal{Y}} \phi_y(y)p(y \mid x)dy.
\]

(1)

Hence, for each value of the conditioning variable \( x \), we obtain an element \( \mu_{Y \mid X = x} \) of \( \mathcal{H}_Y \). Following Song et al. [2013], the conditional mean embedding can be associated with the operator \( \mathcal{C}_{Y \mid X} : \mathcal{H}_X \rightarrow \mathcal{H}_Y \), which satisfies

\[
\mu_{Y \mid X = x} = \mathcal{C}_{Y \mid X} \phi_x(x).
\]

(2)

It can be shown [Song et al., 2013] that we can write \( \mathcal{C}_{Y \mid X} = \mathcal{C}_{Y \mid X} \mathcal{C}_{X \mid X}^{-1} \) where \( \mathcal{C}_{X \mid X} := \mathbb{E}_{X \mid Y} [\phi_y(Y) \otimes \phi_x(X)] \) and \( \mathcal{C}_{X \mid X} := \mathbb{E}_{X \mid X} [\phi_x(X) \otimes \phi_x(X)] \).

As a result, the finite sample estimator of \( \mathcal{C}_{Y \mid X} \) based on dataset \( \{ (x_i, y_i) \}_{i=1}^n \) can be written as

\[
\hat{\mathcal{C}}_{Y \mid X} = \Phi_y(K + \lambda I)^{-1}\Phi_x^T
\]

(3)

where \( \Phi_y := (\phi_y(y_1), \ldots, \phi_y(y_n)) \) and \( \Phi_x := (\phi_x(x_1), \ldots, \phi_x(x_n)) \) are the feature matrices, \( K := \Phi_y \Phi_x^T \) is the kernel matrix with entries \( k_{ij} = k_x(x_i, x_j) := \langle \phi_x(x_i), \phi_x(x_j) \rangle \), and \( \lambda > 0 \) is

\footnote{In particular, CME \( \mathbb{E}[\phi_y(y) \mid x] \) can be used to estimate conditional expectations \( \mathbb{E}[h(y) \mid x] \) for a broad class of functions \( h \), namely functions in the RKHS determined by the feature map \( \phi_y \).}
We note that this expression is already normalized. However, given that we only have approximations, assuming for the moment that the learned probabilistic classifier attains Bayes optimality, we can deduce the point-wise evaluations of the true conditional density \( p(y|x) \). In the next section, we will adopt these ideas to the context of conditional density estimation in the meta-learning setting. In particular, we will build classifiers that are all fed together with their labels (True/Fake) into the classifier. Hence, the data arises from artificial data and the real data. More concretely, assume that the true underlying density of the data \( p \) is \( \kappa \) times more fake examples than the real ones, which are all fed together with their labels (True/Fake) into the classifier. Hence, the data arises from \( \frac{1}{\kappa + 1} p(y) + \frac{\kappa}{\kappa + 1} p_f(y) \) and the probability that any given \( y \) comes from the true distribution is

\[
P(\text{True}|y) = \frac{p(y)}{p(y) + \kappa p_f(y)}.
\]  

Since our goal is to learn the true density \( p(y) \) we can construct the probabilistic classifier where we model \( P(\text{True}|y) \) as \( \sigma(h_\theta(y)) \) where \( \sigma(t) = 1/(1 + e^{-t}) \) is the logistic function and \( \theta \) are the parameters of the classifier, resulting in the corresponding density model \( p_\theta(y) \). Gutmann and Hyvärinen [2012] show empirically that one can model the unnormalized density (say, \( p_0(y) \)) and the corresponding normalizing constant separately, by writing \( p_\theta(y) = p_{h_\theta}(y) \exp(b) \) with \( \theta = \{b, \theta_0\} \), to obtain a normalized density. In the next section, we will adopt these ideas to the context of conditional density estimation in the meta-learning setting. In particular, we will build classifiers that use conditional mean embeddings to model \( P(\text{True}|y) \).

3 Methodology

3.1 Conditional Mean Embeddings for Noise Contrastive Estimation

As described above, the key ingredient of noise contrastive estimation is a classifier which can discriminate between the samples from the true density, in our case the conditional \( p(y|x) \) i.e. \( \{y_i\}_{i=1}^n \), and those from the fake density \( p_f(y) \) i.e. \( \{y_i\}_{i=1}^{\kappa n} \). For a given \( x \), assuming that the classifier observes samples from the mixture \( \frac{1}{\kappa + 1} p(y|x) + \frac{\kappa}{\kappa + 1} p_f(y) \), the probability that \( y \) arises from the true conditional distribution \( p(y|x) \) as opposed to the fake density \( p_f(y) \) is given by:

\[
P_\theta(\text{True}|y, x) = \frac{p_\theta(y|x)}{p_\theta(y|x) + \kappa p_f(y)}.
\]

