Why do networks have negative weights? The answer is: to learn more functions. We mathematically prove that deep neural networks with all non-negative weights are not universal approximators. This fundamental result is assumed by much of the deep learning literature without previously proving the result and demonstrating its necessity.

1 Do networks need both positive and negative weights?

Deep neural networks (DNNs) are universal approximators [1–3]. However, a positive-only DNN (all weights non-negative, abbreviated as DNN$^+$) cannot solve problems as simple as XOR. Below, we will prove by contradiction that DNN$^+$s are not universal approximators (Theorem 1.2); thus, having both positive and negative weights is necessary for universal approximation. We start by defining the problem and then follow with our key observation: DNN$^+$s are composed of only element-wise, dominance-preserving affine transformations (Def 1.3, Lemma 1.1) and monotonically increasing functions; therefore, positive-only DNNs also preserve element-wise dominance (Theorem 1.1).

Definition 1.1 (DNN). Let $W^{(l)} \in \mathbb{R}^{n_l \times n_{l-1}}$, $n_l$ be the number of units in layer $l$, $b^{(l)} \in \mathbb{R}^{n_l}$, for $l \in \{1, \ldots, L\}$. $l = 0$ is the input layer, and $n_0 = \text{dim}(x)$. Further, define:

$$
\sigma(x) = \begin{cases} 
0 & x_j < 0 \\
-x_j & x_j \geq 0 
\end{cases}
$$

$$
\sigma(x) = (\sigma(x_1), \ldots, \sigma(x_{n_l}))
$$

$$
sigmoid(x) = \frac{1}{1 + e^{-x}}.
$$

Let $\sigma^{(l)}(x) = \sigma(W^{(l)}x + b^{(l)})$ be layer $l$. The pre-activation output layer, $P(x)$, is:

$$
P(x) = \sigma^{(L)} \circ \sigma^{(L-1)} \circ \ldots \circ \sigma^{(1)}(x), P(x) \in \mathbb{R}^{n_L}.
$$

(1)

For a binary classification problem, we only need one output unit, i.e., $n_L = 1$. Therefore, $P(x) \in \mathbb{R}$. We can have the prediction $F(x)$ as:

$$
F(x) = \text{sigmoid}(P(x)).
$$

(2)

Definition 1.2 (DNN$^+$). We define DNN$^+$ as DNNs with only non-negative weights allowed, i.e.,

$$
\forall l \in [L], W^{(l)} \in \mathbb{R}^{n_l \times n_{l-1}}_{\geq 0}.
$$

(3)

Definition 1.3 (element-wise dominance). Consider $x, y \in \mathbb{R}^m$ such that,

$$
\text{for all } i \in [m], x_i \geq y_i.
$$

(4)

We say a function $T : x \in \mathbb{R}^m \mapsto x' \in \mathbb{R}^n$ preserves element-wise dominance when,

$$
\text{for all } j \in \{1, \ldots, n\}, x'_j \geq y'_j.
$$

(5)

Lemma 1.1 (element-wise dominance, affine transformation). The affine transformation $T$ defined by

$$
T : x \in \mathbb{R}^m \mapsto Wx + b \in \mathbb{R}^n, W \in \mathbb{R}^{n \times m}_{\geq 0}, b \in \mathbb{R}^n,
$$

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where $W$ is the weight matrix with all non-negative entries, preserves element-wise dominance. That is, for all $x, y \in \mathbb{R}^m$, $i \in \{1, \ldots, m\}$, $j \in \{1, \ldots, n\}$,

$$\text{if } x_i \geq y_i, \text{ then } T(x)_j \geq T(y)_j.$$ 

Furthermore, the strict dominance $T(x)_j > T(y)_j$ holds if there exists $i$ such that $x_i > y_i$ and $w_{j,i} \neq 0$.

See proof on page 5.

Figure 1: **DNNs with only non-negative weights (DNN$^+$s) are NOT universal approximators.** All red colors in the plots indicate changes brought by flipping some weights' polarities to negative such that the binary classification problems on the left can be solved by the DNN. A) DNN$^+$s cannot solve problems where the decision boundaries are composed of segments of both positive and negative slopes (Corollary 1.1.1). Take the 2-hidden-unit network as an example: by flipping a single input weight to negative (notice red decision boundaries), the problem on the left becomes solvable. B) DNN$^+$s cannot solve binary classification problems where there exists a decision boundary that forms a closed shape (Corollary 1.1.2). Take the 4-hidden-unit network as an example: flipping a single input weight for each of the two middle units allows decision boundaries of positive slopes to form, and further, flipping both input weights of the bottom unit allows the activation gradient to flow in the opposite direction (opposite to the element-wise dominance gradient, which is always to the top and/or right). These changes collectively make the closed-shape problem solvable. C) DNN$^+$s cannot solve binary classification problems where the partition formed by the decision boundaries results in a disconnected set for one class (Corollary 1.1.3), e.g., XOR (Lemma 1.2). By flipping a single output weight of a single hidden unit, the top right quadrant can be sculpted out of the pink class, making the network XOR-solvable.
Theorem 1.1 (element-wise dominance, DNN+). A DNN+ preserves element-wise dominance. That is, for all \( x, y \in \mathbb{R}^m, i \in \{1, \ldots, m\}, j \in \{1, \ldots, n_L\} \).

