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Mean-field message-passing equations in the Hopfield model and its generalizations

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Motivated by recent progress in using restricted Boltzmann machines as preprocessing algorithms for deep neural network, we revisit the mean-field equations (belief-propagation and TAP equations) in the best understood such machine, namely the Hopfield model of neural networks, and we explicit how they can be used as iterative message-passing algorithms, providing a fast method to compute the local polarizations of neurons. In the “retrieval phase” where neurons polarize in the direction of one memorized pattern, we point out a major difference between the belief propagation and TAP equations : the set of belief propagation equations depends on the pattern which is retrieved, while one can use a unique set of TAP equations. This makes the latter method much better suited for applications in the learning process of restricted Boltzmann machines. In the case where the patterns memorized in the Hopfield model are not independent, but are correlated through a combinatorial structure, we show that the TAP equations have to be modified. This modification can be seen either as an alteration of the reaction term in TAP equations, or, more interestingly, as the consequence of message passing on a graphical model with several hidden layers, where the number of hidden layers depends on the depth of the correlations in the memorized patterns. This layered structure is actually necessary when one deals with more general restricted Boltzmann machines.

I. INTRODUCTION

The interest into neural networks has been revived recently by a series of practical successes using so-called “deep neural networks” to solve important and difficult problems in artificial intelligence, ranging from image segmentation to speech recognition (see¹ and references therein). The crucial learning phase in these applications is often started by using techniques for unsupervised learning, like restricted Boltzmann machines (RBM)² or auto-encoders³, in order to obtain a first set of synaptic weights that is then optimized in a supervised learning process using back-propagation.

The unsupervised learning in RBMs is an important problem. Its difficulty comes from the necessity to compute the correlation functions of a general spin systems. The correlation functions can be approximated by numerical methods like Monte-Carlo, but this is rather time-consuming. Alternative methods use local estimates of the correlations^{4,5}, or those that can be deduced by message-passing algorithms based on iteration of local mean-field equations. This last approach, which was pioneered in^{6,7}, has received more and more attention recently⁸⁻¹⁰, and it seems that these sophisticated message-passing algorithms can be quite useful in RBM learning. In recent years, message-passing has proved successful, both for analytical studies and for algorithm design, in several important problems of computer science including error correcting codes (for a reviews see for instance¹¹), constraint satisfaction problems (for a review, see for instance¹²), statistical inference (for a review, see for instance¹³), compressed sensing¹⁴⁻¹⁸, or learning in perceptrons¹⁹⁻²¹.

The aim of this paper is to revisit the mean-field equations, and their use as message-passing algorithm, in the Hopfield model of neural networks²². The Hopfield model, a model of binary neurons interacting by pairs, with synaptic weights chosen in such a way that the neurons tend to polarize spontaneously towards one of the memorized “patterns”, can also be seen as a RBM. It is in fact one of the best understood models of neural networks and of RBMs, and it provides an excellent starting point to understand the mean-field message-passing equations and their possible use as algorithms.

The present paper addresses four issues. The first one is the derivation of the various types of mean-field equations in the Hopfield model, the second one is their use as an algorithm, the third one is an analysis of the mean-field equations in a generalized Hopfield model where patterns have a combinatoric type of correlation. The fourth one is the generalization

of the whole approach to RBMs which are of a more general type than the Hopfield model.

It is useful to clarify the mean-field equations in the case of the Hopfield model because several forms of these equations exist, under various names and acronyms:

- Belief Propagation: BP
- Relaxed Belief Propagation: rBP
- Thouless-Anderson Palmer equations: TAP
- Approximate Message Passing: AMP
- Generalized Approximate Message Passing: GAMP

We shall see that each version is useful: BP and rBP form the basis of the statistical analysis called the cavity method²³ (also known as state evolution or density evolution in the recent computer-science literature) which gives the phase diagram of this problem. They can be used to derive TAP equations²⁴, which are also called AMP equations in the recent computer science literature. TAP equations were originally derived in the Hopfield model by²³. Through our derivation of TAP equations as simplifications of the general BP equations (related to the one done in²⁵), we confirm the validity of these equations, in spite of previous claims by²⁶ and²⁷ that they were incorrect. All methods actually lead to the same TAP equations as²³.

An important point which is clarified in the present approach concerns the use of message-passing mean-field equations in the “retrieval phase” of the Hopfield model, the phase where the neurons polarize spontaneously in the direction of one of the stored patterns (and where the model can be used as an associative memory). In this phase, the usual simplification of BP equations into rBP, which assumes that messages have a Gaussian distribution, is incorrect and one must treat separately some of the messages which are associated with the specific pattern where the polarization develops. The equivalent of the rBP equations, taking into account this modification (called rBP-M in the following), are structurally distinct from the usual rBP equations. However this distinction disappears when one writes TAP equation. This makes the TAP equations much better suited for algorithmic applications.

The Hopfield model is a system of binary neurons (or Ising spins), with infinite range pairwise interactions. It is thus intimately related to the infinite range model of spin glasses

of Sherrington and Kirkpatrick (SK)²⁸, but it differs from it in the detailed structure of the interactions between spins. Instead of being independent random variables, the coupling constants between the spins are built from a set of predetermined patterns that one wants to memorize. This structure leads to a modification of the Onsager reaction term in the TAP equations. Our derivation shows that this modification is easily understood by using a representation of the Hopfield model with two layers, a layer of visible neuron-variables, and a layer of hidden pattern-variables. The exchange of messages between these two layers (in which the Hopfield model is seen as a RBM) precisely leads to the modification of the Onsager reaction term. We will show that this structure can actually be iterated. We define a modified Hopfield model where the patterns are not independent random variables, but they are built by combinations of more elementary objects, called features. In this case, we show that the TAP equations can be understood by a neural network with three layers, in which one adds, between the layer of visible neuron-variables and the layer of hidden pattern-variables, another layer of hidden feature-variables. This spontaneous emergence of more hidden layers when one handles a more structured type of problem is interesting in itself: one might hope that it could lead to an explanation of the success of multilayered network and deep learning in practical tasks where the information certainly contains a deep hierarchy of combinatorial correlations.