Assuming for the moment that the learned probabilistic classifier attains Bayes optimality, we can deduce the point-wise evaluations of the true conditional density \( p(y|x) \) directly from expression (7) as

\[
p_\theta(y|x) = \frac{\kappa p_f(y) P_\theta(\text{True}|y, x)}{1 - P_\theta(\text{True}|y, x)}.
\]
In particular, consider the density model given by

\[
p_\theta(y|x) = \frac{\exp(s_\theta(x, y))}{\int \exp(s_\theta(x, y'))dy'} = \exp(s_\theta(x, y) + b_\theta(x)) ,
\]

for some function \( s_\theta : X \times Y \rightarrow \mathbb{R} \), which following terminology in [Mnih and Teh 2012] we will refer to as the scoring function. Here, \( b_\theta(x) = -\log \int \exp(s_\theta(x, y'))dy' \) arises from the normalizing constant for each conditional density \( p_\theta(y|x) \).

After the classifier has been learned, conditional density estimates can simply be read off from (9).

At \( y = \) new, \( \hat{s} \) can be written as

\[
\hat{s}(y) = \frac{\exp(s_\theta(x, y) + b_\theta(x))}{\exp(s_\theta(x, y) + b_\theta(x)) + \kappa p_f(y)} = \sigma(s_\theta(x, y) + b_\theta(x) - \log(\kappa p_f(y))) ,
\]

where \( \sigma(t) = 1/(1 + e^{-t}) \) is the logistic function. Eq.(11) gives us the form of the probabilistic classifier we will adopt, where we will need to construct the scoring function \( s_\theta(x, y) \) appropriately, and, in particular, how it relates to the feature maps \( \phi_x \) and \( \phi_y \). While the contribution \( b_\theta(x) \) is directly determined by the choice of \( s_\theta \), computing it will be intractable for any given \( s_\theta \) and we will hence decouple the two, and model \( b_\theta(x) \) as a separate neural network with input \( x \) and its own set of parameters to be learned (collated into the overall parameter set \( \theta \)).

We will map \( x \) and \( y \) using feature maps \( \phi_x : X \rightarrow H_X \) and \( \phi_y : Y \rightarrow H_Y \). In order to facilitate learning of these feature maps, they will be parametrized using neural networks (with both sets of parameters collated into \( \theta \)). Hence, we use finite-dimensional feature maps here, but other choices are possible. Next, we compute the Conditional Mean Embedding Operator (CMEO) \( \hat{C}_{Y|X} : H_X \rightarrow H_Y \) given in (3).

Given \( \hat{C}_{Y|X} \), we can estimate the conditional mean embedding for any new \( x^* \) using

\[
\hat{\mu}_{Y|X=x^*} = \hat{C}_{Y|X} \phi_x(x^*).
\]

Note that \( \hat{\mu}_{Y|X=x^*} \in H_Y \). We can now compute \( \langle \phi_y(y^*), \hat{\mu}_{Y|X=x^*} \rangle_{H_Y} = \hat{\mu}_{Y|X=x^*}(y^*) \) for any new \( y^* \in \mathcal{Y} \). This is an evaluation of the conditional mean embedding at any given new response. We expect this value to be high when \( y^* \) is drawn from the true conditional distribution \( Y|X = x^* \) and low in cases where \( y^* \) is drawn from the fake distribution and falls in a region where the true conditional density \( p(y|x^*) \) is low. This is readily seen from observing that the true CME evaluated at \( y^* \) can be written as

\[
\mu_{Y|X=x^*}(y^*) = \mathbb{E}[k_y(y^*, Y)|X = x^*] = \int k_y(y^*, y)p(y|x^*)dy ,
\]

where \( k_y(y, y') := \langle \phi_y(y), \phi_y(y') \rangle_{H_Y} \). This suggests the following form of the scoring function:

\[
s_\theta(x^*, y^*) = \langle \phi_y(y^*), \hat{\mu}_{Y|X=x^*} \rangle_{H_Y} .
\]

Given a set of true examples \( \{(x_j, y_j)\}_{j=1}^n \) as well as the fake responses \( \{y_{i,j}^f\}_{i=1}^\kappa \) associated to each input \( x_j \), we can now train the classifier using model (11) by maximizing conditional log-likelihood of the True/Fake labels,

\[
\max_\theta \sum_{j=1}^n \left\{ \log P_\theta(\text{True}|y_j, x_j) + \sum_{i=1}^\kappa \log P_\theta(\text{Fake}|y_{i,j}^f, x_j) \right\}
\]

or, equivalently, by minimizing the logistic loss:

\[
\min_\theta \sum_{j=1}^n \left\{ \log \left( 1 + \frac{\kappa p_f(y_j)}{\exp(s_\theta(x_j, y_j) + b_\theta(x_j))} \right) + \sum_{i=1}^\kappa \log \left( 1 + \frac{\exp(s_\theta(x_j, y_{i,j}^f) + b_\theta(x_j))}{\kappa p_f(y_{i,j}^f)} \right) \right\} .
\]

