ReLUs Regression: Complexity, Exact and Approximation Algorithms

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Abstract

Solving ReLUs regression problems is similar to training a neural network with one node with ReLU activation function, which aims to fit a model where the response is related to the linear combination of input feature variables. We study the ReLU regression problem from the algorithmic complexity perspective. We show that the ReLU regression is NP-hard in general, and when the number of features \( p \) is fixed, there exists an algorithm that achieves the global optimal solution in \( O(n^p) \) running time. We also present an integer programming (IP) framework which can produce dual bounds and feasible upper bounds. Moreover, we present a polynomial-time iterative \( n \)-Approximation Algorithm, which performs well in practice as demonstrated by numerical studies and can be numerically more stable than IP solutions.

1 Introduction

Non-linear regression with a non-convex function has attracted many interests recently (see, e.g., [15, 10]), since they are highly relevant in machine learning problems. However, the theoretical properties of these problems are not well understood due to their non-convex nature.

We study a special form of a non-linear regression problem, which we call the ReLU regression. Such a problem is a basis for logistic regression, sparse logistic regression, and learning a perceptron with noise, which is a building block of a feedforward neural network [12]. Studying such the ReLU regression problem can also provide insight into more complex neural networks. Given \( n \) data points \((X_1, Y_1, t_1), \ldots, (X_n, Y_n, t_n) \in \mathbb{R}^p \times \mathbb{R} \times \mathbb{R} \), for \( i = 1, \ldots, n \), let \( X_i \) be the \( i^{th} \) input variable (each \( X_i \) has \( p \) features), \( Y_i \) be the \( i^{th} \) response variable, and \( t_i \) be the \( i^{th} \) threshold such that \( t_i < Y_i \). Let \( X = (X_1, \ldots, X_n) \in \mathbb{R}^{p \times n} \), let \( Y = (Y_1, \ldots, Y_n)^\top \in \mathbb{R}^{n \times 1} \), and let \( t = (t_1, \ldots, t_n)^\top \in \mathbb{R}^{n \times 1} \) be a vector that contains all threshold. The ReLU regression problem is defined as follows:

\[
\min_{\beta \in \mathbb{R}^p} \| \max\{t, X^\top \beta\} - Y \|_2^2
\]

(ReLU-Regression)
where \( \max \{ t, X^\top \beta \} = (\max \{ t_i, X_i^\top \beta \})_{i=1}^p \in \mathbb{R}^{n \times 1} \). We call it the ReLU Regression problem due to activation function \( \max \{ 0, x \} \), a.k.a., the Rectified linear unit (ReLU) [7].

In machine learning applications, ReLU regression or similar problems involving ReLU functions are usually solved by gradient descent or stochastic gradient descent (see, e.g., [11]). However, gradient descent usually converges slowly, and may not converge to good solutions (although it has been shown that adding random perturbation to gradient direction may help avoid trapping in local solutions). The fundamental question about the algorithmic complexity of ReLU regression (or similar problems) has not been fully addressed.

In this paper, we aim to provide answers to the fundamental question of the algorithmic complexity of ReLU regression. Our contributions include the following. (1) We show that ReLU regression is NP-hard in general. When the number of features \( p \) is fixed, there exists an algorithm that achieves the global optimal solution in \( O(n^p) \) running time. (2) We also present an integer programming (IP) framework, which can produce dual bounds and feasible upper bounds. (3) Moreover, since such a problem is non-convex and combinatoric in nature, finding an efficient approximation algorithm with performance guarantee is important; thus, we present a polynomial-time iterative \( n \)-Approximation Algorithm. Our numerical examples demonstrate that the approximation algorithm performs well in practice and can be numerically more stable than IP solutions.

Literature. Non-linear regression with known non-linear transform has been studied in [15], since in [15] the function is monotonic for their main result to hold; however, the ReLU function we considered here is clearly non-monotonic, and the inverse function does not exist (therefore the analysis in [15] cannot carry through in our case, and the results therein do not apply). Moreover, the gradient-descent like methods are unlikely to have any guarantees (e.g., approximation ratio) in [9] for the general ReLU regression because of its non-convex objective function. The non-linear regression problem has also been studied in [10] as an instance of the non-convex \( M \)-estimator and the landscape properties are studied there, which sheds a different statistical perspective from our algorithmic results here. Compared with (sub-)gradient descent methods and their stochastic versions (see, e.g., [11]), our approximation algorithm can be viewed nearly as a second-order method, which is guaranteed to terminate in a finite number of iterations.

2 Main Theoretical Results

From a computational perspective, the first question to ask is the following: What is the computational complexity of finding an exact solution to the ReLU regression? We can prove that:

**Theorem 1.** ReLU Regression is NP-hard.

We note that there are limited results for NP-hardness of training NNs with ReLU activation function: [4, 8, 3]. Another line of research in understanding the hardness of training ReLU neural networks assumes that data is coming from some distribution [13, 14].

However, the techniques used here are significantly different. To prove Theorem 1, we show that \texttt{ReLU-Regression} is at least as difficult to solve as the so-called \textit{subset sum problem}, which is known to be NP-complete. Details of the proof can be found in Section 4.1.

In view of Theorem 1, we further ask the following important questions:

1. \textit{Fixed parameter tractability}: Are there conditions under which we can solve \texttt{ReLU-Regression} exactly in polynomial time?
2. **Approximation algorithm**: Are there polynomial time algorithms that produce solutions which have performance guarantees?

3. **Greedy heuristics**: Are there reasonable heuristics to explore that produce good solutions in practice for ReLU-Regression?

4. **Integer program**: In view of its discrete optimization nature, can we reformulate ReLU-Regression as an integer programming problem, and solve using standard black-box solvers such as [2]?

In the following sub-sections, we address each of the questions.

