

# Boundary Conditions and Phase Transitions in Neural Networks. Simulation Results

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**Abstract.** This paper gives new simulation results on the asymptotic behaviour of theoretical neural networks on  $\mathbb{Z}$  and  $\mathbb{Z}^2$  following an extended Hopfield law. It specifically focuses on the influence of fixed boundary conditions on such networks. First, we will generalise the theoretical results already obtained for attractive networks in one dimension to more complicated neural networks. Then, we will focus on two-dimensional neural networks. Theoretical results have already been found for the nearest neighbours Ising model in 2D with translation-invariant local isotropic interactions. We will detail what happens for this kind of interaction in neural networks and we will also focus on more complicated interactions, *i.e.*, interactions that are not local, neither isotropic, nor translation-invariant. For all these kinds of interactions, we will show that fixed boundary conditions have significant impacts on the asymptotic behaviour of such networks. These impacts result in the emergence of phase transitions whose geometric shape will be numerically characterised.

*Keywords:* Stochastic neural networks; Hopfield model extension; Phase transitions; Simulations

## 1 Introduction

The objective of this paper is to study the influence of fixed boundary conditions on particular discrete dynamical systems, namely neural networks. This work is motivated by the fact that, in theoretical biology, researches on neural networks and more generally on the structural stability of regulatory networks are more and more deployed to understand their capacity to adapt to natural constraints (see [1,2,3]). Boundary conditions are one of the structural features on which it seems to be of great interest to focus in order to obtain more knowledge about dynamical systems useful to medicine and biology.

In some dynamical systems, the impact of specific parameters expresses itself by the appearance of phase transition. Phase transitions correspond to sharp and sudden changes of the behaviour of systems. They have been intensively studied by physicists, mathematicians and more recently computer scientists [4,5]. They have been shown to have a significant importance in particular in the study of

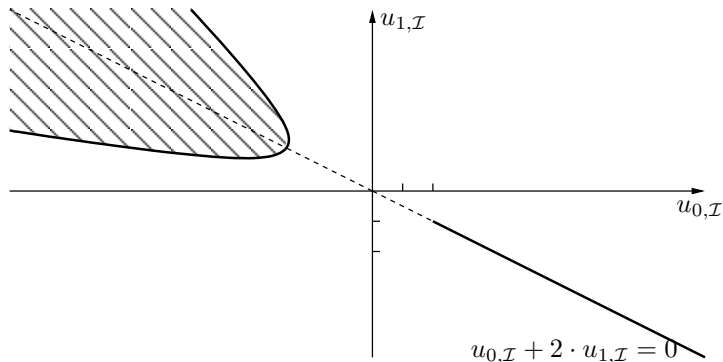
robustness of many systems [6,7,4]. In this paper, we explore phase transitions phenomena in the context of the fixed boundary conditions impact in neural networks.

More precisely, this paper presents complementary results to those presented in [8]. In [8], we theoretically prove that the influence of fixed boundary conditions on one-dimensional attractive neural networks is not significant and does not lead to the emergence of phase transition. Here, we decide to go further and give more general results (resp. new results) on one-dimensional (resp. two-dimensional) neural networks subjected to fixed boundary conditions. Because of the high underlying difficulties of theoretical studies of phase transition, we are going to proceed with simulations. Thus, we will present a computer assisted method to study phase transition phenomena emerging from the influence of fixed boundaries on the thermodynamic behaviour of complex neural networks. Moreover, we will not restrict ourselves to neither attractive nor isotropic and translation-invariant systems since they do not seem to be realistic from the biological point of view. We will hence study the attractive and repulsive form of three kinds of neural networks: the isotropic and translation-invariant ones (called *homogeneous*), the isotropic but non-translation-invariant ones (called *non-translation-invariant*) and the anisotropic and non-translation-invariant ones (called *inhomogeneous*). More precisely, in these different cases, we are going to define the interaction matrix  $W$  depending on two parameters  $u_0$  and  $u_1$  which will be defined in the next section. We will then show that, in homogeneous Hopfield-like neural networks, our results are identical to those obtained in the Ising model. Furthermore, we will numerically highlight the geometrical shapes of emerging phase transitions in the case of more complicated neural networks.

Because of the strong closeness between the networks which will be studied in this paper and the Ising model, we will introduce in Section 2 the most important results about the influence of boundary conditions in the context of ferromagnetic networks. Then, after a presentation in Section 3 of the chosen way to study the influence of fixed boundaries in neural networks, Section 4 will detail the results obtained on different one- and two-dimensional neural networks in order to highlight the emergence (or not) of phase transitions due to boundary conditions. Furthermore, we will show that, by passing from the homogeneous to the inhomogeneous case, despite a significant decrease of the relative weight of boundary conditions, the global behaviour of neural networks significantly depends on these boundary conditions. Eventually, some perspectives of this work will be presented in Section 5.

## 2 Boundary influence and the Ising model

In [9], Ising developed a simple probabilistic model imitating the dynamics of ferromagnetic particles networks of  $n$  elements on a lattice  $R$  of  $\mathbb{Z}^d$ . In this model, a particle  $i$  has two possible states at time  $t$ : up-oriented ( $\sigma_i(t) = +1$ ) or



**Fig. 1.** Parametric conditions on  $u_{0,\mathcal{I}}$  and  $u_{1,\mathcal{I}}$  showing phase transitions for the Ising model in  $\mathbb{Z}^2$  in the isotropic and translation-invariant attractive and repulsive cases. They illustrate the results obtained by Dobrushin and Ruelle. The bottom right corner, that corresponds to the attractive case, shows that the phase transition (in bold) takes place on a part of the straight line  $u_{0,\mathcal{I}} + 2 \cdot u_{1,\mathcal{I}} = 0$ . The upper left corner, relative to the repulsive case, shows that the phase transition (the striped space) can occur on a neighbourhood of this straight line.

down-oriented ( $\sigma_i(t) = -1$ ). Also, a particle gets the influence of an external field on itself and has an interaction on each of its nearest neighbours. Likewise the extended version of the Hopfield law defined in [8], such networks can be entirely described by interaction matrices  $W_{n \times n}$  in which coefficient  $w_{ij}$  indicates the action of the  $j$ -th particle on the  $i$ -th. With  $\mathcal{N}_i$  denoting the neighbourhood of the particle  $i$  (including  $i$  itself), the interaction potential of  $i$  at time  $t$  is defined by:

$$H_{\mathcal{I}}(\sigma_i(t)) = - \sum_{j \in \mathcal{N}_i \setminus \{i\}} w_{ij} \cdot \sigma_i(t) \cdot \sigma_j(t) - h \cdot \sigma_i(t)$$

The state of a ferromagnetic particle at time  $t + 1$  is then defined by:

$$P_{\mathcal{I}}(\sigma_i(t + 1) = +1 \mid \sigma_j(t), j \in \mathcal{N}_i \setminus \{i\}) = \frac{e^{H_{\mathcal{I}}(1)/T}}{1 + e^{H_{\mathcal{I}}(1)/T}}$$

where  $H_{\mathcal{I}}(1) = - \sum_{j \in \mathcal{N}_i \setminus \{i\}} w_{ij} \sigma_j(t) - h$ .

The results obtained in our framework of neural networks that we will expose in the sequel are very close to the results obtained on the Ising model by Dobrushin [10,11] and Ruelle [12,13,14]. It is thus relevant to briefly recall them.

