Boundary Conditions and Phase Transitions in Neural Networks. Theoretical Results

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Abstract. The purpose of this paper is to expose some relevant theoretical results about the asymptotic behaviour of finite neural networks (on lattices) with fixed boundary conditions. This work focus on two different topics that seem to be of interest from the biological point of view. First, it intents to exhibit the links existing between synchronous and asynchronous updating iteration modes in these networks, whatever the number of dimensions is. We will prove that the effects of boundary conditions on a whole neural network do no depend on the updating iteration mode, *i.e.*, if the asymptotic behaviour admits phase transitions, these phase transitions are observable in synchronous and asynchronous networks. Then, we more precisely focus on the one-dimensional case and we show that boundaries have no significant impact on such networks. So, we will present a new mathematical approach that permits the theoretical study of the asymptotic dynamics and of boundary influence characterisation in neural networks. We will also introduce the tools generalising the method to study phase transitions in more complex cases.

Keywords: Stochastic neural networks; Hopfield model extension; Phase transitions.

1 Introduction

In this paper, we focus on the asymptotic behaviour of large scale neural networks when they are regulated by their own components (*i.e.*, the neurons) and also by fixed boundary conditions which correspond to neurons whose state cannot change during the dynamical evolution of the system. Our aim is to show that the influence exerted by boundary conditions does not depend in certain cases on the state values on boundaries. Before going further, it seems to be important to present why we interest in finite networks. From the point of view of biologists, it seems to be too artificial to use periodic or free boundaries because of the nature of living systems. Let us give an example to illustrate this remark: the cytoplasm of a cell of an eukaryotic organism is separated from other cells by the cell membrane, which plays the role of boundary conditions for the inner cell. Furthermore, as flows between cells exist, the membranes have to respect

some biological constraints. So, to respect as well as possible the lifelikeness, it is judicious to interest in finite neural networks with fixed boundaries.

This work is encouraged by the increasing interest researchers get in the questions of dynamical behaviour, structural stability and robustness in complex systems, specifically in biological complex systems. Hence, the comprehension of the common behaviours among synchronous and asynchronous dynamics as well as the impact of boundaries on such dynamical systems are relevant to understand how they reach to adapt to this kind of dynamical and topological variations. Consequently, the first part of this paper deals with the link existing between two kinds of updating iteration modes: we will prove that, whatever the dimension of the underlying lattice is, there is a proportionality relation between the synchronous and the asynchronous modes, *i.e.*, if a phase transition occurs in the synchronous mode, it is also observable in the asynchronous one.

Furthermore, this paper will point out the result that, in one-dimensional neural networks, the influence of boundary conditions is not significant, what brings us to prove that phase transition phenomena cannot emerge from the asymptotic behaviour of one-dimensional neural networks. Thanks to this mathematical study, we give a new theoretical approach which would be useful to develop this work to more complex neural networks. Indeed, we will see that this method is obviously appropriate to permit to exhibit phase transitions phenomena in two-dimensional (or more) networks with more complicated properties that we will discuss.

The case of influence of boundaries was studied in the past in physics for ferromagnetic particles networks following the Ising law. The Ising model [1] was created in order to represent how a particle of a system can modify its behaviour in function of its neighbours. In the one-dimensional case, Ising proved that the dynamics of such networks does not bring to sudden and important change of behaviours. More formally, the behaviour of ferromagnetic particles networks does not admit *phase transition*. We will see in this paper that these past results can be deployed to neural networks following a stochastic version of an extended Hopfield law.

In Section 2, we give preliminary definitions, describe the model of random neural network considered and present some explicit invariant measure expressions, depending on the updating modes and on the boundary conditions. In Section 3, we give indications about parametric conditions of phase transitions and study the asymptotic behaviour of such networks. In Section 4, we open the discussion to more complicated cases of phase transitions in two-dimensional neural networks (the anisotropic case, the not translation invariant case...) and introduce a simulation method to study them.

2 Hopfield-like neural networks

2.1 Definitions

We consider in the following a random version of the Hopfield neural networks [2], whose evolution is defined by a stochastic updating rule. More precisely, we will denote by R a set of $N \times M$ neurons, which are located at vertices of $\mathbb{Z}^2$, each of them having two possible states of activity, defined, if we call $\sigma(t) = (\sigma_i(t))_{i \in R} \in \Omega = \{0, 1\}^{N \times M}$ the current configuration of the network at time t, by the following rule:

$$\sigma_i(t) = \begin{cases} 0 & \text{if the neuron } i \text{ is inactive at time } t, \\ 1 & \text{if the neuron } i \text{ is firing at time } t. \end{cases}$$

In the present study, we will fix the boundary conditions of R instead using classical periodic (toric) or free boundaries; in the following, $\overline{\sigma}$ will denote boundary configuration on the complementary of R in $\mathbb{Z}^2$ ($\mathbb{Z}^2 \backslash R = R^c$) and we will suppose that the origin O of $\mathbb{Z}^2$ belongs to R.