After the classifier has been learned, conditional density estimates can simply be read off from (9). Note that we need to be able to evaluate the fake density pointwise. We will take a closer look at the choices of fake densities in Section 3.3.
We now describe how to train our developed model in the meta-learning setting. Let \( y \) be the set of \( l \) conditional density estimation tasks with \( T_q \) corresponding to the dataset \( D_q = \{(x^q_i, y^q_i)\}_{i=1}^{m_q} \), where \( x^q_i \in \mathcal{X} \) and \( y^q_i \in \mathcal{Y} \) share the same domains across the tasks. We use an approach similar to that of the Neural Process (NP) \cite{Garnelo2018}, where during training we define a context set and a target set. For example, for task \( q \) we use \( m_{cq} \) samples to be context and the remaining \( m_{q} = m_{q} - m_{cq} \) to be target. Conditional mean embedding operator in \( \phi \) will be estimated using the context set, whereas the conditional mean embeddings will be evaluated on the target set, as in Eq. \( 12 \).

Next, for each target example, we sample \( \kappa \) fake samples from \( p_f(y) \) and represent them in \( \mathcal{H}_Y \) using the feature map \( \phi_y \) so that Eq. (11) can be computed for each of these \( \kappa + 1 \) samples \( (1 \text{ true and } \kappa \text{ fakes}) \). By also providing the labels (i.e. True/Fake), we proceed by training the classifier, i.e. learning the parameters \( \theta \) of neural networks \( \phi_x, \phi_y \) and \( b_\theta \) using the objective (16) jointly over all tasks. The resulting feature maps hence generalize across tasks and can be readily applied to a new, previously unseen dataset, where we are simply required to compute the scoring function \( s_\theta(x, y) \) using the conditional mean embedding operator estimated on this new dataset and insert it into Eq. (9).

**Algorithm 1 MetaCDE**

```
1: for \( q = 1, \ldots, l \) do
2:     Estimate the CME \( \tilde{C}_Y|X \) using the context points \( D^q_{\text{context}} \) \( \triangleright \) Eq. (3) 
3:     Generate \( \kappa \) fake samples \( \{y^f_j\}_{j=1}^\kappa \) from the fake distribution \( p_f(y) \)
4:     Evaluate the CME \( \tilde{P}_{Y|X=x^f_j} \) for \( j = 1, \ldots, m_{cq} \) \( \triangleright \) Eq. (12)
5:     Compute feature maps of \( \{y^f_j\} \) as well as \( \{y^f_{ij}\}_{i=1}^\kappa \) using \( \phi_y \) for \( j = 1, \ldots, m_{cq} \)
6:     Optimize the parameters \( \theta \) of neural networks \( \phi_x, \phi_y \) and \( b_\theta \) using SGD and Adam optimizer applied to the logistic loss jointly over all tasks \( \triangleright \) Eq. (16)
7:     Compute the density \( p_\theta(y|x) \) \( \triangleright \) Eq. (9)
```

### 3.3 Choice of the Fake Distribution in NCE

The choice of the fake distribution plays a key role in the learning process here, especially due to the fact that we are interested in conditional densities. In particular, if the fake density is different from the marginal density \( p(y) \), then our model could learn to distinguish between the fake and true samples of \( y \) simply by constructing a “good enough” model of the marginal density \( p(y) \) on a given task while completely ignoring the dependence on \( x \) (this can be achieved by making the feature maps of \( x \) constant). This becomes obvious if, say, the supports of the fake and the true marginal distribution are disjoint, where clearly no information about \( x \) is needed to build a classifier – i.e. the classification problem is “too easy”. Thus, ideally we wish to draw fake samples from the true marginal \( p(y) \) in a given task. While we could achieve this by drawing a \( y \) paired to another \( x \), i.e. from the empirical distribution of pooled \( y_s \) in a given task, recall that we also require existence of a fake density which can be computed pointwise and inserted into Eq. (9). Hence, we propose to use a kernel density estimate (KDE) of \( y_s \) as our fake density in any given task. In particular, kernel density
estimator of \( p(y) \) is computed on all responses \( y \) (context and target). In order to sample from this fake distribution, we simply draw from the empirical distribution of pooled \( y \)s and add Gaussian noise with standard deviation being the bandwidth of the KDE (assuming we are using a Gaussian KDE for simplicity here; other choices of kernel are of course possible with appropriate modification of the type of noise). As our experiments demonstrate, this choice ensures that the fake samples are sufficiently hard to distinguish from the true ones, requiring the model to learn meaningful feature maps which capture the dependence between \( x \) and \( y \) and are informative for the CDE task.