They focused on Ising networks which were attractive ( $w_{ij} < 0$ ) or repulsive ( $w_{ij} > 0$ ) isotropic (for all  $i \in R$ ,  $w_{ij} = w_{ij'}$  for all  $j, j' \in \mathcal{N}_i \setminus \{i\}$ ) and translation-invariant (for all  $i, i'$  such that  $i \neq i'$  and for all  $j_1, \dots, j_k \in \mathcal{N}_i \setminus \{i\}$  and  $j'_1, \dots, j'_k \in \mathcal{N}_{i'} \setminus \{i'\}$ , such that,  $\forall l = 1, \dots, k, j'_l = j_l + i' - i$  (the

vertices  $i$ 's equalling 0 at the top left until  $n - 1$  at the bottom right), we have:  $w_{ii} = w_{i'i'}$  and  $(w_{ij_1}, \dots, w_{ij_k}) = (w_{i'j'_1}, \dots, w_{i'j'_k})$ . They gave general results about phase transitions. The method that they used to obtain their results is judicious and seems to be appropriate in our context. They defined a local potential  $U_{\mathcal{I}}$  by a couple of parameters  $(u_{0,\mathcal{I}}, u_{1,\mathcal{I}})$  that are related to the coefficients of the interaction matrix  $W$  such that:

$$\forall i, j \text{ s.t. } j \in \mathcal{N}_i \setminus \{i\}, u_{0,\mathcal{I}} = h/T \text{ and } u_{1,\mathcal{I}} = w_{ij}/T$$

With this approach, Dobrushin and Ruelle made it possible to study the asymptotic evolution of such networks by only basing on variations of this pair of local potentials  $(u_0, u_1)$ . They exposed some properties of phase transitions emphasising the influence of geometrical boundaries and gave the two following theorems, which are illustrated in Figure 1.

**Theorem 1.** If  $U$  is attractive ( $u_1 < 0$ ), then a phase transition occurs only on the straight line defined by the equation  $u_0 + du_1 = 0$  when the network tends to  $\mathbb{Z}^d$ , below a critical temperature  $T_{c,a}$ .

**Theorem 2.** If  $U$  is repulsive ( $u_1 > 0$ ), then a phase transition can only occur on a particular region of the space  $(u_0, u_1)$  corresponding to a large ‘‘parabolic’’ neighbourhood of the straight line defined by the equation  $u_0 + du_1 = 0$  when the network tends to  $\mathbb{Z}^d$ , below a critical temperature  $T_{c,r}$ .

In this paper, we will extend these specific results to the Hopfield-like networks as those presented in [8]. Their main properties are going to be recalled. So, this study will focus on neural networks whose evolution follows a stochastic version of the Hopfield law. In these networks, if  $\partial_{ext}R$  denotes the boundary of the neural network  $R$  such that  $i \in \partial_{ext}R \Leftrightarrow i \in \mathbb{Z}^d \setminus R, \exists j \in R$  s.t.  $j \in \mathcal{N}_i$ , the interaction potential of a neuron  $i$  is defined by:

$$H(\sigma_i(t)) = \sum_{j \in \mathcal{N}_i \cap R} w_{ij} \cdot \sigma_j(t) + \sum_{j \in \mathcal{N}_i \cap \partial_{ext}R} w_{ij} \cdot \bar{\sigma}_j(t)$$

where  $\bar{\sigma}$  denotes the configuration of the boundary.

The evolution of a neuron from time  $t$  to time  $t + 1$  is then defined by either:

$$P(\sigma_i(t + 1) = 1 \mid \sigma_j(t), j \in \mathcal{N}_i \setminus \{i\}) = \frac{e^{H(1)/T}}{1 + e^{H(1)/T}} \quad (1)$$

or

$$P(\sigma_i(t + 1) = \alpha \mid \sigma_j(t), j \in \mathcal{N}_i) = \frac{e^{\alpha \cdot H(\sigma_i(t))/T}}{1 + e^{H(\sigma_i(t))/T}} \quad (2)$$

The rule 1 corresponds to an external field (threshold like as in [15], where the threshold  $\theta = -w_{ii}$ ) that does not depend on the state of  $i$  at time  $t$  and the rule 2 (a stochastic version of the rule used in [16,17]) corresponds to an external influence depending on the state of  $i$  at time  $t$  (it is the case in neural networks for an axonal or somatic potential modulation depending on the existence of a

previous axonal firing or in genetic regulation networks for a post-transcriptional action like the one of microRNAs which prevents a proteic repression or induction). More precisely, we will use the rule 2 in all the performed simulations and the rule 1 with external field to give a theoretical result about attractive Hopfield-like networks for which both rules give the same minimal energies as the Boltzmann machine for same initial configurations.

Let us eventually notice that the coefficients  $u_1 = w_{ij}/T$  and  $u_0 = w_{ii}/T$  take here the opposite values than in the Ising model.

### 3 Simulation protocol

As it has been discussed in the introduction, the theoretical characterisation of phase transitions in discrete dynamical systems is known to be a difficult problem. In order to bypass the underlying difficulties, it seems to be reasonable to think of this problem in a different way. Indeed, before we try to obtain any theoretical results about phase transitions in complex neural networks, we may wonder whether phase transitions really occur and if they can be highlighted. Thus, in this section, we present a method based on simulations that allows to obtain some significant results on this kind of phenomenon in this framework.

#### 3.1 Preliminary definitions and influence of boundary

As the main definitions for the one-dimensional case are given in [8], we are only going to give here definitions for two-dimensional neural networks.

**Definition 1.** *The eccentricity  $\epsilon(v)$  of a graph vertex  $v$  in a connected graph  $G$  is the maximum  $L1$ -distance between  $v$  and any other vertex  $w$  of  $G$ .*

First of all, in this paper, let us note that we focus on theoretical networks represented by finite square lattices on  $\mathbb{Z}^2$ . We will be concerned by the von Neumann neighbourhood. Then, it is easy to define the boundary of such networks by using the geometrical properties of the lattices. The boundary in  $\mathbb{Z}^2$  of a square lattice  $R$  is thus the set of neurons which do not belong to  $R$  and have one and only one neighbour inside  $R$ , set at which we add the four corner neurons. In the same way, it is easy to define the centre  $C_R$  of  $R$ . Let us notice that  $C_R$  is a set of one or four neurons depending on the parity of the side size of the studied square lattice. Indeed, if the size of the lattice is odd, the centre of  $R$  is defined by a set composed by the neuron whose eccentricity is minimal. Else, if its side size is even, it is easy to split by the median axes the network  $R$  in four square sub-networks  $R_1, R_2, R_3, R_4$  of equal sizes. Each of these sub-networks contains one corner of  $R$  and, in each of them, it is easy to find the neuron  $C_i$  the furthest from the corner. By merging the four sub-networks, we obtain  $R$  and the centre of  $R$  is then the set of these four  $C_i$ 's as illustrated in Figure 2. Thus, according to this definition, the central vertices of a network  $R$  on  $\mathbb{Z}^2$  correspond exactly to the vertices of  $R$  of minimal eccentricity. Let us enumerate

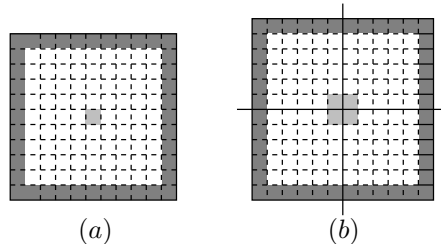
the neurons of the network from 0 to  $n - 1$  from left to right and from top to bottom of the lattice. Then, if we define a configuration of the network at time  $t$  by the following sequence  $\sigma(t) = \{\sigma_0(t), \sigma_1(t), \dots, \sigma_i(t), \sigma_{i+1}(t), \dots, \sigma_{n-1}(t)\}$ , the state of the centre of the network is defined by:

$$\sigma_{C_R}(t) = \sigma_{\frac{n-1}{2}}(t)$$

for an odd side size lattice and by:

$$\begin{aligned} & \sigma_{C_R}(t) \\ & \parallel \\ & \left\{ \sigma_{\frac{n}{2} - \frac{\sqrt{n}}{2} - 1}(t), \sigma_{\frac{n}{2} - \frac{\sqrt{n}}{2}}(t), \sigma_{\frac{n}{2} + \frac{\sqrt{n}}{2} - 1}(t), \sigma_{\frac{n}{2} + \frac{\sqrt{n}}{2}}(t) \right\} \end{aligned}$$

otherwise.