As in [3], we define the boundaries of the networks by means of the following notations where $\mathcal{N}_i$ is the neighbourhood of the neuron i in which the synaptic weight between i and j, denoted w_{ij}, does not vanish ($j \in \mathcal{N}_i \Leftrightarrow w_{ij} \neq 0$):
$\partial_{int}R = \{i \in R; \ \exists j \in R^c, \ j \in \mathcal{N}_i\},$
$\partial_{ext}R = \{i \notin R; \ \exists j \in R, \ j \in \mathcal{N}_i\},$
$\partial R = \{(i, j), \ i \in \partial_{int}R, \ j \in \partial_{ext}R; \ j \in \mathcal{N}_i\}.$

The temporal evolution of the network R is defined by the probability that a neuron i evolves from state $\sigma_i(t)$ to state $\sigma_i(t+1)$ knowing $\sigma(t)$ on $\mathcal{N}_i$ (local updating rule). In our case, we choose the following rule [4]:

$$P(\sigma_i(t+1) = \alpha | \sigma_j(t), j \in \mathcal{N}_i \cup \{i\}) = \frac{e^{\alpha . H_i(\sigma(t))/T}}{1 + e^{\alpha . H_i(\sigma(t))/T}}$$

where:
$\circ$ $\alpha \in \{0, 1\}$,
$\circ$ $H_i(\sigma(t)) = \sum_{j \in (\mathcal{N}_i \cup \{i\}) \cap R} w_{ij}\sigma_j(t) + \sum_{j \in (\mathcal{N}_i \cup \{i\}) \cap \partial_{ext}R} w_{ij}\overline{\sigma_j}(t)$ is the interaction potential of the neuron i with its neighbours in $\mathcal{N}_i$ and
$\circ$ T is the temperature of the network R.

If $T = 0$, we recover the deterministic version of the Hopfield model; on the contrary, if T tends to infinity, we have probability $\frac{1}{2}$ to have state 1 or state 0 in neuron i, whatever the states are in $\mathcal{N}_i$. T increases the randomness (until the uniformity) in the network. The interaction potential $H(\sigma(t))$ of the configuration $\sigma(t)$ at time t is given by: $H(\sigma(t)) = \sum_{i \in R} H_i(\sigma(t)) = \sum_{i \in R}[\sum_{j \in (\mathcal{N}_i \cup \{i\}) \cap R} w_{ij}\sigma_j(t) + \sum_{j \in (\mathcal{N}_i \cup \{i\}) \cap \partial_{ext}R} w_{ij}\overline{\sigma_j}(t)]$. Next we will suppose that the weights are symmetrical: $w_{ij} = w_{ji}$.

With such local updating rules, when the size of the network is finite (which is always the case when working with computer simulations), the asymptotic

behaviour of the system when time tends to infinity is characterised by a probability measure which is uniquely determined, and remains unique in absence of phase transition, when the network size is tending to infinity. Let us now explicit this measure, taking into account the updating modes and the boundaries.

2.2 Invariant measures

It has already been shown that the invariant measure of the network depends on the updating modes: sequential, parallel, or block sequential [4,5]. The interesting result is that in every case, when the size of the network is finite, the stationary measure is unique (thanks to strictly positive terms in the Markovian matrix, whose general term $M(\sigma, \xi)$ is the probability to move from a configuration σ to a configuration ξ in R). We will give now the general expressions for the invariant measures obtained in each case, depending on boundary conditions:

- *Sequential (asynchronous) case:*

The updating is made successively for each neuron. This leads to the following invariant measure expression:

$$\mu_{as}(\sigma) = Z_{as}^{-1} e^{\sum_{i,j \in R} \frac{w_{ij}\sigma_i\sigma_j}{2T} + \sum_{(i,j) \in \partial R} \frac{w_{ij}\sigma_i\overline{\sigma_j}}{T}}$$

where Z_{as}^{-1} is a normalising constant.

- *Parallel (synchronous) case:*

The updating is made simultaneously for each neuron in the whole network. This leads to the following invariant measure expression:

$$\mu_s(\sigma) = Z_s^{-1} \sum_{\xi \in \Omega} e^{\frac{\sum_{(i,j) \in \partial R} w_{ij}(\sigma_i + \xi_j)\overline{\sigma_j} + \sum_{i,j \in R} w_{ij}\sigma_i\xi_j}{T}}$$

where Z_s^{-1} is a normalising constant.

- *Block sequential (partially synchronous) case:*

More generally, we can consider n sub-networks $R_k (k = 1, ...n)$ of the neural network R and the updating is made synchronously into a sub-network, and successively for the sub-networks. This leads to the following invariant measure expression:

$$\mu_{ps}(\sigma) = Z_{ps}^{-1} \sum_{\xi \in \Omega} e^{\frac{<\sigma>+\sigma(\overline{\sigma})+<\xi>+\xi(\overline{\xi})+\ll\sigma,\xi\gg}{T}}$$

where Z_{ps}^{-1} is a normalising constant and:
$< \sigma > = \sum_{i=1,...,n} \sum_{j \in R_i} \sum_{k \in \cup_{j<i} R_j} w_{jk}\sigma_j\sigma_k,$
$\sigma(\overline{\sigma}) = \sum_{j \in R} \sum_{k \in R^c} w_{jk}\sigma_j\overline{\sigma_k},$
$\ll \sigma, \xi \gg = \sum_{i=1,...,n} \sum_{j \in R_i} \sum_{k \in \cup_{j \leq i} R_j} w_{jk}\sigma_j\xi_k.$
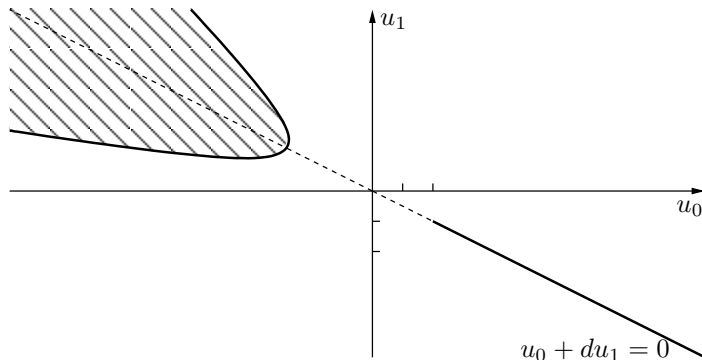
Fig. 1. Parametric conditions on u_0 and u_1 of phase transitions for the Ising model in $\mathbb{Z}^d$ in the isotropic and translation invariant attractive and repulsive cases. They illustrate the results obtained by Dobrushin and Ruelle. The bottom right corner, that corresponds to the attractive case, shows that the phase transition (in bold) can take place on a part of the straight line $u_0 + du_1 = 0$. 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.

