

ABBA Neural Networks: Coping with Positivity, Expressivity, and Robustness

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▶ To cite this version:

Ana-Antonia Neacșu, Jean-Christophe Pesquet, Vlad Vasilescu, Corneliu Burileanu. ABBA Neural Networks: Coping with Positivity, Expressivity, and Robustness. SIAM Journal on Mathematics of Data Science, In press. hal-04386260

HAL Id: hal-04386260

https://hal.science/hal-04386260

Submitted on 10 Jan 2024

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2.6

Abstract. We introduce ABBA networks, a novel class of (almost) non-negative neural networks, which are shown to possess a series of appealing properties. In particular, we demonstrate that these networks are universal approximators while enjoying the advantages of non-negative weighted networks. We derive tight Lipschitz bounds both in the fully connected and convolutional cases. We propose a strategy for designing ABBA nets that are robust against adversarial attacks, by finely controlling the Lipschitz constant of the network during the training phase. We show that our method outperforms other state-of-the-art defenses against adversarial white-box attackers. Experiments are performed on image classification tasks on four benchmark datasets.

- 12 Key words. Neural Networks, Robustness, Optimization, Lipschitz, Image Classification
- 13 MSC codes. 15A48, 68T05, 65K10

1. Introduction. Deep learning methods based on neural network models have received increasing attention in the scientific community, because of their stunning abilities to solve a variety of complex tasks. These powerful systems excel at learning intricate mappings and, in some cases, even surpass human performance. However, deep architectures usually lack interpretability and they may lead to over-parameterized models [13, 37]. Additionally, their robustness is not well-controlled, leaving them exposed to potential adversarial attacks. For instance, [49] demonstrated that by introducing carefully-crafted, low-magnitude adversarial perturbations, neural classifiers could be easily fooled [17]. A way of overcoming the aforementioned challenges consists in introducing some specific constraints in the neural network design. In this article, we are interested in nonnegativity and stability constraints on the network weights.

It is widely accepted that humans possess the innate ability to decompose complex interactions into discrete, intuitive hierarchical categories before analyzing them [26]. Conceptually, this evolution towards part-based representation in human cognition can be linked to non-negativity restrictions on the network weights [7]. This idea, along with other factors, has sparked interest in neural networks with non-negative weights. These networks have drawn attention for several reasons. Firstly, they align with human understandability, making them more interpretable. Secondly, the non-negativity constraint can act as beneficial regularization, effectively reducing overfitting issues. Moreover, recent studies have demonstrated that it is possible to derive a tight Lipschitz bound for such networks. This Lipschitz constant serves as a valuable metric for quantifying the robustness of the network, enabling us to design networks with enhanced resilience to adversarial perturbations during the training process. Despite their advantages, one significant drawback of networks with non-negative weights is that they might be less expressive than networks with arbitrary signed weights. In [54], it is shown that standard non-negative networks are not universal approximators [54], a limitation that

^{*}Part of this work was supported by the French ANR Research and Teaching Chair in Artificial Intelligence BRIDGEABLE.

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our work overcomes.

Approach. In this work, we are interested in neural networks having non-negative weights, except for the first and last linear layers. This class of networks obviously constitutes an extension of those having all their linear layers non-negative-valued. We focus on a particular subclass of these networks for which the weight matrices have a structure of the form

$$\begin{bmatrix} A & B \\ B & A \end{bmatrix},$$

thus enjoying a number of algebraic properties. The corresponding networks are subsequently called ABBA networks. Note that weight matrices A and B are duplicated in ABBA networks, thus allowing us to limit the number of parameters.

Contributions. This paper makes several key contributions, which are as follows:

- We show that we can put any arbitrary signed network in an ABBA form. This property holds for fully connected as well as for convolutional neural networks.
- Universal approximation theorems are derived for networks featuring non-negatively weighted layers.
- We present a method for effectively controlling the Lipschitz constant of ABBA networks¹. The resulting training strategy applies to both fully connected and convolutional cases. Precise Lipschitz bounds are typically NP hard to compute for arbitrary signed networks, but our framework allows us to derive such bounds that are easy to compute.
- Numerical experiments conducted on standard image datasets showcase the excellent performance of ABBA networks for small models. Notably, they exhibit substantial improvements in both performance and robustness compared to networks with exclusively non-negative weights. Moreover, we demonstrate that ABBA networks are competitive with robust networks featuring arbitrarily signed weights, trained using state-of-the-art techniques.

Outline. The rest of the paper is organized as follows. Section 2 offers an overview of the related literature, while in Section 3 our main contributions concerning ABBA architectures are introduced, alongside a list of fundamental properties. Section 4 extends our results to the case of convolutional neural networks and two Lipschitz constant expressions are derived. Section 5 describes the training strategy we employ to generate robust models with respect to adversarial perturbations. Section 6 details the results obtained for different image classification tasks, while Section 7 is dedicated to concluding remarks.

2. Related work. Non-negative neural networks. Inspired by non-negative matrix factorization (NMF) techniques, the work of [7] introduces non-negative restrictions on the weights to create neural networks in which the hidden units correspond to identifiable concepts. [4] showed that Autoencoders (AE) trained under non-negativity constraints are able to derive meaningful representations that unearth the hidden structure of high-dimensional data. Their method showed promising results from both performance and feature interpretation viewpoints on four different classification tasks. [12] presented the first polynomial-time algorithm for Probably Approximately Correct (PAC) learning 1-layer neural networks with positive coefficients. Moreover, ensuring non-negativity has been shown to have a regularization effect, reducing feature overfitting, which is a very common problem, especially

¹A full TensorFlow implementation of our framework can be provided on demand and will be made publicly available upon paper acceptance.

for tasks where the available training data is scarce [35]. Neural networks defining convex functions of their inputs [1] also constitute a subclass of networks with non-negative weights.

Link with other networks. From another perspective, the idea of using redundant weights is reminiscent of siamese networks [6]. These architectures are successfully used to handle similarity learning tasks, such as face verification [50], character recognition [23], and object tracking [19]. Siamese networks compute a similarity metric on the representations of the inputs, after applying the same transformation to each one. Apart from the proven efficiency on solving computer vision tasks, they have lately been employed in NLP problems, e.g., computational argumentation. In [14], it is shown that siamese architectures outperform other baselines trained on convincingness datasets.

Robustness. The robustness of neural networks against possible adversarial attacks is a topic that has received increasing attention since nowadays AI-based solutions are ubiquitous [3, 36]. A sizable body of literature on adversarial attacks and different defense strategies have emerged in recent years as a result of the work in [49]), which revealed the alluring susceptibility of neural networks to adversarial perturbations and proposed a box-constrained L-BFGS algorithm for finding adversarial examples. [15] introduced the FGSM attack as a one-step modification of the input image, following the direction of loss maximization, while [24] incorporated this step into an iterative method known as PGD, seen as an improvement over basic FGSM. DeepFool [33] iteratively searches for the closest adversarial point that directs the optimization towards crossing the decision boundary. DDN [42] and FMN [39] attacks fall into the category of projected-gradient methods, using iterative updates of the perturbation vector towards the minimization of its magnitude.

Defensive strategies have been developed to alleviate this robustness issue. [47] divides adversarial defense methods into three categories: adversarial detection, gradient masking, and robust optimization. Adversarial Training (AT) was first introduced by [15] and later improved by [32]. Recent works on AT [48, 55] have successfully analyzed and refined training techniques, however, no theoretical certificates regarding their behavior in the presence of different adversaries have been established yet. Regularization-based methods, such as [30, 46, 59], include additional terms in their objective, steering the learning process in a direction that leads to better generalization. [40] provides robustness certificates for neural networks with one hidden layer, yielding an upper bound of the error in the presence of any adversary (see [11, 16, 41] for more advanced methods. Randomized smoothing [9, 25, 29, 44, 57] certifies the robustness of a classifier around an input point by measuring the most-likely prediction over Gaussian-corrupted versions of the point.

Lipschitz properties of neural networks. As highlighted by [49], the Lipschitz behavior of a neural model is closely correlated with its robustness against adversarial attacks, providing an upper bound on the response given input perturbations. Controlling the Lipschitz behavior of the network thus offers theoretical stability guarantees. However, computing the exact constant, even for small networks is an NP-hard problem [20], and finding a good approximation in a reasonable time is an open challenge. Several solutions have been proposed lately (see for example: [5, 18, 21, 58]). [45] introduced *deel-lip*, a framework to control the Lipschitz constant of each layer individually, while [2] propose GroupSort networks to ensure robustness. [38] proposed a framework for training fully-connected neural networks using Lipschitz regularized and constrained techniques, proving their effectiveness in the scenario of Gaussian-added perturbation noise. A recent result in [10] showed that in the case of models with non-negative weights a tight Lipschitz bound can be established, making possible the training of neural network models with certified robustness guarantees.

- 119 3. ABBA Neural Networks.
- 3.1. Problem formulation. In the remainder of this paper, $\|\cdot\|$ will denote the ℓ_2 -norm when
- dealing with a vector, and the spectral norm when dealing with a matrix.
- 122 An *m*-layer feedforward neural network can be described by the following model.
- Model 3.1. T is feedforward neural network if there exists $(N_i)_{1 \le i \le m} \in (\mathbb{N} \setminus \{0\})^m$ such that

$$124 \quad \textbf{(3.1)} \qquad \qquad T = T_m \circ \cdots \circ T_1$$

- where, for every layer index $i \in \{1, ..., m\}$, $T_i = R_i(W_i \cdot +b_i)$, $W_i \in \mathbb{R}^{N_i \times N_{i-1}}$ is the weight matrix,
- 126 $b_i \in \mathbb{R}^{N_i}$ the bias vector, and $R_i : \mathbb{R}^{N_i} \to \mathbb{R}^{N_i}$ the activation operator. N_i corresponds to the number
- of inputs at the i-th layer. Such a layer is convolutive if it corresponds to a weight matrix W_i having
- 128 some Taoeplitz (or block Toeplitz) structure.
- We will say that the activation operator R_i is symmetric, if there exists $(c_i, d_i) \in (\mathbb{R}^{N_i})^2$ such that

130 (3.2)
$$(\forall x \in \mathbb{R}^{N_i})$$
 $R_i(x) - d_i = -R_i(-x + c_i).$

- 131 In other words, $(c_i, d_i)/2$ is a symmetry center of the graph of R_i .
- For example, if R_i is squashing function used in CapsNets [43], it is such that

133 (3.3)
$$(\forall x \in \mathbb{R}^{N_i}) \quad R_i(x) = \frac{\mu \|x\|}{1 + \|x\|^2} x.$$

- with $\mu = 8/(3\sqrt{3})$. It thus satisfies the symmetry property (3.2) with $c_i = d_i = 0$. In addition, R_i
- is nonexpansive, i.e. it has a Lipschitz constant equal to 1 [10] Other examples of symmetric and
- nonexpansive activation operators are presented in Appendix SM1 2 .
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- 3.2. ABBA Matrices. We first define ABBA matrices which will be the main algebraic tool
- 139 throughout this article.
- Definition 3.2. Let $(N_1, N_2) \in (\mathbb{N} \setminus \{0\})^2$. A_{N_1, N_2} is the set of ABBA matrices of size $(2N_2) \times (2N_1)$,
- that is $M \in \mathcal{A}_{N_1,N_2}$ if there exist matrices $A \in \mathbb{R}^{N_2 \times N_1}$ and $B \in \mathbb{R}^{N_2 \times N_1}$ such that

142 (3.4)
$$M = \begin{bmatrix} A & B \\ B & A \end{bmatrix}.$$

- 143 The sum matrix associated with M is then defined as $\mathfrak{S}(M) = A + B$.
- We give some of the most relevant properties of these matrices. In particular, we will see that the ABBA structure is stable under standard matrix operations.
- 146 Proposition 3.3. Let $(N_1, N_2, N_3) \in (\mathbb{N} \setminus \{0\})^3$.
- 147 (i). If $M \in \mathcal{A}_{N_2,N_1}$, then its transpose $M^{\top} \in \mathcal{A}_{N_1,N_2}$ and $\mathfrak{S}(M^{\top}) = \mathfrak{S}(M)^{\top}$.
- 148 (ii). If $(M_1, M_2) \in (\mathcal{A}_{N_2, N_1})^2$, then $M_1 + M_2 \in \mathcal{A}_{N_2, N_1}$ and $\mathfrak{S}(M_1 + M_2) = \mathfrak{S}(M_1) + \mathfrak{S}(M_2)$.
- 149 (iii). If $M_1 \in \mathcal{A}_{N_2,N_1}$ and $M_2 \in \mathcal{A}_{N_3,N_2}$, then $M_2M_1 \in \mathcal{A}_{N_3,N_1}$ and 150 $\mathfrak{S}(M_2M_1) = \mathfrak{S}(M_2)\mathfrak{S}(M_1)$.