**Fig. 2.** Definition of the boundary (in dark grey) and the centre (in light grey) of neural network lattices for (a) an odd size and (b) an even size.

In the sequel, we will give a quantitative measure of the influence of fixed boundary conditions on neural networks by focusing only on their impact on the centre. We will denote this measure by  $\bar{S}$ . Since we consider networks on lattices on  $\mathbb{Z}$  or  $\mathbb{Z}^2$ , it is trivial to understand that the highlight of the influence of boundary conditions on the centre is a sufficient condition to prove their influence on the whole network. Indeed, their influence on it implicates the propagation of the states of the boundary vertices through all the vertices separating them from the centre, *i.e.*, through the whole network.

### 3.2 Simulation constraints

Let us remind the result obtained by Onsager [18] proving that the aggregation of ferromagnetic particles states in the Ising model can occur only below a critical temperature. In our framework, as in the Ising model, the phase transitions emerging from the asymptotic behaviour of networks following a Hopfield-like law and resulting from the influence of boundary conditions, if they exist, can

occur only at low temperature too. Indeed, it is easy to prove that the increase of the temperature in such systems augments the randomness until uniformity when the temperature tends to infinity.

Furthermore, let us note that a major difficulty exists when we want to simulate this kind of system: it is impossible to check whether the dynamics of the network has converged or not, whatever the number of iterations of time is. Indeed, in a paper published in 1996 [19] which proposes the algorithm coupled from the past, Propp and Wilson indicate that, even after the system underlying Markov chain has evolved for a long time, there does not exist a method that proves whether the system has converged if (i) the temperature is below the critical one or if (ii) the system is not attractive. So, our work takes place in a difficult framework and we are going to explain what the chosen method is in order to obtain significant results.

### 3.3 Simulation protocol details

In order to numerically highlight and characterise the emergence of phase transitions due to variations of fixed boundary conditions, it is important to analyse the results obtained from a large enough sample of initial conditions. However, because of the time complexity of the protocol, any figure presented in the sequel (see Section 4) corresponds to the results obtained for one initial configuration randomly chosen at the beginning of the simulation and whose density is 0.5, *i.e.*, the probability for a neuron to be activated is 0.5. We will discuss nevertheless the dependence of the results on the choice of initial configurations. Furthermore, the evolution law is normalised on the temperature such that the temperature  $T = 1$ . Moreover, in order to bypass the underlying problem of convergence, we have decided to focus on a specific fixed portion of the orbit of the system. This portion is obtained by letting the neural network evolve during a long enough *transient time*, denoted by  $T_T$  the set of transient iteration times, and by measuring the influence of boundaries during a *sampling time*, denoted by  $T_S$  the set of sampling iteration times. More precisely, the cardinal of  $T_S$  equals the number of iterations during those the computation of the measure is executed.

Let us now detail the quantitative measure  $\bar{S}$  chosen in order to get a good approximation of the influence of the boundary conditions on neural networks. As it has been suggested above,  $\bar{S}$  has to measure the influence of the states of the boundary vertices on the centre. A relevant idea for  $\bar{S}$  is to compute the difference between the activities of the centre, *i.e.*, the difference between the numbers of sampling iterations during which the centre has been activated, observed in a certain domain of the parameters  $u_0$  and  $u_1$  when the boundaries are differently valued. So, if we consider two different boundaries  $\partial_1$  and  $\partial_2$ , it will be easy to compute the two corresponding central activities  $S^{\partial_1}$  and  $S^{\partial_2}$  in order to compare them. Then, a relevant result would be to emphasise that there exist particular zones in the predefined domain of parameters  $u_0$  and  $u_1$  on which there is a significant difference between  $S^{\partial_1}$  and  $S^{\partial_2}$ . Also, it would

be essential to show that these particular zones still exist when the size of the networks increases. Besides, this kind of result will not only lead us to numerically prove the existence of phase transitions as a result of the influence of boundary conditions. It will also allow us to highlight where this influence acts.

More formally, the activity of a neuron  $i$ , *i.e.*, the number of iterations during which  $i$  has been activated (the activity of  $i$ ) over  $|T_S|$  iterations is defined by:

$$S_i = \sum_{t \in T_S} \sigma_i(t)$$

Then, the central activity of the network over these  $|T_S|$  iterations is consequently defined by:

$$S = \sum_{i \in C_R} S_i$$

Now, The influence of the fixed boundary conditions has to be highlighted by comparing the results of the two measures  $\bar{S}$  that depend on two different boundaries. Thus, we are going to define some specific boundary conditions which we will use in the sequel. So, for all  $i \in \partial_{ext}R$ , we have:

$$\overline{\sigma_i^{(0)}} = 0 \tag{3}$$

$$\overline{\sigma_i^{(1)}} = 1 \tag{4}$$

$$\overline{\sigma_i^{(01)}} = \begin{cases} 0 & \text{if } |l_i + c_i| \text{ is even} \\ 1 & \text{otherwise} \end{cases} \tag{5}$$

$$\overline{\sigma_i^{(10)}} = \begin{cases} 0 & \text{if } |l_i + c_i| \text{ is odd} \\ 1 & \text{otherwise} \end{cases} \tag{6}$$

where  $l_i$  (resp.  $c_i$ ) represents the horizontal (resp. vertical) coordinate of the neuron  $i$  of  $\partial_{ext}R$ .

With the previous notations, we can now denote the activity of the central neurons when all the vertices of the boundary are fixed to 0 (resp. 1) by  $S^{(0)}$  (resp.  $S^{(1)}$ ). In the same way, we also denote by  $S^{(01)}$  and  $S^{(10)}$  the activity of the central neurons when the vertices of the boundary follow respectively the rules defined by the equations 5 and 6. Let us remark that the choice of the boundaries makes sense since we will compare the central neurons activities with quite different (equations 3 and 4) and quite similar (equations 5 and 6) boundary conditions.

As we have remarked that the simulation results depend on the attractivity/repulsivity of the network, we have decided to present the results for attractive networks by using the equations 3 and 4 and those for repulsive networks by using the equations 5 and 6. So, the two different measures that we are going to compute are precisely defined by the arithmetic averages (on the number of



sampling iterations and central nodes) of the absolute values of the differences between the activities depending on the chosen boundaries:

$$\overline{S_\alpha} = \frac{|S^{(0)} - S^{(1)}|}{|T_S| \cdot |C_R|}$$

for the attractive case and

$$\overline{S_\beta} = \frac{|S^{(01)} - S^{(10)}|}{|T_S| \cdot |C_R|}$$

for the repulsive case.