This expression holds when $\ll \sigma, \xi \gg \, = \, \ll \xi, \sigma \gg$, which is equivalent to the detailed balance condition (reversibility condition). It is the case for the synchronous $(n = 1)$ and asynchronous cases $(n = N \times M)$, and for the feed-forward modular case, which is a particular mode defined by the synaptic weights: $w_{ij} = 0, \ \forall (i,j); \ i \in R_k, \ j \in R_{k'}, k < k'$. This last mode is of interest because of its biologic relevance in hierarchical systems, with inter-neural connections stabilised in a pyramidal architecture from a master sub-system, with feedback loops present only into the sub-systems, like in the cardio-respiratory regulation [6].

The general term of the Markovian matrix giving the probabilities to move from a configuration σ to a configuration ξ in R after synchronously updating the neurons of a sub-network and successively for the sub-networks $R_k (k = 1, ...n)$, is given by:

$$M(\sigma, \xi) = \frac{e^{(<\xi> + \xi(\overline{\sigma}) + \ll \sigma, \xi \gg)/T}}{\sum_{\xi \in \Omega} e^{(<\xi> + \xi(\overline{\sigma}) + \ll \sigma, \xi \gg)/T}}$$

The proof of the results above can be found in [7,8].

In a case more general than the feed-forward one, we are obliged to calculate the invariant measure by using numerical computations. Note therefore that, in any case above, the number of terms involved in the sums appearing in the formulae is in general too big (if $N \times M$ is large) to calculate exactly the invariant measure probabilities, and hence we must evaluate them by using Monte Carlo methods.

3   Boundaries influence in the Hopfield model

3.1   The problem of the thermodynamic phase transitions and the Ising model

Phase transitions we are concerned with in this paper are thermodynamic phase transitions: these phenomena are observed when the size of the network R tends to infinity (thermodynamic limit). Near parametric conditions of phase transitions, little changes in the parameters lead to great changes in the behaviour of the network, like changes of the asymptotic (when time tends to infinity) characterisation of the system in terms of invariant measure, which remains unique (as given in the previous Section) for fixed boudary conditions, but which can change when these boundary conditions change, *e.g.*, when we make a flip-flop of state 1 to state 0 on the frontier of R. As far as we are concerned, we will see that changing the boundaries will affect the evolution of the network, as in the case of the classical two-dimensional Ising model. In Figure 1, we summarise the results about the Ising model of [9,10,11] by giving conditions of phase transition and, on the contrary, conditions under which no phase transition is observed. These results hold for the isotropic Ising model on $\mathbb{Z}^d$, defined by the synaptic weights: $w_{ii} = Tu_0$, $w_{ij} = Tu1$ if $d(i,j) = 1$ and $w_{ij} = 0$ if $d(i,j) > 1$, where d is the $L1$ distance on $\mathbb{Z}^d$. In the attractive case ($u1 < 0$), phase transitions can occur only when $u0 + du1 = 0$. In the repulsive case ($u1 > 0$), phase transitions are observed in the region of the parametric space $(u0, u1)$ delimited by a neighbourhood of the phase transition line of the attractive case. But there is no particular result concerning the frontier between this region, where phase transitions are observed, and the rest of the parametric space.

The parametric conditions of phase transition were proved for a sequential updating mode. But, thanks to a proportionality relation between partition functions of the invariant measures corresponding to the two updating modes, massively parallel and sequential [12,4,13], these results still hold in the case of the massively parallel (synchronous) updating mode, with fixed boundaries. This assertion will be proved in the next paragraph in the context of our model.

3.2   Parametric conditions of phase transitions in dependence on the updating mode

Parametric conditions of phase transitions are generally obtained for the sequential updating mode, but it is possible to show that for some constraints on the synaptic weights (*i.e.*, weights should simply be symmetrical), these phase transition conditions still hold in the synchronous case. Let us first remember some usual definitions of statistical mechanics. We call:
$\Psi(R, T, W) = -T.\log(Z(R, T, W))$ the free energy of R and
$\psi(T, W) = \lim_{R \to \mathbb{Z}^d} \Psi(R, T, W)/|R|$ the specific free energy of R,
where T is the temperature and W is the matrix of the synaptic weights.

We can observe phase transitions when ψ is not differentiable. We will not discuss here about the existence or differentiability of ψ, but just see if there exists, in certain cases, a proportionality relation between ψ_s and ψ_{as}, respectively the specific free energies in the synchronous and asynchronous updating modes. So the phase transition points are the same in both cases (the result has been confirmed by simulation).