\[
\text{if } x_i \geq y_i, \text{ then } P(x)_j \geq P(y)_j.
\]

For a single output unit DNN, we further have \( F(x) \geq F(y) \). The strict dominance \( P(x)_j > P(y)_j \) and \( F(x) > F(y) \) holds whenever there exists \( i \) such that \( x_i > y_i \) and some weights connecting feature \( i \) and output unit \( j \) are non-zero, such that feature \( i \) and unit \( j \) are connected.

See proof on page 5.

Definition 1.4 (XOR). Let \( x \in \mathbb{R}^2 \) and \( t_1, t_2 \in \mathbb{R} \),

\[
f(x) = \begin{cases} 
0 & \text{if } x_1 \geq t_1 \text{ and } x_2 \geq t_2 \text{ or } [x_1 < t_1 \text{ and } x_2 < t_2] \\
1 & [x_1 \geq t_1 \text{ and } x_2 < t_2] \text{ or } [x_1 < t_1 \text{ and } x_2 \geq t_2].
\end{cases}
\] (6)

Theorem 1.2 (DNN+ cannot solve XOR). DNNs with strictly non-negative weights cannot solve XOR. That is, assume \( W(l) \in \mathbb{R}^{n_l \times n_{l-1}} \) and \( b(l) \in \mathbb{R}^{(l)}, l \in \{1, \ldots, L\} \), where \( n_l \) is the number of nodes in layer \( l \). Then there does not exist a DNN \( F \) such that for any \( \epsilon > 0 \), \( |F(x) - f(x)| < \epsilon \), where \( f \) is the XOR function and \( x \in \mathbb{R}^2 \).

See proof on page 5.

Thus, DNNs with strictly non-negative weights are not universal approximators – they cannot solve XOR because they preserve element-wise dominance. Can we overcome this limitation by flipping the sign of a single weight to make the network XOR-capable? The answer is yes, and we illustrate this result in Figure 1, panel C: in a 3-unit single hidden layer network, flipping one output edge of one hidden unit negates the first quadrant, thus sculpting it out of the pink class region and joining it with the third quadrant.

Based on Theorem 1.1, the element-wise dominance property of DNN+s, we make note of three observations that delineate the types of \( \mathbb{R}^2 \) classification problems that DNN+s fail to solve (Figure 1 left column).

1. Corollary 1.1.1 notes that DNN+s cannot solve problems that require decision boundaries having segments with a positive slope (Figure 1 panel A). This follows from the fact that positive weights can only form decision boundaries that have negative slopes.

2. Corollary 1.1.2 notes that DNN+s cannot solve binary classification problems where there exists a class whose decision boundary forms a closed shape. Element-wise dominance means that for all units in the positive-only DNNs, their activation gradients flow towards the positive directions of all dimensions (top and/or right in \( \mathbb{R}^2 \)). However, for a closed shape decision boundary, it requires the gradient to flow in opposite directions (both towards and away from the partition), which is not doable with positive-only DNNs.

3. Corollary 1.1.3 notes that DNN+s cannot solve binary classification problems where the partition formed by the decision boundaries results in a disconnected set for one class (path-disconnected regions in the input feature space). This is a generalized geometric explanation of why DNN+s cannot solve XOR.

Corollary 1.1.1. (Boundary orientation, in \( \mathbb{R}^2 \)). DNNs with only non-negative weights cannot solve problems where the decision boundaries have segments with a positive slope.

See proof on page 6.

Corollary 1.1.2. (Closed shape, in \( \mathbb{R}^2 \), binary classification) DNNs with only non-negative weights cannot solve binary classification problems (in \( \mathbb{R}^2 \)) where the decision boundaries (or a subset of the decision boundaries) form a closed shape.

See proof on page 6.
Definition 1.5 (path). A path from point $x_1 \in \mathcal{X}$ to point $x_2 \in \mathcal{X}$ is a continuous function $f : [0,1] \mapsto \mathcal{X}$ where $f(0) = x_1$, $f(1) = x_2$.

