An implicit function learning approach for parametric modal regression

Yangchen Pan 1  Ehsan Imani 1  Martha White 1  Amir-massoud Farahmand 2

Abstract
For multi-valued functions—such as when the conditional distribution on targets given the inputs is multi-modal—standard regression approaches are not always desirable because they provide the conditional mean. Modal regression aims to instead find the conditional mode, but is restricted to nonparametric approaches. Such methods can be difficult to scale, and cannot benefit from parametric function approximation, like neural networks, which can learn complex relationships between inputs and targets. In this work, we propose a parametric modal regression algorithm, by using the implicit function theorem to develop an objective for learning a joint parameterized function over inputs and targets. We empirically demonstrate on several synthetic problems that our method (i) can learn multi-valued functions and produce the conditional modes, (ii) scales well to high-dimensional inputs and (iii) is even more effective for certain uni-modal problems, particularly for high frequency data where the joint function over inputs and targets can better capture the complex relationship between them. We then demonstrate that our method is practically useful in a real-world modal regression problem. We conclude by showing that our method provides small improvements on two regression datasets that have asymmetric distributions over the targets.

1. Introduction
The goal in regression is to find the relationship between the input (observation) variable \(X \in \mathcal{X}\) and the output (response) \(Y \in \mathcal{Y}\) variable, given samples of \((X, Y)\). The underlying premise is that there exists an unknown underlying function \(g^* : \mathcal{X} \rightarrow \mathcal{Y}\) that maps the input space \(\mathcal{X}\) to the output space \(\mathcal{Y}\). We only observe a noise-contaminated value of that function: sample \((x, y)\) has \(y = g^*(x) + \eta\) for some noise \(\eta\). If the goal is to minimize expected squared error, it is well known that \(E[Y|x]\) is the optimal predictor (Bishop, 2006). It is common to use Generalized Linear Models (Nelder & Wedderburn, 1972), which attempt to estimate \(E[Y|x]\) for different uni-modal distribution choices for \(p(y|x)\), such as Gaussian \((l_2\) regression) and Poisson (Poisson regression). For multi-modal distributions, however, predicting \(E[Y|x]\) may not be desirable, as it may correspond to rarely observed \(y\) that simply fall between two modes. Further, this predictor does not provide any useful information about the multiple modes. Modal regression is designed for this problem, and though not widely used in the general machine learning community, has been actively studied in statistics. Most of the methods are non-parametric, and assume a single mode (Lee, 1989; Lee & Kim, 1998; Kemp & Silva, 2012; Yu & Aristodemou, 2012; Yao & Li, 2014; Lv et al., 2014; Feng et al., 2017). The basic idea is to adjust target values towards their closest empirical conditional modes, based on a kernel density estimator. These methods rely on the chosen kernel and may have issues scaling to high-dimensional data due to issues in computing similarities in high-dimensional spaces. There is some recent work using quantile regression to estimate conditional modes (Ota et al., 2018), and though promising for a parametric approach, is restricted to linear quantile regression.

A parametric approach for modal regression would enable these estimators to benefit from the advances in learning functions with neural networks. The most straightforward way to do so is to learn a mixture distribution, such as with conditional mixture models with parameters learned by a neural network (Powell, 1987; Bishop, 1994; Williams, 1996; Husmeier, 1997; Husmeier & Taylor, 1998; Zen & Senior, 2014; Ellefsen et al., 2019). The conditional modes can typically be extracted from such models. Such a strategy, however, might be trying to solve a harder problem than is strictly needed. The actual goal is to simply identify the conditional modes, without accurately representing the full conditional distribution. Training procedures for the conditional distribution can be more complex. Methods like EM can be slow (Vlassis & Kroese, 1999) and some approaches have opted to avoid this altogether by discretizing the target and learning a discrete distribution (Weigend & Srivastava, 1995; Feindt, 2004). Further, the mixture requires partic-
In this paper, we propose a new parametric modal regression approach, by developing an objective to learn a parameterized function \( f(x, y) \) on both input feature and target/output. We use the Implicit Function Theorem (Munkres, 1991), which states that if we know the input-output relation in the form of an implicit function, then a general multi-valued function, under certain gradient conditions, can locally be converted to a single-valued function. We learn a function \( f(x, y) \) that approximates such local functions, by enforcing the gradient conditions. We empirically demonstrate that our method can effectively learn the conditional modes on several synthetic problems, and that it scales well when the input is made high-dimensional. We also show an interesting benefit that the joint representation learned over \( x \) and \( y \) appears to improve prediction performance even for uni-modal problems, for high frequency functions where the function values change quickly between nearby \( x \). Finally, we demonstrate the utility of our method on real world dataset for both modal regression and regular regression tasks. The proposed approach to multi-valued prediction is flexible, allowing for a variable number of conditional modes to be discovered for each \( x \), and we believe it is a promising direction in parametric modal regression.

2. Problem Setting

We consider a standard learning setting where we observe a dataset of \( n \) samples, \( S = \{(x_i, y_i)\}_{i=1}^n \). Instead of the standard regression problem, however, we tackle the modal regression problem. The goal in modal regression is to find the set of conditional modes

\[
M(x) = \left\{ y : \frac{\partial p(x, y)}{\partial y} = 0, \quad \frac{\partial^2 p(x, y)}{\partial y^2} < 0 \right\}
\]

(1)

\( M(x) \) is in general a multi-valued function. Consider the example in Figure 1. There are two conditional modes for a given \( x \). For example, for \( x = 0 \), the two conditional modes are \( y_1 = -1.0 \) and \( y_2 = 1.0 \).

The standard approaches to find these conditional modes involve learning \( p(y|x) \) or using non-parametric methods to directly estimate the conditional modes. For example, for a conditional Gaussian Mixture Model, a relatively effective approximation of these modes are the means of the conditional Gaussians. More generally, to get precise estimates, non-parametric algorithms are used, like the mean-shift algorithm (Yizong Cheng, 1995). These algorithms attempt to cluster points based on \( x \) and \( y \), to find these conditional modes. We refer readers to (Chen, 2018; Chen et al., 2014) for a detailed review.