Lemma 1. *Let us suppose that there exist two independent subsets of R, R_1 and R_2, the independence being defined by: $\forall i \in R_1, j \in R_2, w_{ij} = 0$. We have: $\forall \sigma, \eta \in \{0, 1\}^R$, if $R = R_1 \cup R_2$, $H_s(\sigma, \eta) = H_{as}(\sigma_1 \eta_2) + H_{as}(\sigma_2 \eta_1)$, where $\sigma_1 \eta_2$ is the configuration defined by: $(\sigma_1 \eta_2)_i = \sigma_i$ if $i \in R_1$, and $(\sigma_1 \eta_2)_i = \eta_i$ if $i \in R_2$, and where the potentials H_s and H_{as} are defined by $H_s(\sigma, \eta) = \sum_{i,j \in R} w_{ij} \eta_i \sigma_j +$ $\sum_{i \in R, j \in R^c} w_{ij}(\sigma_i + \eta_i)\overline{\sigma_j}$ and $H_{as}(\sigma) = \frac{\sum_{i,j \in R} w_{ij} \sigma_i \sigma_j}{2} + \sum_{i \in R, j \in R^c} w_{ij} \sigma_i \overline{\sigma_j}$.*

Proof. We have:

$$H_{as}(\sigma_1 \eta_2) = \frac{\sum_{i \in R_1, j \in R_2} w_{ij} \sigma_i \eta_j + \sum_{i \in R_2, j \in R_1} w_{ij} \eta_i \sigma_j}{2}$$
$$+ \sum_{i \in R_1, j \in R^c} w_{ij} \sigma_i \overline{\sigma_j}$$
$$+ \sum_{i \in R_2, j \in R^c} w_{ij} \eta_i \overline{\sigma_j}$$

So, since R_1 and R_2 are independent:

$$H_{as}(\sigma_1 \eta_2) = \frac{\sum_{i \in R_1, j \in R_2} (w_{ij} + w_{ji}) \sigma_i \eta_j}{2}$$
$$+ \sum_{i \in R_1, j \in R^c} w_{ij} \sigma_i \overline{\sigma_j}$$
$$+ \sum_{i \in R_2, j \in R^c} w_{ij} \eta_i \overline{\sigma_j}$$

We have supposed above that the weights were symmetrical: $w_{ij} = w_{ji}$. Thus: $H_{as}(\sigma_1 \eta_2) + H_{as}(\sigma_2 \eta_1) = \sum_{i \in R_1, j \in R_2} w_{ij} \sigma_i \eta_j + \sum_{i \in R, j \in R^c} w_{ij}(\sigma_i + \eta_i)\overline{\sigma_j} = H_s(\sigma, \eta)$ and we get the expected result. $\square$

Proposition 1. *For a nearest neighbours model in $\mathbb{Z}^d$, we have $Z_s = (Z_{as})^2$.*

Proof. For a nearest neighbours model on $\mathbb{Z}^d$, it is easy to construct two independent subsets R_1 and R_2 (it suffices to consider that R is made of two subsets R_1 and R_2 separated by a border of neurons disconnecting them). Then we have: $Z_s = \sum_{\sigma, \eta \in \Omega} e^{H_s(\sigma, \eta)/T}$ and $Z_{as} = \sum_{\sigma \in \Omega} e^{H_{as}(\sigma)/T}$. Using the lemma 1 above, we have:

$$Z_s = \sum_{\sigma \in \Omega} \sum_{\eta \in \Omega} e^{(H_{as}(\sigma_1 \eta_2) + H_{as}(\sigma_2 \eta_1))/T}$$
$$= \sum_{\xi \in \Omega} \sum_{\xi' \in \Omega} e^{(H_{as}(\xi) + H_{as}(\xi'))/T}$$
$$= \sum_{\xi \in \Omega} e^{H_{as}(\xi)/T} \sum_{\xi' \in \Omega} e^{H_{as}(\xi')/T}$$

which is the expected result. $\square$

As a consequence of the lemma 1 and the proposition 1, for a nearest neighbours model on $\mathbb{Z}^d$, we have $\psi_s = 2\psi_{as}$. And we have hence the following theorem directly from this proportionality relation between ψ_s and ψ_{as}.

Theorem 1. *Phase transitions are identically observed for sequential and parallel updating modes in Hopfield-like neural networks on $\mathbb{Z}^d$ with fixed boundary conditions.*

This result was already obtained without considering boundaries, in the following cases [12,14,13]:

− Curie-Weiss model on $\mathbb{Z}^d$,

− ferromagnetic Ising model on $\mathbb{Z}^d$,

− Hopfield neural network where synaptic weights are defined via a Hebbian learning rule, and where the two possible states of each neuron are -1 and $+1$.

3.3 A method to exhibit parametric phase transitions conditions

We can define thermodynamic phase transition phenomena by many different ways. A possible approach [9] is to characterise such phenomena by a loss of ergodicity: the invariant measures of the system defined above, depending on updating mode, are not unique, when the size of the network tends to infinity. We apply this definition to exhibit a possible criterion of phase transition.