Finally, we note that while in principle it is possible to consider families of fake distributions which also depend on the conditioning variable \( x \), we do not explore this direction here. This is due to the fact that such approach would require a nontrivial construction of a model of fake conditional densities that is easy to sample from, can be computed pointwise, and according to the same rationale as above, shares the same marginal density with the true conditional model we are interested in.

4 Related Work

NCE for learning representations has been considered before and the closest work to our paper is [Mnih and Teh 2012], which focuses on learning discrete distributions in the context of Natural Language Processing (NLP). They achieve impressive speedups over other word embeddings as they avoid having to compute the normalizing constant thanks to the NCE setup of the optimization. More recently, [Van den Oord et al. 2018] also introduce a NCE method for representation learning, however, they focus on learning an expressive representation in the unsupervised setting, thereby optimizing a mutual information objective instead.

Other methods that also use the idea of fake examples in order to learn an expressive feature map are [Zhang et al. 2018], who train a GAN in order to use the resulting discriminator for few-shot classification.

In terms of using RKHSs in density models, several works, for example [Dai et al. 2018], [Arbel and Gretton 2017] have considered training kernel exponential family models, where the main bottleneck is to compute the normalizing constant. [Dai et al. 2018] exploit the flexibility of kernel exponential families to learn conditional densities and avoid the problem of computing normalizing constants by solving so called nested Fenchel duals. [Arbel and Gretton 2017] train kernel exponential family models using score matching criteria, which allows them to bypass normalizing constant computation. The method however requires computing and storing the first- and second order derivatives of the kernel function for each dimension and each sample and as such requires \( O(n^2d^2) \) memory and \( O(n^3d^3) \) time, where \( n \) is the number of data points and \( d \) the dimension of the problem.

[Sugiyama et al. 2010] propose a method of learning the conditional density by learning a ratio of the joint and the marginal. They model the conditional density as a linear combination of a set of basis functions. This method works well on reasonably complicated tasks, although the optimal choice of basis functions is still unclear.

In terms of few-shot learning, the only paper (to the best of our knowledge) that considers CDE is [Dutordoir et al. 2018]. They propose to extend the inputs with additional latent variables and use a GP to project these extended vectors onto samples from the conditional density. Contrary to our method they do not learn a feature map for the output specifically but rather use a multi-ouput GP onto which they stack a probabilistic projection into the original output space.

5 Experiments

5.1 Experiments on Synthetic Data

We first validate our method on a synthetic dataset. In our experimental setup, we wish to measure how well our method can pick up multimodality and heteroscedasticity in the response variable and so we construct datasets with this in mind as follows: we first sample \( y \sim \text{Uniform}(0, 1) \) and then set \( x = \cos(ay_i + b) + \epsilon_i \), where \( a \) and \( b \) vary between tasks, with noise \( \epsilon_i \sim \mathcal{N}(0, \sigma^2) \). Note that in this case \( x \) can be written as a simple function of \( y \) with added noise, but not vice versa on the whole range of \( x \), leading to the multimodality of \( p(y|x) \). Note also that the marginal distribution of \( Y \) is known and hence using uniform fake samples is sufficient in this case. In Figure 1, we compare our method with a number of alternative conditional density estimations methods. These methods
include $\epsilon$-KDE (KDE applied to the $\epsilon$-neighbourhood of $x$), DDE [Dai et al., 2018], KCEF [Arbel and Gretton, 2017], and LSCDE [Sugiyama et al., 2010].

During meta-learning, we use 50 context points and 80 target points for each task. We also fix $\kappa = 10$ as suggested in [Gutmann and Hyvärinen, 2012]. At testing time, we evaluate the method on 100 new tasks with 50 context/training points each. We simply pass the new context points to our model, which can evaluate the density with a simple forward pass as in (8). The non meta-learning baselines are trained on each of the 100 datasets separately. We have included additional experiments with 15 and 30 context points in the Appendix to illustrate the robustness of the methods with varying training data sizes as well as additional information on the neural network architectures.

In the table below we report the mean log-likelihood over the 100 different datasets. The reason for the high variance in some methods stems from the varying difficulty of tasks. We also report the $p$-values of the one-sided signed Wilcoxon test which confirms that the likelihood of our method, MetaCDE, is significantly higher than all the respective methods we compare against. For more experiments and further clarifications, cf. the Appendix, where the high variance is explained using a histogram of differences in likelihood w.r.t. to MetaCDE.