Definition 1.6 (path-disconnected point pair). For a pair of points $x_1, x_2 \in \mathcal{X}$, $x_1$ and $x_2$ are path-disconnected if there does not exist a path $f : [0,1] \mapsto \mathcal{X}$ where $f(0) = x_1$, $f(1) = x_2$.

Definition 1.7 (disconnected space in $\mathbb{R}^2$). A space $\mathcal{X} \subset \mathbb{R}^2$ is path-disconnected if there exists $x_1, x_2 \in \mathcal{X}$ such that $x_1$ and $x_2$ are path-disconnected.

Corollary 1.1.3. (Disconnected space, in $\mathbb{R}^2$, binary classification.) DNNs with strictly non-negative weights cannot solve a binary classification problem where at least one class is a disconnected space (in $\mathbb{R}^2$).\(^1\)

See proof on page 6.

These three corollaries point to the fundamental flaw of DNN\(^+\)s: however many layers they have, each penultimate layer unit can only form a single continuous decision boundary that is composed of segments having negative slopes. Adding more layers or adding more nodes to each layer of such a network can produce more complex-shaped decision boundaries (Figure 1, panel B, middle column), but cannot form boundaries of more orientations, or form a closed region, or sculpt the input space such that disconnected regions can be joined. Therefore, taking negative weights away from DNNs not only breaks their universality, but it also drastically shrinks their repertoire of representable functions. Thus, for real-world problem solving, it is crucial to have both positive and negative weights in the network.

References and Notes

[1] Kurt Hornik, Maxwell Stinchcombe, and Halbert White. Multilayer feedforward networks are universal approximators. Neural Networks, 2(5):359–366, jan 1989. 1

[2] G. Cybenko. Approximation by superpositions of a sigmoidal function. Mathematics of Control, Signals and Systems 1989 2:4, 2(4):303–314, dec 1989.

[3] Kurt Hornik. Approximation capabilities of multilayer feedforward networks. Neural Networks, 4(2):251–257, jan 1991. 1

\(^1\) An example of disconnected space is the second and forth quadrant that form class 0 in XOR.
A Proofs

Lemma 1.1 (element-wise dominance, affine transformation). The affine transformation $T$ defined by

$$T : x \in \mathbb{R}^m \mapsto Wx + b \in \mathbb{R}^n, \quad W \in \mathbb{R}^{n \times m}_{\geq 0}, b \in \mathbb{R}^n,$$

where $W$ is the weight matrix with all non-negative entries, preserves element-wise dominance. That is, for all $x, y \in \mathbb{R}^m, i \in \{1, \ldots, m\}, j \in \{1, \ldots, n\}$,

$$\text{if } x_i \geq y_i, \quad \text{then } T(x)_j \geq T(y)_j.$$

Furthermore, the strict dominance $T(x)_j > T(y)_j$ holds if there exists $i$ such that $x_i > y_i$ and $w_{j,i} \neq 0$.

Proof of Lemma 1.1. Let $W_j$ be the $j$th row of $W$. Then

$$T(x)_j - T(y)_j = (W_jx + b_j) - (W_jy + b_j) = W_j(x - y) = w_{j,1}(x_1 - y_1) + \cdots + w_{j,m}(x_m - y_m) \geq w_{j,1} \times 0 + \cdots + w_{j,m} \times 0 = 0.$$

If $\exists x_i > y_i$ and $w_{j,i} \neq 0$, then $w_{j,i} \times (x_i - y_i) > 0$, then $T(x)_j > T(y)_j$.

Theorem 1.1 (element-wise dominance, DNN+). A DNN+ preserves element-wise dominance. That is, for all $x, y \in \mathbb{R}^m, i \in \{1, \ldots, m\}, j \in \{1, \ldots, n_L\}$,

$$\text{if } x_i \geq y_i, \quad \text{then } P(x)_j \geq P(y)_j.$$

For a single output unit DNN, we further have $F(x) \geq F(y)$. The strict dominance $P(x)_j > P(y)_j$ and $F(x) > F(y)$ holds whenever there exists $i$ such that $x_i > y_i$ and some weights connecting feature $i$ and output unit $j$ are non-zero, such that feature $i$ and unit $j$ are connected.

Proof of Theorem 1.1. We have that monotonically increasing functions preserve element-wise dominance. Furthermore, composing two functions that preserve element-wise dominance also preserves element-wise dominance.

Now, we have that the affine transformation $T$ as in $T(x) = W^{(l)}x + b^{(l)}$ where $W^{(l)}$ is a non-negative weight matrix preserves element-wise dominance by Corollary 1.1.