If μ is the invariant measure of the infinite system, then we can easily obtain the following relations, where the cylinder $[A, B] = \{\sigma \mid \sigma_i = 1, i \in A; \sigma_i = 0, i \in B\}$:

(i) projective equations:
$$\forall A, B \subset R \mid A \cap B = \emptyset, \forall i \in A, \mu([A, B]) + \mu([A\backslash\{i\}, B \cup \{i\}]) = \mu([A\backslash\{i\}, B])$$

(ii) conditional equations:
$$\forall i \in R, \mu([\{i\}, \emptyset]) = \sum_{A,B \subset R \mid i \notin A,B} \Phi_i(A, B)\mu([A, B]) \text{ (Bayes equation)}$$

where conditional probability $\mu(\sigma_i = 1 \mid [A, B]) = \frac{e^{H(\sigma_i)/T}}{1+e^{H(\sigma_i)/T}} = \Phi_i(A, B)$.

We note $L = R\backslash\{i\}$ and we order the neurons i's of L from 1 to $|L|$; for every subset K of L, j_K denotes the smallest index of the neurons of K. Then we can define the matrix of order $2^{|L|} \times 2^{|L|}$, denoted by M, corresponding to the coefficients of the former equations, in which $\Phi(A, B)$ is just $\Phi_O(A, B)$, O being the origin of $\mathbb{Z}^d$. Let us consider the following matrices $M1$ and $M2$ as blocks of the matrix M:

$$M1 = \begin{pmatrix} 1 & 1 & \dots & 0 \\ 1 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & 0 \\ \Phi(L,\emptyset) & \Phi(L\backslash\{1\},\{1\}) & \dots & \Phi(K, L\backslash K) \end{pmatrix}$$

$$M2 = \begin{pmatrix} 0 & & \dots & 0 \\ 0 & & \dots & 0 \\ \vdots & & \vdots & \vdots \\ 0 & & \dots & 1 \\ \Phi(K\backslash\{j_K\}, L\backslash K \cup \{j_K\}) & & \dots & \Phi(\emptyset, L) \end{pmatrix}$$

We finally have:

$$M = \begin{pmatrix} M1 & M2 \end{pmatrix}$$

First lines of M are the coefficients of the projective equations and the last line corresponds to the coefficients of the conditional equation. Let us denote by Ξ the general cylinder $[K\backslash\{j_K\}, (L\backslash K) \cup \{j_K\}]$. We can then write the system obtained by the equations of type *(i)* and *(ii)* in the following form:

$$M.\begin{pmatrix} \mu([L, \emptyset]) \\ \mu([L\backslash\{1\}, \{1\}]) \\ \mu([L\backslash\{2\}, \{2\}]) \\ \vdots \\ \mu([K, L\backslash K]) \\ \mu(\Xi) \\ \vdots \\ \mu([\{1\}, L\backslash\{1\}]) \\ \mu([\emptyset, L]) \end{pmatrix} = \begin{pmatrix} \mu([L\backslash\{1\}, \emptyset]) \\ \mu([L\backslash\{2\}, \emptyset]) \\ \cdots \\ \vdots \\ \mu([K\backslash\{j_K\}, L\backslash K]) \\ \cdots \\ \vdots \\ \mu([\emptyset, L\backslash\{1\}]) \\ \mu([\{0\}, \emptyset]) \end{pmatrix}$$

Equations of types *(i)* and *(ii)* are generally linearly independent; but, under certain parametric conditions, they are linearly dependent and it is the case under phase transitions conditions (when μ is non unique). When $det M \neq 0$, we can express the matricial equation above with a new matrix of order $2^{|L'|} \times 2^{|L'|}$ and new vectors of dimension $2^{|L'|}$, corresponding to $2^{|L'|}$ new subsets, L' having one element less than L, until we reach the subset of R equal to $L^{(|L|-2d)} = \mathcal{N}_i$.

Lemma 2. [15] *We have:*
$det M = 0 \Leftrightarrow \sum_{K \subset L}(-1)^{|L\backslash K|}\Phi(K, L\backslash K) = 0.$

In the case of our model in its isotropic form in $\mathbb{Z}^d$ defined by $w_{ii} = Tu_0$, and $w_{ij} = Tu_1$, if $d(i,j) = 1$, we can replace L by $\mathcal{N}_i$, and we get from Lemma 2 that $det M = 0$ admits a finite set of solutions among which appears the following one: $u0 + du1 = 0$. So we retrieve the classical equation of phase transition (see Subsection 3.1 and the following example). The pertinence of this specific solution is proven thanks to all the simulation results obtained on isotropic and translation invariant neural networks whatever the initial condition is.

Example 1. Let us consider the one-dimensional Hopfield model and define cylinder subsets: $[\Lambda, \emptyset] = \{\bullet \times \bullet\}$, $[\Lambda\backslash\{1\}, \{1\}] = \{\circ \times \bullet\}$, $[\Lambda\backslash\{2\}, \{2\}] = \{\bullet \times \circ\}$, $[\emptyset, \Lambda] = \{\circ \times \circ\}$, where the symbol $\bullet$ (resp. $\circ$) denotes a fired neuron (resp. an inhibited neuron), and $\times$ denotes the site origin O. Then, M is equal to:

$$M = \begin{pmatrix} 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ \frac{e^{u_0+2u_1}}{1+e^{u_0+2u_1}} & \frac{e^{u_0+u_1}}{1+e^{u_0+u_1}} & \frac{e^{u_0+u_1}}{1+e^{u_0+u_1}} & \frac{e^{u_0}}{1+e^{u_0}} \end{pmatrix}$$