We do not address here the full problem of learning in the Hopfield model or in RBMs. We only study the “direct” problem of determining the polarization of each neuron (from which one can deduce the pair correlations by using linear response). However a good control of this direct problem is an essential ingredient of most unsupervised learning protocols.

The paper is organized as follows:

- Section 2 provides basic definitions of the Hopfield model and recalls its phase diagram.
- Section 3 derives the mean field equations. It starts with the phases where there is no spontaneous polarization of the neurons, and derives successively the BP equations, their rBP simplification using Gaussian messages, and finally the TAP (or AMP) equations. It then studies the modifications of these equations when one works in the retrieval phase. The consistency of the BP equations with the standard replica results (a consistency which had been disputed in²⁷) is then explicitly shown.
- Section 4 explains how the mean-field equations can be turned into algorithms, by iterating them with a careful update schedule.

- Section 5 studies a modified Hopfield model in which the patterns are no-longer independent, but they are built as combinations of more elementary random variables. We work out the modification of BP and TAP equations in this case, using a representation of the problem with two layers of hidden variables, on top of the layer of visible neurons.

- Section 6 derives the message-passing algorithms obtained from mean-field equations (BP, rBP and TAP) in a general model of RBM.

- Section 7 provides some concluding remarks, and perspectives for further studies.

II. THE HOPFIELD MODEL

A. Definitions

In the Hopfield model²², neurons are modeled as N binary spins s_i , $i = 1, \dots, N$, taking values in $\{\pm 1\}$. These spins interact by pairs, the energy of a spin configuration is

$$E = -\frac{1}{2} \sum_{i,j} J_{ij} s_i s_j . \quad (1)$$

This is a spin glass model where the coupling constants J_{ij} take a special form. Starting from p “patterns”, which are spin configurations

$$\xi_i^\mu = \pm 1, \quad i \in \{1, \dots, n\}, \quad \mu \in \{1, \dots, p\} , \quad (2)$$

the coupling constants are defined as

$$J_{ij} = \frac{1}{N} \sum_{\mu} \xi_i^\mu \xi_j^\mu . \quad (3)$$

Given an instance defined by the set of couplings $J = \{J_{ij}\}$, the Boltzmann distribution of the spins, at inverse temperature β , is defined as

$$P_J(s) = \frac{1}{Z} e^{(\beta/2) \sum_{i,j} J_{ij} s_i s_j} . \quad (4)$$

Using a Gaussian transformation, the partition function Z can be re-written as

$$Z = \sum_s \int \prod_{\mu} \frac{d\lambda_{\mu}}{\sqrt{2\pi\beta}} \exp \left[-\frac{\beta}{2} \sum_{\mu} \lambda_{\mu}^2 + \beta \sum_{\mu,i} \frac{\xi_i^{\mu}}{\sqrt{N}} s_i \lambda_{\mu} \right] . \quad (5)$$

This expression shows that the Hopfield model is also a model of N binary spins s_i and P continuous variables with a Gaussian measure, λ_{μ} , interacting through random couplings

ξ_i^μ/\sqrt{N} which are iid random variables taking values $\pm 1/\sqrt{N}$ with probability 1/2. This is nothing but a Restricted Boltzmann Machine in which the visible neurons are binary variables that interact with P hidden continuous variables with a Gaussian distribution. The variable λ_μ can be interpreted as the projection of the spin configuration on the pattern μ , as suggested by the identity relating its mean $\langle \lambda_\mu \rangle$ and the expectations values of the spins:

$$\langle \lambda_\mu \rangle = \frac{1}{\sqrt{N}} \sum_i \xi_i^\mu \langle s_i \rangle . \quad (6)$$

B. Known results

The phase diagram of the Hopfield model has been studied in detail in²⁹³⁰ and subsequent papers. In the thermodynamic limit where the number of neurons N and the number of patterns P go to infinity with a fixed ratio $\alpha = P/N$, the phase diagram is controlled by the temperature $T = 1/\beta$ and the ratio α . One finds three main phases:

- The paramagnetic phase. At high enough temperatures, $T > T_g(\alpha)$, the spontaneous polarization of each neuron vanishes $\langle s_i \rangle = 0$.
- The retrieval phase. In a regime of low enough temperature and low enough α , there exists a retrieval phase, where the neurons have a spontaneous polarization in the direction of one of the stored patterns μ . This means that, in the thermodynamic limit :

$$\frac{1}{N} \sum_i \langle s_i \rangle \xi_i^\mu = M \quad (7)$$

$$\frac{1}{N} \sum_i \langle s_i \rangle \xi_i^\nu = 0 \quad (\nu \neq \mu) \quad (8)$$

For symmetry reasons, there exist two retrieval states one with a polarization $M > 0$ (where M is a function of α, β), one with the polarization $-M$ (pointing opposite to the pattern).

The transition corresponding to the appearance of retrieval states is a first order transition. One should thus distinguish two temperatures: at $T < T_M(\alpha)$, retrieval states first appear as metastable states, at a lower temperature $T < T_c(\alpha)$, they become global minima of the free energy.

- The spin glass phase. In an intermediate range of temperature, or at large α , the neurons acquire a spontaneous polarization, but in some directions which are not in the direction of one of the patterns. In the spin glass phase, the spin-glass order parameter q , defined by

$$q = \frac{1}{N} \sum_i \langle s_i \rangle^2 \quad (9)$$

is strictly positive, while

$$\forall \mu : \frac{1}{N} \sum_i \langle s_i \rangle \xi_i^\mu = 0 \quad (10)$$

The phase diagram is recalled in Fig. 1.

