GENERALIZED QUANTILE LOSS FOR DEEP NEURAL NETWORKS

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ABSTRACT

This note presents a simple way to add a count (or quantile) constraint to a regression neural net, such that given $n$ samples in the training set it guarantees that the prediction of $m < n$ samples will be larger than the actual value (the label). Unlike standard quantile regression networks, the presented method can be applied to any loss function and not necessarily to the standard quantile regression loss, which minimizes the mean absolute differences. Since this count constraint has zero gradients almost everywhere, it cannot be optimized using standard gradient descent methods. To overcome this problem, an alternation scheme, which is based on standard neural network optimization procedures, is presented with some theoretical analysis.

1 Introduction

In many applications, it is often required to predict the conditional probability rather than the conditional mean. Among those applications one can find electricity consumption forecasting [1], short term power load forecasting [2] and financial returns [3] to name some.

Perhaps the most known tool for tackling those problems is the quantile regression [4]. While regular least squares minimization estimates the conditional mean, quantile regression estimates the median or any other quantile. Formally, the model parameters are derived by optimizing:

$$\hat{\beta} = \arg\min_{\beta \in \mathbb{R}^d} \left[ (\tau - 1) \sum_{y_i < x_i^T \beta} (y_i - x_i^T \beta) + \tau \sum_{y_i \geq x_i^T \beta} (y_i - x_i^T \beta) \right]$$

(1)

where $\{x_i\}_{i=1}^n \in \mathbb{R}^d$ are the data points, $\{y_i\}_{i=1}^n \in \mathbb{R}$ are the labels, $0 < \tau < 1$ is the desired quantile and $\beta$ are the model parameters to be determined. Recently, it was suggested to optimize the quantile loss using more complex models and to utilize the quantile loss to estimate uncertainty of neural networks [5]. In this case, $x_i^T \beta$ is replaced by some neural network $N(x_i; \Theta)$ with parameters $\Theta$ and Eq. (1) is used as the loss function, usually reformulated a little bit different.

One of the limitations of general quantile-based predictions is that they are ill-posed, since there is an infinite number of possibilities for fitting a curve to pass between the data points in a way that a certain number of points is above the curve and the rest of the points are below the curve. As for the quantile loss of quantile regression, it minimizes the mean of absolute differences. For example, for predicting the conditional probability of the 50% quantile, substituting $\tau = 0.5$ leads to

$$\hat{\Theta} = \arg\min_{\beta \in \mathbb{R}^d} \sum_{i=1}^n |y_i - N(x_i; \Theta)|.$$  

(2)

Eq. (2) is a standard $l_1$ loss function for minimizing the mean absolute differences (MAD). Therefore, it passes a manifold that separates between the dataset, so half of the dataset is above that manifold and half is in, in such a way that the sum of $l_1$ distances between the manifold and the data points will be minimal. Changing the formulation such that the goal
will be to minimize a different loss function (other than $l_1$) subject to a quantile constraint is not straightforward. In this note, we present a computational flow that generalizes the quantile regression for neural networks, such that the loss function can be almost any loss function and yet to be able to add constraint on the quantile of the model.

2 Problem Formulation

Given a regression loss function of a neural network, and a number (or percentile) of samples, the suggested method optimizes the neural net to minimize the loss function such that only a specified fraction of samples will be above the predicted regression value of the neural network. Formally, given $n$ samples, $x_i \in \mathbb{R}^d$, $i = 1, \ldots, n$ with their corresponding values, $y_i \in \mathbb{R}$ and a number $m \leq n$, the algorithm find weights $\Theta$ in order to optimize:

$$
\text{minimize } \mathcal{L}(N(X, \Theta); Y) \\
\text{such that: } \text{count}_i(y_i \geq y_i) = m
$$

(3)

where $N(X; \Theta)$ is the output of the neural network with parameters $\Theta$ given input data $X$. The predicted value is denoted by $\hat{y}$, i.e. $\hat{y} \triangleq N(x_i; \Theta)$. The count function returns the amount of times the condition inside holds and can be defined via the indicator function, i.e.

$$\text{count}_i(a_i > b_i) = \sum_i \mathbf{1}_{a_i > b_i}
$$

One of the challenges Eq. 3 holds is dealing with the count function, which has no gradients and cannot be optimized directly using standard gradient methods. An example that can be given as a special case of Eq. 3 is to minimize the mean-squared-error (MSE) over $n$ samples, such that the error of 10% of the predicted values will be above the real values:

$$
\text{minimize } \sum_{i=1}^{n} (N(x_i; \Theta) - y_i)^2 \\
\text{such that: } \text{count}_i(N(x_i; \Theta) \geq y_i) = 0.1n
$$