²Appendices with number of the form SMx can be found in the supplementary materials.

- (iv). A_{N_1,N_1} is a ring when equipped with the standard matrix addition and product.
- (v). If A and B are two square matrices of the same size, the eigenvalues of $\begin{bmatrix} A & B \\ B & A \end{bmatrix}$ are those of A + B and A B.
- (vi). If A and B are two matrices having the same dimensions, the spectral norm of $\begin{bmatrix} A & B \\ B & A \end{bmatrix}$ is equal to $\max\{\|A+B\|, \|A-B\|\}$.
- (vii). If $M \in \mathcal{A}_{N_2,N_1}$ has non-negative elements, the spectral norm of M is $\|\mathfrak{S}(M)\|$.
- (viii). Let $A \in \mathbb{R}^{N_2 \times N_1}$ and $B \in \mathbb{R}^{N_2 \times N_1}$, and let $K = \min\{N_1, N_2\}$. Let $(\lambda_k)_{1 \leqslant k \leqslant K}$ (resp. $(\mu_k)_{1 \leqslant k \leqslant K}$) be the singular values of A + B (resp. A B) and let $\{u_k\}_{1 \leqslant k \leqslant K} / \{v_k\}_{1 \leqslant k \leqslant K}$ (resp $\{t_k\}_{1 \leqslant k \leqslant K}$) be associated orthonormal families of left/right singular vectors in $\mathbb{R}^{N_2} / \mathbb{R}^{N_1}$.
- Then, the singular values of $\begin{bmatrix} A & B \\ B & A \end{bmatrix}$ are $(\lambda_k, \mu_k)_{1 \leqslant k \leqslant K}$ and associated orthonormal families of left/right singular vectors are

$$\left\{\frac{1}{\sqrt{2}} \begin{bmatrix} u_k \\ u_k \end{bmatrix}, \frac{1}{\sqrt{2}} \begin{bmatrix} t_k \\ -t_k \end{bmatrix}\right\}_{1 \leqslant k \leqslant K} / \left\{\frac{1}{\sqrt{2}} \begin{bmatrix} v_k \\ v_k \end{bmatrix}, \frac{1}{\sqrt{2}} \begin{bmatrix} w_k \\ -w_k \end{bmatrix}\right\}_{1 \leqslant k \leqslant K}.$$

163 (ix). *If A* and *B* are two matrices having the same dimensions,

164 (3.5)
$$\operatorname{rank}\left(\begin{bmatrix} A & B \\ B & A \end{bmatrix}\right) = \operatorname{rank}(A+B) + \operatorname{rank}(A-B).$$

165 (x). Let f be a function from $\mathbb{R}^{(2N_2)\times(2N_1)}$ to $\mathbb{R}^{(2N_2)\times(2N_1)}$. Assume that either f operates elementwise or it is a spectral function in the sense that there exists a function $\varphi \colon \mathbb{R}_+ \to \mathbb{R}_+$ such that

(3.6)
$$(\forall M \in \mathbb{R}^{(2N_2) \times (2N_1)}) \quad f(M) = \sum_{k=1}^{2K} \varphi(\tilde{\lambda}_k) \tilde{u}_k \tilde{v}_k^{\mathsf{T}}$$

- 168 where $K = \min\{N_1, N_2\}$, $(\tilde{\lambda}_k)_{1 \leqslant k \leqslant 2K}$ are the singular values of M, and $\{\tilde{u}_k\}_{1 \leqslant k \leqslant 2K}$ /
 169 $\{\tilde{v}_k\}_{1 \leqslant k \leqslant 2K}$ are associated orthonormal families of left / right singular vectors in \mathbb{R}^{2N_2} /
 170 \mathbb{R}^{2N_1} . Then f maps any matrix in \mathcal{A}_{N_2,N_1} to a matrix in \mathcal{A}_{N_2,N_1} .
 - (xi). The best approximation of maximum rank $R < \min\{N_1, N_2\}$ (in the sense of the Frobenius norm) to a matrix in A_{N_2,N_1} belongs to A_{N_2,N_1} .
- 173 (xii). The projection onto the spectral ball of center 0 and radius $\rho \in]0, +\infty[$ of an ABBA matrix is an ABBA matrix.
- The proofs of these properties are provided in Appendix SM2.
 - 3.3. Extension to feedforward networks. We will now extend the previous algebraic concepts by introducing the class of ABBA feedforward neural networks. In the following, the structure of an ABBA fully-connected network will be presented from the perspective of investigating its links with standard networks. Such networks make use of weights that respect the structure of ABBA matrices, except for the first and the last layers. More precisely, the first layer maps the input to a twice-higher dimensional space, while the last layer performs a dimension reduction by a factor of 2.

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³This means that (SM2.11) and (SM2.12) hold.

Definition 3.4. Let $m \in \mathbb{N} \setminus \{0\}$. \widetilde{T} is an m-layer ABBA network if 182

183 (3.7)
$$\widetilde{T} = (\widetilde{W}_{m+1} \cdot + \widetilde{b}_{m+1}) \widetilde{T}_m \cdots \widetilde{T}_1 \widetilde{W}_0$$

- with $\widetilde{W}_0 \in \mathbb{R}^{(2N_0) \times N_0}$, $\widetilde{W}_{m+1} \in \mathbb{R}^{N_m \times (2N_m)}$, $\widetilde{b}_{m+1} \in \mathbb{R}^{N_m}$, and 184
- $(\forall i \in \{1, \dots, m\}) \quad \widetilde{T}_i = \widetilde{R}_i(\widetilde{W}_i \cdot + \widetilde{b}_i)$ (3.8)185
- $\widetilde{R}_i \colon \mathbb{R}^{2N_i} \to \mathbb{R}^{2N_i}$ 186 (3.9)
- $\widetilde{b}_i \in \mathbb{R}^{2N_i}$, (3.10)187
- $\widetilde{W}_i \in \mathcal{A}_{N_i, N_{i-1}}$, (3.11)188
- for given positive integers $(N_i)_{0 \le i \le m}$. \widetilde{T} is an m-layer non-negative ABBA network if it is an m-layer 190
- ABBA network as defined above and, for every $i \in \{1, \ldots, m\}$, the elements of \widetilde{W}_i are non-negative.
- In the remainder of this paper, $\mathcal{N}_{m,\mathcal{A}}$ will designate the class of m-layer ABBA networks and $\mathcal{N}_{m,\mathcal{A}}^+$
- will designate the subclass of m-layer non-negative ABBA networks. This latter subclass will be the 193
- main topic of investigation in this work. We will also use the notation $\mathcal{N}_{m,\mathcal{A}}^+(\rho)$ to designate the set of 194
- neural networks in $\mathcal{N}_{m,\mathcal{A}}^+$ where all the activation operators operate componentwise using the same 195
- function $\rho \colon \mathbb{R} \to \mathbb{R}$. 196
- 3.4. Link with standard neural networks. In this section, we show that we can reshape Model 3.1 197
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- as a special case of a non-negative ABBA network. At each layer $i \in \{1,\dots,m\}$ of this model, let $W_i^+ = (W_{i,k,\ell}^+)_{1\leqslant k\leqslant N_i,1\leqslant \ell\leqslant N_{i-1}} \in [0,+\infty[^{N_i\times N_{i-1}}$ be the positive part of matrix $W_i = (W_{i,k,\ell})_{1\leqslant k\leqslant N_i,1\leqslant \ell\leqslant N_{i-1}}$, 199
- 200

201 (3.12)
$$(\forall k \in \{1, \dots, N_i\})(\forall \ell \in \{1, \dots, N_{i-1}\})$$
 $W_{i,k,\ell}^+ = \begin{cases} W_{i,k,\ell} & \text{if } W_{i,k,\ell} > 0 \\ 0 & \text{otherwise.} \end{cases}$

- Let $W_i^- = W_i^+ W_i \in [0, +\infty]^{N_i \times N_{i-1}}$ be the negative part of W_i , where all the positive elements 202
- of W_i have been discarded. Let us now define a non-negative ABBA neural network by using these 203
- 204 quantities.
- Definition 3.5. Let $m \in \mathbb{N} \setminus \{0\}$. Let T be the feedforward neural defined in Model 3.1. \widetilde{T} is a network 205
- in \mathcal{N}_{m-A}^+ associated with T if it satisfies relations (3.7)-(3.11) with 206

207 (3.13)
$$\widetilde{W}_0 = \begin{bmatrix} I_{N_0} \\ -I_{N_0} \end{bmatrix}, \quad \widetilde{W}_{m+1} = \frac{1}{2}[I_{N_m} - I_{N_m}],$$

and 208

209 (3.14)
$$(\forall i \in \{1, \dots, m\})$$
 $\widetilde{R}_i : \begin{bmatrix} x \\ z \end{bmatrix} \mapsto \begin{bmatrix} R_i(x) \\ R_i(z) \end{bmatrix},$

210 (3.15)
$$\widetilde{W}_i = \begin{bmatrix} W_i^+ & W_i^- \\ W_i^- & W_i^+ \end{bmatrix}.$$

- Note that a weight parametrization similar to (3.15) was used in [56] for computing lower and upper 212
- bounds on the output of a deep equilibrium layer, but in this article W_i^- has negative values. 2.13
- As we will show next, the main result is that, if the activation functions are symmetric, network T214
- defined above is identical to network T in terms of input-output relation, for judicious choices of the 215
- 216 biases of \tilde{T} .

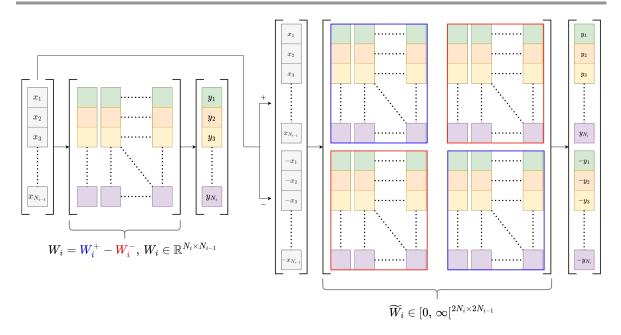


Figure 1: Equivalence between a standard fully-connected layer and its ABBA correspondent.