Looking at the plot in Figure 1, however, a natural idea is to instead directly learn a parameterized function \( f(x, y) \) that captures the relationship between \( x \) and \( y \). Unfortunately, it is not obvious how to do so, nor how to use \( f(x, y) \) to obtain the conditional modes. In the next section, we develop an approach to learn such a parameterized \( f(x, y) \) by using the implicit function theorem.

3. An implicit function learning approach

In this section, we develop an objective to facilitate learning parametric functions for modal regression. The idea is to directly learn a parameterized function \( f(x, y) \) instead of a function taking only \( x \) as input. The approach allows for a variable number of conditional modes for each \( x \). Further, it allows us to take advantage of general parametric function approximators, like neural networks, to identify these modal manifolds that capture the relationship between the conditional modes and \( x \).

3.1. Implicit Function Learning Objective

Consider learning an \( f(x, y) \) such that \( f(x, y) = 0 \) for all conditional modes and non-zero otherwise. For example, for the Circle problem, \( f(x, y) = x^2 + y^2 - 1 \) for all conditional modes. Such a strategy—finding \( f(x, y) = 0 \) for all conditional modes—is flexible in that it allows for a different number of conditional modes for each \( x \). The difficulty with learning such an \( f \), particularly under noisy data, is constraining it to be zero for conditional modes \( y_j \) and non-zero otherwise. To obtain meaningful conditional modes \( y_1, \ldots, y_m \) for \( x \), the \( y \) around each \( y_j \) should be described by the same mapping \( g_j(x) \). The existence of such \( g_j \) is guaranteed by the Implicit Function Theorem (Munkres, 1991) as described below, under one condition on \( f \).

\textbf{Implicit Function Theorem}: Let \( f : \mathbb{R}^d \times \mathbb{R}^k \rightarrow \mathbb{R}^k \) be a continuously differentiable function. Fix a point \( (x, y) \in \mathbb{R}^d \times \mathbb{R}^k \) such that \( f(x, y) = 0 \), for \( 0 \in \mathbb{R}^k \). If the Jacobian matrix \( J \), where the element in the \( i \)th row and \( j \)th column is \( J_{i,j} = \frac{\partial f(x, y)}{\partial y_j} \), is invertible, then there exists open sets \( U, V \) containing \( (x, y) \) such that there exists a unique
continuously differentiable function \( g : \mathcal{U} \to \mathcal{V} \) satisfying \( g(x) = y \) and \( f(x, g(x)) = 0 \).

Consider the one dimensional case (i.e. \( k = 1 \)). The theorem states that if we know the relationship between independent variable \( x \) and dependent variable \( y \) in the form of implicit function \( f(x, y) = 0 \), then under certain conditions, we can guarantee the existence of some function defined locally to express \( y \) given \( x \). For example, a circle on a two dimensional plane can be expressed as \( \{(x, y) | x^2 + y^2 = 1 \} \), but there is no definite expression (single-valued function) for \( y \) in terms of \( x \). However, given a specific point on the circle \((x_0, y_0) \) \( (y_0 \neq 0) \), there exists an explicit function defined locally around \((x_0, y_0)\) to express \( y \) in terms of \( x \).

Notice that at \( y_0 = 0 \), the condition required by the implicit function theorem is not satisfied: \( \frac{\partial (x^2 + y^2 - 1)}{\partial y} = 2y = 0 \) at \( y_0 = 0 \), and so is not invertible.

Obtaining such smooth local functions \( g \) enables us to find these smooth modal manifolds. The conditional modes \( g_1, \ldots, g_m \) satisfy \( f(x, g_j(x)) = 0 \) and \( \frac{\partial f(x, g_j(x))}{\partial y} \neq 0 \). When training \( f \), we can attempt to satisfy both conditions to ensure existence of the \( g_j \). The gradient condition ensures that for \( y \) locally around \( f(x, g_j(x)) \), we have \( f(x, y) \neq 0 \). This encourages the other requirement that \( f(x, y) \) be non-zero for the \( y \) that are not conditional modes. We therefore pursue this simpler objective, which avoids the complications of negative sampling.

Now we derive the full objective, under stochastic targets. To do so, we make some assumptions on the noise around the conditional modes. We assume that the noise around each conditional mode is Gaussian. More precisely, define

\[
\epsilon(X, Y) \overset{\text{def}}{=} g_j(X) - Y \tag{2}
\]

for \( g_j \), the conditional mode for \( Y \). Our goal is to approximate \( \epsilon(x, y) \) with parameterized function \( f_\theta(x, y) \) for parameters \( \theta \). We assume

\[
\epsilon(X, Y) \sim \mathcal{N}(\mu = 0, \sigma^2) = (2\pi\sigma)^{-k/2} \exp \left( -\frac{\epsilon(X, Y)^2}{2\sigma^2} \right) \tag{3}
\]

For this function, for an observed \((x, y)\), we have

\[
\frac{\partial \epsilon(x, y)}{\partial y} = \frac{\partial g_j(x) - y}{\partial y} = -1. \tag{4}
\]

At the conditional modes, we want to ensure \( \frac{\partial \epsilon(x, y)}{\partial y} \neq 0 \), to satisfy the implicit function condition. Therefore, when learning \( f \), we encourage \( \frac{\partial f(x, y)}{\partial y} = -1 \) for all observed \( y \). Putting this together, our goal is to minimize the negative log likelihood of \( f_\theta \) which approximates a zero-mean Gaussian random variable, under this constraint which we encourage with a quadratic penalty term. This gives the following objective, where the goal is to find \( \arg \min_\theta L(\theta) \):

\[
L(\theta) \overset{\text{def}}{=} \sum_{i=1}^n f_\theta(x_i, y_i)^2 + \left( \frac{\partial f_\theta(x_i, y_i)}{\partial y} + 1 \right)^2 \tag{5}
\]

The same objective is used when doing prediction, but now optimizing over \( y \). Given \( x \), we compute a \( y^* \) in the set \( \arg \min_y f_\theta(x^*, y)^2 + \left( \frac{\partial f_\theta(x^*, y)}{\partial y} + 1 \right)^2 \). These \( y^* \) should correspond to the conditional modes, because the objective should be minimal for conditional modes. In all our experiments, we opted for the simple strategy of searching over 200 evenly spaced values in the range of \( y \).