### 2.1 Fixed parameter tractability

We show that although the ReLU-Regression problem is NP-hard, a strong polynomial time algorithm can be obtained, for a fixed number of features $p$. Note that the ReLU-Regression problem can be represented as the following two-phase optimization problem:

$$\min_{\beta \in \mathbb{R}^p} \left\| \max\{t, X^\top \beta\} - Y \right\|_2^2$$

$$= \min_{I \subseteq [n]} \min_{\beta \in P(I)} \sum_{i \in I} (X_i^\top \beta - Y_i)^2 + \sum_{i \in I^C} (t_i - Y_i)^2$$

where

$$P(I) \triangleq \{ \beta \in \mathbb{R}^p : X_i^\top \beta \geq t_i, i \in I; X_i^\top \beta \leq t_i, i \in I^C \}$$

is the set of feasible region of $\beta$ for a given $I$. Given any $I \subseteq [n]$, if $P(I) \neq \emptyset$, let

$$z^*(I) \triangleq \min_{\beta \in P(I)} \sum_{i \in I} (X_i^\top \beta - Y_i)^2 + \sum_{i \in I^C} (t_i - Y_i)^2$$

be the minimum value of inner optimization problem. An important observation is that: Given index set $I \subseteq [n]$, the inner optimization problem

$$\min_{\beta \in P(I)} \sum_{i \in I} (X_i^\top \beta - Y_i)^2 + \sum_{i \in I^C} (t_i - Y_i)^2$$

is convex. Then the only challenge in solving ReLU-Regression problem is to find the optimal set of indices $I$. A natural idea is to check every non-empty set $P(I)$ and find the minimum solution of all non-empty $P(I)$. Thus, we need to count the number of non-empty set $P(I)$. A trivial upper bound of the number of possible set $I \subseteq [n]$ is $2^n$, which is exponential in the number of samples. However, the good news is that we can prove:

**Claim 1.** The number of nonempty distinct $P(I)$ set is polynomial in the number of samples, given a fixed number of features $p$.

As a consequence of the above Claim, we obtain the following result:

**Theorem 2.** If the number of features $p$ is fixed, then ReLU Regression can be solved in polynomial time. See Algorithm [7].

Similar proof techniques have been used recently in the context of Deep neural nets [1, 3]. See Section 4.2 for details of the proof to Theorem 2.
Algorithm 1: Exact Algorithm

1: **Input**: Sample data matrix $X \in \mathbb{R}^{p \times n}$, response vector $Y \in \mathbb{R}^n$, threshold vector $t \in \mathbb{R}^n$.
2: **Output**: A global optimal solution $\beta^*$ to the ReLU-Regression problem.
3: **function** Exact Algorithm($X, Y, t$)
4: Set $H_i \leftarrow \{\beta : X_i^\top \beta = t_i\}$ for $i = 1, \ldots, m$.
5: Generate arrangements of the hyperplanes $\mathcal{A}(H_1, \ldots, H_n) = \{C_1, \ldots, C_m\}$ with $m \leq O(n^p)$.
6: for $i = 1, \ldots, m$ do
7: Solve a convex program $z^*(I_{C_i})$.
8: return The optimal solution $\beta^*$.

2.2 Approximation Algorithm

When $p \geq 3$ and $n \gg p$, the algorithm in Theorem 2 is not tractable in practice. Thus it is natural to consider an efficient Approximation Algorithm, which we describe in the following.

Let

$$f_I^\sigma(\beta) \triangleq \sum_{i \in I} (X_i^\top \beta - Y_i)^2 + \sum_{i \in I^C} \sigma(X_i^\top \beta, t_i, Y_i),$$

where the auxiliary function $\sigma : \mathbb{R}^3 \rightarrow \mathbb{R}$ is defined as

$$\sigma(x, t, y) = \begin{cases} (x - y)^2 & \text{if } x \geq 2y - t \\ (t - y)^2 & \text{if } x \leq 2y - t \end{cases}$$

which is a convex approximation and upper bound of $(\max\{t, x\} - y)^2$ such that $\sigma(x, t, y) - (\max\{t, x\} - y)^2 > 0$ if and only if $x \in (t, 2y - t)$. See Figure 1 for an example. The term $\sigma(x, t, y)$ can be equivalently represented by letting $\sigma(x, t, y) = (y - t + v)^2$ where $x = u + v$ with $u \leq 2y - t$ and $0 \leq v$.

![Auxiliary convex upper approximation: $\sigma(x)$](image)

Figure 1: Function $\sigma(x, t, y)$ with $t = 1, y = 2$

It is easy to show the following property:

**Proposition 1.** $z^\sigma(I) \triangleq \min_\beta f_I^\sigma(\beta) \leq z^*(I)$. 

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Proposition 1 holds, since we can remove the restriction of $\beta \in P(I)$ in the left-hand-side of the above inequality.

Intuition for the Approximation Algorithm is the following. Suppose $\beta^*$ is the optimal solution to a regular regression problem, i.e.,

$$\beta^* \in \arg \min \|X^T \beta - Y\|_2^2$$

and

$$t_i < X^T \beta^*_i$$

for all $i \in \{1, \ldots, n\}$. Then $\beta^*$ is the optimal solution of ReLU-Regression. Therefore, if $t_i \ll Y_i$ for some $i$, then we expect that an optimal solution $\hat{\beta}$ of ReLU-Regression will satisfy $t_i < X^T \hat{\beta}$, i.e., $i \in I^*$.