Proposition 3.6. Let T be the m-layer feedforward network in Model 3.1. Assume that, for every $i \in \{1, \ldots, m\}$, the activation operator R_i in the i-th layer of T satisfies the symmetry relation (3.2) where $c_i \in \mathbb{R}^{N_i}$ and $d_i \in \mathbb{R}^{N_i}$. Let \widetilde{T} be the neural network of $\mathcal{N}_{m,\mathcal{A}}^+$ associated with T whose bias vectors $(\widetilde{b}_i)_{1 \leq i \leq m}$ are linked to those $(b_i)_{1 \leq i \leq m}$ of T by the relations

221 (3.16)
$$(\forall i \in \{1, \dots, m\}) \quad \widetilde{b}_i = \begin{bmatrix} b_i - W_i^- d_{i-1} \\ c_i - b_i - W_i^+ d_{i-1} \end{bmatrix},$$

$$\widetilde{b}_{m+1} = -\frac{d_m}{2},$$

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with $d_0 = 0$. Then, for every input, \widetilde{T} delivers the same output as T.

The proof of this proposition is provided in Appendix A. An illustration of the link between fully-connected layers and ABBA matrices is shown in Figure 1.

3.5. Expressivity of non-negative ABBA networks. One of the main advantages of non-negative ABBA networks with respect to standard networks with non-negative weights is that they are universal approximators. More specifically, we have the following result.

Proposition 3.7. Let $(n_e, n_r) \in (\mathbb{N} \setminus \{0\})^2$. Let $f: \mathbb{R}^{n_e} \to \mathbb{R}^{n_r}$ be a continuous function. Let \mathbb{K} be any nonempty compact subset of \mathbb{R}^{n_e} and let $\epsilon \in]0, +\infty[$.

(i). Let $\rho \colon \mathbb{R} \to \mathbb{R}$ be a symmetric non polynomial activation function. There exists a network $\widetilde{T} \in \mathcal{N}_{1,\mathcal{A}}^+(\rho)$ with $N_0 = n_{\mathrm{e}}$ inputs and $N_2 = n_{\mathrm{r}}$ outputs such that

234 (3.18)
$$(\forall x \in \mathbb{K}) \quad \|\widetilde{T}(x) - f(x)\| < \epsilon.$$

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(ii). Let $\rho \colon \mathbb{R} \to \mathbb{R}$ be a symmetric continuous activation function that is continuously differentiable around at least one point where its derivative is nonzero. Then there exists $m \geqslant 3$ and $\widetilde{T} \in \mathcal{N}_{m,\mathcal{A}}^+(\rho)$ with $N_0 = n_{\rm e}$ inputs, $N_{m+1} = n_{\rm r}$ outputs, and $2N_i = 2(n_{\rm e} + n_{\rm r} + 2)$ neurons in every layer $i \in \{1, \ldots, m\}$ such that (3.18) holds.

Proof. Proposition 3.6 shows that non-negative ABBA networks can be as expressive as signed networks. Combining this fact with existing universal approximation results for signed networks (see [28] for (i) and [22] for (ii)) allows us to deduce these results.

- (i) addresses the case of shallow wide networks where the number of neurons in the hidden layer can be arbitrarily large, while (ii) corresponds to the case of deep networks having a limited number of neurons per layer. An illustration of these results is provided in Appendix SM7.
- 3.6. Lipschitz bounds for ABBA fully-connected networks. As mentioned in the previous sections, the robustness of neural networks with respect to adversarial perturbations can be evaluated through their Lipschitz constant. However, most of the existing techniques for computing a tight estimate of the constant have a high computational complexity for deep or wide networks, whereas simpler upper bounds may turn out to be over-pessimistic.

Nevertheless, in the context of non-negative weighted neural networks [10] proved that tight approximations to the Lipschitz constant can be achieved. In the following, we extend this result and show that we can derive a simple expression for the Lipschitz constant, using a separable bound, for non-negative ABBA networks.

Proposition 3.8. Let $m \in \mathbb{N} \setminus \{0\}$ and let $\widetilde{T} \in \mathcal{N}_{m,\mathcal{A}}^+$ be given by (3.7)-(3.11). Assume that, for every $i \in \{1, \dots, m-1\}$, \widetilde{R}_i is a nonexpansive operator operating componentwise. A Lipschitz constant of \widetilde{T} is

256 (3.19)
$$\theta_m = \|\widetilde{W}_{m+1}\| \|\mathfrak{S}(\widetilde{W}_m) \cdots \mathfrak{S}(\widetilde{W}_1)\| \|\widetilde{W}_0\|.$$

The proof of this result is detailed in Appendix B. Note that this bound expression could be easily extended to other norms based on the results in [10].

A standard separable upper bound for the Lipschitz constant [49] for the ABBA network \widetilde{T} considered in the previous proposition is

$$\overline{\theta}_m = \|\widetilde{W}_{m+1}\| \|\widetilde{W}_m\| \cdots \|\widetilde{W}_1\| \|\widetilde{W}_0\|.$$

262 According to Proposition 3.3(vii), this bound reads also

263 (3.21)
$$\overline{\theta}_m = \|\widetilde{W}_{m+1}\| \|\mathfrak{S}(\widetilde{W}_m)\| \cdots \|\mathfrak{S}(\widetilde{W}_1)\| \|\widetilde{W}_0\|,$$

264 which, by simple norm inequalities, is looser than θ_m .

265 If T is the feedforward network defined in Model 3.1 and we apply Proposition 3.8 to the 266 associated non-negative ABBA network \widetilde{T} of Definition 3.5. We have

267 (3.22)
$$\|\widetilde{W}_0\| = \|\widetilde{W}_0^{\top} \widetilde{W}_0\|^{1/2} = \|2 I_{N_0}\|^{1/2} = \sqrt{2}$$

268 and

269 (3.23)
$$\|\widetilde{W}_{m+1}\| = \|\widetilde{W}_{m+1}\widetilde{W}_{m+1}^{\top}\|^{1/2} = \frac{1}{\sqrt{2}}.$$

270 In turn, for every $i \in \{1, \dots, m\}$,

271 (3.24)
$$\mathfrak{S}(\widetilde{W}_i) = W_i^+ + W_i^- = |W_i|.$$

where $|W_i|$ is the matrix whose elements are the absolute values of W_i . Hence the Lipschitz constant

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of \widetilde{T} in (3.19) reduces to

274 (3.25)
$$\theta_m = |||W_m| \dots |W_1|||.$$

- It then follows from Proposition 3.6 that θ_m is also a Lipschitz constant of T when using symmetric activation functions. Note that this bound was actually already derived in [10, Proposition 5.12].
- 4. Convolutional networks. We will now extend the results presented in Section 3 to convolutional layers.
- 4.1. ABBA convolutional layers. For any $i \in \{1, ..., m\}$, W_i is a convolutional layer with
- 280 $\zeta_{i-1} \in \mathbb{N} \setminus \{0\}$ input channels, ζ_i output channels, kernels $(w_{i,q,p})_{1 \leqslant p \leqslant \zeta_{i-1}, 1 \leqslant q \leqslant \zeta_i}$, and stride $s_i \in \mathbb{N} \setminus \{0\}$.
- The output $(y_q)_{1 \le q \le \zeta_i}$ of this layer (prior applying any activation operation) is linked to its input
- 282 $(x_p)_{1 \le p \le \zeta_{i-1}}$ by

283 **(4.1)**
$$(\forall q \in \{1, \dots, \zeta_i\}) \quad u_q = \sum_{p=1}^{\zeta_{i-1}} w_{i,q,p} * x_p$$

$$y_q = (u_q)_{\downarrow_{s_i}}.$$

- Hereabove, for every $p \in \{1, \dots, \zeta_{i-1}\}$, $x_p = (x_p(\mathbf{n}))_{\mathbf{n} \in \mathbb{Z}^d}$ designates a d-dimensional discrete signal.
- Dimension d=1 corresponds to 1D signals and d=2 to images. A similar notation is used for other
- signals, in particular u_q and $w_{i,q,p}$ with $q \in \{1,\ldots,\zeta_i\}$. The d-dimensional discrete convolution is
- denoted by * and $(\cdot) \downarrow_{s_i}$ is the decimation (or subsampling) by a factor s_i .
- The ABBA convolutional layer \widetilde{W}_i associated with W_i has twice the number of input channels
- and twice the number of output ones. More specifically, its input consists of ζ_{i-1} signals $(\widetilde{x}_p^+)_{1 \leqslant p \leqslant \zeta_{i-1}}$
- and ζ_{i-1} signals $(\widetilde{x}_p^-)_{1\leqslant p\leqslant \zeta_{i-1}}$. Similarly, its output consists of ζ_i signals $(\widetilde{y}_q^+)_{1\leqslant q\leqslant \zeta_i}$ and ζ_i signals
- 293 $(\widetilde{y}_q^-)_{1\leqslant q\leqslant \zeta_i}$. To make the input-output relations more explicit, let us define the kernels $w_{i,q,p}^+$ and $w_{i,q,p}^-$
- analogously to the fully connected case:

$$(\forall \mathbf{n} \in \mathbb{Z}^d) \quad w_{i,q,p}^+(\mathbf{n}) = \begin{cases} w_{i,p,q}(\mathbf{n}) & \text{if } w_{i,p,q}(\mathbf{n}) > 0\\ 0 & \text{otherwise,} \end{cases}$$

286 (4.2)
$$w_{i,q,p}^{-}(\mathbf{n}) = w_{i,q,p}^{+}(\mathbf{n}) - w_{i,p,q}(\mathbf{n}).$$

298 Then the outputs of the ABBA layer are linked to its inputs by the following relations

$$(\forall q \in \{1, \dots, \zeta_i\}) \quad \widetilde{u}_q^+ = \sum_{p=1}^{\zeta_{i-1}} w_{i,q,p}^+ * \widetilde{x}_p^+ + \sum_{p=1}^{\zeta_{i-1}} w_{i,q,p}^- * \widetilde{x}_p^-$$

300 (4.3)
$$\widetilde{u}_{q}^{-} = \sum_{p=1}^{\zeta_{i-1}} w_{i,q,p}^{-} * \widetilde{x}_{p}^{+} + \sum_{p=1}^{\zeta_{i-1}} w_{i,q,p}^{+} * \widetilde{x}_{p}^{-}$$

$$\widetilde{y}_q^+ = (\widetilde{u}_q^+)_{\downarrow_{s_i}}$$

$$\widetilde{y}_q^- = (\widetilde{u}_q^-)_{\downarrow_{s_i}}.$$

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The above equations provide the general form of a convolutional ABBA layer when relaxing (4.2). 304

An alternative formulation of convolutional layers in a matrix form, along with its correspondent d-dimensional spectral representation, is possible (see Appendix SM3). This basically amounts to characterize layer (4.1) by the following matrices

308 (4.4)
$$(\forall \mathbf{n} \in \mathbb{Z}^d) \quad \mathbf{W}_i(\mathbf{n}) = \begin{bmatrix} w_{i,1,1}(\mathbf{n}) & \dots & w_{i,1,\zeta_{i-1}}(\mathbf{n}) \\ \vdots & & \vdots \\ w_{i,\zeta_{i},1}(\mathbf{n}) & \dots & w_{i,\zeta_{i},c_{i-1}}(\mathbf{n}) \end{bmatrix} \in \mathbb{R}^{\zeta_i \times \zeta_{i-1}},$$