### 3.2. Theoretical Support for the Objective

At first glance, the above objective does not appear to constrain the number of conditional modes learned. The function \( f_\theta \) could seemingly learn \( f_\theta(x, y) = 0 \) for many of the observed \( y \). The reason this does not occur is because the regularizer encourages parallel lines through conditional modes, which naturally restricts the function to have a small set of solutions to \( \arg \min_y f_\theta(x^*, y)^2 + \left( \frac{\partial f_\theta(x^*, y)}{\partial y} + 1 \right)^2 \).

Consider the following simple example. We compose a training set by uniformly sampling 4000 data points from a circle: \( \{(x, y) | x^2 + y^2 = 1 \} \) and train our implicit function \( f_\theta(x, y) \). Figure 2 shows the function \( f_\theta(x = 0, y) \), \( y \in [-1.2, 1.2] \) after training. The correct target values at \( x = 0 \) should be \(+1\) and \(-1\). The slope of the function around each of these modes is optimally \(-1\), to satisfy the regularizer \( \left( \frac{\partial f_\theta(x^*, y)}{\partial y} + 1 \right)^2 \) which encourages a slope of \(-1\) through all observed \( y \). To have multiple modes, the function does have to pass through 0 through a spurious point, but the slope of the function here violates the regularizer. The function is not penalized in doing so, because it see few (if any) \( y \) in this region and so is free to pick any slope, including the steep positive slope observed in the figure.

![Figure 2](image-url)  
*The trained function \( f_\theta(x = 0, y) \). The blue point is \((0, 0)\); and the other two black points are the predicted points by \( \arg \min_\theta f_\theta(0, y)^2 + \left( \frac{\partial f_\theta(0, y)}{\partial y} + 1 \right)^2 \).*

We formalize this in the following theorem, and then discuss how this theorem motivates that the implicit function
Let $f(x)$ be a continuously differentiable function on the interval $(a,b)$. Let $x_1 < x_2 \in (a,b)$ and $f(x_1) = f(x_2)$ and $f'(x_1)f'(x_2) > 0$ (i.e. the slopes have the same sign and are nonzero). Then there exist $x_0 \in (x_1,x_2)$ such that $f(x_1) = f(x_2) = f(x_0)$ and $f'(x_0)f'(x_1) \leq 0, f'(x_0)f'(x_2) \leq 0$.

**Proof.** Please see Appendix A.1.

**Corollary 1.** Let $f(x)$ be a continuously differentiable function on the interval $(a,b)$. If there are, in total $n > 1$, $n \in \mathbb{Z}$ points: $a < x_1 < ... < x_n < b$ such that $f(x_1) = f(x_2) = ... = f(x_n)$ and they have the same sign of nonzero derivatives, then there must be another $n-1$ points on $(a,b)$ which have an identical function value with $f(x_i), i = 1,...,n$ with different derivative signs.

**Proof.** This is a direct consequence of applying the above Theorem 1 consecutively across $(x_1,x_2), (x_2,x_3)$ etc.

The corollary tells us that if we have two roots for $f(x) = 0$ on the interval $(a,b)$ and the tangent lines on the two points have the same derivative direction, there must be another root between the two with different derivative sign. Consider $f_0(0,y)$ as the function $f(x)$ in the above Theorem 1. We now have $f_0(0,1) = f_0(0,-1)$ and the derivative at $y = \pm 1$ are almost the same (i.e. hence they have the same sign) since we train the parameters such that $\frac{\partial f_0(0,y)}{\partial y}$ is close to $-1$ at any training point. As one can see that, by Theorem 1, there is one root for $f_0(0,y) = 0$ at $y = 0$.

Now, consider that if there is a wrong prediction $y' \in (-1,1)$ but $f_0(0,y')$ is almost zero and $\frac{\partial f_0(0,y)}{\partial y}$ is very close to $-1$—it has the same sign as the other two correct predictions. By our Corollary 1, this indicates that there are another two roots for $f_0(0,y) = 0$ on $(-1,y'),(y',1)$ respectively—which leads to two more waves on the interval $(-1,1)$. It implies that every time the objective gives one more incorrect prediction, the function $f_0(0,y)$ has two more waves. This would result in a high penalty from the optimizer, and unless the training data reflects such a high frequency pattern, it is unlikely to choose to do so.

### 4. Properties of Implicit Function Learning

In this section, we conduct experiments to investigate the properties of our learning objective. First, by using the Circle datasets, we show its utility for dealing with multimodal distribution, particularly compared to modeling the entire distribution with mixture distributions and the classic kernel density estimation approach. Second, we show that our objective does allow us to leverage the representational power of neural networks, by testing it on high-frequency data.

#### 4.1. Comparison on Simple Synthetic Datasets

We compare the learning performance of our algorithm with two modal regression baselines on a single-circle dataset (two modes), double-circle dataset (four modes), and a high dimensional double-circle dataset (four modes with high dimensional input feature). To evaluate prediction performance on test data, we compute the root mean squared error (RMSE) for the predicted value and the closest of the two or four modes values to that prediction.

We compare to Kernel Density Estimation (KDE) and Mixture Density Networks (MDN). KDE is a non-parametric approach to learn a distribution, which has strong theoretical guarantees for representing distributions. It can, however, be quite expensive in terms of both computation and storage. We use KDE, instead of using the mean-shift algorithm, because it is a strictly stronger competitor. MDN (Bishop, 1994) learns a conditional Gaussian mixture, with neural networks, by maximizing likelihood. For both methods, we use a very fine grid search—400 evenly spaced values in the target space—to find a mode given by the KDE distribution or MDN distribution: $\hat{y} = \arg \max_y \hat{p}(y|x)$. For both our algorithm (Implicit) and MDN, we use a two hidden layer neural network ($16 \times 16$ tanh units) and train using stochastic gradient descent with mini-batches of size 128. We optimize both algorithms by sweeping the learning rate from $\{0.1, 0.01, 0.001, 0.0001\}$.