With this intuition, we develop Algorithm 2:

**Algorithm 2 Approximation Algorithm**

1: **Input**: Sample data matrix $X \in \mathbb{R}^{p \times n}$, response vector $Y \in \mathbb{R}^n$, threshold vector $t \in \mathbb{R}^n$, where we assume (without loss of generality): $Y_1 - t_1 \leq Y_2 - t_2 \leq \cdots \leq Y_n - t_n$.
2: **Output**: A feasible solution $\beta$ for the ReLU-Regression problem.
3: **function** APPROXIMATION ALGORITHM($X,Y,t$)
   4:   **for** $t = 1, \ldots, n + 1$ **do**
   5:     Set $I_t \leftarrow \{t, \ldots, n\}$ when $t \leq n$, and set $I_{t} \leftarrow \emptyset$ when $t = n + 1$.
   6:     Set $\beta^t \leftarrow \arg \min_\beta f^\sigma_{I_t}$.
   7:     Set $t_{\text{approx}} \leftarrow \arg \min_{t \in [n+1]} z^\sigma(I_t)$.
   8: **return** $\beta^t_{\text{approx}}$.

It is clear that we have to sort the values of $Y_i - t_i$'s and then solve $n + 1$ convex optimization problems in running Algorithm 2. Thus, Algorithm 2 is a polynomial-time algorithm. We can prove the following performance guarantee for the quality of solution produced by the Approximation Algorithm:

**Theorem 3.** Algorithm 2 is an $n$-Approximation Algorithm, i.e., if $z_{\text{approx}}$ is the objective function value of the $\beta$ returned by the algorithm, and $z_{\text{opt}}$ of ReLU-Regression then:

$$z_{\text{opt}} \leq z_{\text{approx}} \leq nz_{\text{opt}}.$$  

Proof of Theorem 3 can be found in Section 4.3.

### 2.3 Greedy Heuristic

Now we present a greedy heuristics for ReLU-Regression

**Definition 1.** Given any $\beta$, let $I(\beta) \triangleq \{i \mid 2Y_i - t_i \geq X_i^T \beta > t_i\}$.

We can prove the following simple result, which will define an improving step in our heuristic algorithm.

**Proposition 2.** Given $I \subseteq \{1, \ldots, n\}$, let $\beta_I \in \arg \min_\beta f^\sigma_{I}$. Then

$$z^\sigma(I(\beta_I)) \leq z^\sigma(I).$$
Proposition 2 is core to developing an improving step: initializing with an \( I \), we obtain \( I(\beta_I) \) and set this as the new \( I \). Then repeat until \( I = I(\beta_I) \). Now there remain two questions: (1) How should we initialize the algorithm and (2) Will the algorithm terminate in a finite number of iterations. We choose to initialize the algorithm using the solution to a regular regression (i.e., using the least-square solution). This ensures that we can obtain solutions that are least as good as the least square solutions.

Algorithm 3 Greedy Heuristic

1: **Input**: Sample data matrix \( X \in \mathbb{R}^{p \times n} \), response vector \( Y \in \mathbb{R}^n \), threshold vector \( t \in \mathbb{R}^n \).
2: **Output**: A feasible solution \( \beta \) for the ReLU-Regression problem.
3: **function** \text{Greedy Heuristic}(X, Y, t, I_0)
4: Initialize the index set \( I_0 \leftarrow \{i \in [n]: X_i^\top \beta_0 > t_i\} \) where \( \beta_0 \leftarrow \arg \min_\beta \|X_i^\top \beta - Y_i\|_2^2 \).
5: while \( I_{t+1} \neq I_t \) do
6: Set \( \hat{\beta} \leftarrow \arg \min_\beta f_{\sigma_{I_t}}(\beta) \).
7: Set \( I_{t+1} \leftarrow \{i \in [n]: X_i^\top \hat{\beta} > t_i\} \).
8: return \( \beta_\text{fix} \leftarrow \hat{\beta} \).

We can also prove that

**Theorem 4.** Algorithm 3 terminates in finite number of iterations.

Proofs to Proposition 2 and Theorem 4 can be found in Section 4.4.

2.4 Integer Programming Formulation

We now show that ReLU-Regression can be cast as an integer programming (IP) problem. By solving the IP, the dual lower bounds and the upper bounds (based on feasible solutions) can be obtained. Notice that solving integer programming exactly may take an exponential running time. However, in numerical experiment, we found it sometime suffices to stop in a fixed number of iterations. However, this may leads to lower accuracy for the IP solution; an Approximation Algorithm that we will present in the next section can sometimes obtain better empirical results.

A key requirement of developing an integer programming formulation is to be able to bound all the \( \beta \) variables. To achieve this, we prove the following structural result regarding optimal solutions of ReLU-Regression.

**Theorem 5.** Let \( \beta^* \) be a global optimal solution to ReLU-Regression problem. Let \( I_+ \triangleq \{i : X_i^\top \beta^* > t_i\} \). Using the singular value decomposition, we obtain \( X_{I_+} = U_{I_+} \Sigma_{I_+} V_{I_+}^\top \in \mathbb{R}^{|I_+| \times p} \) where \( U_{I_+} \in \mathbb{R}^{|I_+| \times |I_+|} \) is unitary, \( \Sigma_{I_+} \) is diagonal, and \( V_{I_+} \in \mathbb{R}^{p \times p} \) is unitary. Let \( \beta' = (X_{I_+} X_{I_+}^\top)^\dagger X_{I_+} Y_{I_+} \in \arg \min_\beta \|X_{I_+}^\top \beta - Y_{I_+}\|_2^2 \). then \( \beta' \) is an optimal solution to ReLU-Regression.