- defining the so-called MIMO impulse response of W_i , which plays a prominent role in dynamical
- system theory [52]. The MIMO impulse response of the ABBA layer $\widetilde{\mathcal{W}}_i$ is then characterized by ABBA 310
- 311 matrices:

312 (4.5)
$$(\forall \mathbf{n} \in \mathbb{Z}^d) \quad \widetilde{\boldsymbol{W}}_i(\mathbf{n}) = \begin{bmatrix} \boldsymbol{W}_i^+(\mathbf{n}) & \boldsymbol{W}_i^-(\mathbf{n}) \\ \boldsymbol{W}_i^-(\mathbf{n}) & \boldsymbol{W}_i^+(\mathbf{n}) \end{bmatrix} \in [0, +\infty[^{(2\zeta_i) \times (2\zeta_{i-1})},$$

- where $\boldsymbol{W}_{i}^{+}(\mathbf{n}) = (w_{i,q,p}^{+}(\mathbf{n}))_{1\leqslant q\leqslant \zeta_{i},1\leqslant p\leqslant \zeta_{i-1}} \in [0,+\infty[^{\zeta_{i}\times\zeta_{i-1}} \text{ and } \boldsymbol{W}_{i}^{-}(\mathbf{n}) = (w_{i,q,p}^{-}(\mathbf{n}))_{1\leqslant q\leqslant \zeta_{i},1\leqslant p\leqslant \zeta_{i-1}} \in [0,+\infty[^{\zeta_{i}\times\zeta_{i-1}} \text{ This alternative view will be useful in the following } \boldsymbol{W}_{i}^{-}(\mathbf{n})$
- 315 sections.
- 4.2. Lipschitz bounds for convolutional networks. In this section, we establish bounds on 316
- the Lipschitz constant of an m-layer convolutional neural network T. Each linear operator W_i 317
- corresponding to layer $i \in \{1, ..., m\}$ will be defined by (4.1). We also define a variable 318

319 (4.6)
$$\sigma_i = \prod_{l=1}^i s_l$$

- aggregating strides from layer 1 to layer i. Subsequently, we will assume that, for every $i \in \{1, \dots, m\}$, 320
- the activation operators $(R_i)_{1 \le i \le m}$ are nonexpansive operators. Moreover, these operators are applied 321
- componentwise (see Appendix SM1). This means that, for every $i \in \{1, \dots, m-1\}$, there exists a 322
- function ρ_i from $\mathbb R$ to $\mathbb R$ such that 323

$$(\forall \mathbf{x} \in \mathcal{H}_i) \quad \mathbf{y} = R_i(\mathbf{x})$$

325 (4.7)
$$\Leftrightarrow (\forall p \in \{1, \dots, c_i\})(\forall \mathbf{n} \in \mathbb{Z}^d) \quad y_p(\mathbf{n}) = \rho_i(x_p(\mathbf{n})).$$

- In Appendix SM4, we derive frequency-based expressions allowing us to calculate bounds on 327
- the Lipschitz constant of T. For accurate numerical evaluations, the frequency transform in these 328 expressions has to be replaced by a Discrete Fourier Transform involving a significant number of 329
- frequency bins (e.g., 128^d). Due to this fact, a computation bottleneck occurs when MIMO filters 330
- are characterized by a large number of input/output channels (e.g., for 2D applications). In the 331
- following, we provide an alternative lower-complexity formulation for computing bounds of the 332
- Lipschitz constant. In the case of non-negative kernels, we show that this bound is tight. 333
- Theorem 4.1. Let $(\sigma_i)_{1 \leq i \leq m}$ be the aggregated stride factors of network T, as defined by (4.6), and 334
- let 335

336 (4.8)
$$W = (W_m)_{\uparrow \sigma_{m-1}} * \cdots * (W_2)_{\uparrow \sigma_1} * W_1$$

337 where $(W_i)_{1\leqslant i\leqslant m}$ are the MIMO impulse responses of each layer of network T and, for every $i\in$

338 $\{2,\ldots,m\}$, $(\mathbf{W}_i)_{\uparrow\sigma_{i-1}}$ is the interpolated sequence by a factor σ_{i-1} of \mathbf{W}_i (see (SM3.9)). For every

339 $\mathbf{j} \in \mathbb{S}(\sigma_m) = \{0, \dots, \sigma_m - 1\}^d$, we define the following matrix:

340 (4.9)
$$\overline{W}^{(\mathbf{j})} = \sum_{\mathbf{n} \in \mathbb{Z}^d} W(\sigma_m \mathbf{n} + \mathbf{j}) \in [0, +\infty[^{\zeta_m \times \zeta_0}].$$

341 Then

342 (4.10)
$$\theta_m = \left\| \sum_{\mathbf{j} \in \mathbb{S}(\sigma_m)} \overline{\boldsymbol{W}}^{(\mathbf{j})} (\overline{\boldsymbol{W}}^{(\mathbf{j})})^\top \right\|^{1/2}$$

- is a lower bound on the Lipschitz constant estimate of network T. In addition, if for every $i \in \{1, \ldots, m\}$,
- 344 $p \in \{1, \ldots, \zeta_{i-1}\}$, and $q \in \{1, \ldots, \zeta_i\}$, $w_{i,q,p} = (w_{i,q,p}(\mathbf{n}))_{\mathbf{n} \in \mathbb{Z}^d}$ is a non-negative kernel, then θ_m is a
- 345 *Lipschitz constant of* T.
- 346 The proof of Theorem 4.1 is given in Appendix C.
- The constant θ_m in (D.4) is actually equal to the one calculated in Appendix SM4. The following majorization if thus obtained (see (SM4.4)):

349 (4.11)
$$\theta_m \leqslant \overline{\theta}_m = \|\mathcal{W}_m\| \cdots \|\mathcal{W}_1\|.$$

- 350 By applying Theorem 4.1 to each individual layer $(W_i)_{1 \le i \le m}$ assumed to be with non-negative kernels,
- 351 we get the following expression for the upper-bound:

352 (4.12)
$$\overline{\theta}_m = \prod_{i=1}^m \left\| \sum_{\mathbf{j} \in \mathbb{S}(s_i)} \overline{\boldsymbol{W}}_i^{(\mathbf{j})} (\overline{\boldsymbol{W}}_i^{(\mathbf{j})})^\top \right\|^{1/2},$$

353 where

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354 (4.13)
$$(\forall i \in \{1, \dots, m\}) (\forall \mathbf{j} \in \mathbb{S}(s_i)) \qquad \overline{\boldsymbol{W}}_i^{(\mathbf{j})} = \sum_{\mathbf{n} \in \mathbb{Z}^d} \boldsymbol{W}_i(s_i \mathbf{n} + \mathbf{j}).$$

- The bound $\bar{\theta}_m$ is generally more tractable than θ_m since it separates the influence of each layer and does not require to compute the global matrix sequence W as expressed by (4.8). However, such
- separable bounds are usually loose. According to our observations, it turns out that, in the special
- case of convolutional layers with non-negative kernels, θ_m and $\overline{\theta}_m$ are quite close (see numerical tests in Appendix SM5).
- To illustrate these results, the computation of the Lipschitz bound of a layer corresponding to an average pooling is presented as an example in Appendix SM6.
 - 4.3. Bounds for ABBA convolutional networks. Let us extend the previous results to the ABBA context. The linear operators of the considered ABBA network \widetilde{T} are denoted by $(\widetilde{\mathcal{W}}_i)_{0\leqslant i\leqslant m+1}$. The weights in $\widetilde{\mathcal{W}}_0$ and $\widetilde{\mathcal{W}}_{m+1}$ are signed, whereas $(\widetilde{\mathcal{W}}_i)_{1\leqslant i\leqslant m}$ are convolutional layers with d-dimensional non-negative kernels. More precisely, we assume that, for every $i\in\{1,\ldots,m\}$, the i-th layer of the ABBA network has $2\zeta_{i-1}$ input channels, $2\zeta_i$ output channels, and stride $s_i\in\mathbb{N}\setminus\{0\}$. The MIMO impulse response of such a layer is of the form (4.5). We make the same assumptions of nonexpansiveness and separability for the activation operators as in the previous section. We recall that $(\boldsymbol{W})_{\uparrow\sigma}$ denotes the interpolated version by a factor σ of a MIMO impulse response $\boldsymbol{W}=\left(\boldsymbol{W}(\mathbf{n})\right)_{\mathbf{n}\in\mathbb{Z}^d}$. The following result is then established in Appendix D:

Theorem 4.2. Under the above assumptions on the convolutional ABBA network \widetilde{T} , let

372 (4.14)
$$(\forall i \in \{1, \dots, m\}) (\forall \mathbf{j} \in \mathbb{S}(s_i)) \quad \Omega_i^{(\mathbf{j})} = \sum_{\mathbf{n} \in \mathbb{Z}^d} \mathfrak{S}(\widetilde{\boldsymbol{W}}_i(s_i \mathbf{n} + \mathbf{j})) \in [0, +\infty[^{\zeta_i \times \zeta_{i-1}}, \mathbf{n}])$$

373 where $(\widetilde{\boldsymbol{W}}_i(\mathbf{n}))_{n\in\mathbb{Z}}$ is the MIMO impulse response of the ABBA layer of index i. Then a Lipschitz constant 374 of \widetilde{T} is

375 (4.15)
$$\overline{\theta}_m = \|\widetilde{W}_{m+1}\| \left(\prod_{i=1}^m \left\| \sum_{\mathbf{j} \in \mathbb{S}(s_i)} \Omega_i^{(\mathbf{j})} \left(\Omega_i^{(\mathbf{j})} \right)^\top \right\| \right)^{1/2} \|\widetilde{W}_0\|,$$

- where $\|\widetilde{W}_{m+1}\|$ (resp. $\|\widetilde{W}_0\|$) is the spectral norm of the linear operator employed in the last (resp. first layer).
- The bound (4.15) will be subsequently used to control the Lipschitz constant of non-negative ABBA networks during their training.
 - 5. Lipschitz-constrained training. The theoretical bounds established in the previous sections provide a relatively easy way of computing a tight estimate of the global Lipschitz constant. We propose a simple approach to control it during the training phase. Since our networks contain mostly layers having non-negative weights and a few layers having arbitrary-signed weights, their Lipschitz constant will be controlled separately and different constraint sets will be handled for each case.

To train a robust ABBA network, we employ a projected version of the well-known ADAM optimizer. Each layer i is parameterized by a vector Ψ_i . In the case of a dense layer, Ψ_i is a vector gathering the elements of weight matrix \widetilde{W}_i , the components of the associated bias \widetilde{b}_i , and a possible additional parameter that will be introduced hereafter. For an ABBA layer, Ψ_i is thus a vector of dimension $2N_i(N_{i-1}+1)$ or $2N_i(N_{i-1}+1)+1$. In the context of a 2D convolutional layer, an array w_i of scalar convolutional kernels is substituted for the weight matrix. In the ABBA case, we have $2\zeta_i\zeta_{i-1}$ such kernels. To ensure nonnegativity (if needed) and Lipschitz bound conditions on the weight operator, we project Ψ_i onto a suitable closed and convex constraint set. Considering pairs $(z_k)_{1\leqslant k\leqslant K}$ of inputs images and their associated labels, the operations performed at each epoch n>0 to minimize a loss function ℓ are presented in Algorithm 5.1. After each iteration t of the optimizer, we perform a projection $\operatorname{proj}_{S_{i,t}}$ onto a constraint set $S_{i,t}$ The definition of this set and the corresponding method for managing the projection is detailed in the following, according to the network type.