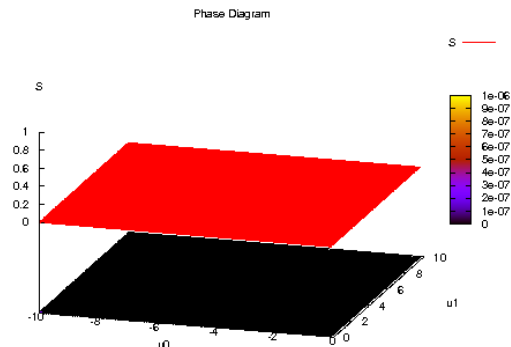
### 3.4 Studied lattices and reading of the results

All the simulations performed aim at showing if the dynamics of the central neurons of such systems evolving with a parallel updating iteration mode change their behaviour according to the activating, inhibiting or double nature of boundaries influencing them. They consist also in a precise computation of the strength of this influence. Moreover, usually in physics, to numerically prove the existence of a thermodynamic phase transition in the behaviour of a dynamical system, it is necessary to obtain identical results on this system for three sizes of different order of magnitude. Thus, in the one-dimensional case, we have performed simulations on neural networks where  $n = 53$ ,  $n = 503$  and  $n = 5003$ . In the two-dimensional case, we have chosen the three following sizes:  $n = 11 \times 11$  (*i.e.*, 121 neurons),  $n = 37 \times 37$  (*i.e.*, 1369 neurons), and  $n = 131 \times 131$  (*i.e.*, 17161 neurons) for which we will present and discuss the results. These numbers may appear to be small but the execution time of the simulations has prevented us to go further. However, these lattices sizes give a sample in respect with the physicist method to argue the emergence of phase transitions. Let us also notice that all these sizes are prime numbers to avoid side effects such as periodicity as much as possible.

Finally, the presentation of the results will be done with three-dimensional graphics on which the vertical axis named  $S$  corresponds to the quantitative measure of boundaries influence and the horizontal plane represents the domain of the two parameters  $u_0$  and  $u_1$  on which the measure is computed. Moreover, in these graphics will be exposed two surfaces: the first one (in red dominance) gives the exact values of the measure obtained by computation and the second one (in black dominance) gives a maybe more readable indication on the measure level (*i.e.*, its normalised altitude).

## 4 Simulation results

In this section, first, we are going to give the major definitions. Then, we will illustrate and generalise the theoretical results obtained in [8] by showing that the



**Fig. 3.** Simulation results obtained for all one-dimensional Hopfield-like network cases where the size of the network is  $n = 53$ ,  $n = 503$  or  $n = 5003$ .

asymptotic behaviour of one-dimensional neural networks does not depend on fixed boundaries. Eventually, in the third part, we will focus on the case of two-dimensional neural networks and show the non-uniqueness of the quantitative measure discussed in the previous section.

#### 4.1 Definitions

Before presenting simulation results in three different kinds of one- and two-dimensional neural networks, we are going to give more details about the notions of homogeneity, non-translation-invariance and inhomogeneity. As it is said in the introduction of the paper, our goal is to numerically characterise phase transitions phenomena by conserving the Dobrushin’s and Ruelle’s approach. Because it seems to be relevant to go further than to just work with homogeneous networks in a biological context, we will formally define the interactions in underlying graphs depending on the two parameters  $u_0$  and  $u_1$  on which we want our study to be based. The formal definition of homogeneous interactions being given in Section 1, here, we give those corresponding to non-translation-invariant and inhomogeneous networks.

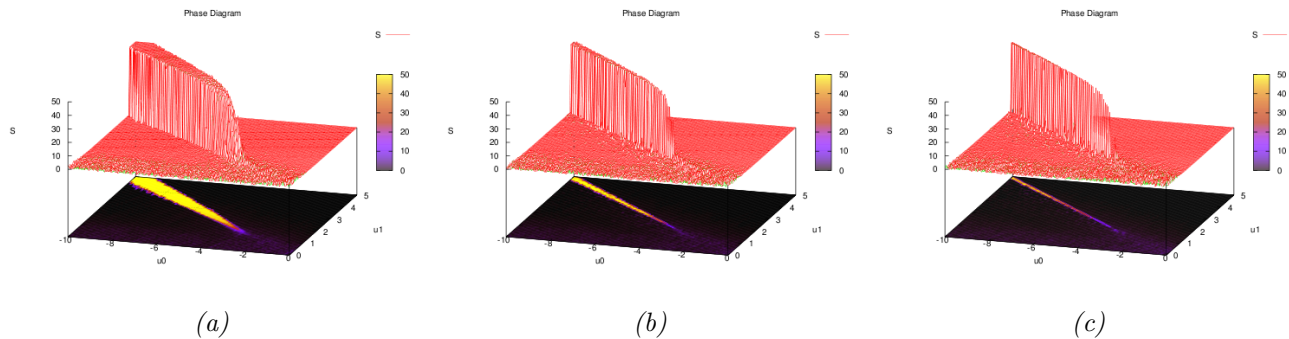
First of all, let us remind the formal definition of isotropy and translation-invariance properties.

**Definition 2.** *A system is isotropic (or rotation-invariant) if it exhibits the same characteristics in all directions. Consequently, a Hopfield-like network  $R$  is called isotropic if, for all neuron  $i$  of  $R$ , all the interaction coefficients that its neighbours have on it are identical. Formally, we have:*

$$\forall i \in R, \forall j, j' \in \mathcal{N}_i \setminus \{i\}, w_{ij} = w_{ij'}$$

**Definition 3.** Let  $(w_{ij_1}, \dots, w_{ij_k})$  be the interaction coefficients the  $k$  neighbours of the neuron  $i$  have on  $i$ . A Hopfield-like network  $R$  is translation-invariant if such coefficient sequences are identical for all  $i$ 's whatever their place in the grid is. Formally, we have, if  $j'_s = j_s + (i' - i), \forall s = 1, \dots, k$ :

$$\forall i, i' \in R, (w_{ij_1}, \dots, w_{ij_k}) = (w_{i'j'_1}, \dots, w_{i'j'_k}).$$



**Fig. 4.** Simulation results of the homogeneous attractive case when the neural network is respectively represented by a grid (a)  $11 \times 11$ , (b)  $37 \times 37$  and (c)  $131 \times 131$ . The results are presented on the domain of parameters  $u_0 = [-10, 0]$  and  $u_1 = [0, 5]$  with a resolution of 0.05.

Let us now discuss non-translation-invariant neural networks that seem to be closer to biological systems. In this kind of system, the synaptic weights corresponding to the actions that a neuron  $i$  receives from its neighbours are defined by a function of the L1-distance between the neuron  $i$  and the closest neuron belonging to the centre of the network. More formally, we define:

$$w_{ij} = \begin{cases} u_0 & \text{if } j = i, \\ \frac{u_1}{1 + \eta \cdot d(i, C_R)} & \text{if } j \in \mathcal{N}_i \setminus \{i\}, \\ 0 & \text{otherwise.} \end{cases}$$

where  $\eta$  takes values in  $[0, 1]$ . When this parameter is equal to 0, the system follows a homogeneous extended stochastic Hopfield rule. When it is greater than 0, it permits to include more and more non-translation-invariance and, thus, to give specific information about the effects of this non-translation-invariance introduction in neural networks. We will see in the sequel that the differences between the obtained results for “simple” ( $\eta = 0$  or  $\eta = 1$ ) attractive neural networks have led us to use this parameter in order to have more details on the influence of non-translation-invariance in the specific case of attractive networks.