![Image of a figure with red and green dots]

**Figure 1:** In Order (synthetic dataset): MetaCDE (ours), DDE, LSCDE, KCEF, $\epsilon$-KDE

The red dots are the context/training points and the green dots are points from the true density.

| Method      | Mean over 100 log-likelihoods | P-value for Wilcoxon test |
|-------------|-------------------------------|---------------------------|
| MetaCDE     | $197.36 \pm 25.26$           | NA                        |
| DDE         | $162.98 \pm 68.67$           | $< 2.2e-16$               |
| LSCDE       | $44.95 \pm 74.36$           | $< 2.2e-16$               |
| KCEF        | $-388.30 \pm 699.65$        | $< 2.2e-16$               |
| $\epsilon$-KDE | $116.31 \pm 235.80$       | $1.92e-07$                |

Table 1: Average held out log-likelihood on 100 different synthetic cos tasks. We also compute the $p$-value for the one sided signed Wilcoxon test w.r.t to MetaCDE

### 5.2 Experiments on Ramachandran plots for molecules

Finding all energetically favourable conformations for flexible molecular structures in both bound and unbound state is one of the biggest challenge in computational chemistry [Hawkins, 2017] as the number of possibilities increases exponentially with the dimension. Knowledge about the distributions of dihedral angles in molecules (represented using Ramachandran plots [Mardia, 2013]) is used in different sampling schemes and it is currently limited by the library curated by chemists. Here, we attempt to apply MetaCDE in order to learn richer relationships between dihedral angles, which can lead to an improved performance in the molecule sampling scheme.

The data we have used in our experiments was extracted from crystallography database [Gražulis et al., 2011]. The multimodality of the dataset arises from the molecular symmetries such as reflection and rotational symmetry. Namely, when we rotate the molecule around the symmetry axis or reflect along the plane of symmetry, it results in a conformation indistinguishable from the original.

In our experiments we consider the cases where we have 80 data points per task during training and only 20 at testing time. In our meta-learning setup we are going to take 20 context and 60 target points. We again fix $\kappa = 10$ [Gutmann and Hyvärinen, 2012] and evaluate our method using log-likelihood.
on 100 examples for pairs of dihedral angles, which have not been seen during training. As in the previous experiment, we perform a one-sided signed Wilcoxon test to confirm that MetaCDE achieves a significantly higher held-out log-likelihood than other methods.

![Figure 2: In Order (Real dataset): MetaCDE (ours), DDE, LSCDE, KCEF, $\epsilon$-KDE](image)

The red dots are the context/training points and the green dots are points from the true density.

|                      | MetaCDE         | DDE          | LSCDE         | KCEF          | $\epsilon$-KDE |
|----------------------|-----------------|--------------|---------------|----------------|----------------|
| Mean over 100 Log-likelihoods | -297.58 ± 67.63 | -315.49 ± 204.82 | -335.85 ± 192.09 | -396.95 ± 871.97 | -422.99 ± 346.46 |
| P-value for Wilcoxon test | NA              | 4.932e-05    | 2.692e-05    | 1.397e-05      | 9.49e-07       |

Table 2: Average held out log-likelihood on 100 different configurations of molecules. We also compute the p-value for the one sided signed Wilcoxon test w.r.t to MetaCDE.

Further clarifications and illustrations are given in the Appendix. Note that one could take into account that the data itself lies on a torus by simply pre-processing the angles $x$ and $y$ into $[\cos(x), \sin(x)]$ and $[\cos(y), \sin(y)]$, respectively. This is sensible and easily implemented in our method.

5.3 Experiments on NYC taxi data

Lastly, we illustrate our algorithm on the NYC taxi dataset from January 2016 that contains over one million data points\footnote{Data has been taken from: https://www1.nyc.gov/site/tlc/about/tlc-trip-record-data.page}. We are interested in estimating conditional densities $p_{\text{pickup}}(\text{dropoff}|\text{tips})$. Hence, we use different pickup locations as determining our tasks and our goal is to model the dropoff density conditionally on the tip amount. In this case, different tasks will correspond to different pickup locations and hence the conditional density will change accordingly.

At testing time, we give the model 200 datapoints of unseen pickup locations and model the conditional density based on those. In Figure 3, we illustrate one testing case and show how the density evolves as the tip amount increases. The pickup location in Brooklyn (red dot) is not seen by the method. In particular, we see that as the tip amount increases, the trips become more likely to end in Manhattan. We illustrate additional unseen pickup locations in the Appendix as well as additional information on these experiments.

6 Conclusions and Future Work

We introduced a novel method for conditional density estimation in a meta-learning setting. We applied our method to a variety of synthetic and real-world data, with strong performance on an application in computational chemistry and an illustrative example using NYC Taxi data. Owing to the meta-learning framework, experiments indicate that the developed method is able to capture correct density structure even when presented with small sample sizes at testing time. Similarly to the neural process [Garnelo et al., 2018b], our method is able to construct a task embedding. In our case however, embedding of each task takes the form of a conditional mean embedding operator, computed with feature maps learned using noise contrastive estimation. Further study
Figure 3: CDE of the dropoff locations as the tip amount increases. The trips start in Brooklyn (red dot)

could involve other choices of fake distribution $p_f(y)$, including those depending on the conditioning variable. An interesting avenue of applications would be in modelling conditional distributions in the reinforcement learning setting. In particular, [Lyle et al., 2019] and [Bellemare et al., 2017] have shown the benefits of using distributional perspective on reinforcement learning as opposed to only modelling expectations of returns received by the agents.