Handling Lipschitz constants for fully-connected layers. Consider the network defined by Model (3.5). In the case of fully connected networks, the Lipschitz constant is given by Proposition 3.8, which basically splits the bound into three terms: the first and the last account for the starting and ending layers, respectively, while the middle one encompasses all the ABBA layers. For the two former arbitrary-signed layers, we control the Lipschitz constants individually during training, by imposing a bound on each weight matrix spectral norm. This defines the following two constraints:

403 (5.1)
$$(\forall i \in \{0, m+1\}) \quad ||\widetilde{W}_i|| \leqslant \overline{\theta}_{m,i},$$

where $\overline{\theta}_{m,i}$ is the imposed Lipschitz bound for the *i*-th layer. To deal with this constraint, we decompose the weight matrix as $\widetilde{W}_i = \overline{\theta}_{m,i}\widetilde{W}'_i$, which yields the constraint set

406 (5.2)
$$(\forall i \in \{0, m+1\})$$
 $S_{i,t} = \{\widetilde{W}'_i \mid ||\widetilde{W}'_i|| \le 1\}.$

The projection onto $S_{i,t}$ is performed by clipping the singular values of \widetilde{W}'_i to 1.

In our proposed training procedure, we set $\overline{\theta}_{m,0}\overline{\theta}_{m,m+1}=1$. This gives the network one degree of freedom to automatically adapt the value of the Lipschiz constant of these two layers. To do so, we adopt the following parametrization

411 (5.3)
$$\overline{\theta}_{m,0} = \exp(\alpha), \quad \overline{\theta}_{m,m+1} = \exp(-\alpha),$$

- where $\alpha \in \mathbb{R}$ is a trainable parameter. It constitutes an extra component of the vector Ψ_i when $i \in \{0, m+1\}$.
- In the case of ABBA dense layers, we need to handle two requirements: ensure that, for every $i \in \{1,\ldots,m\}$, \widetilde{W}_i is a non-negative ABBA matrix, and to constrain the product of all the weight matrices to be such that $\|\widetilde{W}_m \cdots \widetilde{W}_1\| \leq \overline{\theta}_m$. Since $\overline{\theta}_{m,0}\overline{\theta}_{m,m+1} = 1$, $\overline{\theta}_m$ corresponds to the target
- Lipschitz bound for the ABBA network.

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For every $i \in \{1, ..., m\}$, \widetilde{W}_i is parameterized by W_i^+ and W_i^- . We define the following two constraint sets:

420 (5.4)
$$\mathcal{D}_i = \{ (W_i^+, W_i^-) \in (\mathbb{R}^{N_i \times N_{i-1}})^2 \mid W_i^+ \geqslant 0 \text{ and } W_i^- \geqslant 0 \},$$

421 (5.5)
$$C_{i,t} = \left\{ (W_i^+, W_i^-) \in (\mathbb{R}^{N_i \times N_{i-1}})^2 \mid \left\| A_{i,t} \begin{bmatrix} W_i^+ & W_i^- \\ W_i^- & W_i^+ \end{bmatrix} B_{i,t} \right\| \leqslant \overline{\theta}_m \right\}.$$

- Here-above, matrix $A_{i,t}$ (resp. $B_{i,t}$) is an ABBA matrix, which is the product of the weight matrices for the posterior (resp. previous layers). In this case, $S_{i,t} = \mathcal{D}_i \cap C_{i,t}$. To perform the projection onto the intersection of these two sets, we use an instance of the proximal algorithm presented in [35], which alternates between elementary projections onto \mathcal{D}_i and projections onto the spectral ball with center 0 and radius $\bar{\theta}_m$. Because of Proposition 3.3(xii), the latter projection allows us to keep the structure of ABBA matrices.
- Handling Lipschitz constants for convolutional layers. In the case of convolutional ABBA networks, we derived the bound in (4.15) which consists of the product of m+2 terms. The Lipschitz bound constraint is managed by introducing auxiliary variables $(\overline{\theta}_{m,i})_{0\leqslant i\leqslant m+1}$ defining upper bounds for each layer. At iteration t of the algorithm estimates $(\overline{\theta}_{m,i,t})_{0\leqslant i\leqslant m+1}$ of the auxiliary bounds are updated. Similarly to the fully connected case, we use two different types of constraints.
- For the *i*-th ABBA convolutional layer with $i \in \{1, ..., m\}$, we consider the constraint set

435 (5.6)
$$C_{i,t} = \{ \mathcal{W}_i \mid \left\| \sum_{\mathbf{j} \in \mathbb{S}(s_i)} \Omega_i^{(\mathbf{j})} \left(\Omega_i^{(\mathbf{j})} \right)^\top \right\| \leqslant \overline{\theta}_{m,i,t}^2 \}$$

- 436 where matrices $(\Omega_i^{(\mathbf{j})})_{\mathbf{j} \in \mathbb{S}(s_i)}$ are linked to the convolution kernels by the linear relation (4.14). By
- concatenating all these s_i^d matrices horizontally, we obtain a rectangular matrix Ω_i which allows us to
- 438 reexpress (5.6) in the simpler form:

439 (5.7)
$$C_{i,t} = \{ \mathcal{W}_i \mid ||\Omega_i|| \leqslant \overline{\theta}_{m,i,t} \}.$$

- 440 We also have to impose the non-negativity of the filters alongside the stability bound. This corresponds
- 441 to a constraint set \mathcal{D}_i . Projecting onto $\mathcal{S}_{i,t} = \mathcal{C}_{i,t} \cap \mathcal{D}_i$ is performed by using the same iterative proximal
- 442 algorithm as previously.

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457 458 For the first and the last layers, we impose similarly that $\|\mathcal{W}_i\| \leq \overline{\theta}_{m,i,t}$ with $i \in \{0, m+1\}$. Since the kernels are signed, we resort a frequency formulation (see (SM4.18)) to estimate the spectral norm of the convolutional operator. The procedure we use is described in Appendix SM8.

Convolutional layers are usually succeeded by an ABBA fully connected network. This part will be handled as explained previously. However, we need to set the upper bounds $(\bar{\theta}_{m,i,t})_{0 \leqslant i \leqslant m+1}$ used in the convolutional part and the upper bound of the ABBA fully connected part. With a slight abuse of notation, let us denote this latter bound by $\bar{\theta}_{m,m+2,t}$, while the target Lipschitz constant for the global network is still denoted by $\bar{\theta}_m$. We have to deal with the following constraint:

451 (5.8)
$$\prod_{i=0}^{m+2} \overline{\theta}_{m,i,t} = \overline{\theta}_m.$$

We proceed by computing the Lipschitz constants $(\widetilde{\theta}_{m,i,t})_{0 \leqslant i \leqslant m+2}$ of the layers after the ADAM update.

453 Then, we set

$$(\forall i \in \{0, \dots, m+2\}) \quad \overline{\theta}_{m,i,t} = \widetilde{\theta}_{m,i,t} \left(\frac{\overline{\theta}_m}{\prod_{i'=0}^{m+2} \widetilde{\theta}_{m,i',t}}\right)^{\frac{1}{m+3}},$$

which guarantees that (5.8) holds. Update (5.9) can be interpreted as the orthogonal projection onto the constraint set defined by (5.8) after a logarithmic transform of the auxiliary variables. The benefit of such a transform is to convexify the constraint.

Algorithm 5.1 Projected ADAM Algorithm $\Psi_{i,t}$ – weights of layer i at iteration t $(z_k)_{1 \leqslant k \leqslant K}$ – set of input image-label pairs β_1, β_2 – ADAM hyperparameters Partition $\{1, \dots, K\}$ into mini-batches $(\mathbb{M}_{q,n})_{1 \leqslant q \leqslant Q}$ t = (n-1)Q + q# sweep mini-batches for $q \in \{1, ..., Q\}$ do **for** layer i **do** $g_{i,t} = \sum_{k \in \mathbb{M}_{q,n}} \nabla_i \ell(z_k, (\Psi_{i,t})_{1 \le i \le m})$ $\mu_{i,t} = \beta_1 \mu_{i,t-1} + (1 - \beta_1) g_{i,t}$ $\nu_{i,t} = \beta_2 \nu_{i,t-1} + (1 - \beta_2) g_{i,t}^2$ $\gamma_t = \gamma \sqrt{1 - \beta_2^t} / (1 - \beta_1^t)$ $\widetilde{\Psi}_{i,t} = \Psi_{i,t} - \gamma_t \mu_{i,t} / (\sqrt{\nu_{i,t}} + \epsilon)$ end for **for** layer i **do** $\Psi_{i,t+1} = \operatorname{proj}_{\mathcal{S}_{i,t}}(\widetilde{\Psi}_{i,t})$ end for end for

Dataset	Network	Architecture	Accuracy [%]
MNIST	ABBA	Dense	98.33
		Conv	98.70
	Non-Negative	Dense	94.95
		Conv	93.27
	Baseline	Dense	98.35
		Conv	98.68
FMNIST	ABBA	Dense	90.02
		Conv	90.17
	Non-Negative	Dense	84.56
		Conv	83.09
	Baseline	Dense	90.00
		Conv	90.20
RPS	ABBA	Conv	99.08
	Non-Negative	Conv	67.30
	Baseline	Conv	98.86
CelebA	ABBA	Conv	90.21
	Non-Negative	Conv	61.04
	Baseline	Conv	90.17

Table 1: Comparison between ABBA, full non-negative and arbitrary-signed (baseline) networks.

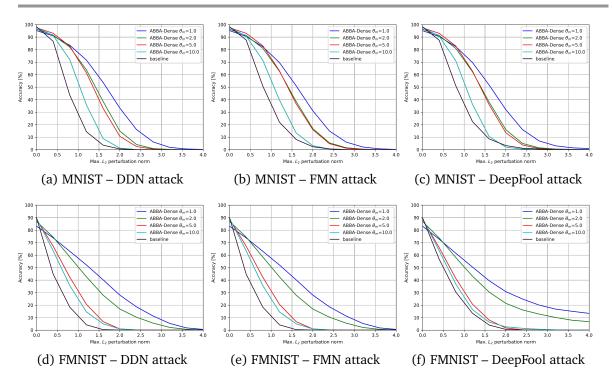


Figure 2: Accuracy vs. Perturbation for different Lipschitz constants – Dense Architecture.

- 6. Experiments. In this section, we show the versatility of ABBA neural networks in solving classification tasks. The objective of our experiments is three-fold:
 - (i). First, we compare positive ABBA structures with their classic non-negative counterparts and check that our method yields significantly better results in all considered cases.
 - (ii). We then train ABBA models constrained to different Lipschitz bound values and evaluate their robustness against several adversarial attacks.
 - (iii). Finally, we compare our proposed approach with three other well-established defense strategies, namely *Adversarial Training* (AT), *Trade-off-inspired adversarial defense* (TRADES) [59], *Deel-Lip* proposed by [45], and *orthonormalization* [2].