#### 4.1.1. Dataset Description

**Single-circle.** The training set is acquired by uniformly sampling 4000 data points from a circle: $\{ (x, y)| x^2 + y^2 = 1 \}$. Since we add zero mean Gaussian noise with standard deviation $\sigma = 0.1$ to targets, we can interpret the conditional probability distribution $p(y|x)$ as a two-component mixture Gaussian $p(y|x) = 0.5N(y; \sqrt{1-x^2}, \sigma^2) + 0.5N(y; -\sqrt{1-x^2}, \sigma^2)$ as shown in Figure 1.

**Double-circle.** The same number of training points, 4000, are randomly sampled from two circles (i.e. $\{ (x, y)| x^2 + y^2 = 1 \}, \{ (x, y)| x^2 + y^2 = 4 \}$) and the targets are contaminated by the same Gaussian noise as in the single-circle dataset. This is a challenging dataset where $p(y|x)$ can be considered as a piece-wise mixture of Gaussian: there are four components on $x \in (-1,1)$ and two components on $x \in (-2, -1) \cup (1, 2)$. The purpose of using this dataset is to examine how the performances of different algorithms change when we increase the number of modes.

**High dimensional double-circle.** We further increase the difficulty of learning by projecting the one dimensional feature value to 128 dimensional binary feature through tile
coding\footnote{We refer readers to \url{http://www.incompleteideas.net/tiles.html} for more details about tile coding. It is a frequently used feature generation method in reinforcement learning.}: $\phi : [-2, 2] \mapsto \{0, 1\}^{128}$. The purpose of using this dataset is to examine how different algorithms can scale to high dimensional case. Scaling to high dimensionality is a desired property in many practical problems.

### 4.1.2. Empirical Results

The learning curves on the above three datasets are shown in Figure 3. We plot the RMSE as a function of number of mini-batch updates for the two parametric methods MDN and Implicit. KDE is shown as a constant line since it directly uses the whole training set as input. For MDN, we show its performances with a different number of mixture components, which is an important and typically sensitive parameter. With only two components, MDN performs poorly, even when the true number of modes is two; therefore, we include 3, 4 and 6 mixture components. From Figure 3, one can see that: 1) although (a) and (b) have low dimensional feature, MDN with only 3 and 4 components degrades significantly when we increase the number of modes of the training data from two to four. 2) KDE scales poorly with both the number of modes and input feature dimension. We also found that it is quite sensitive to the kernel type and bandwidth parameter. 3) Our algorithm Implicit achieves stable performances across all the datasets and performs the best on the high dimensional double-circle dataset. In contrast, MDN performs poorly even with 6 mixture components for the high dimensional binary features.

In order to verify that our approach indeed provides meaningful predictions, we plot the predictions of our algorithm in Figure 4 on the single-circle dataset. We report both taking the top prediction and the top 4 predictions, when testing 200 values in a grid search. The purpose of showing multiple predictions for each $x$ is to show that our algorithm is capable of predicting multiple modes, instead of a single one, and that it does not easily produce spurious modes. For example, on the interval $[0.2, 0.5]$, Figure 4(b) shows that the algorithm is able to predict both modes while there is no point in the middle, which indicates the two modes are among the 4 predictions we made and the additional 2 predictions are also accurate.

### 4.2. Robustness to high frequency data

The above circle example can be thought of as an extreme case where the underlying true function has extremely high, or even unbounded frequency (i.e. when the input changes a little, there is a sharp change for the true target). In this section, we investigate if our parametric approach to modal regression does provide an advantage to extracting complex interaction between $x$ and $y$. We do so by testing it on a unimodal high-frequency dataset, and comparing the solution found by Implicit it to standard $\ell_2$ regression.

We generate a synthetic dataset by uniformly sampling $x \in [-2.5, 2.5]$ and using the below underlying procedure to compute the targets:

$$
    y = \begin{cases} 
        \sin(8\pi x) + \xi & x \in [-2.5, 0) \\
        \sin(0.5\pi x) + \xi & x \in [0, 2.5] 
    \end{cases}
$$

---

*Figure 3. (a)(b) shows learning curves on single-circle and double-circle datasets respectively. MDN-3 indicates mixture density network trained with 3 components. All results are averaged over 30 random seeds and the shaded area indicates standard error.*

*Figure 4. (a)(b) shows the predictions of our algorithm on the single-circle dataset by making 1 prediction and making 4 predictions for each $x$ respectively.*
where $\xi$ is zero-mean Gaussian noise with variance $\sigma^2$. This function has relatively high frequency when $x \in [-2.5, 0)$ and has a relatively low frequency when $x \in [0, 2.5]$.

**Significance of this artificial dataset.** The dataset is designed to be difficult to learn, because several existing works (Smale & Zhou, 2004; 2005; Jiang, 2019; Pan et al., 2020) indicate that the bandwidth limit of the underlying true function strongly affects the sample efficiency of a learning algorithm. Intuition about why high frequency functions (large bandwidth limit) are difficult to learn can be gained from the Shannon sampling theorem (Zayed, 1993): the sampling rate$^2$ should exceed twice of the maximum frequency of the signal to guarantee perfect signal reconstruction.

**Examining the learning behaviour.** We use $16 \times 16$ hidden tanh units NN for our algorithm. For the $l_2$ regression, we use the same size NN and perform extensive parameter sweep to optimize its performance: activation function type swept over tanh and relu, learning rate swept over $\{0.1, 0.01, 0.001, 0.0001, 0.00001\}$. For both algorithms, we used a mini-batch size of 128. Note the only difference between the two NNs is that Implicit has one more input unit, i.e. the target $y$.