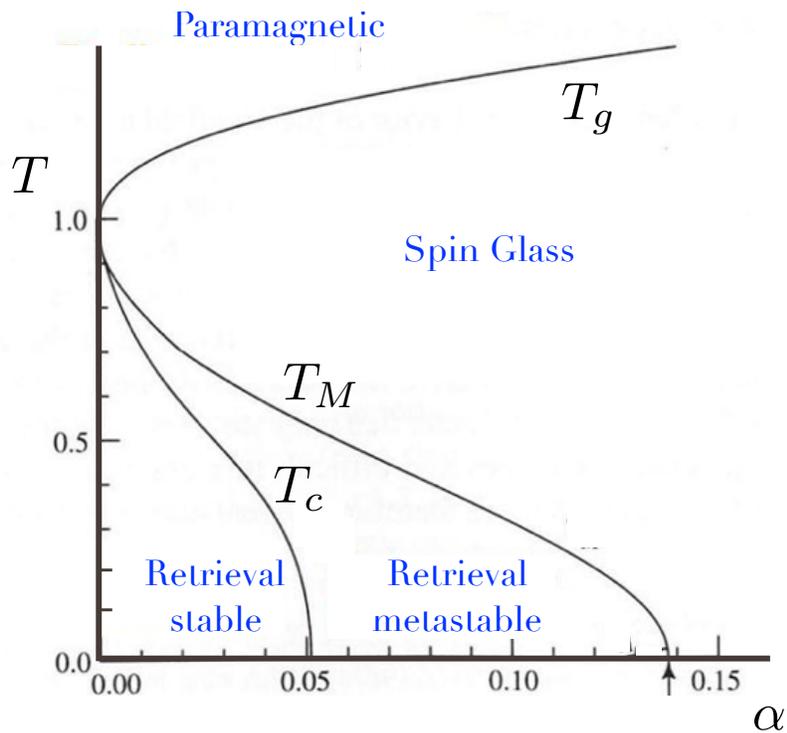


FIG. 1. Phase diagram of the Hopfield model, from³⁰

III. MEAN-FIELD EQUATIONS

A. Belief propagation

We use the representation (5) of the Hopfield model. Figure 2 shows the factor graph for this problem. The BP equations are written using the standard procedure (see for instance¹²). For the Hopfield model, this approach was first used by²⁵. The BP equations are expressed in terms of four types of messages: $m_{i \rightarrow \mu}(s_i)$, $m_{\mu \rightarrow i}(\lambda_\mu)$, $\hat{m}_{\mu \rightarrow i}(s_i)$, $\hat{m}_{i \rightarrow \mu}(\lambda_\mu)$. The message $m_{i \rightarrow \mu}(s_i)$, being a probability of a binary variable, can be parameterized in terms of a single number $h_{i \rightarrow \mu}$, denoted ‘‘cavity field’’, defined by:

$$m_{i \rightarrow \mu}(s_i) \cong e^{\beta h_{i \rightarrow \mu} s_i} , \quad (11)$$

(in this paper, the symbol ‘ \cong ’ denotes equality up to a constant : if $p(\cdot)$ and $q(\cdot)$ are two measures on the same space -not necessarily normalized-, we write $p(x) \cong q(x)$ if there exists $C > 0$ such that $p(x) = C q(x)$). Similarly:

$$\hat{m}_{\mu \rightarrow i}(s_i) \cong e^{\beta \hat{h}_{\mu \rightarrow i} s_i} . \quad (12)$$

The BP equations are:

$$h_{i \rightarrow \mu} = \sum_{\nu(\neq \mu)} \hat{h}_{\nu \rightarrow i} \quad (13)$$

$$\hat{m}_{\mu \rightarrow i}(s_i) \cong \int d\lambda_\mu m_{\mu \rightarrow i}(\lambda_\mu) \exp\left((\beta/\sqrt{N})\xi_i^\mu s_i \lambda_\mu\right) \quad (14)$$

$$\hat{m}_{i \rightarrow \mu}(\lambda_\mu) \cong \cosh \beta \left(h_{i \rightarrow \mu} + (\xi_i^\mu/\sqrt{N})\lambda_\mu \right) \quad (15)$$

$$m_{\mu \rightarrow i}(\lambda_\mu) \cong e^{-(\beta/2)\lambda_\mu^2} \prod_{j(\neq i)} \hat{m}_{j \rightarrow \mu}(\lambda_\mu) \quad (16)$$

Notice that in this notation the message $\hat{m}_{i \rightarrow \mu}$ is not a normalizable distribution of λ_μ . This is not a problem because it appears in the equations only through the combination (16) which is normalizable thanks to the presence of the local Gaussian measure $e^{-(\beta/2)\lambda_\mu^2}$.

B. Relaxed BP equations

The general BP equations are not very useful because the messages $m_{\mu \rightarrow i}$ and $\hat{m}_{i \rightarrow \mu}$ are functions of the continuous variables λ_μ . However the messages can be simplified, by noticing that, in the thermodynamic limit, they are actually Gaussian distributions and

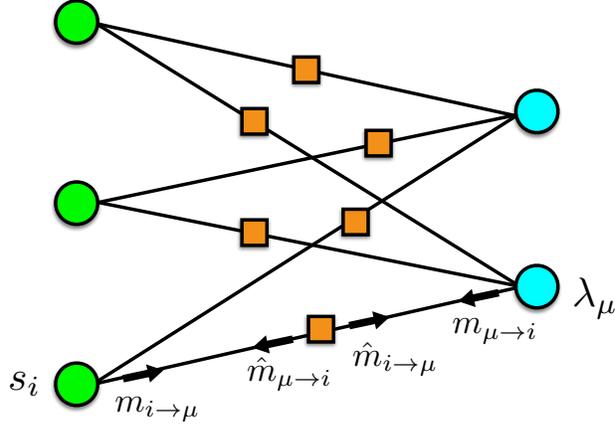


FIG. 2. Factor graph of the Hopfield model, in the representation using spin-variables (s_i , left circles) and pattern-variables (λ_μ , right circles). For each pair of spin-variable and pattern-variable, there is an interaction factor (squares). The graph also defines the messages used in belief propagation

can be parameterized by just two moments. This simplification leads to equations that are usually called “relaxed BP” (rBP) in the literature. It was first used in the cavity method for systems with long-range interactions⁽²³⁾, and has been developed in various problems of communication theory^{31–34}.

We shall first work out this simplification in the phase where there is no condensation on any pattern. Technically, this means that the distributions $m_{\mu \rightarrow i}(\lambda_\mu)$ are dominated by values of λ_μ which are finite (in the large N limit). It is easy to see that, in this case, (15) can be expanded around $\lambda_\mu/\sqrt{N} = 0$ and the BP equations (13-16) close under the hypothesis that the messages $m_{\mu \rightarrow i}(\lambda_\mu)$ are Gaussian distributions.

