Fixed points of nonnegative neural networks

Tomasz Piotrowski [1] **Renato L. G. Cavalcante** [2] **Mateusz Gabor** [3]

[1]Nicolaus Copernicus University [2]Fraunhofer Heinrich Hertz Institute [3]Wrocław University of Science and Technology

Introduction

We consider the existence of fixed points of nonnegative neural networks, i.e., neural networks that take as an input and produce as an output nonnegative vectors. We first show that nonnegative neural networks with nonnegative weights and biases can be recognized as monotonic and (weakly) scalable functions within the framework of nonlinear Perron-Frobenius theory. This fact enables us to provide conditions for the existence of fixed points of nonnegative neural networks, and these conditions are weaker than those obtained recently using arguments in convex analysis.

Preliminaries

The nonnegative cone and its interior (i.e., the positive cone) are denoted as $\mathbb{R}^n_+ := \{x \in \mathbb{R}^n \mid x \geq 0\}$ and $\mathrm{int}(\mathbb{R}^n_+) := \{x \in \mathbb{R}^n \mid x > 0\}$, respectively. Let $x, y \in \mathbb{R}^n_+$. The partial ordering induced by the nonnegative cone is denoted as $x \leq y \Leftrightarrow y - x \in \mathbb{R}^n_+$. Similarly, for $x \neq y$, $x < y \Leftrightarrow y - x \in \mathbb{R}^n_+$, and $x \ll y \Leftrightarrow y - x \in \mathrm{int}(\mathbb{R}^n_+)$. The fixed point set of a function $f : X \to Y$ with Y and X being subsets of a given set S is denoted as

$$\mathrm{Fix}(f) = \{x^\star \in X \mid f(x^\star) = x^\star\}.$$

Nonnegative mappings

A continuous mapping $f : \mathbb{R}^s_+ \to \mathbb{R}^p$ is said to be

1. *nonnegative* if
$$\forall x \in \mathbb{R}^s_+ \quad f(x) \in \mathbb{R}^p_+, \tag{1}$$
2. *monotonic* if
$$\forall x, \tilde{x} \in \mathbb{R}^s_+ \quad x \leq \tilde{x} \implies f(x) \leq f(\tilde{x}), \tag{2}$$
3. *weakly scalable* if
$$\forall x \in \mathbb{R}^s_+ \quad \forall \rho \geq 1 \quad f(\rho x) \leq \rho f(x), \tag{3}$$
4. *scalable* if
$$\forall x \in \mathbb{R}^s_+ \quad \forall \rho > 1 \quad f(\rho x) \ll \rho f(x). \tag{4}$$

Neural network model

Let $T_i \colon \mathbb{R}^{k_{i-1}} \to \mathbb{R}^{k_i}$ of the form $T_i(x_{i-1})\sigma_i(W_i x_{i-1} + b_i)$ be the i-th layer of an n-layered feed forward neural network, $i = 1, \ldots, n$, where $x_{i-1} \in \mathbb{R}^{k_{i-1}}$ is the input to the layer, $W_i \colon \mathbb{R}^{k_{i-1}} \to \mathbb{R}^{k_i}$ is the linear weight operator (matrix), $b_i \in \mathbb{R}^{k_i}$ is the bias, and $\sigma_i \colon \mathbb{R}^{k_i} \to \mathbb{R}^{k_i}$ is the activation function. A neural network T is then the composition

$$T = T_n \circ \cdots \circ T_1, \tag{5}$$

Hereafter, we assume that the input and output layers have the same dimension $k_0 = k_n$,

Classes of mappings

We use the convention that each subscript applied to A refer to one of the above properties, so that, for example:

- continuous and nonnegative mappings are (A_0)-mappings;
- continuous, nonnegative, and monotonic mappings are $(A_{0,1})$-mappings;
- continuous, nonnegative, monotonic, and weakly scalable mappings are $(A_{0,1,2})$-mappings; and
- continuous, nonnegative, monotonic, and scalable mappings are $(A_{0,1,2,3})$-mappings.

We note that the above classes of mappings satisfy $A_{0,1,2,3} \subset A_{0,1,2} \subset A_{0,1} \subset A_0$.

Activation Functions

The following two lists provide examples of widely-used continuous scalar concave activation functions (with their domains restricted to $\mathbb{R}_+$), and, hence, $(A_{0,1,2})$-scalar activation functions.

1. (L1) continuous scalar concave activation functions satisfying $\lim_{\xi \to \infty} \sigma'(\xi) = 0$:
   - (ReLU6) $x \mapsto \min\{x, 6\}$
   - (hyperbolic tangent) $x \mapsto \tanh x$
   - (softsign) $x \mapsto \frac{x}{1+x}$
   - (sigmoid) $x \mapsto \frac{1}{1+\exp(-x)}$
2. (L2) continuous scalar concave activation function satisfying $\lim_{\xi \to \infty} \sigma'(\xi) = 1$:
   - (ReLU) $x \mapsto x$

Asymptotic mapping

Let $T : \mathbb{R}^k_+ \to \mathbb{R}^k_+$ be an $(A_{0,1,2})$-neural network of the form (5). The asymptotic mapping associated with T is the mapping defined by

$$T_\infty : \mathbb{R}^k_+ \to \mathbb{R}^k_+ : x \mapsto \lim_{p \to \infty} \frac{1}{p} T(px). \tag{6}$$

We recall that the above limit always exists.