The matrix equation of the dynamics becomes:

$$M. \begin{pmatrix} \mu([\Lambda, \emptyset]) \\ \mu([\Lambda\backslash\{1\}, \{1\}]) \\ \mu([\Lambda\backslash\{2\}, \{2\}]) \\ \mu([\emptyset, \Lambda]) \end{pmatrix} = \begin{pmatrix} \mu([\Lambda\backslash\{1\}, \emptyset]) \\ \mu([\Lambda\backslash\{2\}, \emptyset]) \\ \mu([\emptyset, \{2\}]) \\ \mu([\{0\}, \emptyset]) \end{pmatrix}$$

Vanishing the determinant of M leads to the following equation:

$DetM = 0 \Leftrightarrow -(e^{u_0} + 2e^{2u_0+2u_1} - 2e^{u_0+u_1} - e^{2u_0+3u_1} - e^{2u_0+u_1} + e^{u_0+2u_1})/((1+ e^{u_0})(1 + e^{u_0+u_1})(1 + e^{u_0+2u_1})) = 0$

which admits a set of two solutions: $\{u_1 = 0; u_0 + u_1 = 0\}$. So, we obtain the following relation:

$u_0 + u_1 = 0 \Rightarrow DetM = 0$

that exactly corresponds to the results obtained by Ruelle in the context of ferromagnetic networks.

Definition 1. *[16,17] Let us consider an interaction potential H on R and identify a configuration $\sigma \in \{0,1\}^R$ with the subset S of R on which the value of σ_i is 1.*
Then H is called strongly super-modular *potential if $\forall A_i \subset R, i = 1, \ldots, n$ then the Poincaré's inequality [3] holds;*
H is called super-modular, *if the Poincaré's inequality holds for $n = 2$;*
H is called attractive, *if we have: $\forall A \subset R, |A| \geq 2 \Rightarrow \sum_{B \subset A}(-1)^{|A\backslash B|}H(B) = 0$.*

Proposition 2. [16] *H is strongly super-modular if and only if it is attractive.*

Proposition 3. [17] *If a potential H on R is super-modular, then phase transition occurs if and only if there exists i in R, such that $\mu^-([\{i\}, \emptyset]) \neq \mu^+([\{i\}, \emptyset])$, where μ^- (resp. μ^+) is the limit (when R tends to $\mathbb{Z}^d$) of the measure observed when all states are fixed at 0 (resp. 1) on the boundary of R.*

Note that the proposition 3 holds if H is attractive, in particular in the case of neural networks with positive weights.

Proposition 4. *In the one-dimensional case of the stochastic version of the Hopfield model with isotropy and translation invariance underlying properties, $\mu^-([\{i\}, \emptyset]) = \mu^+([\{i\}, \emptyset])$ for any i in R, when $detM = 0$.*

Proof. Let us suppose that $R = [-r, +r]$ and denote:
$\forall A, B \subset R \mid A \cap B = \emptyset, \ \mu^+([A, B]) = \lim_{R \to \mathbb{Z}} \mu([A, B] \mid [\{-(r + 1), r + 1\}, \emptyset]),$
$a^+ = \mu^+([\{-1, 1\}, \emptyset]),$

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[3] The Poincaré's inequality is defined by: $H(\cup_{i=1,\ldots,n} A_i) \geq \sum_{i=1,\ldots,n} H(A_i) - \sum_{i<j} H(A_i \cap A_j) + \ldots + (-1)^k \sum_{i_1 < \ldots < i_k} H(\cap_{j=1,\ldots,k} A_{i_j}) + \ldots + (-1)^n H(\cap_{i=1,\ldots,k} A_i)$

$b^+ = \mu^+([\{-1\}, \{1\}]) = \mu^+([\{1\}, \{-1\}])$ (for symmetry reasons) and
$x^+ = \mu^+([\{0\}, \emptyset])$ where $0 \notin A \cup B$.

With these previous notations, the equations *(i)* and *(ii)* above reduce here to:
• $a^+ + b^+ = \mu^+([\{-1\}, \emptyset]) = x^+$ because of the hypothesis of translation invariance and
• $x^+ = \Phi(\{-1, 1\}, \emptyset).a^+ + 2\Phi(\{-1\}, \{1\}).b^+ + \Phi(\emptyset, \{-1, 1\}).(1 - a^+ - 2b^+)$

We consequently get:
$\forall A, B \subset R \mid A \cap B = \emptyset, 0 \notin A \cup B, \mu^+(\sigma_0 = 1 \mid [A, B]) = \frac{e^{H(\sigma)/T}}{1 + e^{H(\sigma)/T}} = \Phi(A, B)$,
where $\sigma_i = 1$, for $i \in A \cup \{0\}$ and $\sigma_i = 0$, for $i \in B$, and where $\Phi(A, B)$ denotes $\Phi_0(A, B)$.

When $det M = 0$, there exists a link between two lines of M, hence we have an equation determining the value of x^+:
$det M = 0 \Leftrightarrow (\Phi(\{-1, 1\}, \emptyset) - \Phi(\emptyset, \{-1, 1\})).x^+ + \Phi(\emptyset, \{-1, 1\}) = x^+$, hence:
$x^+ = \frac{\Phi(\emptyset, \{-1, 1\})}{1 - \Phi(\{-1, 1\}, \emptyset) + \Phi(\emptyset, \{-1, 1\})}$

Because $x^+ = x^-$ (we have: $\mu^-(\sigma_0 = 1 \mid [A, B]) = \Phi(A, B)$ and the same equations as above by replacing $+$ by $-$ lead to the same final value for x^+ and x^-), we get:
$\mu^+([\{0\}, \emptyset]) = \mu^-([\{0\}, \emptyset])$ and the results follows from the translation invariance. $\square$