Under this assumption, one can parameterize these messages in terms of their two first moments. This leads to the so-called rBP equations. We define:

$$a_{\mu \rightarrow i} = \int d\lambda_\mu m_{\mu \rightarrow i}(\lambda_\mu) \lambda_\mu \quad (17)$$

$$c_{\mu \rightarrow i} = \int d\lambda_\mu m_{\mu \rightarrow i}(\lambda_\mu) \lambda_\mu^2 - a_{\mu \rightarrow i}^2 \quad (18)$$

In order to derive the rBP equations, we first derive the asymptotic form of the function $\hat{m}_{i \rightarrow \mu}(\lambda_\mu)$ in the large N limit:

$$\hat{m}_{i \rightarrow \mu}(\lambda_\mu) = \exp \left(\beta \frac{\xi_i^\mu}{\sqrt{N}} \lambda_\mu \tanh(\beta h_{i \rightarrow \mu}) + \frac{\beta^2}{2N} \lambda_\mu^2 [1 - \tanh^2(\beta h_{i \rightarrow \mu})] \right) \quad (19)$$

Inserting this expression into (16) we get:

$$c_{\mu \rightarrow i} = \frac{1}{\beta} \frac{1}{1 - (\beta/N) \sum_{j(\neq i)} [1 - \tanh^2(\beta h_{j \rightarrow \mu})]} \quad (20)$$

$$a_{\mu \rightarrow i} = \frac{1}{\sqrt{N}} \frac{\sum_{j(\neq i)} \xi_j^\mu \tanh(\beta h_{j \rightarrow \mu})}{1 - (\beta/N) \sum_{j(\neq i)} [1 - \tanh^2(\beta h_{j \rightarrow \mu})]} \quad (21)$$

Eqs. (13) and (14) can be re-written as:

$$h_{i \rightarrow \mu} = \sum_{\nu(\neq \mu)} \frac{\xi_i^\nu}{\sqrt{N}} a_{\nu \rightarrow i} \quad (22)$$

Equations (21) and (22) form a set of $2NP$ equations for the $2NP$ variables $a_{\mu \rightarrow i}$ and $h_{i \rightarrow \mu}$. These are the rBP equations for the Hopfield model.

C. TAP (or AMP) equations

The rBP equations relate messages propagated along the edges of the factor graph (in the language of spin glasses they are “cavity-equations”). In the large N limit it is possible, and very useful for algorithmic purpose, to simplify these rBP equations and turn them into a set of equations which relate “site”-quantities associated with the variable-nodes of the factor graph. This allows to go from $2NP$ variables to $N + P$ variables, and leads to an effective reduction of computer time and memory. The equations that relate them are analogous to those found in²⁴ for spin glasses, hence the name TAP equations. In computer science, they are often called approximate-message-passing (AMP) equations^{14,16–18,35–37}. To avoid confusion, notice that, in their paper on the Hopfield model²⁵, Kabashima and Saad use the same word (TAP equations) both for the rBP equations and what we call TAP equations.

We prefer to use two different terms, in line with the terminology which is presently most common in information theory.

The site-variables are local fields defined as:

$$H_i = \sum_{\nu} \frac{\xi_i^{\nu}}{\sqrt{N}} a_{\nu \rightarrow i} \quad (23)$$

$$A_{\mu} = \frac{1}{\sqrt{N}} \frac{\sum_j \xi_j^{\mu} \tanh(\beta h_{j \rightarrow \mu})}{1 - (\beta/N) \sum_j [1 - \tanh^2(\beta h_{j \rightarrow \mu})]} \quad (24)$$

They give the expectation values of the variables:

$$\langle s_i \rangle = M_i = \tanh(\beta H_i) \quad (25)$$

$$\langle \lambda_{\mu} \rangle = A_{\mu} \quad (26)$$

We shall derive here a closed set of $N + P$ equations that relate these $N + P$ variables.

The main idea of the derivation of TAP equations comes from the observation that the rBP message $a_{\mu \rightarrow i}$ should be nearly equal to A_{μ} , up to small corrections that can be handled perturbatively in the large N limit. Similarly, $h_{i \rightarrow \mu}$ is nearly equal to H_i , up to small corrections. Let us work out the explicit form of these corrections. We define

$$q = \frac{1}{N} \sum_i \tanh^2(\beta H_i) \quad (27)$$

We first notice that

$$h_{j \rightarrow \mu} = H_j - \frac{\xi_j^{\mu}}{\sqrt{N}} a_{\mu \rightarrow j} \quad (28)$$

Therefore:

$$\frac{1}{N} \sum_j [1 - \tanh^2(\beta h_{j \rightarrow \mu})] \simeq 1 - q \quad (29)$$

up to corrections which vanish when $N \rightarrow \infty$. Therefore :

$$A_{\mu} \simeq \frac{1}{1 - \beta(1 - q)} \frac{1}{\sqrt{N}} \sum_j \xi_j^{\mu} \tanh(\beta h_{j \rightarrow \mu}) \quad (30)$$

and:

$$a_{\mu \rightarrow i} \simeq A_{\mu} - \frac{1}{1 - \beta(1 - q)} \frac{1}{\sqrt{N}} \xi_i^{\mu} \tanh(\beta h_{i \rightarrow \mu}) \quad (31)$$

In this last expression, the second term is a correction of order $1/\sqrt{N}$. In this correction we can substitute $h_{i \rightarrow \mu}$ by H_i , the difference would give a contribution of order $O(1/N)$ to $a_{\mu \rightarrow i}$, which can be neglected. Therefore :

$$a_{\mu \rightarrow i} \simeq A_{\mu} - \frac{1}{1 - \beta(1 - q)} \frac{1}{\sqrt{N}} \xi_i^{\mu} \tanh(\beta H_i) \quad (32)$$

Substituting this expression in the definition (23) of H_i we get:

$$H_i \simeq \sum_{\nu} \frac{\xi_i^{\nu}}{\sqrt{N}} A_{\nu} - \frac{\alpha}{1 - \beta(1 - q)} \tanh(\beta H_i) \quad (33)$$