We also have that the multidimensional ReLU function $\sigma$ (applying the one-dimensional ReLU in each dimension) is also monotonically increasing in each dimension and hence preserves element-wise dominance. Thus $\sigma^{(l)}$ preserves element-wise dominance for all $l \in \{1, \ldots, L\}$.

The pre-activation output $P$ is the composition of the functions $\sigma^{(l)}$ from 1 to $L$. Thus as each $\sigma^{(l)}$ preserves element-wise dominance, so does $P$. Finally, we have that the output of the DNN $F$ is the composition of $P$ and the sigmoid, which is monotonically increasing and hence preserves element-wise dominance. Thus a DNN+ preserves element-wise dominance, as desired.

Theorem 1.2 (DNN+ cannot solve XOR). DNNs with strictly non-negative weights cannot solve XOR. That is, assume $W^{(l)} \in \mathbb{R}_{>0}^{n_{l-1} \times n_l}$ and $b^{(l)} \in \mathbb{R}^{n_l}$, $l \in \{1, \ldots, L\}$, where $n_l$ is the number of nodes in layer $l$. Then there does not exist a DNN $F$ such that for any $\epsilon > 0, |F(x) - f(x)| < \epsilon$, where $f$ is the XOR function and $x \in \mathbb{R}^2$.

Proof of Theorem 1.2. This will be a proof by contradiction.

Assume we have a DNN+ $F$ such that for all $x \in \mathbb{R}^2, |F(x) - f(x)| < \epsilon$, where $\epsilon = 0.1$. Now take the following three points $A, B, C \in \mathbb{R}^2$ such that $A_i < C_i < B_i$ for $i \in \{1, 2\}$ (meaning $C$ dominates $B$ which dominates $A$). Let $A$ and $B$ be in class 1 and $C$ be in class 0 (Figure 1).
Since a DNN\(^+\) preserves element-wise dominance, we have that \(F(A) \leq F(C) \leq F(B)\). However, given the class labelings we have assigned, we have that \(f(A) = f(B) = 1\) and \(f(C) = 0\). Thus \(f(A) > f(C)\).

For \(\epsilon = 0.1\), we must have that \(|F(A) - f(A)| < 0.1\), which implies \(F(A) > 0.9\), which implies \(F(C) > 0.9\), but this contradicts \(|F(C) - f(C)| < 0.1\) which implies \(F(C) < 0.1\).

Thus there does not exist \(F\) that is \(\epsilon = 0.1\) close to \(f\), and hence we cannot find a DNN\(^+\) to be \(\epsilon\) close to \(f\) for all \(\epsilon\), which is the desired result.

**Corollary 1.1.4.** (Boundary orientation, in \(\mathbb{R}^2\).) **DNNs with only non-negative weights cannot solve problems where the decision boundaries have segments with a positive slope.**

**Proof of Corollary 1.1.1.** Consider a situation where we have a segment in the decision boundary with a positive slope. Choose 3 points \(A, B, C \in \mathbb{R}^2\) around the boundary with following conditions: \(A, C\) are class 0, \(B\) is class 1, that \(x^A_1 = x^B_1 < x^C_1\) and \(x^A_2 < x^B_2 = x^C_2\).

An example would be \(A = (0, 1, 0), B = (0, 1, 1), C = (1, 1, 1)\), and the decision boundary is the function \(f(w) = 2w\).

It is always possible to pick three such points for the following reason: assume we have a line segment forming a decision boundary with positive slope \(m > 0\). Let \(d = (d_1, d_2)\) be a point on the segment. Let \(\epsilon > 0\) be some small value. Construct \(w, v, u\) such that

\[
\begin{align*}
w &= (d_1 + \epsilon, d_2) \\
u &= (d_1 + \epsilon, d_2 + 2m\epsilon) \\
v &= (d_1 + 3\epsilon, d_2 + 2m\epsilon) \\
\end{align*}
\]

Then we have \(w\) and \(v\) will be in class 0 and \(u\) will be in class 1. Furthermore, by construction, \(v\) element-wise dominates \(u\) which in turn element-wise dominates \(w\).

Now a DNN\(^+\) preserves element-wise dominance so we must have that \(F(w) \leq F(u) \leq F(v)\). However, \(f(v) = f(w) < f(u)\). Thus by the same reasoning as for theorem (1.2), we have that a DNN\(^+\) cannot solve problems where the decision boundary contains a positive line segment.