Proposition 5. *In the one-dimensional case of the stochastic version of the isotropic and translation invariant Hopfield model, $\mu^+([\{-r, r\}, \emptyset])$ (resp. $\mu^-([\{-r, r\}, \emptyset])$) has the same limit than $(\mu^+([\{-r\}, \emptyset]))^2$ (resp. $((\mu^-([\{-r\}, \emptyset]))^2)$, when $R = [-r, r]$ tends to $\mathbb{Z}$.*

Proof. Let us note:
• $\alpha_R^+ = \mu([\{-r, r\}, \emptyset] \mid [\{-(r+1), r+1\}, \emptyset])$,
• $\alpha^+ = \lim_{R \to \mathbb{Z}} \alpha_R = \mu^+([\{-r, r\}, \emptyset])$,
• $\beta_R^+ = \mu([\{-r\}, \{r\}] \mid [\{-(r+1), r+1\}, \emptyset])$,
• $\beta^+ = \lim_{R \to \mathbb{Z}} \beta_R = \mu^+([\{-r\}, \{r\}]) = \mu^+([\{r\}, \{-r\}])$ (for symmetry reason),
• $y_R^+ = \mu([\{-r\}, \emptyset] \mid [\{-(r+1), r+1\}, \emptyset])$,
• $y^+ = \lim_{R \to \mathbb{Z}} y_R = \mu^+([\{-r\}, \emptyset]) = \mu^+([\{r\}, \emptyset])$ (for symmetry reason).

We will in the following develop the numerator and the denominator of the fractions α_R^+, β_R^+ and y_R^+, in order to make explicit their common parts (the Λ's below) and also the differences for being able to give a majoration of $\alpha_R^+ - y_R^{+2}$.

The proof will be done, if $|\alpha_R^+ - y_R^{+2}|$ tends to 0, when R tends to $\mathbb{Z}$. We denote:
○ $\Lambda_{r,1} = \sum_{\sigma \in \{0,1\}^R \mid \sigma(-(r-1))=1, \sigma((r-1))=1} e^{H(\sigma(t))}$,
○ $\Lambda_{r,2} = \sum_{\sigma \in \{0,1\}^R \mid \sigma(-(r-1))=1, \sigma((r-1))=0} e^{H(\sigma(t))}$ (and we have, for symmetry reason,
○ $\Lambda_{r,2} = \sum_{\sigma \in \{0,1\}^R \mid \sigma(-(r-1))=0, \sigma((r-1))=1} e^{H(\sigma(t))}$),
○ $\Lambda_{r,3} = \sum_{\sigma \in \{0,1\}^R \mid \sigma(-(r-1))=0, \sigma((r-1))=0} e^{H(\sigma(t))}$),
○ $\Upsilon_\alpha = e^{2u_0 + 2u_1}.(e^{2u_1}.\Lambda_{r,1} + 2e^{u_1}.\Lambda_{r,2} + \Lambda_{r,3})$,

○ $\Upsilon_\beta = e^{u_0+u_1}.[e^{u_1}.(\Lambda_{r,1}+\Lambda_{r,2})+\Lambda_{r,2}+\Lambda_{r,3}]$ and
○ $Z_R = e^{2u_0+2u_1}.(e^{2u_1}.\Lambda_{r,1}+2e^{u_1}.\Lambda_{r,2}+\Lambda_{r,3})+2e^{u_0+u_1}.[e^{u_1}.(\Lambda_{r,1}+\Lambda_{r,2})+\Lambda_{r,2}+\Lambda_{r,3}]+\Lambda_{r,1}+2\Lambda_{r,2}+\Lambda_{r,3}$.

We have then:
$$\begin{aligned}
\Lambda_{r,1}\Lambda_{r,3}-\Lambda_{r,2}^2 &= ((1-e^{u_1}).e^{u_0+u_1})^2 \\
&\quad \times(\Lambda_{r-1,1}\Lambda_{r-1,3}-\Lambda_{r-1,2}^2) \\
&= \ldots \\
&= ((1-e^{u_1}).e^{u_0+u_1})^{2(r-1)} \\
&\quad \times(\Lambda_{1,2}^2-\Lambda_{1,1}\Lambda_{1,3}) \\
&= ((1-e^{u_1}).e^{u_0+u_1})^{2r}.e^{u_0}
\end{aligned}$$

$$\alpha_R^+ = \frac{\Upsilon_\alpha}{Z_R}$$

$$\beta_R^+ = \frac{\Upsilon_\beta}{Z_R}$$
$$y_R^+ = \alpha_R^+ + \beta_R^+$$

Hence:
$$\begin{aligned}
\alpha_R^+ - y_R^{+2} &= \frac{(1-e^{u_1})^2.(\Lambda_{r,1}\Lambda_{r,3}-\Lambda_{r,2}^2)}{Z_R^2} \\
&= \frac{((1-e^{u_1}).e^{u_0+u_1})^{2r}.e^{u_0})}{Z_R^2}
\end{aligned}$$

We have also:
$Z_R \le (1+e^{u_0+u_1})^2.(\Lambda_{r,1}+2\Lambda_{r,2}+\Lambda_{r,3}) \le \ldots \le (1+e^{u_0+u_1})^{2r}.(\Lambda_{1,1}+2\Lambda_{1,2}+\Lambda_{1,3}) = K.(1+e^{u_0+u_1})^{2r}$, and $Z_R^2 \le K^2.(1+e^{u_0+u_1})^{4r}$.