Considering now the definition (24) of A_{μ} we can expand it as

$$\begin{aligned} A_{\mu} &= \frac{1}{1 - \beta(1 - q)} \sum_j \frac{\xi_j^{\mu}}{\sqrt{N}} \tanh \left[\beta \left(H_j - \frac{\xi_j^{\mu}}{\sqrt{N}} a_{\mu \rightarrow j} \right) \right] \\ &\simeq \frac{1}{1 - \beta(1 - q)} \sum_j \frac{\xi_j^{\mu}}{\sqrt{N}} \tanh \left[\beta \left(H_j - \frac{\xi_j^{\mu}}{\sqrt{N}} A_{\mu} \right) \right] + O(1/N) \\ &\simeq \frac{1}{1 - \beta(1 - q)} \sum_j \frac{\xi_j^{\mu}}{\sqrt{N}} \left[\tanh(\beta H_j) - \beta \frac{\xi_j^{\mu}}{\sqrt{N}} (1 - \tanh^2(\beta H_j)) A_{\mu} \right] \end{aligned} \quad (34)$$

This gives:

$$A_{\mu} = \frac{1}{\sqrt{N}} \sum_j \xi_j^{\mu} \tanh(\beta H_j) \quad (35)$$

Equations (33) and (35), together with the definition (27), are the TAP (or AMP) equations which relate the $N + P$ variables H_i and A_{μ} . It turns out that they are linear in A_{μ} , and these variables can thus be eliminated (notice however that this is a specific feature of the Hopfield model, due to the Gaussian nature of variables λ_{μ} : as we shall see in Sect. 6, this is no longer true for more general RBMs, where the measure on λ_{μ} is non-Gaussian). Eliminating A_{μ} , we write closed equations for the N local fields H_i

$$H_i = \frac{1}{N} \sum_j J_{ij} \tanh(\beta H_j) - \frac{\alpha}{1 - \beta(1 - q)} \tanh(\beta H_i) \quad (36)$$

An alternative presentation of these TAP equations are in terms of the local magnetizations $M_i = \tanh(\beta H_i)$:

$$M_i = \tanh \left[\beta \sum_j J_{ij} M_j - \frac{\alpha \beta}{1 - \beta(1 - q)} M_i \right] \quad (37)$$

$$= \tanh \left[\beta \sum_{j(\neq i)} J_{ij} M_j - \frac{\alpha \beta^2 (1 - q)}{1 - \beta(1 - q)} M_i \right] \quad (38)$$

$$q = \frac{1}{N} \sum_i M_i^2 \quad (39)$$

These TAP equations were first derived in²³ using the cavity method. The re-derivation that we have presented here uses a different approach, namely the BP equations and their simplification at large N , and obtains the same result.

The claims in²⁶ and²⁷ according to which these equations are wrong were probably based on their misunderstanding of the presence of diagonal terms in (37). Actually the TAP equations that they derive agree with ours, and with the original finding in²³, as can be seen explicitly in the form (38).

While²³ claimed (without writing the proof) that the TAP equations (39) reproduce the known equilibrium properties of the Hopfield model found with replicas, it was stated in²⁶ and²⁷ that they do not give the well known value of the spin glass transition temperature T_c , and that they disagree with the result of the replica method. These statements are not correct. We provide below the explicit proof that our rBP and TAP equations are in perfect agreement with the replica result, and therefore with the known value of T_c , as stated in²³. The following derivation also gives a useful pedagogical example of how the equilibrium results can be obtained from the mean-field equations : the critical temperature can be analysed through a study of the TAP equations, while the replica result for the order parameter can be obtained from a statistical analysis of the rBP equations.

D. rBP and TAP (AMP) equations in the retrieval phase

Let us work out the modifications that take place in the retrieval phase, when the measure condenses on one pattern (a similar analysis can be carried out easily in the mixed phase where the condensation takes place on a finite number of patterns, we shall keep here to the retrieval phase). In the retrieval phase corresponding to pattern $\mu = 1$, one expects that the distribution of λ_1 will be dominated by values close to $\lambda_1 = M\sqrt{N}$. When deriving BP equations, the message $\hat{m}_{i \rightarrow 1}(\lambda_1)$ takes the form:

$$\hat{m}_{i \rightarrow 1}(M) = \cosh \beta \left(h_{i \rightarrow 1} + M \xi_i^1 \right) . \quad (40)$$

Therefore :

$$m_{1 \rightarrow i}(M) \cong e^{N\psi_{1 \rightarrow i}(M)} , \quad (41)$$

where

$$\psi_{1 \rightarrow i}(M) = -\frac{\beta}{2}M^2 + \frac{1}{N} \sum_{j(\neq i)} \log \cosh \left[\beta \left(h_{j \rightarrow 1} + M \xi_j^1 \right) \right] \quad (42)$$

In the large N limit, the measure $m_{1 \rightarrow i}(M)$ is dominated by the maximum of the function

$\psi_{1 \rightarrow i}(M)$. One should notice that in the large N limit this function converges to

$$\psi(M) = -\frac{\beta}{2}M^2 + \frac{1}{N} \sum_j \log \cosh \left[\beta \left(h_{j \rightarrow 1} + M \xi_j^1 \right) \right] \quad (43)$$

The maximum of $\psi(M)$ can be either in $M = 0$ or in $M = \pm M^*$, where M^* is the largest solution of the equation

$$M = \frac{1}{N} \sum_j \xi_j^1 \tanh \left[\beta \left(h_{j \rightarrow 1} + M \xi_j^1 \right) \right] \quad (44)$$

The retrieval phase is the phase where the maximum is obtained at $M = \pm M^*$. In this case the rBP equations (21-22) are modified, because the messages $m_{1 \rightarrow i}$, instead of being Gaussian distributions with finite means and variances, become dominated by values of λ_1 close to $M\sqrt{N}$. The new set of equations obtained in this regime will be denoted rBP-M (for relaxed belief propagation - magnetized) equations.

$$a_{\mu \rightarrow i} = \frac{1}{\sqrt{N}} \frac{\sum_{j(\neq i)} \xi_j^\mu \tanh(\beta h_{j \rightarrow \mu})}{1 - (\beta/N) \sum_{j(\neq i)} [1 - \tanh^2(\beta h_{j \rightarrow \mu})]} \quad , \quad \mu \geq 2 \quad (45)$$

$$h_{i \rightarrow \mu} = \sum_{\nu(\neq \mu, 1)} \frac{\xi_i^\nu}{\sqrt{N}} a_{\nu \rightarrow i} + M \xi_i^1 \quad , \quad \mu \geq 2 \quad (46)$$

$$h_{i \rightarrow 1} = \sum_{\nu(\neq 1)} \frac{\xi_i^\nu}{\sqrt{N}} a_{\nu \rightarrow i} \quad (47)$$

The rBP-M equations in the retrieval phase with condensation on pattern 1 are given by (44-47).