The last kind of neural networks studied is the *inhomogeneous* one. The definition of these systems is really close to the one that corresponds to the non-translation-invariant ones. The difference is that anisotropy is added. To do that, the synaptic weights  $w_{ij}$  are defined by a function of the L1-distance between the neuron  $j$  and the closest neuron belonging to the centre of the network. Formally, we have:

$$w_{ij} = \begin{cases} u_0 & \text{if } j = i, \\ \frac{u_1}{1+\eta \cdot d(j, C_R)} & \text{if } j \in \mathcal{N}_i \setminus \{i\}, \\ 0 & \text{otherwise.} \end{cases}$$

## 4.2 One-dimensional neural networks

This subsection aims at illustrating and generalising to other kinds of neural networks the theoretical result of [8]. This result shows that the behaviour of one-dimensional attractive neural networks does not admit phase transition as a consequence of the influence of fixed boundary conditions. Indeed, there exists a property of constant probability for the centre to be activated or inhibited at the asymptotics whatever the boundaries of the network are. Here, since we focus on one-dimensional networks, we only fix the boundary states values to 0 and 1 and compute  $\overline{S_\alpha}$ . To numerically prove that different fixed boundary conditions have the same influence on the whole network, the simulation results must present a phase diagram whose the surface of  $\overline{S_\alpha}$  values is null whatever the  $u_0$  and  $u_1$  are.

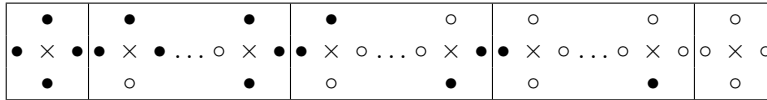
We have seen that such results are observed in all cases of large one-dimensional attractive and repulsive neural networks. As illustrated in Figure 3, the quantitative measure  $\overline{S_\alpha}$  vanishes whatever the values of the parameters  $u_0$  and  $u_1$  are. That corroborates the fact that there is no phase transition in the one dimensional case. Indeed, the probability for the centre to be activated is the same whatever the boundaries and the kind of interactions are. Let us finally notice that the results given by the simulation of the dynamics of such neural networks are a first step in the direction of the validation of our simulator.

## 4.3 Two-dimensional neural networks

In this subsection, we give results about three different kinds of interactions in two-dimensional neural networks. We respectively name these kinds of networks homogeneous, non-translation-invariant and inhomogeneous networks. Thus, we give the results obtained on attractive neural networks and then, we expose what happens in the repulsive ones. More precisely, for these two different kinds of networks, we will present the sub-cases of homogeneity, non-translation-invariance and inhomogeneity.

$$M = \begin{pmatrix} 1 & 1 & 0 & \dots & 0 & 0 \\ 1 & 0 & 1 & \dots & 0 & 0 \\ 1 & 0 & 0 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 0 & 1 \\ \frac{e^{u_0+4u_1}}{1+e^{u_0+4u_1}} & \frac{e^{u_0+3u_1}}{1+e^{u_0+3u_1}} & \frac{e^{u_0+3u_1}}{1+e^{u_0+3u_1}} & \dots & \frac{e^{u_0+u_1}}{1+e^{u_0+u_1}} & \frac{e^{u_0}}{1+e^{u_0}} \end{pmatrix}$$

**Fig. 5.** Matrix of projectivity  $M$  for nearest-neighbours two-dimensional neural networks.



**Table 1.** Possible neighbourhoods of the centre of a neural network where a “•” corresponds to a firing neuron and a “○” corresponds to an inactive one.

### Attractive neural networks

- Results on homogeneous networks

Figure 4 illustrates the values of  $u_0$  and  $u_1$  for which the effects of boundary conditions can be observed. Thus, we can see that the influence of fixed boundary conditions takes place in a small neighbourhood of the straight line defined by  $u_0 + 2u_1 = 0$ . Let us note that this neighbourhood tends to reduce exactly to the straight line  $u_0 + 2u_1 = 0$  by increasing the lattice size such that it is highlighted by Figure 4 (c). This result has been checked for all the executed simulations.

Furthermore, the three presented phase diagrams show that the influence of fixed boundary conditions happens after a certain value of the parameter  $u_0$ . This value is identical whatever the size of the lattice is and is approximately equal to  $-3$ . Consequently, this threshold is critical for the appearance of a significant value of the measure  $\overline{S}_\alpha$ . Since the phenomenon of influence of fixed boundary conditions appears at a specific value of a parameter whatever the size of the system is, we can argue that it corresponds to a phase transition.

Now, let us discuss in a more formal way the existence of this phase transition characterising the influence of fixed boundary conditions on homogeneous attractive neural networks (this step will allow to validate our simulator).

**Proposition 1.** *In two-dimensional attractive stochastic Hopfield-like networks (with the rule with external field), the emergence of phase transition resulting from the influence of fixed boundary conditions can occur on the straight line defined by  $u_0 + 2u_1 = 0$ , which is the condition of linear dependence between*

*projective and conditional equations defining the probability of the activity of the network centre [8].*

*Proof.* In order to prove that  $u_0 + 2u_1 = 0$  is a linear dependence condition, it seems useful to focus on a simplification of the Markovian character of the system. To do that, let us use the general mathematical method described in [8]. Then, we can easily obtain a matrix  $M$  of size  $2^4 \times 2^4$  (see Figure 5) that contains the coefficients of the projective and conditional equations describing the  $2^4$  possible states of the 4 strict neighbours of a central neuron given in Table 1. The objective is to prove that  $u_0 + 2u_1 = 0 \Rightarrow \text{Det}M = 0$ . Indeed, if the determinant of  $M$  is not null, it means that all the unknowns can be expressed as a function of the probability of the centre to be activated; thus, an independent equation allows a unique determination of the probabilities of activity in boundary cylinders as a function of the probability of activity in the centre. This kind of parametric condition prevents phase transitions observations because of the uniqueness of the invariant measure.

The determinant of this matrix is defined by:

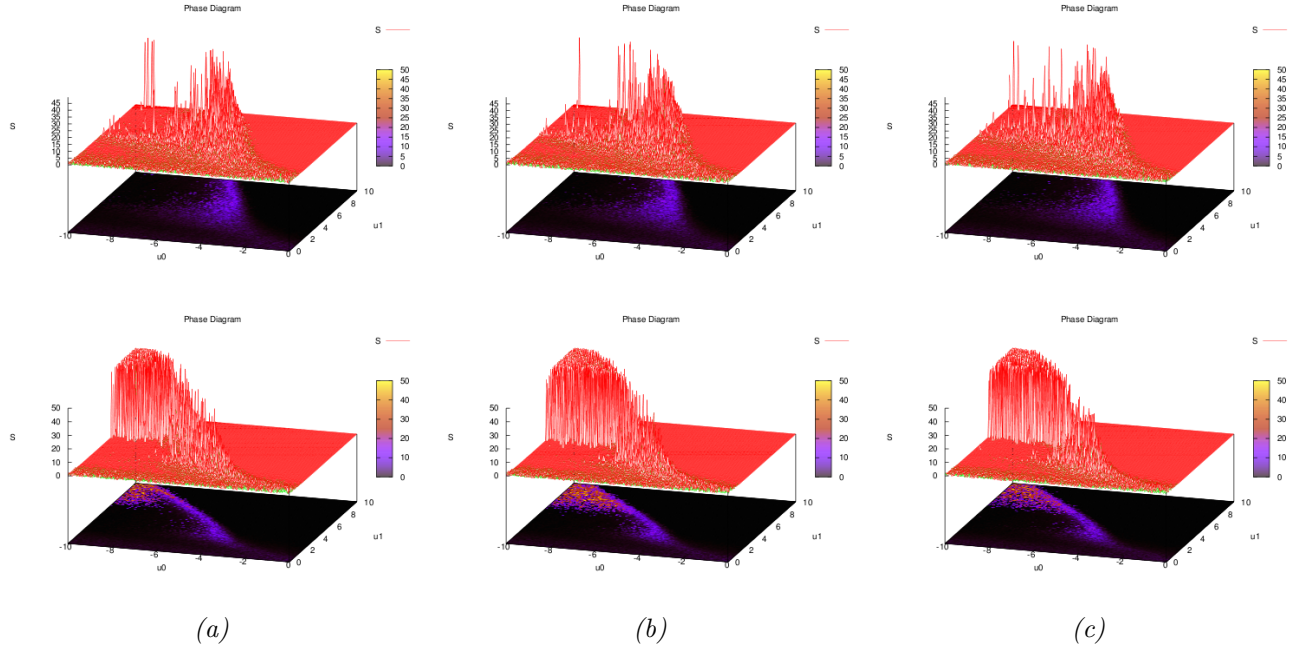
$$\begin{aligned} \text{Det}M = & (-e^{4u_0+10u_1} + 4e^{4u_0+9u_1} - 6e^{4u_0+8u_1} + 4e^{4u_0+7u_1} \\ & - e^{4u_0+6u_1} + 3e^{3u_0+9u_1} - 7e^{3u_0+8u_1} + e^{3u_0+7u_1} \\ & + 6e^{3u_0+6u_1} + e^{3u_0+5u_1} - 7e^{3u_0+4u_1} + 3e^{3u_0+3u_1} \\ & - 3e^{2u_0+7u_1} + 7e^{2u_0+6u_1} - e^{2u_0+5u_1} - 6e^{2u_0+4u_1} \\ & - e^{2u_0+3u_1} + 7e^{2u_0+2u_1} - 3e^{2u_0+u_1} + e^{u_0+4u_1} \\ & - 4e^{u_0+3u_1} + 6e^{u_0+2u_1} - 4e^{u_0+u_1} + e^{u_0}) \\ & / [(1 + e^{u_0+4u_1})(1 + e^{u_0+3u_1})(1 + e^{u_0+2u_1})(1 + e^{u_0+u_1})(1 + e^{u_0})] \end{aligned}$$

The vanishing equation of the determinant:  $\text{Det}M = 0$  admits a set of four solutions among which appears  $u_0 = -2u_1$ . We get the expected result.  $\square$

Consequently, theoretically, we prove that phase transition in attractive Hopfield-like networks can occur on the straight line  $u_0 + 2u_1 = 0$ . Let us remark that this equation is the one corresponding to the only observed phase transition with simulations independently of the initial conditions, which validates the simulator and show that phase transitions only occur on this straight line. Ruelle proved this result in 1972 for Ising networks by using the pressure differentiability (see [20]).

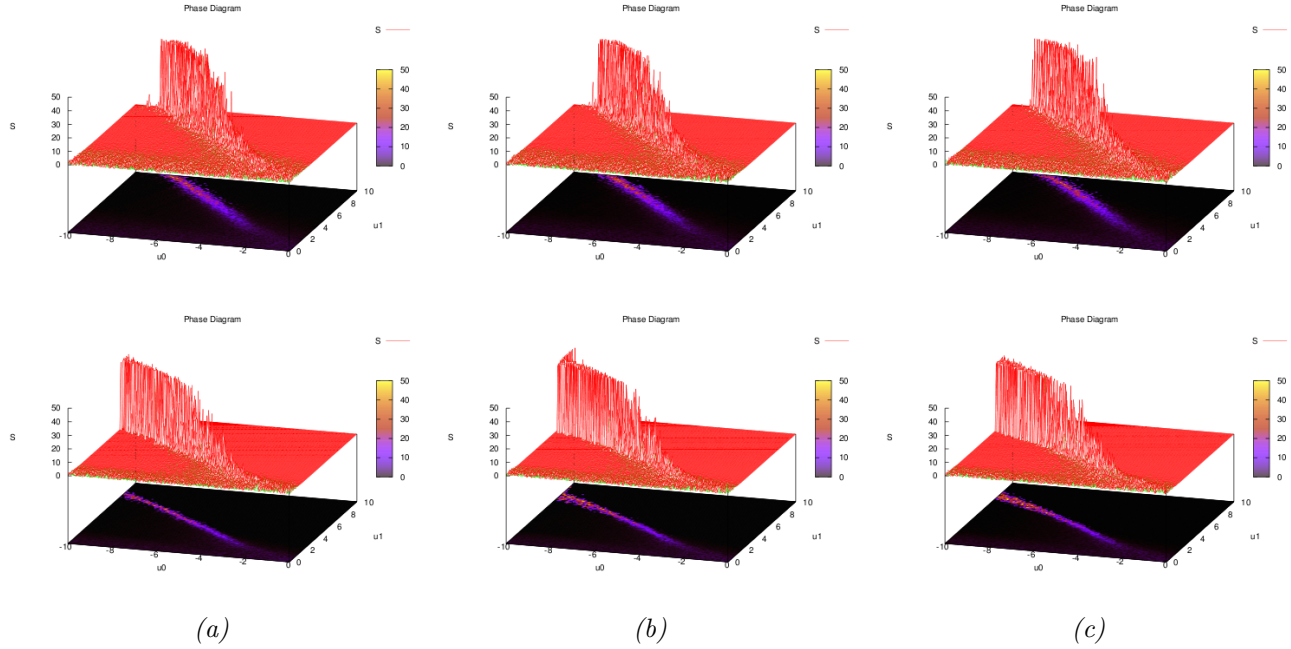
- Results on non-translation-invariant networks

The study of non-translation-invariant attractive neural networks gives significant results about the influence of boundaries in large networks as Figure 6 shows. The introduction of non-translation-invariance in a homogeneous neural network does not only change the position of the parametric domain of phase transition but also the shape of this domain.



**Fig. 6.** Simulation results of the non-translation-invariant attractive case when the neural network is respectively represented by a grid (a)  $11 \times 11$ , (b)  $37 \times 37$  and (c)  $131 \times 131$ . The first (resp. second) line of this figure presents the results when  $\eta = 1$  (resp.  $\eta = 0.5$ ).