In particular, Theorem 5 says that there exists an optimal solution to ReLU-Regression which is exactly the solution to the regular regression, on a subset of the rows of \( X \) and \( Y \). Since we can bound the size of optimal solutions of regular regression, we can bound the size of at least one optimal solution to ReLU-Regression. Now we develop the following integer programming formulation. For each \( i \in [n] \), let \( X_i^\top \beta = u_i + v_i \), where \( u_i \triangleq \min\{t_i, X_i^\top \beta\} \leq t_i \) and \( v_i \triangleq \ldots \)

\(^\dagger\) stands for psuedo-inverse.
Thus, \( X_i^T \beta - \min\{t_i, X_i^T \beta \} \geq 0 \). Thus, \( \max\{t_i, X_i^T \beta \} = t_i + v_i \). Let \((z_i)_{i=1}^n \in \{0, 1\}^n\) be a set of binary variables such that:

\[
\begin{cases}
  z_i = 1 & \text{if } X_i^T \beta \geq t_i \\
  z_i = 0 & \text{if } X_i^T \beta \leq t_i
\end{cases}
\begin{align*}
  u_i &= t_i, \quad v_i \geq 0 \\
  u_i &= X_i^T \beta, \quad v_i = 0
\end{align*}
\]

\( \Leftrightarrow \)

\[
\begin{cases}
  v_i \geq 0 \\
  v_i \leq (X_i^T \beta - t_i) z_i \\
  u_i \leq t_i \\
  u_i - t_i \geq (X_i^T \beta - t_i)(1 - z_i) \\
  X_i^T \beta = u_i + v_i
\end{cases}
\] (QIP-precase)

Let \( m_i \) and \( M_i \) be the upper and lower bounds of \( X_i^T \beta \), respectively. We obtain the following: the constraints (QIP-precase) are equivalent to:

\[
\begin{cases}
  v_i \geq 0 \\
  v_i \leq (M_i - t_i) z_i \\
  u_i \leq t_i \\
  u_i - t_i \geq (m_i - t_i)(1 - z_i) \\
  X_i^T \beta = u_i + v_i
\end{cases}
\] (QIP-case)

Therefore, we obtain an equivalent quadratic integer programming formulation for ReLU-Regression as follows:

\[
\min_{\beta, z, u, v} \sum_{i=1}^n (t_i + v_i - Y_i)^2
\] (QIP)

\[
\begin{align*}
  v_i \geq 0 & \quad i \in [n] \\
  v_i \leq (M_i - t_i) z_i & \quad i \in [n] \\
  u_i \leq t_i & \quad i \in [n] \\
  u_i - t_i \geq (m_i - t_i)(1 - z_i) & \quad i \in [n] \\
  X_i^T \beta = u_i + v_i & \quad i \in [n] \\
  X_i^T \beta \in [m_i, M_i] & \quad i \in [n] \\
  z_i \in \{0, 1\} & \quad i \in [n]
\end{align*}
\]

where the upper and lower bounds \( m_i \) and \( M_i \) can be found using Theorem 5. See Section 4.5 for details on how \( m_i \) and \( M_i \) are determined.

## 3 Numerical Experiments

In this section, we present some numerical examples of ReLU regression problem, in comparing the Approximation Algorithm, greedy heuristic, and the IP formulation (which is solved using the quadratic integer programming solver). All numerical experiments are implemented with hardware: MacBookPro13 with 2 GHz Intel Core i5 CPU and 8 GB 1867 MHz LPDDR3 Memory; and software: Python 3.5 and Gurobi 7.0.2.

We use the recovery error and the prediction error as our performance metrics. The \( \ell_2 \) recovery error is \( \| \hat{\beta} - \beta^* \|_2 \), where \( \beta^* \) is the true parameter that we pick in the simulation, and \( \hat{\beta} \) is the solution that we obtained from various approaches. The prediction error is \( \| \max\{t, X^T \beta\} - Y \|_2 \) which is square root of the objective function of the ReLU-Regression.
The simulated data are generated as follows. Let \( X \in \mathbb{R}^{p \times n} \) be a matrix with \( n \) samples \( x_1, \ldots, x_n \in \mathbb{R}^p \), where each sample \( x_i \) is generated independently from normal distribution \( N(0, \Sigma) \), where \( \Sigma \in \mathbb{R}^{p \times p} \) is a Toeplitz matrix with \( \Sigma_{jk} = 0.95^{|j-k|} \). Let the true \( \beta^* \) be chosen arbitrarily. Let the random noise \( \epsilon \) be \( N(0, \sigma^2) \). Given any threshold vector \( t \in \mathbb{R}^n \), the observation vector \( Y \in \mathbb{R}^n \) is generated as \( Y = \max\{t, X^\top \beta^*\} + \epsilon \).

We run our Approximation Algorithm with the following settings. Let \( p = 200 \) and the number of samples \( n = 400 \). Consider an arbitrary picked vector \( \beta^* \) be generated from \( N(0, tI_p) \) (with \( t = 20 \) in our setting), and vary \( \sigma \) from 0 to 10. For each fixed set of parameters \((p, n, \beta^*, \sigma)\), we generate \( Y = \max\{t, X^\top \beta^*\} + \epsilon \) four times. The results are reported in Figure [2, 3].

![Figure 2: Recovery error of three methods](image)

![Figure 3: Prediction error of three methods](image)

We can make the following observations for the numerical results in Figure [2, 3]:

1. Integer Programming (IP) approach: The recovery error of IP method can be larger than the heuristic. Since we have to solve an IP with very large big-M coefficients \((m_i, M_i)\) which leads to instability (numerical errors) of the commercial solver; Gurubi is not able to obtain a very good
solution within few hours. Although the objective value of IP method is comparable with greedy heuristic, the run-time of this approach is the worst among all methods and it take on average 40 min per instance.

(2) Greedy heuristic: The greedy heuristic performs well empirically. As the noise variance $\sigma$ increases, the recovery error grows. We can see that this method has the best objective value among all methods. Although we cannot verify a polynomial running time for the Greedy heuristic, it is the most efficient in terms of run-time in our experiments. (9 min per instance in average).

(3) Approximation Algorithm: The recovery error of Approximation Algorithm is small when the noise is small, when the noise increases, the approximation algorithm cannot find a good solution since the optimal set of indices appear not to be close to $\hat{J}$ (See Section 4.3). The run-time of the Approximation Algorithm (30 ~ 40 min per instance on average) is slower than the greedy heuristic.