**Acknowledgements**

We would like to thanks Anthony Caterini, Qinyi Zhang, Emilien Dupont, David Rindt, Robert Hu, Leon Law, Jin Xu, Edwin Fong and Kaspar Martens for helpful discussions and feedback. JFT is supported by the EPSRC and MRC through the OxWaSP CDT programme (EP/L016710/1). YWT and DS are supported in part by Tencent AI Lab and DS is supported in part by the Alan Turing Institute (EP/N510129/1). YWT’s research leading to these results has received funding from the European Research Council under the European Union’s Seventh Framework Programme (FP7/2007-2013) ERC grant agreement no. 617071.
References

Michael Arbel and Arthur Gretton. Kernel conditional exponential family. *arXiv preprint arXiv:1711.05363*, 2017.

Marc G Bellemare, Will Dabney, and Rémi Munos. A distributional perspective on reinforcement learning. In *Proceedings of the 34th International Conference on Machine Learning-Volume 70*, pages 449–458. JMLR. org, 2017.

Bo Dai, Hanjun Dai, Arthur Gretton, Le Song, Dale Schuurmans, and Niao He. Kernel exponential family estimation via doubly dual embedding. *arXiv preprint arXiv:1811.02228*, 2018.

Vincent Dutordoir, Hugh Salimbeni, James Hensman, and Marc Deisenroth. Gaussian process conditional density estimation. In *Advances in Neural Information Processing Systems*, pages 2385–2395, 2018.

Marta Garnelo, Dan Rosenbaum, Chris J Maddison, Tiago Ramalho, David Saxton, Murray Shanahan, Yee Whye Teh, Danilo J Rezende, and SM Eslami. Conditional neural processes. *arXiv preprint arXiv:1807.01613*, 2018a.

Marta Garnelo, Jonathan Schwarz, Dan Rosenbaum, Fabio Viola, Danilo J Rezende, SM Eslami, and Yee Whye Teh. Neural processes. *arXiv preprint arXiv:1807.01622*, 2018b.

Saulius Gražulis, Adriana Daškevič, Andrius Merkys, Daniel Chatteigner, Luca Lutterotti, Miguel Quiros, Nadezhdha R Serebryanaya, Peter Moeck, Robert T Downs, and Armel Le Bail. Crystallography open database (cod): an open-access collection of crystal structures and platform for world-wide collaboration. *Nucleic acids research*, 40(D1):D420–D427, 2011.

Michael U Gutmann and Aapo Hyvärinen. Noise-contrastive estimation of unnormalized statistical models, with applications to natural image statistics. *Journal of Machine Learning Research*, 13(Feb):307–361, 2012.

Paul C. D. Hawkins. Conformation Generation: The State of the Art. *Journal of Chemical Information and Modeling*, 57(8):1747–1756, 2017. doi: 10.1021/acs.jcim.7b00221. URL [https://doi.org/10.1021/acs.jcim.7b00221](https://doi.org/10.1021/acs.jcim.7b00221) PMID: 28682617.

Clare Lyle, Pablo Samuel Castro, and Marc G Bellemare. A comparative analysis of expected and distributional reinforcement learning. *arXiv preprint arXiv:1901.11084*, 2019.

Kanti V. Mardia. Statistical approaches to three key challenges in protein structural bioinformatics. *Journal of the Royal Statistical Society: Series C (Applied Statistics)*, 62(3):487–514, 2013.

Andriy Mnih and Yee Whye Teh. A fast and simple algorithm for training neural probabilistic language models. In *Proceedings of the 29th International Conference on Machine Learning*, pages 1751–1758, 2012.

Krikamol Muandet, Kenji Fukumizu, Bharath Sriperumbudur, Bernhard Schölkopf, et al. Kernel mean embedding of distributions: A review and beyond. *Foundations and Trends® in Machine Learning*, 10(1-2):1–141, 2017.

Le Song, Kenji Fukumizu, and Arthur Gretton. Kernel embeddings of conditional distributions: A unified kernel framework for nonparametric inference in graphical models. *IEEE Signal Processing Magazine*, 30(4):98–111, 2013.

Bharath K. Sriperumbudur, Kenji Fukumizu, and Gert R. G. Lanckriet. Universality, characteristic kernels and rkhs embedding of measures. *J. Mach. Learn. Res.*, 12:2389–2410, July 2011. ISSN 1532-4435.

Masashi Sugiyama, Ichiro Takeuchi, Taiji Suzuki, Takafumi Kanamori, Hirotaka Hachiya, and Daisuke Okanohara. Least-squares conditional density estimation. *IEICE Transactions on Information and Systems*, 93(3):583–594, 2010.