Let us first focus on the case where  $\eta = 1$ . Significant values of  $\overline{S_\alpha}$  are observed in a triangular domain of  $(u_0, u_1)$  which is defined by the two straight lines:  $u_0 + 2u_1 = 0$  and  $u_0 + \frac{2}{5}u_1 = -2$ . More precisely, we can remark that the influence of fixed boundary conditions is strong in the neighbourhood of the line  $\frac{2}{5}u_1 = -2$  and tends to disperse and to be weakened by approaching the line  $u_0 + 2u_1 = 0$  for low values of the couple of parameters  $(u_0, u_1)$ . Furthermore, let us note that this value tends to vanish in the triangular domain for high values of the couple of parameters  $(u_0, u_1)$ . We can also notice that this domain stays the same by increasing the size of the lattice. Furthermore, significant values of  $\overline{S_\alpha}$  start for the same specific value of  $u_0$  than in the homogeneous case, *i.e.*, approximatively  $u_0 = -3$ . Therefore, we can argue that the influence of boundary conditions in the attractive non-translation-invariant case leads to the emergence of a phase transition. More generally, if we execute simulations on a large number of different initial configurations, we obtain the same kind of results. However, the phase transition line on which the measure  $\overline{S_\alpha}$  is strong is not always  $u_0 + \frac{2}{5}u_1 = -2$  but is always included in the triangular domain of parameters described above. In this case, the dispersion of the measure takes



**Fig. 7.** Simulation results of the inhomogeneous attractive case when the neural network is respectively represented by a grid (a)  $11 \times 11$ , (b)  $37 \times 37$  and (c)  $131 \times 131$ . The first (resp. second) line of this figure presents the results when  $\eta = 1$  (resp.  $\eta = 0.5$ ).

place around the straight line in the direction of the characteristic straight lines delimiting the domain of phase transition.

Now, if we focus on a smaller introduction of non-translation-invariance ( $\eta = 0.5$ ), we can highlight the same kind of phenomenon although the characteristic straight lines delimiting the phase transition domain are  $u_0 + 2u_1 = 0$  and  $u_0 + \frac{5}{4}u_1 = 0$ . Here also, the value of  $u_0$  for which the phase transition appears is  $u_0 = -3$ . Here too, if we execute a large number of simulations on different initial configurations, we remark a possible rotation of the second phase transition line in this triangular domain.

In conclusion, we can say that the loss of translation-invariance changes the occurrence of phase transition in attractive neural networks. The results stay coherent with those obtained in the homogeneous attractive case. Indeed, phase transitions can occur in a neighbourhood of a straight line which corresponds to a rotation of the one observed in homogeneous neural networks. What seems also to be important is the appearance of a larger parametric domain of boundaries influence which increases when we introduce more non-translation-invariance.



Consequently, it would be of interest to study more precisely these rotation and dispersion phenomena induced by the introduction of non-translation-invariance.

- Results on inhomogeneous networks

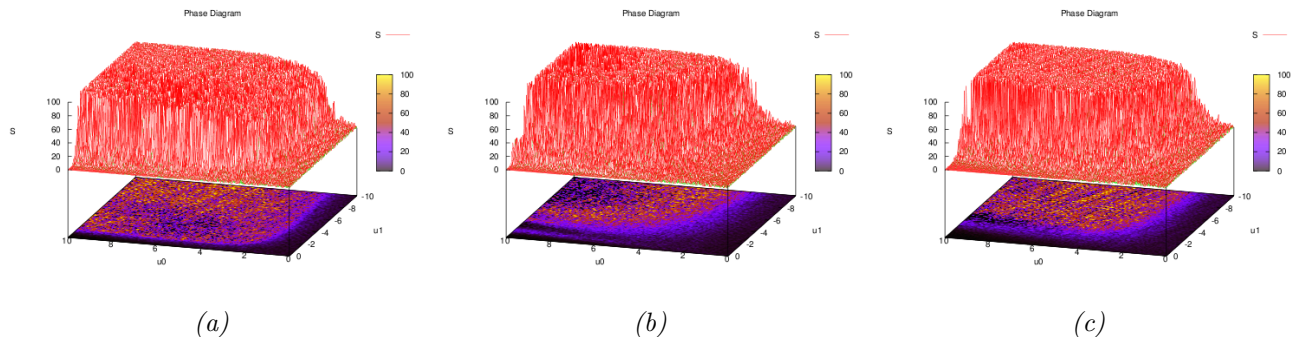
Let us focus on the first line of Figure 7. First, we can observe that the introduction of anisotropy leads to different results than those obtained on non-translation-invariant neural networks. In inhomogeneous networks, being given an initial configuration, the influence of fixed boundary conditions is observable on a straight line and there is no dispersion of the measure  $\overline{S_\alpha}$ . Indeed, the presented phase diagrams show that the fixed boundary conditions have an impact on the straight line defined by  $u_0 + \frac{4}{5}u_1 = 0$ . We can note that the results stay the same with the increasing of the size of the grid. Moreover, like in all the previous cases, it is important to remark that the value of  $u_0$  from which a significant value of  $\overline{S_\alpha}$  is obtained is  $u_0 = -3$ . Thus, we can also conclude here that the influence of fixed boundary conditions leads to the emergence of phase transition.

Now, by considering the second line of Figure 7, we reach the same conclusion, except that the phase transition straight line is defined by  $u_0 + \frac{5}{4}u_1 = 0$ . In this case also, the results are identical whatever the size of the lattice is and the critical value of  $u_0$  is  $-3$ .

Finally, from a more global point of view, in these two cases, if we consider a large number of simulations on different randomly chosen initial configurations, a small rotation of the phase transition can happen depending on the initial configuration. That is why we argue that, in inhomogeneous neural networks, phase transitions can appear in a small triangular domain of parameters  $(u_0, u_1)$  which corresponds to a neighbourhood of the phase transition straight lines previously defined. Thus, the introduction of anisotropy reduces the dispersion of the significant values of  $\overline{S_\alpha}$  and, consequently, the appearance of phase transitions in inhomogeneous networks happens in a smaller domain of  $(u_0, u_1)$ , which allows to increase the robustness of non-translation-invariant neural networks against the influence of fixed boundary conditions.

**Repulsive neural networks** The objective of this subsection is to give simulation results on repulsive neural networks. The interest of this specific study comes directly from the natural properties of regulation networks, which always present a significant proportion of inhibition and even can be totally inhibited like in the case of the  $n$ -switches [21,22].

First of all, let us focus on repulsive homogeneous networks. The influence exerted by fixed boundary conditions on these networks is more complex than the influence observed in attractive networks. The domain of parameters under which the influence can occur is not a straight line but a parabolic domain in which the symmetric of the straight line obtained in the attractive case is included. Thus,



**Fig. 8.** Simulation results of the repulsive case when the neural network is respectively (a) homogeneous, (b) non-translation-invariant and (c) inhomogeneous. The phase diagrams presented are those obtained for lattices  $131 \times 131$  when  $\eta = 1$ .

the action of fixed boundary conditions in such neural networks is quite similar to the one observed on ferromagnetic systems described by the Ising model. As we can see in Figure 8 (a), the influence of the boundary conditions takes place in a large neighbourhood of the straight line  $u_0 + 2u_1 = 0$  which seems to be delimited by the two following lines :  $u_0 \approx 1$  and  $u_1 \approx -1$ . By performing simulations on lattices of different sizes with a random choice of initial configurations, we have remarked that the results obtained are always qualitatively identical, which allows to conclude in the existence of a phase transition.

Now, let us consider the adding of non-translation-invariance and/or anisotropy. Just like in the repulsive homogeneous case, the study of the influence of boundary conditions in no longer translation-invariant and/or anisotropic repulsive neural networks shows phase transitions in a certain domain of parameters ( $u_0, u_1$ ) (see Figure 8 (b) & (c)). This phenomenon is quasi similar to the one discussed in the previous paragraph. Indeed, here again, certain values of the measure  $\overline{S_\beta}$  are significantly far from 0, allowing the phenomenon of phase transition to occur in a large domain of parameters that cannot be reduced to a straight line.

However, some small differences with the homogeneous case can be pointed out. Then, one can notice that, for these two different kinds of neural networks, the slope is the same for the two lines delimiting the phase transition domain but is different from the one observed in the homogeneous case (whose influence domain slope is significantly more important). Finally, we have to notice that the two domains of boundary conditions influence are included in the domain observed in the homogeneous case.

