

Universal Approximation Theorem for Interval Neural Networks

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Abstract. One of the main computer-learning tools is an (artificial) neural network (NN); based on the values $y^{(p)}$ of a certain physical quantity y at several points $x^{(p)} = (x_1^{(p)}, \dots, x_n^{(p)})$, the NN finds a dependence $y = f(x_1, \dots, x_n)$ that explains all known observations and predicts the value of y for other $x = (x_1, \dots, x_n)$. The ability to describe an arbitrary dependence follows from the *universal approximation* theorem, according to which an arbitrary continuous function of a bounded set can be, within a given accuracy, approximated by an appropriate NN.

The measured values of y are often only known with interval uncertainty. To describe such situations, we can allow interval parameters in a NN and thus, consider an *interval NN*. In this paper, we prove the universal approximation theorem for such interval NN's.

Neural networks. At present, one of the main computer learning tools is an (artificial) *neural network* that simulates, on the level of neurons, human ability to learn (see, e.g., [2]). One of the most widely used neural networks is based on a neuron which takes n input signals x_1, \dots, x_n and returns the output $y = f(w_1 \cdot x_1 + \dots + w_n \cdot x_n + w_0)$, where w_i are real numbers called *weights*, and $f(x)$ is, usually, either a so-called *logistic* function $f_0(x) = 1 / (1 + \exp(-x))$ (for *non-linear* neurons), or an identity function $f(x) = x$ (for *linear* neurons). To form a *neural network*, we send the output of these neurons as inputs to other neurons. Two types of neural architecture are most widely used: 3-layer and 4-layer. In both architectures:

- the first layer (called *input layer*) inputs the signals x_i ;
- each intermediate layer consists of non-linear neurons that process the outputs of the previous layer:
 - the second layer consists of K non-linear neurons, each of which ($k = 1, \dots, K$) transforms the inputs x_1, \dots, x_n into an output

$$y_k = f_0(w_{k1} \cdot x_1 + \dots + w_{kn} \cdot x_n + w_{k0});$$

- in a 4-layer network, the third layer consists of L non-linear neurons, each of which transforms the inputs y_1, \dots, y_K into a signal

$$z_l = f_0(w'_{l1} \cdot y_1 + \dots + w'_{lK} \cdot y_K + w'_{l0}).$$

- the last layer (called *output layer*) contains a single linear neuron that combines the results of the previous layer into an output y :
 - for a 3-layer network, we get $y = W_1 \cdot y_1 + \dots + W_K \cdot y_K + W_0$;
 - for a 4-layer network, we get $y = W_1 \cdot z_1 + \dots + W_L \cdot z_L + W_0$.

For each set of weights w_{ki} , w'_{lk} , W_j , these formulas lead to a function that describes y in terms of x_1, \dots, x_n . For a 3-layer network, we have

$$y = f_{NN}(x_1, \dots, x_n) = \sum_{k=1}^K W_k \cdot f_0 \left(\sum_{i=1}^n w_{ki} \cdot x_i + w_{k0} \right) + W_0. \quad (1)$$

For a 4-layer network, we have

$$y = f_{NN}(x_1, \dots, x_n) = \sum_{l=1}^L W_l \cdot f_0 \left(\sum_{k=1}^K w'_{lk} \cdot y_k + w'_{l0} \right) + W_0, \quad (2)$$

where

$$y_k = f_0 \left(\sum_{i=1}^n w_{ki} \cdot x_i + w_{k0} \right). \quad (3)$$

We are usually given some *patterns* $(x_1^{(p)}, \dots, x_n^{(p)}, y^{(p)})$, and we want to find the weights for which, for each pattern, $y^{(p)} \approx f_{NN}(x_1^{(p)}, \dots, x_n^{(p)})$. Finding such weights is called *learning*.

The fact that such weights always exist (for appropriate K and/or L) follows from the result known as the *universal approximation theorem* [3]–[5], [7], [8]: For every continuous function $f(x_1, \dots, x_n)$ on a compact set $M \subset R^n$ and for every $\varepsilon > 0$, there exist weights for which for every $(x_1, \dots, x_n) \in M$, $|f(x_1, \dots, x_n) - f_{NN}(x_1, \dots, x_n)| < \varepsilon$. This result is true both for 3-layer and for 4-layer networks.