Brian L Trippe and Richard E Turner. Conditional density estimation with bayesian normalising flows. *arXiv preprint arXiv:1802.04908*, 2018.
Aaron Van den Oord, Yazhe Li, and Oriol Vinyals. Representation learning with contrastive predictive coding. *arXiv preprint arXiv:1807.03748*, 2018.

Ruixiang Zhang, Tong Che, Zoubin Ghahramani, Yoshua Bengio, and Yangqiu Song. Metagan: An adversarial approach to few-shot learning. In *Advances in Neural Information Processing Systems*, pages 2365–2374, 2018.
Appendices

A Synthetic dataset setup and further experiments

In this experiment we are given a variable number of context points during testing time ranging from 15, 30 and 50. Each of the non meta learning models DDE, KCEF, ε-KDE, LSCDE are trained on the new datasets. Our MetaCDE is trained with 15, 30 and 50 context points on the tasks respectively and with 80 target points. At testing time, we simply pass the data through our model without having to retrain on the new unseen dataset. Note that we report again the p-values of the Wilcoxon signed one-sided test and we can see that as we decrease the context points, our methods is significantly outperforming the other methods.

A.1 Model specifications

For our MetaCDE we used a 3-hidden layer Neural Network with tanh activation functions and Adam optimizer for all of our feature maps. We cross validate on held out dataset, over 32 and 64 hidden nodes per layer and λ = 1.0, 0.1 for the regularization parameter. We fix the learning rate at 1e-3. We also set κ = 10.

- KCEF: we used the CV function that was built in their Github repository
- LSCDE: We CV for σ in logspace(−3, 5, 20) and λ in logspace(−5, 5, 20)
- ε-KDE: We CV over ε in linspace(0.1, 1, 15) and bandwidth in linspace(0.01, 1, 15)
- DDE: We CV over the bandwidth of 0.5 and 1.0
A.2 Using 50 context points

|               | MetaCDE     | DDE         | LSCDE        | KCEF         | ε-KDE        |
|---------------|-------------|-------------|--------------|--------------|--------------|
| 100 Log-likelihood | 197.36 ± 25.26 | 162.98 ± 68.67 | 44.95 ± 74.36 | -388.30 ± 699.65 | 116.31 ± 235.80 |
| P-value for Wilcoxon test | NA          | 9.681e-06    | <2.2e-16      | <2.2e-16     | 1.92e-07     |

Table 3: Average held out log-likelihood on 100 different synthetic \( \cos \) tasks. We also compute the p-value for the one sided signed Wilcoxon test w.r.t to MetaCDE.

Figure 4: In Order (synthetic dataset): MetaCDE (ours), DDE, LSCDE, KCEF, \( \epsilon \)-KDE
The red dots are the context/training points and the green dots are points from the true density.
Table 4: Average held out log-likelihood on 100 different synthetic \( \cos \) tasks. We also compute the \( p \)-value for the one sided signed Wilcoxon test w.r.t to MetaCDE.

|          | MetaCDE  | DDE      | LSCDE    | KCEF     | \( \epsilon \)-KDE |
|----------|----------|----------|----------|----------|---------------------|
| Log-likelihood | 114.92 ± 17.25 | 64.61 ± 54.33 | -23.02 ± 65.31 | -233.38 ± 528.99 | 29.64 ± 194.51 |
| P-value   | NA       | 4.017e-14 | <2.2e-16 | <2.2e-16 | 1.389e-13 |

A.3 Using 30 context points

Figure 5: In Order (synthetic dataset): MetaCDE (ours), DDE, LSCDE, KCEF, \( \epsilon \)-KDE. The red dots are the context/training points and the green dots are points from the true density.
A.4 Using 15 context points

|                      | MetaCDE   | DDE       | LSCDE     | KCEF      | $\epsilon$-KDE |
|----------------------|-----------|-----------|-----------|-----------|----------------|
| 100 Log-likelihoods  | 46.99 ± 12.24 | 0.58 ± 40.70 | -57.99 ± 59.13 | -142.19 ± 259.59 | -87.80 ± 224.13 |
| P-value for Wilcoxon test | NA       | < 2.2e-16 | < 2.2e-16 | < 2.2e-16 | < 2.2e-16 |

Table 5: Average held out log-likelihood on 100 different synthetic $\cos$ tasks. We also compute the p-value for the one sided signed Wilcoxon test w.r.t to MetaCDE.