Figure 5(a-c) shows the evaluation curve on testing set for the above two algorithms as the noise variance increases. The learning curve is plotted by evaluating the testing error every 10k number of iterations (i.e. mini-batch updates) averaged over 30 random seeds. We show the testing error on the entire testing set, on high frequency area ($x \leq 0$) and low frequency area ($x \geq 0$) respectively. We run into 1 million iterations to make sure each algorithm is sufficiently trained and both early and late learning behaviour can be examined.

Notice that, trained without observation noise (i.e. $\xi \equiv 0$), our implicit function learning approach achieves a much lower error (at the order of $10^{-2}$) than the $l_2$ regression does (at the order of $10^{-1}$). As noise increases, the targets become less informative and hence our algorithm’s performance decreases to be closer to the $l_2$ regression. Unsurprisingly, for both algorithms, the high frequency area is much more difficult to learn and is a dominant source of the testing error. After sufficient training, our algorithm can finally reduce the error of both the high and low frequency regions to a similar level.

---

$^2$In signal processing, sampling refers to the reduction of a continuous-time signal to discrete time signal. Sampling rate refers to number of samples per second.

---

**Figure 5.** Figure (a)(b)(c) show performances of Implicit (red) and $l_2$ regression L2 (black) objective as we increase the Gaussian noise variance. We show the testing error measured by RMSE on entire testing set (solid line), on high frequency region (i.e. $x \in [-2.5, 0)$, dashed line) and on low frequency region ($x \in [0.0, 2.5]$, dotted line). The results are averaged over 30 random seeds.

---

**Figure 6.** (a) Approximated and true functions. (b) The distance matrix showed in heat map computed by hidden layer representation learned by L2 (left) and Implicit (right) method.
Examining the neural network representation. We further investigate the performance gain of our algorithm by examining the learned NN representation. We plot the predictions in figure 6(a) and the corresponding NN representation through heatmap in figure 6(b). In a trained NN, we consider the output of the second hidden layer as the learned representation, and investigate its property by computing pairwise distances measured by $l_2$ norm between 161 different evenly spaced points on the domain $x \in [-2.5, 2.5]$. That is, a point $(x, x')$ on the heatmap in figure 6(b) denotes the corresponding distance measured by $l_2$ norm between the NN representations of the two points (hence the heatmap shows symmetric pattern w.r.t. the diagonal). For our algorithm, the target input is given by minimizing our implicit learning objective.

The representations provide some insight into why Implicit outperformed the $l_2$ regression. In figure 6(a), the $l_2$ regression fails to learn one part of the space around the interval $[-2.25, -1.1]$. This corresponds to the black area in the heatmap, implying that the $l_2$ distance between NN representations among those points are almost zero. Additionally, one can see that the heatmap of our approach shows a clearly high resolution on the high frequency area and a low resolution on the low frequency area, which coincides with our intuition for a good representation: in the high frequency region, the target value would change a lot when $x$ changes a little, so we expect those points to have finer representations than those in low frequency region. This experiment shows that given the same NN size, our algorithm can better leverage the representation power of the NN.

5. Results on Real World Datasets

In this section, we first conduct a modal regression case study on a real world dataset. Then we show the general utility of our implicit function learning approach on two regression datasets; our method incorporates information from the target space, which should be beneficial even for regular regression tasks. Appendix A.2 includes details for reproducing the experiments and dataset information.

5.1. Modal Regression: Predicting Insurance Cost

To the best of our knowledge, the existing modal regression literature rarely use real world datasets. This is likely because it is difficult to evaluate the predictions from modal regression algorithms. We propose a simple way to construct a dataset from real data that is suitable for testing modal regression algorithms. The idea is to take a dataset with categorical features, that are related to the target, and permute the categorical variables to acquire new target values. Afterwards, we remove those categorical features from the dataset, so that each instance can have multiple possible target values. We construct our dataset using this approach with the Medical Cost Personal Datasets Lantz (2013). We turn it into a modal regression dataset by the following steps.

1. We determined that the “smoker” categorical variable is significantly relevant to the insurance charge. This can be seen from our Boxplot 7(a).
2. An $l_2$ regression model is trained to predict the insurance charges.
3. We flip the “smoker” variable of all examples and query the trained $l_2$ model to acquire a new target for each instance in the dataset.
4. We augment the original dataset with these new generated samples.
5. Remove the “smoker” variable from the dataset to form the modal regression dataset.

Since each instance has two possible targets, and $l_2$ regression can only produce one output, we compute the error between the predicted value and the closest of the two modes. We report both root mean squared error (RMSE) and mean absolute error (MAE). Figure 7(b)(c) shows the learning curves of different algorithms. It can be seen that: 1) $l_2$ regression performs the worst. This suggests the conditional

![Boxplot: smoke v.s. insurance cost](image1)

![RMSE](image2)

![MAE](image3)
We now show the general utility of our algorithm, in that it we consider hidden unit types as meta-parameter and we neural network (NN) (Fallah et al., 2009).

The mean of the Poisson is parameterized by a linear function in term of input feature. We use this algorithm Ordinary linear regression, where the prediction is linear in term of input features. We use this algorithm again slightly outperforms $\ell_2$ regression. One can see from Table 2 that our algorithm achieves slightly better performance.

Next we use the Song year dataset (Bertin-Mahieux et al., 2011), where the task is to predict a song’s release year by using audio features of the song. The dataset has a target distribution that is clearly not Gaussian, though it is not clear which generalized linear model is appropriate. Hence we only include $\ell_2$. One can see from Table 2 that our algorithm again slightly outperforms $\ell_2$ regression.

### 6. Conclusion and Discussion

The paper introduces a parametric modal regression, using a simple but powerful implicit function learning approach. We show that it can handle datasets where the conditional distribution $p(y|x)$ is multimodal, and is particularly useful when the underlying true mapping has a large bandwidth limit. We also illustrate that our algorithm achieves competitive performance on real world datasets for both modal regression and regular regression. An important next step highlighted by this work is to better identify how to evaluate modal regression approaches on real data, including how to determine the number of modes to obtain and how to evaluate them.
References

Abadi, M., Agarwal, A., Barham, P., and et al. TensorFlow: Large-scale machine learning on heterogeneous systems, 2015. Software available from tensorflow.org.