It should be noticed that they involve a completely different estimate for the message $a_{1 \rightarrow i}$ when compared to the rBP equations without condensation. In particular, they cannot be obtained from (21,22) by just assuming that $a_{1 \rightarrow i}$ becomes of order \sqrt{N} (such a procedure is unable to reproduce eqn(44)). The reason is that the condensation is a first order transition, and the rBP equations in the retrieval phase correspond to a solution $M > 0$ to Eq.(44) that is different from the usual one with $M = 0$ (in which case one needs to consider the $O(1/\sqrt{N})$ corrections as in (21)). The main drawback of these rBP-M equations is that one must use a different set of equations depending on the pattern towards which the system polarizes. This is quite inefficient for algorithmic applications : if one does not know a priori which pattern is being retrieved, one should run in parallel $P = \alpha N$ different algorithms, each one testing the possible polarization towards one of the patterns, and compare the results.

Fortunately, the situation is much better when considering TAP equations. It is straightforward to go from these rBP-M equations to the TAP (or AMP) equations for the retrieval phase. One gets:

$$H_i = \sum_{\nu \geq 2} \frac{\xi_i^\nu}{\sqrt{N}} A_\nu - \frac{\alpha}{1 - \beta(1 - q)} \tanh(\beta H_i) + M \xi_i^1 \quad (48)$$

$$A_\mu = \frac{1}{\sqrt{N}} \sum_j \xi_j^\mu \tanh(\beta H_j) \quad , \quad \mu \geq 2 \quad (49)$$

$$M = \frac{1}{N} \sum_j \xi_j^1 \tanh(\beta H_j) \quad (50)$$

It turns out that these TAP equations are exactly the ones that would be obtained from the usual TAP equations (33,35), assuming that $A_1 = \sqrt{N}M$. This is rather remarkable considering the fact that the rBP-M equations in the retrieval phase cannot be obtained continuously from the rBP equations without retrieval (because of the first order phase transition discussed above). The discontinuity in the set of rBP equations when going from the uncondensed to the retrieval phase thus disappears when one uses instead the TAP (GAMP) equations. This makes the TAP equations a much better choice for algorithmic applications.

E. Consistency with the replica results

1. Critical temperature

The paramagnetic solution of the TAP equations (37,39) is the solution with zero local magnetizations, $\forall i : M_i = 0$. The spin glass transition is a second order phase transition, therefore its temperature $T_c = 1/\beta_c$ is the largest temperature where a solution with non-zero local magnetization exists. It can be found by linearizing the TAP equations (37,39) and identifying their instability point. Explicitly, the linearization gives:

$$M_i = \beta \sum_j J_{ij} M_j - \frac{\alpha\beta}{1 - \beta} M_i + O(M^3) \quad (51)$$

The direction of instability is the one of the eigenvector of the J matrix with largest eigenvalue. Denoting by λ_{\max} this largest eigenvalue, the value of β_c is given by:

$$1 = \beta_c \lambda_{\max} - \frac{\alpha\beta_c}{1 - \beta_c} \quad (52)$$

By definition, λ_{\max} is the largest eigenvalue of the matrix $N \times N$ matrix $J = (1/N)\xi\xi^T$, where the $N \times P$ matrix ξ has iid random entries taking values ± 1 with probability $1/2$. In fact the distribution of the largest eigenvalue of J concentrates around

$$\lambda_{\max} = (1 + \sqrt{\alpha})^2 . \quad (53)$$

This result can be derived using the replica method or the cavity method. An easy way to obtain it is to realize that the value of λ_{\max} depends only on the first two moments of the distribution of the matrix elements ξ_i^μ . In particular it is the same as the one which would be obtained if the entries of ξ were iid with a normal distribution of mean 0 and variance 1. This last case is very well known since the work of Marcenko and Pastur³⁸, and it gives the value of λ_{\max} written in (53).

Using (53), the value of β_c obtained from (52) is

$$\beta_c = \frac{1}{1 + \sqrt{\alpha}} . \quad (54)$$

This agrees with the well known result of³⁰ for the critical temperature: $T_c = 1 + \sqrt{\alpha}$.

2. *Order parameter*

The cavity or BP equations can be used in two distinct ways: on a single instance they can be solved by iteration, and if a fixed point is found, this idea may be used as an algorithm for estimating the local magnetizations. But in the case where the instances are generated from an ensemble (like the case that we study here, where the ξ_i^μ are iid random variables), one can also perform a statistical analysis of the equation. This is the essence of the cavity method, and is also known in the litterature on message passing as the density evolution.

We will show that this statistical analysis of the cavity equations give the same results as the replica method, as claimed in²³, and contrary to the statements of²⁷. For simplicity, we keep here to the “replica symmetric” approximation.