Interval neural networks. From the mathematical viewpoint, a neural network is an extrapolation tool. For example, in geophysics, if we measure the density d at several depths and locations, we can use a neural network to extrapolate this data and thus, to predict the density at all possible depths and locations.

The data from which we extrapolate is often known with a reasonable inaccuracy: instead of a single value of density, we usually have an *interval* $\mathbf{d} = [\underline{d}, \bar{d}]$ of possible values of density. It is therefore desirable to predict, for all other depths and locations, not just a single value, but the *interval* of possible values of density (so that we not only have the prediction, but also the accuracy of this prediction). In other words, we want to extrapolate the *interval-valued* function $\mathbf{d}(x_1, \dots, x_n) = [\underline{d}(x_1, \dots, x_n), \bar{d}(x_1, \dots, x_n)]$.

From the mathematical viewpoint, an interval-valued function can be viewed as two real-valued functions \underline{d} and \bar{d} . Therefore, we can use two different neural networks to describe these two functions (a similar idea was proposed in [9]). The disadvantage of this approach is that, even if take the patterns from the functions \underline{f} and \bar{f} for which always $\underline{f}(x_1, \dots, x_n) \leq \bar{f}(x_1, \dots, x_n)$, due to approximate character of neural network approximations ($\underline{f}_{NN} \approx \underline{f}$ and $\bar{f}_{NN} \approx \bar{f}$), we sometimes end up with $\underline{f}_{NN}(x_1, \dots, x_n) > \bar{f}_{NN}(x_1, \dots, x_n)$, in which case

$$[\underline{f}_{NN}(x_1, \dots, x_n), \bar{f}_{NN}(x_1, \dots, x_n)]$$

is *not* a meaningful interval.

To solve this problem, a notion of an *interval neural network* was invented [6] (see also [10]), in which, instead of two different neural networks, we have a single network, but with interval-valued weights \mathbf{w}_{ki} , \mathbf{w}'_{lk} , and \mathbf{W}_j . For a 3-layer network, we have

$$\begin{aligned} \mathbf{y} &= \mathbf{f}_{NN}(x_1, \dots, x_n) = [\underline{f}_{NN}(x_1, \dots, x_n), \bar{f}_{NN}(x_1, \dots, x_n)] \\ &= \sum_{k=1}^K \mathbf{W}_k \cdot f_0 \left(\sum_{i=1}^n \mathbf{w}_{ki} \cdot x_i + \mathbf{w}_{k0} \right) + \mathbf{W}_0, \end{aligned} \quad (4)$$

where all the operations with intervals are understood in the sense of interval arithmetic (see, e.g., [1]).

For a 4-layer network, we have

$$\begin{aligned} \mathbf{y} &= \mathbf{f}_{NN}(x_1, \dots, x_n) = [\underline{f}_{NN}(x_1, \dots, x_n), \bar{f}_{NN}(x_1, \dots, x_n)] \\ &= \sum_{l=1}^L \mathbf{W}_l \cdot f_0 \left(\sum_{k=1}^K \mathbf{w}'_{lk} \cdot \mathbf{y}_k + \mathbf{w}_{l0} \right) + \mathbf{W}_0, \end{aligned} \quad (5)$$

where

$$\mathbf{y}_k = f_0 \left(\sum_{i=1}^n \mathbf{w}_{ki} \cdot x_i + \mathbf{w}_{k0} \right). \quad (6)$$

With these formulas, for all possible weight combinations, and for all possible values x_1, \dots, x_n , we get an interval.

There exists methods of training such a network, which are experimentally rather successful [6]. However, in contrast to real-valued neural networks, we did not have a universal approximation theorem that would guarantee that such weights can be found. This theorem is proven in this paper.