We have the expected result by remarking that: $\frac{|e^{u_0+2u_1}-e^{u_0+u_1}|}{(e^{2u_0+2u_1}+2e^{u_0+u_1}+1)} < 1$. The same proof can be used for showing that $|\alpha_R^- - y_R^{-2}|$ tends to 0, when R tends to $\mathbb{Z}$. $\square$

Proposition 6. *We have: $\lim_{r\to+\infty}\mu^+([\{r\},\emptyset]) = \lim_{r\to+\infty}\mu^-([\{r\},\emptyset])$ in the one-dimensional case of the stochastic version of the isotropic and translation invariant Hopfield model, when $\det M \ne 0$.*

Proof. From the equations *(i)* and *(ii)* above, we have:
$\forall R \subset \mathbb{Z}, \alpha_R^+ + \beta_R^+ = y_R^+$, thus $\alpha^+ + \beta^+ = x^+$
and
$x^+ = \Phi^+(\{-r,r\},\emptyset).a^+ + 2\Phi^+(\{-r\},\{r\}).b^+ + \Phi^+(\emptyset,\{-r,r\}).(1-a^+-2b^+)$,
where
$\forall A,B \subset R \mid A \cap B = \emptyset, \Phi_R^+(A,B) = \mu^+([A,B] \mid [\{-(r+1),r+1\},\emptyset])$
and
$\Phi^+(A,B) = \lim_{R\to\mathbb{Z}}\Phi_R(A,B)$.

Finally, we have the three following equations:
(1) Projection equation
$\alpha^+ + \beta^+ = x^+$,

(2) Conditional equation
$$x^+ = \Phi^+(\{-r, r\}, \emptyset).a^+ + 2\Phi^+(\{-r\}, \{r\}).b^+ + \Phi^+(\emptyset, \{-r, r\}).(1 - a^+ - 2b^+),$$
(3) Independence equation
$$\alpha^+ = x^{+2},$$
from which we deduce the value of x^+. We can do the same for x^-, and we get the same value than for x^+, because $\Phi^-(A, B) = \Phi^+(A, B)$ due to the spatial Markovian character of the measures μ^+ and μ^-. $\square$

From the propositions above, we obtain the following theorem:

Theorem 2. *One-dimensional extended stochastic Hopfield networks does not admit phase transition in respect to the influence of fixed boundary conditions.*

Note that the same type of reasoning could be used for the Hopfield model in two dimensions or even in n dimensions, in which we observe an occurrence of phase transition inside the domain of vanishing of $detM$, if the absolute values of the synaptic weights are sufficiently far from 0. Unfortunately, the equations of type *(1)*, *(2)* and *(3)* above are becoming rapidly numerous (we need for example five equations in two dimensions) to be used for proving the uniqueness of $\mu([\{0\}, \emptyset])$ and we will use only simulations in a further paper for studying the influence of boundaries on the asymptotic behaviour of the neural network.

4   Conclusion

After having explicated the links existing between some updating modes, what seems to be of great interest when the studied object is a dynamical system, this paper has given some results emphasizing the links existing between physical and biological systems, namely ferromagnetic particles networks and neural networks. Indeed, it has been shown that the studied random version of the Hopfield model, that is relevant to study neural networks, admits a good closeness with the Ising model, that has been well studied in the past in statistical physics. We have so proven that the asymptotic behaviour of one-dimensional neural networks face to fixed boundary conditions cannot be associated to phase transition phenomena, what is a first step to characterise the general influence of fixed boundaries in such networks. Besides, it is interesting to see the effect of different boundaries on the evolution of the network. Usually, authors do not consider fixed boundaries but prefer periodic boundaries, which is often not relevant in biological applications. Fixed boundaries permit us to consider biological and physical applications for a large scale of finite neural networks, in which the boundary conditions can be considered as an external magnetic field, or as a chemical potential, or as an external synaptic activity exerted on the considered neuronal population.

The problem is now to see if we can show the existence of phase transitions for more general models of neural networks. In the general n-dimensional Ising model, we know that the phase transition conditions in the attractive case

still occurs for parametric conditions on synaptic weights [18] where $detM$ vanishes. The question is thus to know if neural networks following the rules of the generalised version of the Hopfield model admit the same properties (or close properties). So, we will first focus on simple two-dimensional neural networks, *i.e.*, with isotropy and translation invariance underlying features, before interesting in more complicated cases by breaking these underlying features and, so, by making anisotropic and not translation invariant networks. We could go further by breaking the locality property off and consequently studying networks where the interaction potentials received by a neuron are not only depending on the state of its nearest neighbours.

In order to study this kind of two-dimensional neural networks, it seems important to introduce simulation tools permitting to bypass the theoretical method presented here because of its rapidly increasing complexity and the difficulties to integrate in this method the notions of anisotropy, non translation invariance and globality. In a next article, we will give details about the chosen simulation method based on the computation of the absolute difference $|\mu^+([\{0\},\emptyset]) - \mu^-([\{0\},\emptyset])|$ when the size of the network R is tending to infinity. If this limit does not vanish, we will say that phase transition occurs. We will then give the obtained phase diagram representing the value of this measure in function of the two parameters u_0 and u_1. When it will be possible, we will compute the value of the determinant of the matrix M, in order to evaluate the domain of validity of the co-occurrence of phase transition and of vanishing for $detM$.

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