Nonlinear spectral radius

Let $T : \mathbb{R}^k_+ \to \mathbb{R}^k_+$ be an $(A_{0,1,2})$-neural network of the form (5). The spectral radius of the corresponding asymptotic mapping T_∞ is defined by

$$\rho(T_\infty) = \max\{\lambda \in \mathbb{R}_+ : \exists\, x \in \mathbb{R}^k_+ \backslash \{0\}, \ \text{s.t. } T_\infty(x) = \lambda x\} \in \mathbb{R}_+. \tag{7}$$

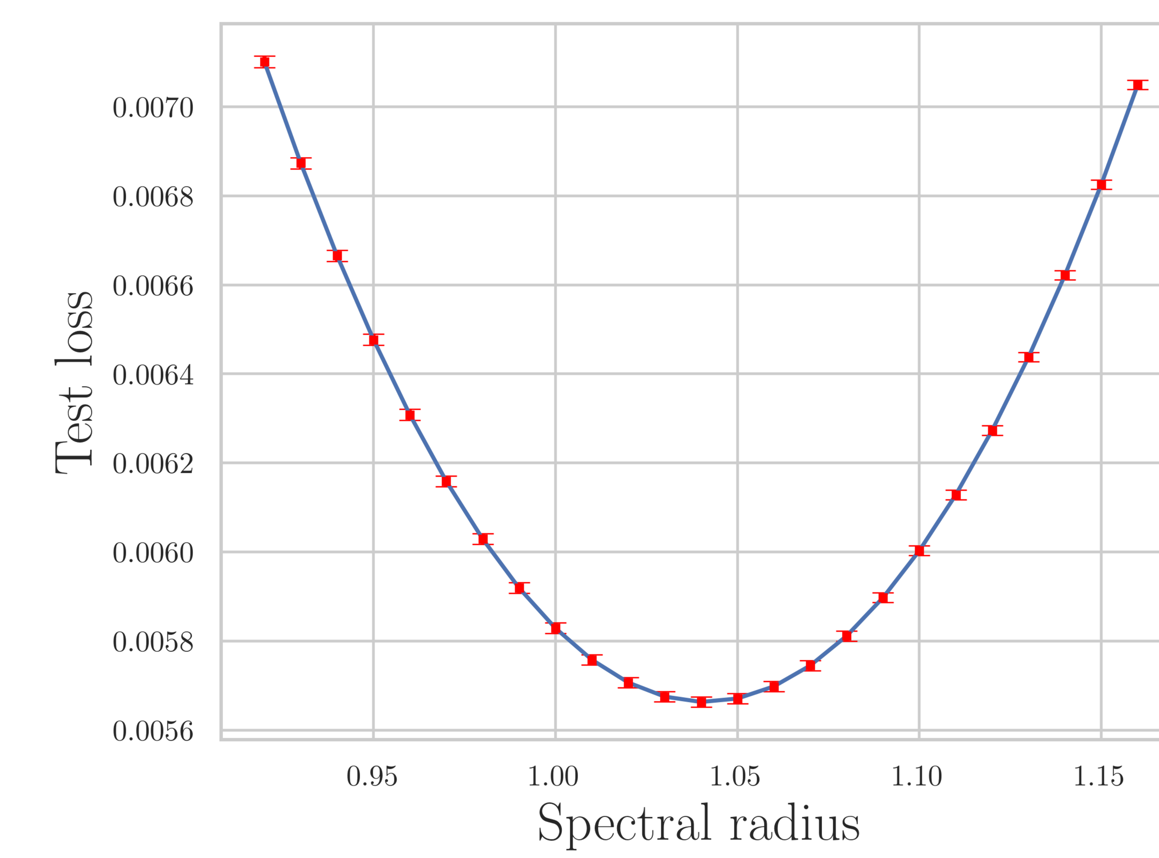
If all layers use activation function from (L2), then $\rho(T_\infty) = \rho(\Pi^1_{i=n} W_i)$. On the other hand, of at least one layer of T uses activation function from list (L1), then $\rho(T_\infty) = 0$.

Fixed points

- If T is $(A_{0,1,2,3})$ and $\rho(T_\infty) < 1$, then the fixed point exists, is unique, and the fixed point iteration of T converges to the fixed-point for any $x_1 \in \mathbb{R}^n_+$.
- If T is $(A_{0,1,2})$ and $\rho(T_\infty) < 1$, then the fixed point exists and the fixed point iteration of T converges to the least fixed point from $x_1 = 0$. If T is also primitive ($T^m(0) \gg 0$), then the fixed point set $\mathrm{Fix}(T)$ is an interval and the fixed point iteration of T converges to $x^\star \in \mathrm{Fix}(T)$ for any $x_1 \in \mathrm{int}(\mathbb{R}^n_+)$.
- If T is $(A_{0,1})$, then assume that there exists T_2 which is $(A_{0,1,2})$. If $\forall x \in \mathbb{R}^n_+ \; T(x) \leq T_2(x)$ and the fixed point exists for T_2, then for T the fixed point also exists and the fixed point iteration of T converges to the least fixed point from $x_1 = 0$.
- If T is (A_0), then assume that there exists T_2 which is $(A_{0,1})$. If $\forall x \in \mathbb{R}^n_+ \; T(x) \leq T_2(x)$ and the fixed point exists for T_2, then for T the fixed point also exists.

Scaling spectral radius

For neural network T (autoencoder) which is $(A_{0,1,2})$ with $\rho(T_\infty) > 0$, we can modify the spectral radius to be close to 1, which is an optimal value of slow convergence to the fixed point, which results in to lower loss.



JMLR reference

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