THEOREM. *For every continuous interval-valued function*

$$\mathbf{f}(x_1, \dots, x_n) = [\underline{f}(x_1, \dots, x_n), \bar{f}(x_1, \dots, x_n)]$$

on a compact set $M \subset \mathbb{R}^n$ and for every $\varepsilon > 0$, there exist weights for which for every $(x_1, \dots, x_n) \in M$,

$$|f(x_1, \dots, x_n) - \underline{f}_{NN}(x_1, \dots, x_n)| \leq \varepsilon \quad \text{and} \\ |\bar{f}(x_1, \dots, x_n) - \bar{f}_{NN}(x_1, \dots, x_n)| \leq \varepsilon.$$

Comment. In other words, 4-layer interval neural networks are universal approximators for interval-valued functions.

We could not prove a similar result for 3-layer networks; moreover, since learning algorithms often fail for 3-layer neural networks, we conjecture that 3-layer networks may not be universal approximators after all.

Proof. We will approximate the given interval-valued function by a 4-layer neural network in which the third layer has two neurons, and in which all the weights are real numbers (degenerate intervals) except for the weight $\mathbf{W}_2 = [0, 1]$. To be more precise, we want to use a neural network for which

$$\mathbf{f}_{NN}(x_1, \dots, x_n) = [1, 1] \cdot z_1(x_1, \dots, x_n) + [0, 1] \cdot z_2(x_1, \dots, x_n),$$

where $z_j = f_0(u_j)$, and

$$u_j(x_1, \dots, x_n) = \sum_{k=1}^K w'_{jk} \cdot f_0 \left(\sum_{i=1}^n w_{ki} \cdot x_i + w_{k0} \right) + w'_{j0}.$$

To guarantee that this network produces an ε approximation to the original interval-valued function, it is sufficient to guarantee that z_1 is $(\varepsilon/3)$ -close to \underline{f} , and z_2 is $(\varepsilon/3)$ -close to $\Delta f = \bar{f} - \underline{f} + \varepsilon/3$. Indeed, if these closeness conditions are satisfied, then, from $\Delta f \geq \varepsilon/3$, and from the fact that z_2 is $(\varepsilon/3)$ -close to Δf , we can conclude that $z_2 \geq 0$ and therefore, that $\underline{f}_{NN} = z_1$ and $\bar{f}_{NN} = z_1 + z_2$.

- $\underline{f}_{NN} = z_1$ is $(\varepsilon/3)$ -close to \underline{f} , and therefore, ε -close too.
- Since z_1 is $(\varepsilon/3)$ -close to \underline{f} , and z_2 is $(\varepsilon/3)$ -close to $\Delta f = \bar{f} - \underline{f} + \varepsilon/3$, we can conclude that $z_1 + z_2$ is $(2\varepsilon/3)$ -close to $\underline{f} + \Delta f = \bar{f} + \varepsilon/3$. Therefore, the sum $\bar{f}_{NN} = z_1 + z_2$ is ε -close to \bar{f} .

The function $f_0(x)$ is uniformly continuous, hence, there exists a $\delta > 0$ such that if $|x - x'| \leq \delta$, then $|f_0(x) - f_0(x')| \leq \varepsilon/3$. Therefore, to guarantee that $z_1 = f_0(u_1)$ is $(\varepsilon/3)$ -close to \underline{f} , it is sufficient to guarantee that u_1 is δ -close to the function $F_1(x_1, \dots, x_n) = f_0^{-1}(\underline{f}(x_1, \dots, x_n))$. Similarly, to guarantee that $z_2 = f_0(u_2)$ is $(\varepsilon/3)$ -close to Δf , it is sufficient to guarantee that u_2 is δ -close to the function $F_2(x_1, \dots, x_n) = f_0^{-1}(\Delta f(x_1, \dots, x_n))$.

The expressions for u_1 and u_2 are exactly the expressions for the 3-layer neural network, so, the existence of the weights for which u_1 is δ -close to $F_1(x_1, \dots, x_n)$ follows from the universal approximation theorem for 3-layer real-valued neural networks. Similarly, we can prove the existence of weights that compute the desired u_2 . \square

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