We validate our ABBA networks on four benchmark image classification datasets: MNIST, its more complex variant Fashion MNIST ⁴, a variant ⁵ of the Rock-Paper-Scissors (RPS) dataset [34], and a binary classification on CelebA [31]. For the last dataset, inspired from [45] where eyeglass detection is performed, we specialized our models on a different attribute, namely to identify whether a person is bald or not. To explore the features of different ABBA network topologies, we experiment with two main types of ABBA architectures: one having only fully-connected layers, further referred to as *ABBA Dense*, and another one which includes a convolutional part for feature extraction, followed by a fully connected classification module, *ABBA Conv*. Depending on the dataset, the particularities of each

⁴https://github.com/zalandoresearch/fashion-mnist

⁵https://github.com/DrGFreeman/rps-cv

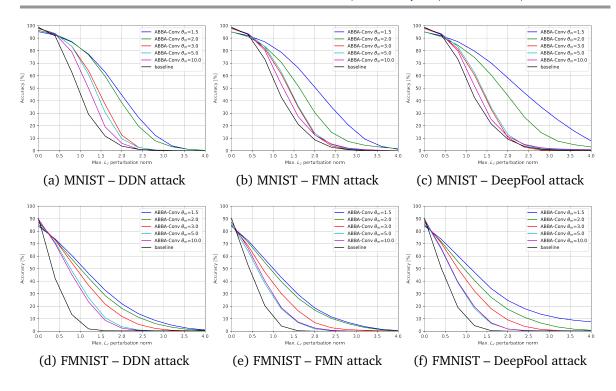


Figure 3: Acc. vs. Perturbation for different Lipschitz constants ABBA Conv Architectures – MNIST and FMNIST.

architecture are slightly different. A detailed description of all the small networks employed in this work, as well as other training details, are provided in Appendix SM9. For all experiments, the input images were scaled in the [-1,1] interval.

ABBA networks vs. non-negative networks. First, we compare our non-negative ABBA networks with standard ones trained under non-negativity constraints. We consider standard neural networks having the same number of parameters as their ABBA equivalent. The results are summarized in Table 1, indicating that ABBA neural networks yield far superior results, in all cases. In the case of fully connected architectures, the difference in terms of accuracy is around $\sim 3\%$ and $\sim 5\%$ for MNIST and FMNIST, respectively. The difference is even higher when we consider Conv architectures (e.g. $\sim 5\%$, $\sim 7\%$, $\sim 31\%$ and $\sim 32\%$ for MNIST, FMNIST, RPS, and CelebA, respectively). This shows that standard non-negative convolutional kernels are often suboptimal for extracting relevant information from image data. On the other hand, training standard neural networks having arbitrary-signed weights gives results very similar to their ABBA equivalents in all the cases, showing that ABBA networks do not suffer from these shortcomings. These results are in agreement with Proposition 3.6.

Stability vs. Performance. According to the "no free lunch" theorem [51], stability guarantees may impact the system performance on clean data. In this work, we train several models by following the approach described in Section 5. The Lipschitz constant of the network is varied in an effort to find the optimal trade-off between robustness and classification accuracy. This compromise is usually use-case specific, depending on the architecture complexity and on the dataset particularities, so the

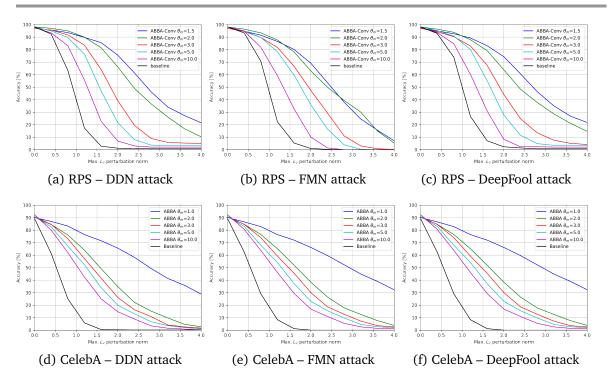


Figure 4: Acc. vs. Perturbation for different Lipschitz constants ABBA Conv Architectures – RPS and CelebA.

tightness of the imposed stability bound must be chosen accordingly. In our experiments, we limited the maximum Lipschitz constant we impose, so that the drop in performance does not exceed 5% of the baseline model accuracy (i.e., the model trained without robustness constraints).

Adversarial attack validation. We train several robust ABBA models by varying the global Lipschitz bound $\overline{\theta}_m$. We then evaluate their robustness against inputs corrupted with different levels of adversarial perturbations, by studying their influence on the overall performance of the system. To create the adversarial perturbations, we use three white-box attackers as described next. **DDN** [42] is a gradient-based ℓ_2 adversarial attack method that seeks to decouple the direction and norm of the additive perturbation. By doing so, this attack is able to generate effective examples, while requiring fewer iterations than other methods. **DeepFool** [33] considers a linear approximation to the model and refines the attack sample iteratively, by selecting the point that would cross the decision boundary with minimal effort in the logit space. The **FMN** [39] attack improves the approach in DDN by introducing adaptive norm constraints on the perturbation, in order to balance the trade-off between the magnitude of the perturbation and the level of miss-classification. This results in a powerful attack that is able to generate adversarial examples with small perturbation levels.

For a given maximum ℓ_2 perturbation norm, we ran each attack for 300 steps, using the default hyperparameters for each of the three attackers. Although all images are normalized in the [-1,1] range, we report the robust accuracy w.r.t. ℓ_2 perturbation measured in [0,1] range, which is the common practice in the literature.

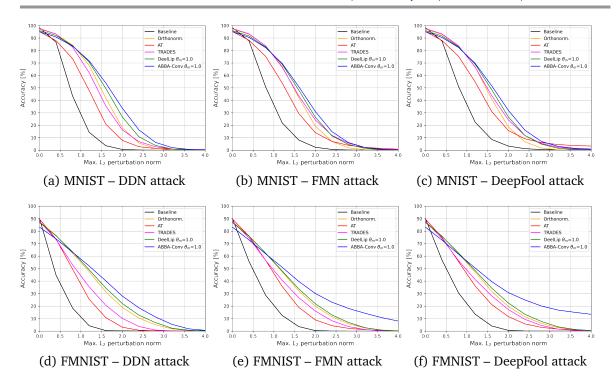


Figure 5: Comparisons with other defense techniques Dense Architectures

The results are summarized in Figures 2, 3, and 4 which show the robustness of MNIST, FMNIST, RPS, and CelebA ABBA models, w.r.t. increasing ℓ_2 norm perturbation, generated with DDN, FMN, and DeepFool attacks. A baseline model, trained without stability constraints and arbitrary-signed weights, is provided as a reference. These graphs could be interpreted as the expected performance of the model if the attack is allowed to influence the input image with an ℓ_2 -norm less than ϵ , where the level of perturbation ϵ varies. For a better understanding of the adversarial perturbation effect, some visual examples of the attacked inputs, for all the datasets, are presented in Appendix SM10.

It can be observed that our robust ABBA models are significantly less affected by adversarial inputs than the undefended baseline. This demonstrates that carefully controlling the Lipschitz constant during training improves the network stability against adversarial attacks. Naturally, as the imposed bound gets lower, the system becomes more robust. Although the difference in robustness between similar values of the Lipschitz constant depends on the intrinsic structure of the dataset, our results show that a good trade-off between robustness and performance can be achieved in all cases.

Comparison with other defense strategies. In the following, we compare our method for training robust models using ABBA networks with other defense strategies. *Deel-Lip*, developed in [45], is a popular Lipschitz-based approach, which uses the spectral normalization of each layer to offer robustness certificates during training. We have also made comparisons with another popular technique to ensure 1-Lipschitz weights, via *orthonormalization* [2, 8]. For our experiments, we

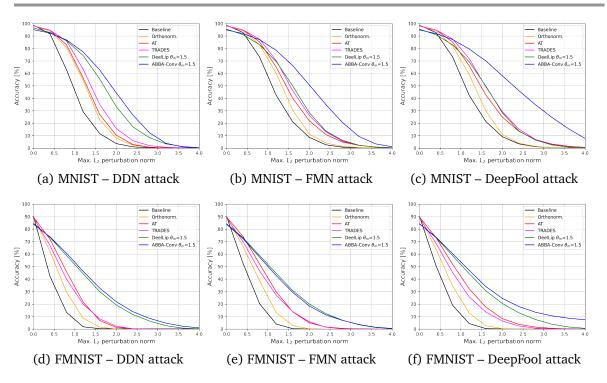


Figure 6: Comparisons with other defense techniques Conv Architectures – MNIST and FMNIST.

trained models from scratch, using the implementation provided by [2] 6 , in order to enforce an l_2 -norm equal to 1 using *Bjorck Orthonormalization*, while also preserving the gradient norm through *GroupSort. TRADES* [59] introduces a robustness regularization term into the training objective. This regularizer encourages the network to have similar predictions on both the original input and its adversarial counterparts. On the other hand, *Adversarial Training* (AT) implies augmenting the training data with adversarial samples, increasing the network generalization capabilities to different input alterations. However, this technique offers weak theoretical stability guarantees, as it is mainly dependent on the strength of the adversary used during training.

For all experiments regarding AT, we used Projected Gradient Descent (PGD) attack to generate the adversarial samples with a perturbation level $\epsilon=0.5$ and then employed the scheduling strategy introduced by [32]. Concerning TRADES, we set $\lambda=1$ for MNIST and FMNIST, and $\lambda=1/2$ for RPS and CelebA datasets. For all the presented techniques we considered the equivalent baseline to each ABBA network.

Comparisons, in the same adversarial set-up as before, are depicted in Figures 5, 6, and 7. We observe that using our theoretically certified Lipschitz bound yields models which are generally more robust than AT and TRADES. For simple datasets, such as MNIST and FMNIST, robust ABBA and Deel-lip models exhibit similar behavior for low-magnitude adversarial attacks, but as we increase the maximum perturbation ϵ , our method performs better. In the case of real-world datasets (RPS and

⁶https://github.com/cemanil/LNets/tree/master

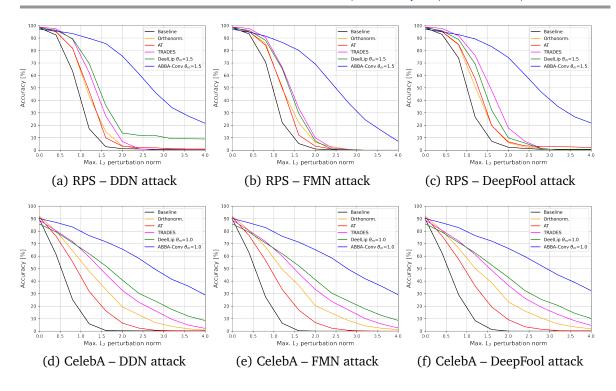


Figure 7: Comparisons with other defense techniques Conv Architectures – RPS and CelebA.

CelebA), ABBA models exhibit high robustness properties against all the tested attacks, showing that our approach allows us to train neural models to reach great stability properties, without losing their generalization power.

Limitations. The main limitation of our method is that non-negative ABBA operators require more parameters to meet the universal approximation conditions. More precisely, for given depth m and number of neurons $(N_i)_{0\leqslant i\leqslant m}$ per layer, a network $\widetilde{T}\in\mathcal{N}_{m,\mathcal{A}}$ has the same number of inputs and outputs as the standard feedfoward network T in Model 3.1. All the layers of \widetilde{T} , except the first one, have however twice more inputs than T. Exact training times are showcased in SM11. Because of the ABBA structure of the weight matrices in (3.11), the maximum number of parameters of \widetilde{T} is $2(N_0^2+\sum_{i=1}^m N_i(N_{i-1}+1)+N_m^2)$ while the number of parameters of T is $\sum_{i=1}^m N_i(N_{i-1}+1)$. By storing $\widetilde{W}_1'=\widetilde{W}_1\widetilde{W}_0\in\mathbb{R}^{(2N_1)\times N_0}$ instead of \widetilde{W}_1 and \widetilde{W}_0 separately, the maximum number of parameters is reduced to $2(\sum_{i=1}^m N_i(N_{i-1}+1)+N_m^2)$. Moreover, since the weights are non-negative, the model does not necessarily require signed representations storage, so the memory space occupied by \widetilde{T} could also be reduced.