Figure 6: In Order (synthetic dataset): MetaCDE (ours), DDE, LSCDE, KCEF, $\epsilon$-KDE
The red dots are the context/training points and the green dots are points from the true density.
A.5 Plotting the histogram of the difference in log-likelihoods

Next we will illustrate why the variance in the log-likelihood estimates are that big. In order to illustrate the idea, we will plot the difference between the log-likelihood of MetaCDE and the other methods including DDE, LSCDE, KCEF, $\epsilon$-KDE.
B Further illustration of the Ramachandran plots

B.1 Additional information on the experimental setup

In this experiment, we look into the Ramachandran plots for molecules. Each plot indicates the energetically stable region of a pair of correlated torsion in the molecule. Specifically, we are interested in estimating the distributions of these correlated dihedral angles. In the experiment, we compute the conditional density for each correlated torsion, given 20 context points at testing time. For our meta-learning training we use 20 context points and 60 targets points.

Note that the data was extracted from crystallography database [Gražulis et al., 2011]. It is possible that some specific pairs of dihedral angles are rarely seen in the dataset. Hence, we may obtain a conditional density with high probability on the region without any observations in some cases. This is reasonable as the database covered only a small part of the chemical space and some potential area could be overlooked. Given that we assume that the support of our conditioning variable $x$ ranges from $[-\pi, \pi)$, we will inevitable also compute conditional distribution on areas where the configurations are not defined and hence the densities in those areas can be safely ignored as a computational biologist would not have queried these configurations in the first place.

B.2 Model specifications

For our MetaCDE we used a 3hidden layer NN with $tanh$ activation functions for all of our feature maps. We cross validate over 32 and 64 hidden nodes per layer and $\lambda = 1.0, 0.1$ for the regularization parameter. We fix the learning rate at $1e^{-3}$. We also set $\kappa = 10$.

- KCEF: we used the CV function that was built in their Github repository
- LSCDE: We CV for $\sigma$ in logspace$(-3, 5, 20)$ and $\lambda$ in logspace$(-5, 5, 20)$
- $\epsilon$-KDE: We CV over $\epsilon$ in linspace$(0.5, 3, 15)$ and bandwidth in linspace$(0.01, 3, 15)$
- DDE: We CV over bandwidth of 0.5 and 1.0
B.3 Additional illustration on the Ramachandran plots

Figure 7: In Order (synthetic dataset): MetaCDE (ours), DDE, LSCDE, KCEF, $\epsilon$-KDE
The red dots are the context/training points and the green dots are points from the true density.
B.4 Plotting the histogram of the difference in log-likelihoods

Next we will illustrate why the variance in the log-likelihood estimates are that big. In order to illustrate the idea, we will plot the difference between the log-likelihood of MetaCDE and the other methods including DDE, LSCDE, KCEF, $\epsilon$-KDE.

B.5 Note on the results

We note that some of the times that the non-meta learning methods do insignificantly better than our method. After investigating the dataset in more detail, we see that the cases where the non meta learning versions are better are cases where the data looks like the plot below. Our proposed method seems to be a lot more conservative on these datasets, by having a higher variance, whereas other methods are able to focus all there mass on those lines. Nevertheless, MetaCDE does recognize that the data follows a line. There lines however are less useful to scientists are they are more interested in more complicated structures. See Figure (8)

Furthermore it looks like our method is not able to always capture the true trend given the limited amount of data. However, it seems to be able to capture some interesting patterns that would be useful to scientist to include in their models. Recently, there has been work done on these Ramachandran plots for Molecules but handcrafting the density maps. Our model would allow us to compute the density maps without prior knowledge.
C Further illustration of the NYC taxi dataset

C.1 Experimental Setup

We have extracted the publicly available dataset from the website\footnote{Data has been taken from: https://www1.nyc.gov/site/tlc/about/tlc-trip-record-data.page}. We have first of all restricted ourselves to dropoff locations in from $-74.1$ to $-73.7$ in longitude and $40.6$ to $40.9$ in latitude. Next we have given our meta learning model 200 datapoints for context during training and 300 for target. At testing time we are presented with 200 context points and are required to compute the conditional density given a tip. Again, we are using a 3-hidden layer NN with 128 nodes and CV over $\lambda = 0.1$ and 1.0. We use the Adam optimizer and fixed the learning rate to $1e^{-3}$. We also set $\kappa = 10$.

C.2 Note on the dataset

In the main text we have seen how the dropoff density changes as we increase the amount of tips. This move of density illustrates well the data itself, as one is more likely to pay higher tips for longer journeys. Below we have plotted the dropoff locations of one specific pickup location colored with the respective tips paid.

Figure 8: Cases where MetaCDE does not seem to perform better than conventional methods
Figure 9: Dropoff locations given a pickup location

Figure 10: CDE of the dropoff locations as the tip amount increases. The trips starts at the red dot

Figure 11: CDE of the dropoff locations as the tip amount increases. The trips starts at the red dot
Figure 12: CDE of the dropoff locations as the tip amount increases. The trips starts at the red dot.

Figure 13: CDE of the dropoff locations as the tip amount increases. The trips starts at the red dot.

Figure 14: CDE of the dropoff locations as the tip amount increases. The trips starts at the red dot.