Remark 2.1. The accuracy for satisfying the count-constraint is implemented up to some tolerance $\delta$, so that the constraint in Eq. 3 is now $|\text{count}_i(\hat{y}_i \geq y_i) - m| \leq \delta$

$$
\text{minimize } f(N(X; \Theta), Y) \\
\text{such that: } |\text{count}_i(\hat{y}_i \geq y_i) - m| \leq \delta
$$

2.1 Description of the Algorithm

The algorithm consists of optimizing Eq. 3 using alternations. The alternations can be viewed as a non-linear and non-orthogonal projection operators. The first type of alternation moves from the current weights $\Theta$ to the closest set of weights $\hat{\Theta}$ which is a local minima of the loss function. This operator is denoted by $\mathcal{P}_\mathcal{M}$.

Definition 2.1. Given a training dataset $X$, a neural net $N(\Theta, X)$ with weights $\Theta$ and a loss function $\mathcal{L}(\Theta, X; Y)$ with a set of local minima $\mathcal{M}$, then $\mathcal{P}_\mathcal{M}\Theta$ returns weights that are the nearest local minimum:

$$\mathcal{P}_\mathcal{M}\Theta = \underset{\mathcal{L}(N(\Theta, X); Y) \in \mathcal{M}}{\text{argmin}} \|\Theta - \hat{\Theta}\|_2
$$

(4)

Definition 2.2. Let $\mathcal{C}$ be the set of all possible weights of a loss function $\mathcal{L}(N(\Theta, X); Y)$, such that the predictions of the neural net, $\{\hat{y}_i\}_{i=1}^{n}$, will be above the real values $\{y_i\}_{i=1}^{n}$ for $m$ points in the training dataset, up to tolerance $\delta$. Formally:

$$\mathcal{C} = \left\{ \Theta \mid |\text{count}_i(N(\Theta, x_i) \geq y_i) - m| \leq \delta \right\}
$$

(5)

Definition 2.3. Given a training dataset $X$, a neural net $N(\Theta, X)$ with weights $\Theta$ and a set of valid count-constraint points $\mathcal{C}$ (Def. 2.2), then $\mathcal{P}_C(\Theta)$ returns the closest weights in $\mathcal{C}$:
\[ \mathcal{P}_C(\Theta) = \arg\min_{\Theta \in \mathcal{C}} \|\Theta - \hat{\Theta}\|_2 \]  

(6)

**Remark 2.2.** Note that \( \mathcal{P}_C \) does not depend on the loss function \( \mathcal{L} \)

Both \( \mathcal{P}_C \) and \( \mathcal{P}_M \) are implemented using stochastic gradient optimizers (specifically, in this paper Adam optimizer was used). The implementation of \( \mathcal{P}_M \) is a standard neural network optimization. \( \mathcal{P}_C \) is implemented by drifting iteratively from the current point \( \Theta \) to a valid point \( \mathcal{P}_C\Theta \in \mathcal{C} \), such that if \( \text{count}_i(\hat{y}_i > y_i) \) is too large, \( \Theta \) is moved against the direction of the gradient of \( \mathcal{N}(\hat{\Theta}, X) \) to reduce the count value or with the direction of the gradient to increase the count function, if the count value is too small.

In practice, implementation of the above operators such that they return the nearest minimum is impossible in general, since it depends on the data, the architecture of the network and the loss function, which is typically a high-dimensional non-convex manifold. However, since the operators are implemented using stochastic gradient descent (or other optimizers), it is likely to assume that the weights returned by the operators are close (probably among the closest) to the point the operator started from.

Optimizing the loss function subject to a count constraint, can be done by the following alternating scheme, which is approximately implemented by Algorithm 1

\[
\Theta^M_i \leftarrow \mathcal{P}_M\Theta^C_i
\]

(7)

\[
\Theta^C_{i+1} \leftarrow \mathcal{P}_C\Theta^M_i
\]

(8)

where \( \Theta^C_0 \) is an arbitrary starting point (random initialization of the weights).

**Algorithm 1** Satisfy count constraint, implementation of \( \mathcal{P}_C \) operator

**Require:** \( \mathcal{N}(\Theta, X) \) - neural network, \( \Theta \) - current network weights, \( \mathbf{Y} = \{y_1, \ldots, y_n\} \in \mathbb{R} \) - labels, \( \mathbf{X} = \{x_1, \ldots, x_n\} \in \mathbb{R}^d \) - Input data, \( m \) - Number of samples to satisfy count constraint, \( \delta \) - Tolerance for the count error, \( \mu \) - Learning rate, MaxIter - Maximal number of iterations.