Bertin-Mahieux, T., Ellis, D. P., Whitman, B., and Lamere, P. The million song dataset. In International Conference on Music Information Retrieval, 2011.

Bishop, C. M. Mixture density networks. Technical Report NCRG/94/001, 1994.

Bishop, C. M. Pattern Recognition and Machine Learning. Springer, 2006.

Chen, Y.-C. Modal regression using kernel density estimation: A review. Wiley Interdisciplinary Reviews: Computational Statistics, pp. e1431, 2018.

Chen, Y.-C., Genovese, C. R., Tibshirani, R. J., and Wasserman, L. Nonparametric modal regression. arXiv:1412.1716, 2014.

Ellefsen, K. O., Martin, C. P., and Tørresen, J. How do mixture density rns predict the future? arXiv:1901.07859, 2019.

Fallah, N., Gu, H., Mohammad, K., Seyyedsalehi, S. A., Nourijelyani, K., and Eshraghian, M. R. Nonlinear poisson regression using neural networks: a simulation study. Neural Computing and Applications, 18(8):939, Jul 2009.

Fanaee-T, H. and Gama, J. Event labeling combining ensemble detectors and background knowledge. Progress in Artificial Intelligence, pp. 1–15, 2013.

Feindt, M. A Neural Bayesian Estimator for Conditional Probability Densities. arXiv:0402093, 2004.

Feng, Y., Fan, J., and Suykens, J. A. K. A statistical learning approach to modal regression. 2017.

Glorot, X. and Bengio, Y. Understanding the difficulty of training deep feedforward neural networks. In International Conference on Artificial Intelligence and Statistics, pp. 249–256, 2010.

Husmeier, D. Modelling conditional probability densities with neural networks. 1997.

Husmeier, D. and Taylor, J. G. Neural networks for predicting conditional probability densities: Improved training scheme combining em and rvfl. Neural Networks, 11: 89–116, 1998.

Jiang, H. A new perspective on machine learning: How to do perfect supervised learning. arXiv:1901.02046, 2019.

Kemp, G. C. and Silva, J. S. Regression towards the mode. Journal of Econometrics, 170(1):92 – 101, 2012.

Kingma, D. P. and Ba, J. Adam: A method for stochastic optimization. International Conference on Learning Representations, 2015.

Lantz, B. Machine Learning with R. Packt Publishing, 2013.

Lee, M.-j. Mode regression. Journal of Econometrics, pp. 337–349, 1989.

Lee, M.-J. and Kim, H. Semiparametric econometric estimators for a truncated regression model: a review with an extension. Statistica Neerlandica, 52(2):200–225, 1998.

Lv, Z., Zhu, H., and Yu, K. Robust variable selection for nonlinear models with diverging number of parameters. Statistics & Probability Letters, pp. 90–97, 2014.

Munkres, J. R. Analysis On Manifolds. Boca Raton: CRC Press, 1991.

Nelder, J. A. and Wedderburn, R. W. M. Generalized linear models. Journal of the Royal Statistical Society. Series A (General), pp. 370–384, 1972.

Ota, H., Kato, K., and Hara, S. Quantile regression approach to conditional mode estimation. arXiv:1811.05379, 2018.

Pan, Y., Mei, J., Farahmand, A.-m., and White, M. Frequency-based search-control in dyna. In International Conference on Learning Representations, 2020.

Powell, M. J. D. Algorithms for approximation. chapter Radial Basis Functions for Multivariable Interpolation: A Review, pp. 143–167. Clarendon Press, 1987.

Smale, S. and Zhou, D.-X. Shannon sampling and function reconstruction from point values. Bulletin of The American Mathematical Society, pp. 279–306, 2004.

Smale, S. and Zhou, D.-X. Shannon sampling ii: Connections to learning theory. Applied and Computational Harmonic Analysis, 19(3):285–302, 2005.

Vlassis, N. and Krose, B. Mixture conditional density estimation with the em algorithm. In International Conference on Artificial Neural Networks, pp. 821–825, 1999.

Weigend, A. S. and Srivastava, A. N. Predicting conditional probability distributions: a connectionist approach. International Journal of Neural Systems, 06:109–118, 1995.

Williams, P. M. Using neural networks to model conditional multivariate densities. Neural Computation, 8(4):843–854, 1996.
Yao, W. and Li, L. A new regression model: Modal linear regression. *Scandinavian Journal of Statistics*, 41(3): 656–671, 2014.

Yizong Cheng. Mean shift, mode seeking, and clustering. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 17(8):790–799, 1995.

Yu, K. and Aristodemou, K. Bayesian mode regression. *arXiv:1208.0579*, 2012.

Zayed, A. *Advances in Shannon’s Sampling Theory*. Taylor & Francis, 1993.

Zen, H. and Senior, A. Deep mixture density networks for acoustic modeling in statistical parametric speech synthesis. In *International Conference on Acoustics, Speech and Signal Processing*, pp. 3844–3848, 2014.
A. Appendix

The appendix includes the proof for Theorem 1 in Section A.1, additional experimental results in Section A.3, and all experimental details for reproducible research in Section A.2.

A.1. Proof for Theorem 1

Theorem 1. Let \( f(x) \) be a continuously differentiable function on the interval \((a, b)\). Let \( x_1 < x_2 \in (a, b) \) and \( f(x_1) = f(x_2) \) and \( f'(x_1) f'(x_2) > 0 \) (i.e. the slopes have the same sign and are nonzero). Then \( \exists x_0 \in (x_1, x_2) \) such that \( f(x_1) = f(x_2) = f(x_0) \) and \( f'(x_0) f'(x_1) \leq 0, f'(x_0) f'(x_2) \leq 0 \).