**Corollary 1.1.5.** (Closed shape, in \(\mathbb{R}^2\), binary classification) **DNNs with only non-negative weights cannot solve binary classification problems (in \(\mathbb{R}^2\)) where the decision boundaries (or a subset of the decision boundaries) form a closed shape.**

**Proof of Corollary 1.1.2.** Assume we have a classification problem where the decision boundary forms a closed shape. Inside the shape is class 1 and outside the shape is class 0. Lay a horizontal line across this closed shape and choose 3 points \(A = (x^A_1, x^A_2), B = (x^B_1, x^B_2), C = (x^C_1, x^C_2)\) in \(\mathbb{R}^2\) on this line that are co-linear such that \(x^A_1 < x^B_1 < x^C_1, x^A_2 = x^B_2 = x^C_2\). \(A, C\) are outside the shape and hence in class 0, and \(y\) is inside the shape and hence in class 1. Thus \(f(A) = f(C) < f(B)\). A DNN\(^+\) preserves element-wise dominance, hence \(F(A) \leq F(B) \leq F(C)\). This contradicts \(f(A) = f(C) < f(B)\) and by the same reasoning as in theorem (1.2), a DNN\(^+\) cannot solve problems where the decision boundary forms a closed shape.

**Corollary 1.1.6.** (Disconnected space, in \(\mathbb{R}^2\), binary classification.) **DNNs with strictly non-negative weights cannot solve a binary classification problem where at least one class is a disconnected space (in \(\mathbb{R}^2\)).**

**Proof of Corollary 1.1.3.** We name class 0 and 1 for our binary classification problem. Without loss of generality, we assume class 0 is path-disconnected, then it has at least two regions where the points are path-disconnected between regions. Draw a line segment \(AB\) that connects the two path-disconnected regions, then \(AB\) must pass through class 1 by definition 1.7.

\(^2\)An example of disconnected space is the second and forth quadrant that form class 0 in XOR.
**Case 1**  
$AB$ is a line of horizontal, vertical or positive slope. Pick 3 points $x, y, z$ to be co-linear, lie on $AB$ and follow the class labels: $f(x) = f(z) = 0 < f(y) = 1$. In any of the three slope cases of $AB$ (horizontal, vertical, positive), we get that there is element-wise dominance amongst the 3 co-linear points $x, y, z$ because they always follow one of the following 3 cases.

1. $\begin{cases} x_1 = y_1 = z_1 \\ x_2 < y_2 < z_2 \end{cases}$
2. $\begin{cases} x_1 < y_1 < z_1 \\ x_2 = y_2 = z_2 \end{cases}$
3. $\begin{cases} x_1 < y_1 < z_1 \\ x_2 < y_2 < z_2 \end{cases}$

Since a DNN$^+$ preserves element-wise dominance, we will get that $F(x) \leq F(y) \leq F(z)$. The class labels assigned to each point imply that $f(x) = f(z) < f(y)$. Using the same reasoning as in lemma (1.1), we get thus that a DNN$^+$ cannot solve this classification problem.

**Case 2**  
Only exist $AB$ of negative slope. This means, any possible $AB$ that connects the disconnected regions of class 0 is of negative slope. This is only possible when the range of the two regions ($\mathbb{P}_A, \mathbb{P}_B$) do not overlap and without loss of generality, follows $\begin{cases} a_1 \leq t_1 < b_1 \\ a_2 \geq t_2 > b_2 \end{cases}, \forall \begin{cases} a = (a_1, a_2) \in \mathbb{P}_A, \\ b = (b_1, b_2) \in \mathbb{P}_B \end{cases}$. This is because if there is range overlap between $\mathbb{P}_A, \mathbb{P}_B$, i.e. $\exists a_1 = b_1$, or $a_2 = b_2$, then one can always find horizontal or vertical $AB$ that connects $\mathbb{P}_A, \mathbb{P}_B$ (Case 1). It suffices to consider this case when class 0 is exhaustively composed of $\mathbb{P}_A, \mathbb{P}_B$.

Then for our binary classification problem, $\forall x \in (\mathbb{R}^2 - \mathbb{P}_A - \mathbb{P}_B)$, we have $f(x) = 1$. Now we pick points $x, a, z$ such that $a \in \mathbb{P}_A, x, z \not\in (\mathbb{P}_A + \mathbb{P}_B)$:

$\begin{cases} x_1 < a_1 \leq t_1 < z_1 \\ x_2 < t_2 \leq a_2 < z_2 \end{cases} \implies f(a) = 0 < f(x) = f(z) = 1$

Since a DNN$^+$ preserves element-wise dominance, we will get that $F(x) \leq F(a) \leq F(z)$. This contradicts with $f(a) < f(x) = f(z)$. Using the same reasoning as in lemma (1.1), we get thus that a DNN$^+$ cannot solve this classification problem.

\[\square\]