Eventually, it is important to notice that the results presented in Figure 8 are those for which we have obtained the larger domains of phase transitions. Indeed, depending on the initial condition, other kinds of phase transitions can occur. However, the essential point is that all these domains are always contained in the presented ones. Thus, these numerical results allow us to conclude that, if phase transitions occur in repulsive neural networks, they are observable in domains corresponding to a large parabolic neighbourhood of the domains obtained in attractive neural networks.

## 5 Conclusion and perspectives

This paper has presented new numerical results on phase transitions inherent to the influence of fixed boundary conditions on complex neural networks. The existence (or the absence) of phase transitions has been confirmed by identical qualitative and quantitative results obtained for networks sizes of different orders of magnitude.

Thus, simulations have confirmed the fact that no phase transition phenomenon can occur when the network is one-dimensional. Moreover, in two-dimensional networks, we observe a certain robustness of the qualitative shape of the phase transition parametric set with respect to the isotropy breaking or translation-invariance breaking. Despite the appearance of a triangular parametric domain under which phase transitions can occur in non-translation-invariant and inhomogeneous attractive networks, the three different kinds of attractive neural networks studied show that the emergence of phase transitions can happen in the neighbourhood of a straight line. On the contrary, the shape of this parametric domain for repulsive neural networks is closer to a parabolic one. Nevertheless, we have seen that the effect of the networks features can be quite different according to the nature of the networks. Indeed, attractive networks are more sensitive to isotropy/anisotropy and translation-invariance/non-translation-invariance than repulsive networks. The latter keep similar localisation in the parametric space when their features vary. These results are of particular interest because neural networks are generally composed by an important proportion of repulsive interactions.

There exists a lot of perspectives to this work. First of all, the first point that seems interesting to study is what are the properties of the influence of boundaries in graphs that correspond to the reality of biological networks. In this research, we have voluntarily reduced the problem to simple networks that have classical properties. However, different studies [23,24] have shown that the shape of biological networks such as neural networks or protein networks is not close to the one of a cellular automaton on  $\mathbb{Z}^2$ . They rather have a lot of common properties with complex networks such as scale-free or small-world networks. We would like to know if the theoretical and simulation results that we have obtained in this work can be applied in such more general cases.

Furthermore, what also seems to be judicious is to focus on the link between the stochastic version and the deterministic version of the Hopfield model, by decreasing progressively the temperature in order to let it tend to 0.

Finally, we would like to go further in the characterisation of these mentioned phase transitions in respect to the influence of boundary conditions. Indeed, it would be of interest to know if there exist links between boundary influence and the percolation theory for example. We would also like to generalise our theoretical method to the more complicated kinds of neural networks studied here with only a computer-based approach. Another perspective would be to focus on more realistic updating rules, *e.g.*, which are block-parallel (see definition in [8]) with each block having its own dynamics, *i.e.*, each block does not wait the end of the updating of all blocks to restart a new sequential updating, when the blocks are distinct.

## References

1. Albert, R., Barabási, A.L.: Statistical Mechanics of Complex Networks. *Reviews of Modern Physics* **74** (2002)
2. Barabási, A.L., Oltvai, Z.N.: Network Biology: Understanding the Cell's Functional Organization. *Nature Reviews Genetics* **5** (2004) 101–113
3. Kitano, H.: Biological Robustness. *Nature Reviews Genetics* **5** (2004) 826
4. Hinrichsen, H.: Nonequilibrium Critical Phenomena and Phase Transitions into Absorbing States. *Advances in Physics* **49** (2000) 815–958
5. Berry, H.: Nonequilibrium Phase Transition in a Self-Activated Biological Network. *Physical review E* **67** (2003) 031907
6. Fatès, N., Morvan, M.: Perturbing the Topology of the Game of Life Increases its Robustness to Asynchrony. In: *Proceedings of the 6th International Conference on Cellular Automata for Research and Industry. Volume 3305 of Lecture Notes in Computer Science.*, Springer (2004) 111–120
7. Fatès, N., Morvan, M.: An Experimental Study of Robustness to Asynchronism for Elementary Cellular Automata. *Complex systems* **16**(1) (2005) 1–27
8. Demongeot, J., Jézéquel, C., Sené, S.: Boundary Conditions and Phase Transitions in Neural Networks. *Theoretical Results*. Submitted to *Neural Networks* (2008)
9. Ising, E.: Beitrag zur Theorie des Ferromagnetismus. *Zeitschrift fur Physics* **31** (1925) 253–258
10. Dobrushin, R.L.: Existence of Phase Transition in Models of a Lattice Gas. In: *Proceedings of the Fifth Berkeley Symposium on Mathematical Statistics and Probability. Volume 3.*, University of California Press (1966) 73–87
11. Dobrushin, R.L.: The Problem of Uniqueness of a Gibbsian Random Field and the Problem of Phase Transitions. *Functional Analysis and its Applications* **2**(4) (1968) 302–312
12. Ruelle, D.: *Statistical Mechanics: Rigorous Results*. W. A. Benjamin (1969)
13. Spitzer, F.L.: Introduction aux Processus de Markov à Paramètre dans  $\mathbb{Z}_\nu$ . In: *École d'été de probabilités de Saint-Flour de 1973. Volume 390 of Lecture Notes in Mathematics.*, Springer (1974) 112–189
14. Ruelle, D.: *Thermodynamic Formalism: the Mathematical Structure of Equilibrium Statistical Mechanics*. Cambridge Mathematical Library (1984)

15. Ackley, D.H., Hinton, G.E., Sejnowski, T.J.: A Learning Algorithm for Boltzmann Machines. *Cognitive Science* **9**(1) (1985) 147–169
16. Athithan, G., Dasgupta, C.: On the Problem of Spurious Patterns in Neural Associative Memory Models. *IEEE Transactions on Neural Networks* **8**(6) (1997) 1483–1491
17. Hassoun, M.H., Watta, P.B.: Alternatives to Energy Function-Based Analysis of Recurrent Neural Networks. In: *Computational Intelligence: A Dynamical System Perspective*, IEEE Computer Society Press (1995) 46–67
18. Onsager, L.: Crystal Statistics. I. A Two-Dimensional Model with an Order-Disorder Transition. *Physical Review* **65** (1944) 117–149
19. Propp, J.G., Wilson, D.B.: Exact Sampling with Coupled Markov Chains and Applications to Statistical Mechanics. *Random Structures and Algorithms* **9**(1-2) (1996) 223–252
20. Ruelle, D.: On the Use of "Small External Fields" in the Problem of Symmetry Breakdown in Statistical Mechanics. *Annals of Physics* **69**(2) (1972) 364–374
21. Cinquin, O., Demongeot, J.: Positive and Negative Feedback: Striking a Balance Between Necessary Antagonists. *Journal of Theoretical Biology* **216**(2) (2002) 229–241
22. Cinquin, O., Demongeot, J.: High-Dimensional Switches and the Modelling of Cellular Differentiation. *Journal of Theoretical Biology* **233**(3) (2005) 391–411
23. Montoya, J.M., Solé, R.V.: Small World Patterns in Food Webs. *Journal of Theoretical Biology* **214** (2002) 405–412
24. Watts, D.J., Strogatz, S.H.: Collective Dynamics of "Small-World" Networks. *Nature* **393**(6684) (1998) 440–442