4 Proofs of main results

4.1 ReLU Regression is NP-hard

In order to prove Theorem 1 we show that the subset sum problem can be polynomially reduced to a special case of ReLU-Regression problem. We begin a definition to the subset sum problem.

**Definition 2. Subset sum problem:** Given $p + 1$ natural numbers $a_1, \ldots, a_p$ and $b$, the subset sum problem is to find out whether there exists a subset $S \subseteq [p]$ such that $\sum_{i \in S} a_i = b$.

Now we show the equivalence between subset sum problem and a special case of ReLU-Regression problem. Consider the following auxiliary function $\theta(x) = (\max\{1/2, x\} - 1)^2 + (\max\{-1/2, -x\} - 0)^2$ which has two exactly strict global minimum point at $x = 0, 1$ and $\min_{x \in \mathbb{R}} \theta(x) = 1/4$. See Figure 4.

![Auxiliary function: $\theta(x)$](image)

Figure 4: Function $\theta(x)$

Therefore, we construct our ReLU-Regression problem as follows:

$$\min_{\beta \in \mathbb{R}^p} \left( \max\left\{0, \sum_{i=1}^{p} a_i \beta_i \right\} - b \right)^2 + \sum_{i=1}^{p} \theta(\beta_i).$$

(subset-sum-ReLU)
• If the subset sum problem has a solution $S$, then set $\beta_i = 1, i \in S$ and $\beta_i = 0, i \notin S$. In this case, $(\max \{0, \sum_{i=1}^{p} a_i\beta_i\} - b)^2 = 0$ and each $\theta(\beta_i)$ achieves its global minimum. Then this ReLU regression achieves its global minimum $\frac{p}{4}$.

• If the subset sum problem does not have a solution, then we have two cases:

1. If we set $\beta_i \in \{0, 1\}$ for all $i \in [p]$. Still for each $i \in [p]$, the function $\theta(\beta_i)$ achieves their global minimum, but $(\max \{0, \sum_{i=1}^{p} a_i\beta_i\} - b)^2 > 0$, the global minimum of subset-sum-ReLU is strictly greater than $\frac{p}{4}$.

2. If some $\beta_i \notin \{0, 1\}$. Under this case, $(\max \{0, \sum_{i=1}^{p} a_i\beta_i\} - b)^2 \geq 0$, however, for that $i$, we have $\theta(\beta_i) > \frac{1}{4}$, thus the global minimum of subset-sum-ReLU is strictly greater than $\frac{p}{4}$.

Therefore, we have the subset sum problem has a feasible solution if and only if the global minimum of subset-sum-ReLU problem is $\frac{p}{4}$. Since subset sum problem is NP-hard and it can be polynomial reduction to our ReLU regression problem, then ReLU-Regression is NP-hard.

4.2 Fixed parameter tractability

In the following, we outline a proof to Theorem 2. To prove Claim 1 we need the following definitions: In $\mathbb{R}^p$, define hyperplane $H_i$ as $H_i = \{\beta \in \mathbb{R}^p : X_i^\top \beta = t\}$ for all $i \in [n]$. Thus the whole space $\mathbb{R}^p$ is separated into a family of polyhedrons by $H_1, \ldots, H_n$. In computational geometry, people call the above family of polyhedrons as the hyperplane arrangements generated from $H_1, \ldots, H_n$, denoted as $A(H_1, \ldots, H_n)$. Moreover, we call each non-empty polyhedron $C \in A(H_1, \ldots, H_n)$ a cell of $A(H_1, \ldots, H_n)$, and note that each cell $C$ can be represented as $C = P(J)$ for some $J \subseteq [n]$. Thus we have the following propositions from [6, 5]:

**Proposition 3.** The maximum number of cells that separated by $n$ hyperplanes in $\mathbb{R}^p$ is less than or equal to $\sum_{i=0}^{p} \binom{n}{i} = O(n^p) \ll 2^n$ when $p$ is fixed and $p \ll n$.

**Proposition 4.** There is a polynomial algorithm $O(n^d)$ that enumerates every cells in Proposition 3.

Now we are ready to prove Theorem 2. Therefore, let $A(H_1, \ldots, H_n) = \{C_1, \ldots, C_m\}$ with $m \leq O(n^p)$ where each $C_i$ corresponds to a non-empty polyhedron $P(I_{C_i})$. Then the ReLU-Regression problem can be solved by solving each convex optimization problem $z^*(I_{C_i})$ for $i = 1, \ldots, m$ and take the minimum of them.

4.3 Approximation Algorithm

Without loss of generality, by sorting the indices, let $Y_1 - t_1 \leq Y_2 - t_2 \leq \cdots \leq Y_n - t_n$. Let $\beta^*$ be the global optimal solution of ReLU-Regression. Let $J^* = \{i : X_i^\top \beta^* > t_i\}$. Let $i^*$ be the maximum
index that does not belong to \( J^* \). Let \( \hat{J} \triangleq \begin{cases} \{ i^* + 1, i^* + 2, \ldots, n \} \subseteq J^* & \text{if } i^* \text{ exists} \\ \emptyset & \text{o.w.} \end{cases} \). Then

\[
\begin{align*}
\quad z^\sigma(\hat{J}) &= \min_{\beta \in \mathbb{R}^p} \sum_{i \in \hat{J}} (X_i^T \beta - Y_i)^2 + \sum_{i \notin \hat{J}} \sigma(X_i^T \beta, t_i, Y_i) \\
&\leq \sum_{i \in \hat{J}} (X_i^T \beta^* - Y_i)^2 + \sum_{i \notin \hat{J}} \sigma(X_i^T \beta^*, t_i, Y_i) \\
&= \sum_{i \in \hat{J}} (X_i^T \beta^* - Y_i)^2 + \sum_{i \in J^* \setminus \hat{J}} \sigma(X_i^T \beta^*, t_i, Y_i) + \sum_{i \in (J^*)^C} (t_i - Y_i)^2.
\end{align*}
\]