While our method does not provide any certification regarding the accuracy of the classifier in adversarial environments, it delivers a certified value for the Lipschitz constant of the network.

7. Conclusions. In this paper, we introduce ABBA networks, a novel class of neural networks where the majority of weights are non-negative. We demonstrate that these networks are universal approximators, possessing all the expressive properties of conventional signed neural architectures.

Additionally, we unveil their remarkable algebraic characteristics, enabling us to derive precise Lipschitz bounds for both fully-connected and convolutive operators. Leveraging these bounds, we construct robust neural networks suitable for various classification tasks.

 The main advantage of ABBA networks is that they enjoy all the properties of non-negative networks (e.g., they are easier to interpret and less prone to overfitting), without suffering from the shortcomings of standard ones (e.g., lack of expressivity). Additionally, we showed that ABBA structures allow tight Lipschitz bounds to be estimated, without requiring to solve an NP-hard problem as for conventional neural networks.

For future research, it would be intriguing to explore the application of ABBA networks in regression problems, where controlling the Lipschitz constant may present more challenges. Also, extending our theoretical bounds to different structures, such as recurrent or attention-based networks, holds promise for further advancements. Moreover, it would be interesting to study if using Lipschitz-constrained ABBA neural networks can improve certified robustness strategies like GloRoNets [27].

Finally, we recognize the necessity of investigating the scalability of the proposed training method to deep architectures. One of the main hurdles in this endeavor is the increased number of parameters that deep ABBA architectures entail.

Acknowledgments. We would like to thank Dr. Jérôme Rony and Prof. Ismail Ben Ayed from ETS Montréal for fruitful discussions and insightful suggestions.

For every $i \in \{1, ..., m\}$, let $x_i = T_i(x_{i-1})$ where Appendix A. Proof of Proposition 3.6. 587 $x_0 \in \mathbb{R}^{N_0}$ is an arbitrary input of network T and $x_m \in \mathbb{R}^{N_m}$ its corresponding output. By using the 588 symmetry properties of the activation operators, for every $i \in \{1, ..., m\}$, we have 589

590
$$(\forall i \in \{1, \dots, m\}) \qquad x_i = R_i(W_i x_{i-1} + b_i)$$
591 **(A.1)**
$$= R_i(W_i^+ x_{i-1} - W_i^- x_{i-1} + b_i),$$
592
$$-x_i = -R_i(W_i x_{i-1} + b_i)$$
593
$$= R_i(-W_i x_{i-1} - b_i + c_i) - d_i$$
584 **(A.2)**
$$= R_i(W_i^- x_{i-1} - W_i^+ x_{i-1} - b_i + c_i) - d_i.$$

By making use of notation (3.14), (A.1) and (A.2) can be rewritten more concisely as 596

597 (A.3)
$$(\forall i \in \{1, \dots, m\}) \quad \begin{bmatrix} x_i \\ -x_i \end{bmatrix} = \widetilde{R}_i \left(\begin{bmatrix} W_i^+ & W_i^- \\ W_i^- & W_i^+ \end{bmatrix} \begin{bmatrix} x_{i-1} \\ -x_{i-1} \end{bmatrix} + \begin{bmatrix} b_i \\ c_i - b_i \end{bmatrix} \right) - \begin{bmatrix} 0 \\ d_i \end{bmatrix}.$$

Let us define, for every $i \in \{0, \dots, m\}$, 598

599 (A.4)
$$\widetilde{x}_i = \begin{bmatrix} x_i \\ -x_i + d_i \end{bmatrix}.$$

Altogether (3.16), (3.11), (3.15), and (A.3) yield

601
$$(\forall i \in \{1, \dots, m\}) \quad \widetilde{x}_i = \widetilde{R}_i \left(\begin{bmatrix} W_i^+ & W_i^- \\ W_i^- & W_i^+ \end{bmatrix} \left(\widetilde{x}_{i-1} - \begin{bmatrix} 0 \\ d_{i-1} \end{bmatrix} \right) + \begin{bmatrix} b_i \\ c_i - b_i \end{bmatrix} \right)$$
602 (A.5)
$$= \widetilde{R}_i \left(\widetilde{W}_i \widetilde{x}_{i-1} + \widetilde{b}_i \right).$$

- This shows that, if $(\widetilde{T}_i)_{1\leqslant i\leqslant m}$ are given by (3.8), $\widetilde{x}_m=\widetilde{T}_m\cdots\widetilde{T}_1(\widetilde{x}_0)$. By using the forms of \widetilde{W}_0 and
- W_{m+1} in (3.13), we deduce that

606 (A.6)
$$x_m = \widetilde{W}_{m+1}\widetilde{x}_m + \widetilde{b}_{m+1} = \widetilde{T}(x_0).$$

Appendix B. Proof for Proposition 3.8. According to [53] [10, Proposition 5.5], 607

608 **(B.1)**
$$\vartheta_{m} = \sup_{\Lambda_{1} \in \mathscr{D}^{2N_{1}}_{\{-1,1\}}} \|\widetilde{W}_{m+1}\Lambda_{m}\widetilde{W}_{m} \cdots \Lambda_{1}\widetilde{W}_{1}\widetilde{W}_{0}\|.$$

$$\vdots$$

$$\Lambda_{m} \in \mathscr{D}^{2N_{m}}_{\{-1,1\}}$$

- where, for every $i \in \{1,\ldots,m\}$, $\mathscr{D}^{2N_i}_{\{-1,1\}}$ designates the space of diagonal matrices of size $(2N_i) \times (2N_i)$ with diagonal entries equal to -1 or 1. For every $(\Lambda_1,\ldots,\Lambda_m) \in \mathscr{D}^{2N_1}_{\{-1,1\}} \times \cdots \times \mathscr{D}^{2N_m}_{\{-1,1\}}$, 610

611 **(B.2)**
$$\|\widetilde{W}_{m+1}\Lambda_{m}\widetilde{W}_{m}\cdots\Lambda_{1}\widetilde{W}_{1}\widetilde{W}_{0}\| \leqslant \|\widetilde{W}_{m+1}\|\|\widetilde{W}_{m}\Lambda_{m-1}\widetilde{W}_{m-1}\cdots\Lambda_{2}\widetilde{W}_{2}\Lambda_{1}\widetilde{W}_{1}\|\|\widetilde{W}_{0}\|.$$

- On the other hand, for every $i \in \{1, ..., m\}$, $\widetilde{W}_i \in [0, +\infty[^{(2N_i)\times(2N_{i-1})}]$. It then follows from [10,
- Proposition 5.10] that 613

614 **(B.3)**
$$\sup_{\substack{\Lambda_1 \in \mathscr{D}_{\{-1,1\}}^{2N_1} \\ \vdots \\ \Lambda_{m-1} \in \mathscr{D}_{\{-1,1\}}^{2N_{m-1}}}} \|\widetilde{W}_m \Lambda_{m-1} \widetilde{W}_{m-1} \cdots \Lambda_2 \widetilde{W}_2 \Lambda_1 \widetilde{W}_1\| = \|\widetilde{W}_m \widetilde{W}_{m-1} \cdots \widetilde{W}_2 \widetilde{W}_1\|.$$

According to Proposition 3.3(iii), $\widetilde{W}_m \widetilde{W}_{m-1} \cdots \widetilde{W}_2 \widetilde{W}_1 \in \mathcal{A}_{N_m,N_0}$. Since this matrix has nonnegative elements, we deduce from Proposition 3.3(vii) that

617
$$\vartheta_{m} \leqslant \|\widetilde{W}_{m+1}\| \|\widetilde{W}_{m} \cdots \widetilde{W}_{1}\| \|\widetilde{W}_{0}\|$$
618
$$= \|\widetilde{W}_{m+1}\| \|\mathfrak{S}(\widetilde{W}_{m} \cdots \widetilde{W}_{1})\| \|\widetilde{W}_{0}\|$$
619
$$= \|\widetilde{W}_{m+1}\| \|\mathfrak{S}(\widetilde{W}_{m}) \cdots \mathfrak{S}(\widetilde{W}_{1})\| \|\widetilde{W}_{0}\|,$$

- where the last equality is also a consequence of Proposition 3.3(iii). This leads to the Lipschitz bound in (3.19).
- 623 Appendix C. Proof of Theorem 4.1.
- Before giving the proof of our main result, we will introduce a link between the Fourier and the spatial representations for a nonnegative convolutional kernel.
- Lemma C.1. Let $(c, c') \in (\mathbb{N} \setminus \{0\})^2$ and let

627 (C.1)
$$(\forall \mathbf{n} \in \mathbb{Z}^d) \quad \boldsymbol{H}(\mathbf{n}) = (h_{q,p}(\mathbf{n}))_{1 \leqslant q \leqslant c', 1 \leqslant p \leqslant c} \in [0, +\infty[^{c' \times c}]$$

- 628 where, for every $p \in \{1, ..., c\}$ and $q \in \{1, ..., c'\}$, $h_{q,p} \in \ell^1(\mathbb{Z}^d)^{-7}$. Then, the Fourier transform \widehat{H} of
- 629 $(\boldsymbol{H}(\mathbf{n}))_{\mathbf{n}\in\mathbb{Z}^d}$ is such that

630 (C.2)
$$\sup_{\boldsymbol{\nu} \in [0,1]^d} \|\widehat{\boldsymbol{H}}(\boldsymbol{\nu})\| = \Big\| \sum_{\mathbf{n} \in \mathbb{Z}^d} \boldsymbol{H}(\mathbf{n}) \Big\|.$$

631 *Proof.* For every $\nu \in [0,1]^d$,

632 (C.3)
$$\widehat{\boldsymbol{H}}(\boldsymbol{\nu}) = \sum_{\mathbf{n} \in \mathbb{Z}^d} \boldsymbol{H}(\mathbf{n}) \exp\left(-i2\pi\pi\mathbf{n}^{\top}\boldsymbol{\nu}\right).$$

633 For every $\mathbf{u} = [u_1, \dots, u_c]^{\top} \in \mathbb{C}^c$, by using the triangle inequality,

634
$$\|\widehat{\boldsymbol{H}}(\boldsymbol{\nu})\mathbf{u}\|^{2} = \sum_{q=1}^{c} \left| \sum_{p=1}^{c} [\boldsymbol{H}(\boldsymbol{\nu})]_{q,p} u_{p} \right|^{2}$$
635
$$= \sum_{q=1}^{c'} \left| \sum_{p=1}^{c} \sum_{\mathbf{n} \in \mathbb{Z}^{d}} h_{q,p}(\mathbf{n}) \exp\left(-i2\pi\mathbf{n}^{\top}\boldsymbol{\nu}\right) u_{p} \right|^{2}$$
636
$$\leqslant \sum_{q=1}^{c'} \left(\sum_{p=1}^{c} \sum_{\mathbf{n} \in \mathbb{Z}^{d}} h_{q,p}(\mathbf{n}) |u_{p}| \right)^{2}$$
637
$$= \left\| \sum_{\mathbf{n} \in \mathbb{Z}^{d}} \boldsymbol{H}(\mathbf{n}) |\mathbf{u}| \right\|^{2}$$
638
$$\leqslant \left\| \sum_{\mathbf{n} \in \mathbb{Z}^{d}} \boldsymbol{H}(\mathbf{n}) \right\|^{2} \left\| |\mathbf{u}| \right\|^{2}$$
639 (C.4)
$$= \left\| \sum_{\mathbf{n} \in \mathbb{Z}^{d}} \boldsymbol{H}(\mathbf{n}) \right\|^{2} \|\mathbf{u}\|^{2},$$