**Ensure:** \( \hat{\Theta} \) - optimized network weights

1: \( i \leftarrow 0 \)
2: \( \hat{\mathbf{Y}} \leftarrow \mathcal{N}(\Theta, X) \) # Compute predicted labels
3: \( \hat{m} \leftarrow \text{count}_i(\hat{y}_i > y_i) \)
4: while \( (|\hat{m} - m| > \delta) \) AND \( (i < \text{MaxIter}) \) do
5: \( \text{if } \hat{m} > m \text{ then} \) # Not enough samples passed, increase value
6: \( L \leftarrow -\frac{1}{n} \sum_{i=1}^{m} \hat{y}_i \)
7: else
8: \( L \leftarrow -\frac{1}{n} \sum_{i=1}^{n} \hat{y}_i \)
9: \( \Theta \leftarrow \Theta - \mu \nabla \Theta L \) # Optimize over batch
10: \( i \leftarrow i + 1 \)
11: return \( \hat{\Theta} \)

**Proposition 2.1.** Let \( \Theta^C \) and \( \Theta^M \) \((i \geq 1)\) be a set of points (weights) obtained by a consecutive application of the alternation scheme (Eqs. 7 and 8), then the series \( \|\Theta^C_i - \Theta^M_i\| \) converges.

**Proof.** Since \( i \geq 1 \), then according to Eq. 8, \( \Theta^C_i \in \mathcal{C} \) (Def. 2.2). By the definition of \( \mathcal{P}_M \), \( \Theta^M_i \) is the closest local minima to \( \Theta^C_i \) and by the definition of \( \mathcal{P}_C \), \( \Theta^C_{i+1} \) is the closest valid count-constraint point to \( \Theta^M_i \). Since \( \Theta^C_i \in \mathcal{C} \) and \( \Theta^C_{i+1} \in \mathcal{C} \) is the closest point to \( \Theta^M_i \)

\[
\|\Theta^M_i - \Theta^C_i\| \leq \|\Theta^M_i - \Theta^C_{i+1}\|. 
\]

(9)

By the definition of \( \mathcal{P}_M \), \( \Theta^M_{i+1} \in \mathcal{M} \) is the closest local minima to \( \Theta^C_{i+1} \). Since \( \Theta^M_i \in \mathcal{M} \)

\[
\|\Theta^C_{i+1} - \Theta^M_i\| \leq \|\Theta^M_i - \Theta^C_{i+1}\| 
\]

(10)

Combining Eqs. 8 and 10 gives

\[
\|\Theta^M_{i+1} - \Theta^C_{i+1}\| \leq \|\Theta^M_i - \Theta^C_i\|. 
\]

Since \( \|\Theta^M_i - \Theta^C_i\| \) is monotonically decreasing and bounded it converges, which completes the proof. □
Proposition 2.1 states that the distance between a valid count-constraint point and a local minima point is monotonically decreasing and eventually converges. An interesting observation from the proposition is that it tells us where to look for the next minima/valid count-constraint point, which enables to decrease the step size of the SGD proportionally to the distance between the two points. The proposition is illustrated in Fig. 1.

Additionally, the following observations infer directly from Proposition 2.1:

- Since the distance between a valid count-constraint point and a local minimum converges, then eventually it means (excluding pathological cases of points having exactly the same distance) that the algorithm iterates between one local minimum and one valid count-constraint point. Therefore, it converges to a specific local minimum/count-constraint point.

- The difference in model’s performance between those two points, depends on the distance and the Lipschitz constant of the neural network [6]. So if the distance is small (and hopefully the Lipschitz constant), then stopping in count-constraint point or in a local minimum should not make a big difference.

3 Results

3.1 Motorcycle Dataset

In this subsection, the algorithm was applied to the motorcycle dataset [7] to minimize the MSE over several percentiles: 25%, 40% and 60%. The neural network is a simple two layers fully connected layers, the first hidden layer has 50 neurons with tanh activation function, following by a layer with 10 neurons followed by a ReLU activation function.

| % Above Data | RMSE |
|--------------|------|
| 10%          | 29.8 |
| 25%          | 25.1 |
| 75%          | 23.22|
| 90%          | 31.6 |

Table 1: RMSE Error of the curves from Figure 2 with respect the real data

Table 1 shows the error between the model and the real data, i.e. RMSE = \( \sqrt{\frac{1}{n} \sum_{i=1}^{n} (\hat{y}_i - y_i)^2} \)
Figure 2: A variety of curves that minimizes the MSE under different quantile constraints, and regular least squares minimization.

4 Conclusion

This note presented an algorithm that trains a neural network to minimize a general loss function under quantile constraint, which is difficult to implement straightforward since it has no gradients. The note presented the formulation of the problem, an algorithmic description and some theoretical analysis of why the method converges. Finally, we presented results on a small toy dataset, demonstrating the performance of the algorithm.

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