Set \( D \triangleq \sum_{i \in J^*} (X_i^T \beta^* - Y_i)^2 \). Observe that:

\[
\begin{align*}
\sum_{i \in \hat{J}} (X_i^T \beta^* - Y_i)^2 &+ \sum_{i \in J^* \setminus \hat{J}} \sigma(X_i^T \beta^*, t_i, Y_i) \\
&= \sum_{i \in \hat{J}} (X_i^T \beta^* - Y_i)^2 + \sum_{i \in J^* \setminus \hat{J}} \max \left\{ (X_i^T \beta^* - Y_i)^2, (t_i - Y_i)^2 \right\} \\
&\leq \sum_{i \in \hat{J}} (X_i^T \beta^* - Y_i)^2 + \sum_{i \in J^* \setminus \hat{J}} (X_i^T \beta^* - Y_i)^2 + \sum_{i \in J^* \setminus \hat{J}} (t_i - Y_i)^2 \\
&= D + \sum_{i \in J^* \setminus \hat{J}} (t_i - Y_i)^2.
\end{align*}
\]

Thus,

\[
\begin{align*}
z^\sigma(\hat{J}) \leq D + \sum_{i \in J^* \setminus \hat{J}} (t_i - Y_i)^2 &+ \sum_{i \in (J^*)^C} (t_i - Y_i)^2 \\
&= D + \sum_{j \in C} (t_i - Y_i)^2 \leq D + i^* \cdot (t_i - Y_i^*)^2.
\end{align*}
\]

Moreover, from the definition of \( D \), we have: \( z^{opt} \geq D + (t_i - Y_i^*)^2 \). Therefore, the approximation ratio is upper bounded by:

\[
\frac{z^{approx}}{z^{opt}} \leq \frac{z(\hat{J})}{z^{opt}} \leq \frac{D + i^* \cdot (t_i - Y_i^*)^2}{D + (t_i - Y_i^*)^2} \leq i^* \leq n.
\]

### 4.4 Greedy Heuristic

**Proof of Proposition**

Let \( A \leftarrow I \backslash \mathcal{I}(\beta_I), \ B \leftarrow I \cap \mathcal{I}(\beta_I), \ C \leftarrow \mathcal{I}(\beta_I) \backslash I, \ D \leftarrow I^C \cap \mathcal{I}(\beta_I)^C \). Then

\[
\begin{align*}
z^\sigma(I) &= \sum_{i \in A} (X_i^T \beta_I - Y_i)^2 + \sum_{i \in B} (X_i^T \beta_I - Y_i)^2 \\
&\quad + \sum_{i \in C} \sigma(X_i^T \beta_I, t_i, Y_i) + \sum_{i \in D} \sigma(X_i^T \beta_I, t_i, Y_i) \\
&\geq \sum_{i \in A} \sigma(X_i^T \beta_I, t_i, Y_i) + \sum_{i \in B} (X_i^T \beta_I - Y_i)^2 \\
&\quad + \sum_{i \in C} (X_i^T \beta_I - Y_i)^2 + \sum_{i \in D} \sigma(X_i^T \beta_I, t_i, Y_i) \geq z^\sigma(\mathcal{I}(\beta_I)).
\end{align*}
\]
Proof of Theorem \ref{theo:finite}. Finite Number of Iterations. Since there are a finite number of choices \( I \), it is sufficient to positive decreasing in every iteration. The algorithm terminates if and only if \( \mathcal{I}(\beta_1) \neq I \), i.e., the set \( B \leftarrow I \cap \mathcal{I}(\beta_1) \) or \( C \leftarrow \mathcal{I}(\beta_1) \setminus I \) are not empty.

- When set \( B \neq \emptyset \), then we have \( X_i^T \beta_1 < t_i \) for some \( i \in B \), that is \( (X_i^T \beta_1 - Y_i)^2 > \sigma(X_i^T \beta_1, t_i, Y_i) \).
- When set \( C \neq \emptyset \), then we have \( 2Y_i - t_i \geq X_i^T \beta_1 \geq t_i \) for some \( i \in C \), that is \( \sigma(X_i^T \beta_1, t_i, Y_i) > (X_i^T \beta_1 - Y_i)^2 \).

In summary, we have in each step, the heuristic provides a positive decreasing.

4.5 Integer Programming Approach

Proof of Theorem \ref{theo:integer}. Let \( \beta^* \) be a global optimal solution of ReLU-Regression problem. Based on this global minimizer \( \beta^* \), define the following three sets of indices as:

\[
I_+ \triangleq \{ i : X_i^T \beta^* > t_i \} \quad \text{positive set},
\]
\[
I_A \triangleq \{ i : X_i^T \beta^* = t_i \} \quad \text{active set},
\]
\[
I_- \triangleq \{ i : X_i^T \beta^* < t_i \} \quad \text{negative set}.
\]

Now suppose the above three sets of indices \( I_+, I_A, I_- \) are given, the ReLU-Regression problem turns to be:

\[
\min_{\beta \in \mathcal{F}} \sum_{i \in I_+} (X_i^T \beta - Y_i)^2 + \sum_{i \in I_A} (X_i^T \beta - Y_i)^2 + \sum_{i \in I_-} (t_i - Y_i)^2 \quad \text{(Fix-index)}
\]

where the feasible region \( \mathcal{F} \) is defined as:

\[
\mathcal{F} \triangleq \left\{ \beta \in \mathbb{R}^p : \begin{array}{l}
X_i^T \beta > t_i, \quad i \in I_+ \\
X_i^T \beta = t_i, \quad i \in I_A \\
X_i^T \beta < t_i, \quad i \in I_-
\end{array} \right\}.
\]

Let \( \beta^* \) be an optimal solution. Moreover, we can replace the feasible region \( \mathcal{F} \) with its topological closure, \( \bar{\mathcal{F}} \), which does not change the optimal solution \( \beta^* \).