We start from the rBP equations. Considering first the equation (22) giving the cavity field $h_{i \rightarrow \mu}$, we notice that, as the variables ξ_i^μ are iid, provided that the correlations of the messages $a_{\nu \rightarrow i}$ are small enough (this is the essence of the replica symmetric approximation - see²³ and¹²), the cavity field $h_{i \rightarrow \mu}$ has a gaussian distribution with mean 0 and a variance which is independent of the indices i and μ and that we denote by $\overline{h^2}$. Similarly, $a_{\nu \rightarrow i}$ has a

gaussian distribution with mean 0 and a variance which is independent of the indices i and ν and that we denote by $\overline{a^2}$. The rBP equations (21) and (22) relate these two variances:

$$\overline{h^2} = \alpha \overline{a^2} \quad (55)$$

$$\overline{a^2} = \frac{q}{[1 - \beta(1 - q)]^2} \quad (56)$$

We thus obtain:

$$q = \overline{\tanh^2(\beta h)} = \int \frac{dh}{\sqrt{2\pi\Phi}} e^{-h^2/(2\Phi)} \tanh^2(\beta h) , \quad (57)$$

where :

$$\Phi = \frac{\alpha q}{[1 - \beta(1 - q)]^2} , \quad (58)$$

Eqs. (57,58) are exactly the well known equations³⁰ that allow to compute the spin glass order parameter q in the spin glass phase of the Hopfield model, in the replica-symmetric framework.

In the retrieval phase, the same reasoning can be applied starting from the rBP-M equations (44-47). One finds:

$$q = \overline{\tanh^2(\beta h + \xi M)} \quad (59)$$

$$M = \xi \overline{\tanh(\beta h + \xi M)} \quad (60)$$

where the overline denotes the average with respect to the field h , which has a Gaussian distribution of variance Φ , and the binary variable ξ which takes values ± 1 with probability $1/2$. These are precisely the equations obtained in the retrieval phase with the replica method³⁰.

IV. ALGORITHMS : ITERATIONS AND TIME INDICES

Mean-field equations are usually solved by iteration, and interpreted as message-passing algorithms. Turning a set of mean-field equations into an iterative algorithm involves a certain degree of arbitrariness concerning the way the equations are written and the “time indices” concerning the update. A proper choice of time indices may result in an algorithm with much better convergence properties, as underlined for instance in^{39,13}. Here we review the most natural choice for AMP iterations and their consequences.

A. rBP equations

The rBP equations (21,22) are usually iterated as follows :

$$a_{\mu \rightarrow i}^{t+1} = \frac{1}{\sqrt{N}} \frac{\sum_{j(\neq i)} \xi_j^\mu \tanh(\beta h_{j \rightarrow \mu}^t)}{1 - (\beta/N) \sum_{j(\neq i)} [1 - \tanh^2(\beta h_{j \rightarrow \mu}^t)]} \quad (61)$$

$$h_{i \rightarrow \mu}^{t+2} = \sum_{\nu(\neq \mu)} \frac{\xi_i^\nu}{\sqrt{N}} a_{\nu \rightarrow i}^{t+1} \quad (62)$$

There exist various types of update schemes. One can distinguish two main classes:

- In the parallel update, starting from a configuration of the h messages at time t , one computes all the a messages using (61). Then one computes all the new h messages at time $t + 2$ using (62), with the a messages of time $t + 1$ (therefore the h -messages are defined at even times, the a -messages are defined at odd times). In two time-steps, all the messages are updated.
- In an update in series, one picks up a message at random (or, better, one can use a random permutation of all messages to decide on the sequence of updates), and one updates it using either (61)-if the message is an a message- or (62). In the case of random permutations, all messages are updated after $2NP$ time steps.

In the parallel update scheme, one can easily follow the evolution in time of the overlap q^t . Using (61,62), one can perform again the analysis of Sect.III E 2 keeping the time indices. This gives:

$$q^{t+2} = \int \frac{dh}{\sqrt{2\pi\Phi^t}} e^{-h^2/(2\Phi^t)} \tanh^2(\beta h) \quad (63)$$

where

$$\Phi^t = \frac{\alpha q^t}{[1 - \beta(1 - q^t)]^2} . \quad (64)$$

It is easy to see that these equations converge (to $q = 0$) when $T > T_g = 1 + \sqrt{\alpha}$.

B. TAP equations

We can now repeat the previous derivation of the TAP equations keeping track of the time indices that were written in the previous subsection. We keep here to the case of parallel

update. Defining:

$$A_\mu^{t+1} = \frac{1}{\sqrt{N}} \frac{\sum_j \xi_j^\mu \tanh(\beta h_{j \rightarrow \mu}^t)}{1 - (\beta/N) \sum_j [1 - \tanh^2(\beta h_{j \rightarrow \mu}^t)]} \quad (65)$$

$$H_i^{t+2} = \sum_\nu \frac{\xi_i^\nu}{\sqrt{N}} a_{\nu \rightarrow i}^{t+1} \quad (66)$$

One gets:

$$A_\mu^{t+1} = \frac{1}{1 - \beta(1 - q^t)} \frac{1}{\sqrt{N}} \sum_j \xi_j^\mu \tanh(\beta H_j^t) - \frac{\beta(1 - q^t)}{1 - \beta(1 - q^t)} A_\mu^{t-1} \quad (67)$$

$$H_i^{t+2} = \sum_\nu \frac{\xi_i^\nu}{\sqrt{N}} A_\nu^{t+1} - \frac{\alpha}{1 - \beta(1 - q^t)} \tanh(\beta H_i^t) \quad (68)$$

Equations (67,68) give the algorithmic version of TAP equations, used through a parallel iteration. Again, the A variables can be eliminated from these equations, leaving the TAP equations written in terms of local field H_i^t or the magnetization $M_i^t = \tanh(\beta H_i^t)$. Defining $u^t = \beta(1 - q^t)$, and $\tau = t/2$ we get:

$$H_i^{\tau+1} = \frac{1}{1 - u^\tau} \left[\sum_j J_{ij} M_j^\tau - \alpha M_i^\tau - u^\tau H_i^\tau - \frac{\alpha u^\tau}{1 - u^{\tau-1}} M_i^{\tau-1} \right] \quad (69)$$

This final form of the iterative algorithm corresponding to TAP equation involves a kind of memory term (the polarization of neuron i at time τ is obtained from the magnetizations at time $\tau - 1$ and from its magnetization at times $\tau - 1$ and $\tau - 2$), a phenomenon that was first found in the context of TAP equations for the SK model³⁹, and used in¹³.

This algorithm has many advantages. It involves only N fields, therefore its iteration is fast, and above all it can develop a spontaneous polarization towards one of the stored patterns (while in the rBP equations one would need to use a different equation for each of the patterns).