Proof. Part I. We firstly show \( \exists x_0 \in (x_1, x_2) \) such that \( f(x_1) = f(x_2) = f(x_0) \). Without loss of generality, let \( f'(x_1), f'(x_2) < 0 \). The positive case can be proved in exactly the same way. Since \( f'(x_2) < 0 \), one can choose a \( \epsilon_1 \) such that \( 0 < \epsilon_1 < \frac{\epsilon_2 - \epsilon_1}{2} \) and \( f(x_2 - \epsilon_1) > f(x_2) \). Similarly, since \( f'(x_1) < 0 \), one can choose a \( \epsilon_2 \) such that \( 0 < \epsilon_2 < \frac{\epsilon_2 - \epsilon_1}{2} \) and \( f(x_1 + \epsilon_2) < f(x_1) = f(x_2) \). Since the function is a continuously differentiable function, applying intermediate value theorem yields \( \exists x_0 \in [x_1 + \epsilon_2, x_2 - \epsilon_1], s.t. f(x_0) = f(x_1) = f(x_2) \).

Part II. To show the second part \( f'(x_0) f'(x_1) < 0, f'(x_0) f'(x_2) < 0 \), consider the first case where such \( x_0 \) is unique. Then it implies that there exists no other \( x' \in (x_1, x_2), x \neq x_0 \) such that \( f(x') = f(x_1) = f(x_2) = f(x_0) \). We can prove by contradiction. Assume \( f'(x_0) f'(x_1) > 0 \). Then we can replace \( x_1 \) by \( x_0 \) in Part I’s argument, and this gives another \( x_0' \in (x_0, x_2) \subset (x_1, x_2) \) and it contradicts with the prerequisite that \( x_0 \) is unique. Hence, \( f'(x_0) f'(x_1) \leq 0 \).

Consider the case where there are multiple points: \( x_1 < x_0 < x_0' < x_1' < ... < x_2 \) such that \( f(x_0) = f(x_0') = f(x_1) = f(x_2) = f(x_0) \). Then the first case’s result directly applies: one can choose \( x_0', x_1' \), i.e. the first closest point and the second closest point to \( x_1 \); then \( f'(x_0') f'(x_1') \leq 0 \).

The above two parts complete the proof. \( \square \)

A.2. Reproduce experiments in the paper

In this section, we provide additional information about datasets we used and experimental details for reproducing all results in this paper. Our implementation is based on Python 3.3.6. Our deep learning implementation is based on Tensorflow 1.14.0 (Abadi et al., 2015). All of our algorithms are trained by Adam optimizer (Kingma & Ba, 2015) with mini-batch size 128 and all neural networks are initialized by Xavier (Glorot & Bengio, 2010). For our implicit function learning algorithm, we use tanh units for all nodes in neural network.\(^3\) We search over 200 evenly spaced values for prediction except on song year dataset where we use 100. Best parameter settings used to reproduce experiment on each dataset are showed in figure 8. The best parameters are chosen according to the testing error at the end of learning.

A.2.1. Circle and double circle experiment

Circle dataset is generated by uniformly sampling \( x \in [-1, 1] \) first and then \( y = \sqrt{1 - x^2} \) or \( y = -\sqrt{1 - x^2} \) with equal probability. Double circle dataset is generated by uniformly sampling an angle \( \alpha \in [0, 2\pi] \) then use polar expression to compute \( x = r \cos \alpha, y = r \sin \alpha \) where \( r = 1.0 \) or \( r = 2.0 \) with equal probability. High dimensional double dataset is generated by mapping the original \( x \) to \( \{0, 1\}^{128} \) dimensional space. We refer to http://www.incompleteideas.net/tiles.html for tile coding software. The setting of tile coding we used to generate feature is: memory size is 128, 8 tiles and 4 tilings. We keep the neural network size the same as we used in low dimensional case, i.e. 16 \( \times \) 16 tanh units.

For mixture density network (MDN), we use tanh hidden layers and three mixture components on single circle examples, four mixture components on double-circle example. We sweep over learning rate from \{0.01, 0.001, 0.0001\} and the best it chooses is 0.001. The maximization is done by using MLE, the method described in the original paper (Bishop, 1994).

For KDE model, we use the implementation from https://github.com/statsmodels/statsmodels. On the high-dimensional double-circle dataset, we consider the features as categorical. We input the whole training data to build KDE model. We use normal reference rule of thumb for bandwidth selection. We use grid search in the target space to find out the mode. That is, \( \hat{y} = \arg \max_x \hat{p}(y|x) = \arg \max_x \hat{p}(x, y) \) given testing point \( x \). Note that the classic mean-shift algorithm for mode seeking attempts to do hill climbing (i.e. gradient ascent) on a KDE model with multiple initial values, which may still get a local optimum. We opt to directly use a very fine grid search (from 400 evenly spaced values in the target space) to find out the mode given a KDE model.

A.2.2. High frequency data experiment

The dataset is generated by uniformly sampling \( x \in [-2.5, 2.5] \) and then compute targets according to the equa-

\(^3\)Rigorously, to satisfy the assumption that \( f_0(X, Y) \) is Gaussian distributed, linear output unit should be used. However, we observe large error rarely happens. In fact, in our case, it is easy to see that assuming the distribution to be truncated Gaussian (then using tanh is justified) would yield the same optimization objective.
| Algorithms & datasets | Bike sharing | Song year | frequency test, eq(6) | circle/double circle | inverse problem |
|-----------------------|--------------|-----------|-----------------------|---------------------|-----------------|
| L2 regression         | learning rate = 0.0001, 64-by-64 tanh units | learning rate = 0.0001, 64-by-64 tanh units | learning rate=0.01, 16-by-16 tanh units NN | - | - |
| Implicit              | learning rate = 0.0001, 64-by-64 tanh units | learning rate = 0.0001, 64-by-64 tanh units | learning rate = 0.01, 16-by-16 tanh units NN | learning rate = 0.01, 16-by-16 tanh units NN | learning rate = 0.01, 16-by-16 tanh units NN |
| LinearReg             | learning rate = 0.0001 | learning rate = 0.0001 | - | - | - |
| PoissonReg            | learning rate = 0.01 | - | - | - | - |
| NN-Poisson            | learning rate = 0.0001, 64-by-64 tanh units, linear output unit | - | - | - | - |

Figure 8. Best parameter setting for reproducing experiments.