 $^{^{7}\}ell^{1}(\mathbb{Z}^{d})$ is the space of summable *d*-dimensional sequences

where $|\mathbf{u}|$ denotes the vector of moduli of the components of vector \mathbf{u} . This shows that 641

642 (C.5)
$$\|\widehat{\boldsymbol{H}}(\boldsymbol{\nu})\| \leqslant \|\sum_{\mathbf{n} \in \mathbb{Z}^d} \boldsymbol{H}(\mathbf{n})\|.$$

and, consequently, 643

644 (C.6)
$$\sup_{\boldsymbol{\nu} \in [0,1]^d} \|\widehat{\boldsymbol{H}}(\boldsymbol{\nu})\| \leqslant \|\sum_{\mathbf{n} \in \mathbb{Z}^d} \boldsymbol{H}(\mathbf{n})\|.$$

In addition, the upper bound is attained since 645

646 (C.7)
$$\widehat{\boldsymbol{H}}(\mathbf{0}) = \sum_{\mathbf{n} \in \mathbb{Z}^d} \boldsymbol{H}(\mathbf{n}).$$

Next, we derive the proof for Theorem 4.1 in light of Lemma C.1. 647

648

- *Proof.* W being the impulse response of the MIMO filter with the frequency response given by 649 (SM4.1), it follows from Noble identities [52] that W is equivalent to a convolution with W followed 650
- 651 by a decimation by a factor σ_m . Let $\mathbf{x} \in \mathcal{H}_0$. Let the σ_m -polyphase representation of \mathbf{x} (resp. \mathbf{W}) be
- defined as 652

653 (C.8)
$$(\forall \mathbf{j} \in \mathbb{S}(\sigma_m))(\forall \mathbf{n} \in \mathbb{Z}^d) \quad \mathbf{x}^{(\mathbf{j})}(\mathbf{n}) = \mathbf{x}(\sigma_m \mathbf{n} - \mathbf{j})$$

(C.9)
$$\left(\text{resp. } \boldsymbol{W^{(j)}(n)} = \boldsymbol{W}(\sigma_m \mathbf{n} + \mathbf{j})\right).$$

Then, as a result of multirate digital filtering, y = Wx if and only if 656

657 (C.10)
$$\mathbf{y} = \sum_{\mathbf{j} \in \mathbb{S}(\sigma_m)} \mathbf{W}^{(\mathbf{j})} * \mathbf{x}^{(\mathbf{j})}.$$

This sum of MIMO convolutions can be reformulated as a single one 658

659 (C.11)
$$y = H * e$$

- where H is the $c_m imes \sigma_m^d c_0$ MIMO impulse response obtained by stacking rowwise the polyphase 660
- MIMO impulse responses $(W^{(j)})_{j \in \mathbb{S}(\sigma_m)}$ and e is the $\sigma_m^d c_0$ -component d-dimensional signal obtained 661
- by stacking columnwise the polyphase signal components $(\mathbf{x}^{(j)})_{\mathbf{i} \in \mathbb{S}(\sigma_m)}$. For example, if d = 2, we 662
- have 663

$$(\forall \mathbf{n} \in \mathbb{Z}^2)$$

$$\textbf{\textit{M}}(\mathbf{n}) = [\boldsymbol{W}^{(0,0)}(\mathbf{n}), \dots, \boldsymbol{W}^{(\sigma_m-1,0)}(\mathbf{n}), \dots, \boldsymbol{W}^{(0,\sigma_m-1)}(\mathbf{n}), \dots, \boldsymbol{W}^{(\sigma_m-1,\sigma_m-1)}(\mathbf{n})]$$

667 and

668 (C.13)
$$(\forall \mathbf{n} \in \mathbb{Z}^2) \quad \mathbf{e}(\mathbf{n}) = \begin{bmatrix} \mathbf{x}^{(0,\sigma_m-1)}(\mathbf{n}) \\ \vdots \\ \mathbf{x}^{(\sigma_m-1,\sigma_m-1)}(\mathbf{n}) \\ \vdots \\ \mathbf{x}^{(\sigma_m-1,\sigma_m-1)}(\mathbf{n}) \end{bmatrix} .$$

25

669 Note that, according to (C.8),

670
$$\|\mathbf{e}\|^{2} = \sum_{\mathbf{n} \in \mathbb{Z}^{d}} \|\mathbf{e}(\mathbf{n})\|^{2}$$
671
$$= \sum_{\mathbf{n} \in \mathbb{Z}^{d}} \sum_{\mathbf{j} \in \mathbb{S}(\sigma_{m})} \|\mathbf{x}^{(\mathbf{j})}(\mathbf{n})\|^{2}$$
672
$$= \sum_{\mathbf{n} \in \mathbb{Z}^{d}} \|\mathbf{x}(\mathbf{n})\|^{2}$$
673 (C.14)
$$= \|\mathbf{x}\|^{2}.$$

675 This equality and (C.11) imply that

676 (C.15)
$$\|\mathcal{W}\| = \sup_{\boldsymbol{\nu} \in [0,1]^d} \|\widehat{\boldsymbol{H}}(\boldsymbol{\nu})\|.$$

677 We thus deduce from Lemma C.1 that

678 (C.16)
$$\|\mathcal{W}\| = \left\| \sum_{\mathbf{r} \in \mathbb{Z}^d} \mathbf{H}(\mathbf{r}) \right\|.$$

679 On the other hand, by using (C.9),

680
$$\left\| \sum_{\mathbf{n} \in \mathbb{Z}^d} \mathbf{H}(\mathbf{n}) \right\|$$
681
$$= \left\| \left(\sum_{\mathbf{n} \in \mathbb{Z}^d} \mathbf{H}(\mathbf{n}) \right) \left(\sum_{\mathbf{n} \in \mathbb{Z}^d} \mathbf{H}(\mathbf{n}) \right)^{\top} \right\|^{1/2}$$
682
$$= \left\| \sum_{\mathbf{j} \in \mathbb{S}(\sigma_m)} \left(\sum_{\mathbf{n} \in \mathbb{Z}^d} \mathbf{W}^{(\mathbf{j})}(\mathbf{n}) \right) \left(\sum_{\mathbf{n} \in \mathbb{Z}^d} \mathbf{W}^{(\mathbf{j})}(\mathbf{n}) \right)^{\top} \right\|^{1/2}$$
683 (C.17)
$$= \left\| \sum_{\mathbf{j} \in \mathbb{S}(\sigma_m)} \overline{\mathbf{W}}^{(\mathbf{j})} (\overline{\mathbf{W}}^{(\mathbf{j})})^{\top} \right\|^{1/2}.$$

Appendix D. Proof of Theorem 4.2.

This result is a consequence of Theorem 4.1, which provides a Lipschitz bound for nonnegative convolutional neural networks. By following a similar reasoning to Appendix B, a Lipschitz constant of the ABBA network is

689 (D.1)
$$\theta_m = \|\widetilde{W}_{m+1}\| \|\widetilde{W}_m \circ \dots \circ \widetilde{W}_1\| \| \|\widetilde{W}_0\|.$$

690 Let

686

687 688

691 (D.2)
$$\widetilde{W} = (\widetilde{W}_m)_{\uparrow \sigma_{m-1}} * \cdots * (\widetilde{W}_2)_{\uparrow \sigma_1} * \widetilde{W}_1$$

692 and let

693 (D.3)
$$(\forall \mathbf{j} \in \mathbb{S}(\sigma_m)) \quad \Omega^{(\mathbf{j})} = \sum_{\mathbf{n} \in \mathbb{Z}^d} \mathfrak{S}(\widetilde{\mathbf{W}}(\sigma_m \mathbf{n} + \mathbf{j})) \in [0, +\infty[^{\zeta_m \times \zeta_0}].$$

Since $(\widetilde{W}_i)_{1\leqslant i\leqslant m}$ are convolutional operators with nonnegative kernels, it follows from Theorem 4.1

695

715

720

721

722

696 (D.4)
$$\theta_m = \|\widetilde{W}_{m+1}\| \left\| \sum_{\mathbf{j} \in \mathbb{S}(\sigma_m)} \overline{\boldsymbol{W}}^{(\mathbf{j})} (\overline{\boldsymbol{W}}^{(\mathbf{j})})^\top \right\|^{1/2} \|\widetilde{W}_0\|.$$

where, for every $\mathbf{j} \in \mathbb{S}(\sigma_m)$, 697

698 (D.5)
$$\overline{W}^{(\mathbf{j})} = \sum_{\mathbf{n} \in \mathbb{Z}^d} \widetilde{W}(\sigma_m \mathbf{n} + \mathbf{j}) \in [0, +\infty[^{(2\zeta_m) \times (2\zeta_0)}].$$

- On the other hand, for every $\mathbf{n} \in \mathbb{Z}^d$, $\widetilde{\boldsymbol{W}}_i(\mathbf{n})$ is an ABBA matrix. Since $\widetilde{\boldsymbol{W}}(\mathbf{n})$ is obtained by 699 multiplication and addition of such matrices, it follows from Proposition 3.3(ii) and (iii) that it is
- also an ABBA matrix. We deduce that, for every $\mathbf{j} \in \mathbb{S}(\sigma_m)$, $\overline{m{W}}^{(\mathbf{j})}$ is an ABBA matrix and, by using 701
- Proposition 3.3(i), $\overline{W}^{(j)}(\overline{W}^{(j)})^{\top}$ is ABBA. By invoking now Proposition 3.3(i)-(iii) and (vii), we deduce that 703

704
$$\left\| \sum_{\mathbf{j} \in \mathbb{S}(\sigma_{m})} \overline{W}^{(\mathbf{j})} (\overline{W}^{(\mathbf{j})})^{\top} \right\| = \left\| \mathfrak{S} \left(\sum_{\mathbf{j} \in \mathbb{S}(\sigma_{m})} \overline{W}^{(\mathbf{j})} (\overline{W}^{(\mathbf{j})})^{\top} \right) \right\|$$
705
$$= \left\| \sum_{\mathbf{j} \in \mathbb{S}(\sigma_{m})} \mathfrak{S} \left(\overline{W}^{(\mathbf{j})} \right) \mathfrak{S} \left(\overline{W}^{(\mathbf{j})} \right)^{\top} \right\|$$
706 (D.6)
$$= \left\| \sum_{\mathbf{j} \in \mathbb{S}(\sigma_{m})} \Omega^{(\mathbf{j})} (\Omega^{(\mathbf{j})})^{\top} \right\|.$$

This shows that a Lipschitz constant of the ABBA network \widetilde{T} is 708

709 (D.7)
$$\theta_m = \|\widetilde{W}_{m+1}\| \left\| \sum_{\mathbf{j} \in \mathbb{S}(\sigma_m)} \Omega^{(\mathbf{j})} \left(\Omega^{(\mathbf{j})}\right)^\top \right\|^{1/2} \|\widetilde{W}_0\|,$$

Similarly to the derivation of (4.12), we deduce that $\theta_m \leq \overline{\theta}_m$ where $\overline{\theta}_m$ is given by (4.15).

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