By the singular value decomposition, \( X_{I_+}^T = U_{I_+} \Sigma_{I_+} V_{I_+}^T \in \mathbb{R}^{I_+ \times |I_+|} \) where \( U_{I_+} \in \mathbb{R}^{I_+ \times |I_+|} \) be unitary, \( \Sigma = \mathbb{S} \oplus 0 \in \mathbb{R}^{|I_+| \times p} \) be diagonal, \( V_{I_+} \in \mathbb{R}^{p \times \mathcal{F}} \) be unitary. Now we have the following claim to complete the proof:

Claim 2. Let \( \beta' = (X_{I_+} X_{I_+}^T)^\dagger X_{I_+} Y_{I_+} \in \arg \min_{\beta} \| X_{I_+} \beta - Y_{I_+} \|_2^2 \), we have there exists a global optimal solution \( \beta^* \) of ReLU-Regression problem that satisfies \( \beta^* = \beta' \).

Proof. Let \( d \triangleq \beta^* - \beta' \), and let \( \beta_0 \leftarrow \beta' + \alpha d \) with \( \alpha \in \mathbb{R} \). Recall \( \beta^* = \beta_1 \) and \( \beta' = \beta_0 \). Let \( f(\alpha), g(\alpha), h(\alpha) \) be functions defined as:

\[
f(\alpha) \triangleq \| \max \{ t_{I_+}, X_{I_+}^T \beta_0 \} - Y_{I_+} \|_2^2,
\]
\[
g(\alpha) \triangleq \| \max \{ t_{I_A}, X_{I_A}^T \beta_0 \} - Y_{I_A} \|_2^2,
\]
\[
h(\alpha) \triangleq \| \max \{ t_{I_-}, X_{I_-}^T \beta_0 \} - Y_{I_-} \|_2^2.
\]
therefore, the objective function of Fix-index (constrained in the affine line of $\beta^*$ and $\beta'$) can be represented as a function $\text{obj}(\alpha) \triangleq f(\alpha) + g(\alpha) + h(\alpha)$. Note that when $\alpha = 1$, objective function $\text{obj}(\alpha)$ achieves the global minimum of ReLU-Regression problem (so as Fix-index) and when $\alpha = 0$, the function $f(\alpha)$ achieves its global minimum.

We show Claim 2 holds by contradiction, suppose there does not exist a $\beta^*$ such that $\beta^* = \beta'$, then $d \neq 0$.

Observe that for any $\delta > 0$, there exists an $1 > \epsilon > 0$, set $\alpha = 1 - \epsilon$, if $t$ is chosen to be $t < \min_{i \in [n]} Y_i$, we have:

$$
\begin{align*}
    t_i &\leq X_i^T \beta_{1-\epsilon} & i \in I_+, \\
    t_i - \delta &\leq X_i^T \beta_{1-\epsilon} \leq Y_i, & i \in I_A, \\
    X_i^T \beta_{1-\epsilon} &\leq t_i, & i \in I_-.
\end{align*}
$$

Therefore, when we pick $\epsilon > 0$ sufficiently small and $\alpha = 1 - \epsilon$, we have: $g(1) \geq g(1 - \epsilon)$ and $h(1) = h(1 - \epsilon)$. For the function $f(\alpha)$, since $\epsilon > 0$ small enough, then:

$$
f(\alpha) = \|X_{I_+}^T \beta_\alpha - Y_{I_+}\|^2_2 = \alpha^2 d^T X_{I_+} X_{I_+}^T d + 2 \alpha \left( d^T X_{I_+} X_{I_+}^T \beta' - Y_{I_+} X_{I_+}^T d \right)_{=0}^{=A} + \left( \beta'^T X_{I_+} X_{I_+}^T \beta' - 2 Y_{I_+} X_{I_+}^T \beta' \right)_{=C}.
$$

Here we have two cases:

1. If $A > 0$, then $f(\alpha)$ is a strictly convex one variable quadratic function with unique global minimizer $\alpha = 0$. Thus $f(1) > f(1 - \epsilon)$. Therefore,

$$
\text{obj}(1) = f(1) + g(1) + h(1) > f(1 - \epsilon) + g(1 - \epsilon) + h(1 - \epsilon) = \text{obj}(1 - \epsilon).
$$

Note that $\text{obj}(1)$ is the global minimum, then contradicts, therefore $\beta^* = \beta'$.

2. If $A = 0$, then $f(\alpha) = 2B \alpha + C$, and when $B \neq 0$, the function $f(\alpha)$ does not have a finite minimizer, therefore $B = 0$. In this case, $f(\alpha) = C$ be a constant function for all $\alpha \in \mathbb{R}$. Thus $f(1) = f(0)$, therefore $\beta^* = \beta_1 \in \arg\min_\alpha f(\alpha)$. By the definition of $\beta' = \beta_0$, we have $\beta^* = \beta'$.

To show $\beta^* = \beta' = (X_{I_+} X_{I_+})^T Y_{I_+}$, we need the following observations: First, observe that, under case 2, for any $\delta > 0$, there exists an $1 > \epsilon = \epsilon(\delta) > 0$, for any $\alpha \in (1 - \epsilon, 1 + \epsilon)$, if $t_i < Y_i$ for all $i = 1, \ldots, n$, we have:

$$
\begin{align*}
    t_i &< X_i^T \beta_\alpha, & i \in I_+, \\
    t_i - \delta &\leq X_i^T \beta_\alpha \leq Y_i, & i \in I_A, \\
    X_i^T \beta_\alpha &< t_i, & i \in I_-.
\end{align*}
$$
Since in case 2, $f(\alpha) \equiv C$ be a constant and for ant $\alpha \in (1-\epsilon, 1+\epsilon)$, $\max\{t_i, X_i^T \beta\} = t_i$, then it is sufficient to consider the function $g(\alpha)$.