We sweep over \( \{0.1, 0.01, 0.001, 0.0001, 0.00001\} \) to optimize stepsize for both the \( l_2 \) regression and our algorithm, while we additionally sweep over hidden unit and output unit type for the \( l_2 \) regression from \{tanh, relu\}. The best parameter is chosen according to the testing error at the end of training, and the testing error is averaged over 30 runs and at each run, the data is randomly split into training and testing sets. Since the best learning rate chosen by the \( l_2 \) regression is 0.01 when our algorithm chooses 0.001, in figure 9, we also plot the learning curve with learning rate 0.001 to make sure that the performance difference is not due to a slower learning rate of our algorithm.

### A.2.3. Experiments on real world datasets

The Medical Cost Personal Datasets by Lantz (2013) can be downloaded from https://github.com/stedy/Machine-Learning-with-R-datasets/blob/master/insurance.csv. We standardize the age and bmi variables and perform logarithmic transformation for the target variable insurance charge due to its wide range and large values; and hence we actually predict the logarithm of the target variable.

The bike sharing dataset (Fanaee-T & Gama, 2013) (https://archive.ics.uci.edu/ml/datasets/bike+sharing+dataset) and song year dataset (Bertin-Mahieux et al., 2011) (https://archive.ics.uci.edu/ml/datasets/yearpredictionmsd) information are presented in figure 11. Note that the two datasets have very different target distributions as shown in figure 10. On all the three real world dataset, our implicit learning algorithm uses 64 × 64 tanh hidden units and sweep over learning rate from \( \{0.01, 0.001, 0.0001\} \) and find the optimal learning rate as 0.0001. For MDN, we set number of mixture components as 6 and sweep the same range and find the optimal learning rate 0.0001. Note that for all competitors of Implicit, we sweep hidden unit type \{ReLU, tanh\} and find tanh work better. When we report the RMSE/MAE on those real world datasets, we choose the average of the best 5 consecutive evaluation testing errors to report. At each run, we evaluate the testing errors every 10k training steps (i.e. mini-batch updates) and we train each algorithm up to 200k steps.

### A.3. Additional experimental results

In this section, we provide additional experimental results on a classic inverse problem and on the song year dataset.

#### A.3.1. A Classic Inverse Problem

One important type of applications of multi-value function prediction is inverse problem. We now show additional results on a classical inverse function domain as used in (Bishop, 1994). The learning dataset is composed as following.

\[
x = y + 0.3 \sin(2\pi y) + \xi, \quad y \in [0, 1] \quad (7)
\]

where \( \xi \) is a random variable representing noise with uniform distribution \( U(-0.1, 0.1) \). We generate 80k training examples. In Figure 12, we plot the training dataset, and predictions by our implicit function learning algorithm with...
Figure 9. In (a) we repeat the figure shown in previous Section 6.

![Graph showing L2 with learning rate 0.01 and Implicit L2](a) 

![Graph showing L2 with learning rate 0.001 and Implicit L2](b)

Figure 10. Bike sharing targets show a clear Poisson distribution while song year dataset’s target distribution is not intuitive.

(a) Bike sharing dataset target distribution  
(b) Song year dataset target distribution

\[
\text{arg min}_y f_\theta(x, y)^2 + \left( \frac{\partial f_\theta(x, y)}{\partial y} + 1 \right)^2.
\]

We search over 200 evenly spaced \( y \)s in \([0, 1]\) for 200 evenly spaced \( x \in [0, 1] \) to get points in the form of \((x, y)\)s.

### A.3.2. ADDITIONAL RESULT ON SONG YEAR DATASET

Notice that the contributor of song year dataset suggests using the last 51630 as testing set (Bertin-Mahieux et al., 2011), hence we also report this additional result in table 3. The relative performance is actually quite similar to that by random split, except that it has an even lower standard error on testing set (as it is fixed).
### Dataset and preprocessing information

|                       | Number of instances | Train size | Test size | Input feature dimension after preprocessing | Input feature preprocess | Target preprocess |
|-----------------------|---------------------|------------|-----------|-----------------------------------------------|--------------------------|------------------|
| **Bike sharing**      | 17379               | 13903      | 3476      | 114                                           | remove attributes: date, index, year, weather situation 4 and weekday 7; registered, casual; use one-hot encoding for all categorical variables | Scale to [0, 1] except for poisson regression algorithms; scaled back when compute test error |
| **Song Year**         | 515345              | 412276 or 463715 | 103069 or 51630 | 90                                              | standardize to zero-mean unit variance; statistics acquired by using training set | Scale to [0, 1]; scaled back when compute test error |

*Figure 11.* Data preprocessing information.

![Figure 12](image-url)  
(a) Training data  
(b) Implicit

*Figure 12.* Figure (a) shows what the training data looks like. (b) shows the predictions of our implicit learning approach.

*Table 3.* Prediction errors on song year dataset with author suggested train-test split. All numbers are multiplied by $10^2$. The randomness comes from neural network initialization and stochastic mini-batch update.

| Algorithms  | Train RMSE    | Train MAE    | Test RMSE    | Test MAE    |
|-------------|---------------|--------------|--------------|-------------|
| LinearReg   | 959.38(±1.06) | 682.35(±1.2) | 953.08(±0.45) | 681.21(±0.72) |
| L2          | 852.44(±2.27) | 563.65(±2.42)| 892.06(±0.84)| 614.01(±2.16) |
| MDN         | 1032.87(±7.02)| 622.58(±3.48)| 1034.37(±6.76)| 631.92(±3.52) |
| MDN(best 5) | 889.86(±3.68) | 448.48(±2.25)| 891.88(±4.73)| 455.82(±2.68) |
| Implicit    | 862.74(±2.16) | 590.98(±3.13)| 888.72(±0.64)| 458.4(±1.99) |
| Implicit(best 5) | 749.49(±1.86) | 438.9(±2.5) | 774.22(±0.76) | 458.4(±1.99) |