Note that obj(1) is the global optimal, then $g(1) \leq \min\{g(1-\epsilon'), g(1+\epsilon')\}$ with $\epsilon > \epsilon' > 0$. Thus for $i \in I_A$, we have $X_i^T \beta_{1-\epsilon'} = X_i^T \beta^* - \epsilon' X_i^T d \leq t_i$ and $X_i^T \beta_{1+\epsilon'} = X_i^T \beta^* + \epsilon' X_i^T d \leq t_i$ which implies $X_i^T d = 0$. Now $d$ satisfies that: $X_{I_A}^T d = 0$ and $X_{I_A}^T d = 0$.

Consider the value of $X_i^T \beta$ for $i \in I_-$. By assumption, we have $X_i^T \beta^* < t_i$ for all $i \in I_-$, let $I_-$ be partitioned as follows:

$I_1^+ \leftarrow \{i \in I_- : X_i^T \beta' > t_i\}$,
$I_2^+ \leftarrow \{i \in I_- : X_i^T \beta' = t_i\}$,
$I_3^+ \leftarrow \{i \in I_- : X_i^T \beta' < t_i\}$,

i.e., $I_- = I_1^+ + I_2^+ + I_3^+$. Thus by assumption, we have $X_i^T d < 0$ for all $i \in I_1^+ \cup I_2^+$. Let $\alpha^*$ be the optimal solution of the following linear optimization problem:

$$\min \alpha \quad \alpha \in [0, 1 + \epsilon)$$

s.t. $2Y_i - t_i > X_i^T \beta' + \alpha X_i^T d \quad i \in I_1^+$

$x_i^T \beta' + \alpha X_i^T d > t_i \quad i \in I_2^+$

$x_i^T \beta' + \alpha X_i^T d < t_i \quad i \in I_3^+ \cup I_2^+$

(set-alpha)

Note that when $\alpha = 1$, $X_i^T \beta + X_i^T d < t_i$ holds for all $i \in I_-$, then by linearity, the formulation set-alpha is non-empty. But note that when $\beta_{\alpha^*}$ is chosen, if $I_1^+ \neq \emptyset$, the function $\text{obj}(\alpha^*) < \text{obj}(1)$ where $\text{obj}(1)$ is a global optimal which contradicts. Thus $I_1^+ = \emptyset$, which implies $\text{obj}(1) = \text{obj}(0)$ and $\beta^*$ is $(X_{I_+} X_{I_+}^T)^{-1} X_{I_+}^T Y_{I_+}$.

Thus the claim holds.

Bounding $X_i^T \beta^*$. The upper and lower bound $m_i, M_i$ can be found as follows. Let $M \leftarrow \min_\beta ||X^T \beta - Y||_2$, since we have $\min_\beta \|\max\{t, X^T \beta\} - Y\|_2^2 \leq \min_\beta \|X^T \beta - Y\| = M$, then for any optimal solution $\beta^*$ of ReLU-Regression and any $i \in [n]$, we have $(max\{t_i, X_i^T \beta^*\} - Y_i)^2 \leq M$. Therefore, the upper and lower bound of $X_i^T \beta^*$ can be obtained in the following:

- For any $i \in \{i \in [n] : X_i^T \beta^* \geq t_i\}$, the constraint $\max\{t_i, X_i^T \beta^*\} - Y_i)^2 \leq M$ implies $X_i^T \beta^* \leq \sqrt{M + |Y_i|}$.

- For any $i \notin \{i \in [n] : X_i^T \beta^* \geq t_i\}$, by Cauchy-Schwarz inequality, $X_i^T \beta^* \geq -\sum_{j=1}^p |X_j||\beta_j|$. Thus it is sufficient to get the upper bounds $\beta^*_j$ for each $j = 1, \ldots, p$. Based on Theorem 7 there exists an index set $I \subseteq [n]$ such that the global optimal solution $\beta^* = (X_I X_I^T)^{-1} X_I Y_I$. Since $X_I X_I^T$ and $X_I^T X_I$ has the same non-zero eigenvalues, and the Hermitian matrix $X_I^T X_I$ is a submatrix of $X^T X$, then by interlacing theorem the eigenvalues of $X_I^T X_I$ are upper and lower bounded by the eigenvalues of $X^T X$. Let $U_I \Sigma_I V_I^T$ be the singular value decomposition of $X_I$. Therefore, for any $j = 1, \ldots, p$, let $U_j$ be the upper bound of $\beta^*_j$, we have: $U_j \leq \max_{\|v\|_2 = 1} ||(X_I X_I^T)^{-1} X_I Y_I||_2 = [U_I]\Sigma_I V_I^T Y_I$ and thus

$$U_j \leq \| [U_I]\Sigma_I V_I^T \|_2 \|Y_I\|_2 \leq \|\Sigma_I^2\|_2 \|Y_I\|_2 \leq \|\Sigma^2\|_2 \|Y\|_2$$
where $\sigma_I, \sigma$ is the vector of all singular values of $X_I, X$ respectively, and $\sigma^\dagger_I, \sigma^\dagger$ is the vector of all non-zero reciprocals of $\sigma_I, \sigma$ respectively.

Hence the upper and lower bound of $X_i^\top \beta^*$ can be set as $m_i \leftarrow -\sum_{j=1}^p X_{ji} U_j$ and $M_i \leftarrow \sqrt{M} + |Y_i|$ for each $i = 1, \ldots, n$. \hfill $\square$

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