C. Numerical results

The iteration of TAP equations (67,68), or equivalently their expression in terms of the H fields only (69) is a fast algorithm for solving the Hopfield model (in the sense of obtaining the local polarizations of the neuron-variables). We have tested it in the retrieval phase, starting from a configuration with overlap M_0 with one randomly chosen pattern μ_0 , which means that the initial spin configuration s_i^0 satisfies

$$M_0 = \frac{1}{N} \sum_i s_i^0 \xi_i^{\mu_0} . \quad (70)$$

Fig.3 shows the probability that the iteration of these equations converges to a fixed point with a value of overlap with μ_0 larger than .95 (the convergence is defined by the fact that, in (69), the average value of $|H_i^{\tau+1} - H_i^\tau| < 10^{-6}$). The simulations were carried out with networks of $N = 1000$ neurons. The maximal number of iterations was fixed to 200, but in practice we notice that when the algorithm converges it does so in a few iterations, of order 10 to 20.

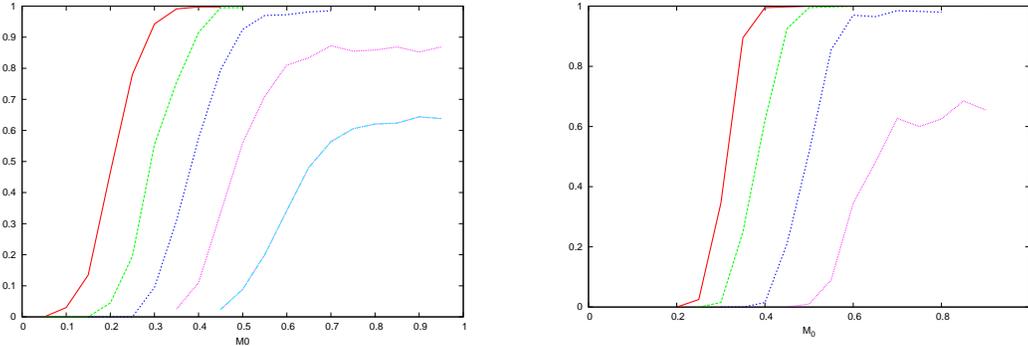


FIG. 3. Iteration of TAP equations using (69). The probability of convergence is plotted versus the overlap to a randomly chosen initial pattern μ_0 . Left-hand figure: temperature $T = 0.01$, simulation with $N = 1000$ neurons and $P = 40, 60, 80, 100, 120$ patterns (from left to right). Right-hand figure: temperature $T = 0.3$, simulation with $N = 1000$ neurons and $P = 40, 60, 80, 100$ patterns (from left to right).

It should be noticed that the iteration of simpler versions of the mean-field equations, either the naive mean-field equations or the SK-TAP equations with the correct time indices of³⁹, also converge when initialized in the same conditions. Actually the basin of attraction for convergence to an overlap $> .95$ with the pattern is larger for naive mean-field than it is for SK-TAP, and the one for SK-TAP is larger than for the correct Hopfield TAP equations. This is probably due to the fact, noticed in²⁵, that the fixed point reached by naive mean-field is actually closer to the pattern than the fixed point reached by SK-TAP, which is itself closer to the pattern than the one obtained by iterating TAP equations. However, the TAP equations have one major advantage : they give the values of the polarizations of neurons which become exact in the thermodynamic limit.

V. MODIFIED HOPFIELD MODEL: CORRELATED PATTERNS WITH COMBINATORIAL STRUCTURE

From its definition (1), the Hopfield model is a type of spin glass. It differs from the SK model by the structure of couplings. In the SK model one draws each J_{ij} (for $i < j$) as an independent random variable with mean zero and variance $1/N$. In the Hopfield model one builds the J_{ij} coupling constants as bilinear superposition of patterns, see (3). It turns out that this modification has a crucial modification on the TAP equations. In the SK model, the TAP equations are²⁴:

$$M_i = \tanh \left[\beta \sum_{j(\neq i)} J_{ij} M_j - \beta^2(1-q)M_i \right] \quad (71)$$

The structure is the same in the Hopfield model, but the precise form of the second term (the so-called Onsager reaction term) is different. For an instructive comparison, it is useful to rescale the interactions of the Hopfield model in such a way that the variance of the couplings are $1/N$, defining thus $J_{ij} = \frac{1}{\sqrt{\alpha}} \frac{1}{N} \sum_{\mu} \xi_i^{\mu} \xi_j^{\mu}$. This simple rescaling can be absorbed in a rescaling of β , and our TAP equations (37) become, in this rescaled Hopfield model:

$$M_i = \tanh \left[\beta \sum_{j(\neq i)} J_{ij} M_j - \frac{\beta^2(1-q)}{1 - \beta(1-q)/\sqrt{\alpha}} M_i \right] \quad (72)$$

Therefore the change of structure of the J_{ij} random variables leads to a modification of the TAP equations, where the Onsager term acquires a denominator $1/[1 - \beta(1-q)/\sqrt{\alpha}]$. Clearly, in the large α limit one recovers the TAP equations of the SK model, as it should be, since the correlations between the J_{ij} become irrelevant in this limit.

The fact that the TAP equations depend on the type of structure of the couplings J_{ij} poses a challenge for their use in practical applications, where one does not really know the structure of these couplings. One elegant way out consists in adapting the reaction term to the concrete set of couplings to which one is applying the method^{7,40}. Our approach in the present paper considers instead an alternative representation of the Hopfield model, in which the visible neuron-variables interact with a hidden layer of pattern-variables. In this expanded representation, the couplings between the visible and the hidden units are nothing but the patterns, which are independent random variables. Therefore the message passing equations (BP, rBP, and eventually TAP) can be written safely and give the result.

The standard results of the Hopfield model hold as long as the ξ_i^μ are independent identically distributed (iid) random variables with zero mean and unit variance. We would like to test our approach by studying a generalization of the Hopfield model in which the patterns are no longer independent random variables. We shall study the case where the patterns have a correlation, created from the following structure:

$$\xi_i^\mu = \frac{1}{\sqrt{\gamma N}} \sum_{r=1}^{\gamma N} u_i^r v_\mu^r \quad (73)$$

where the u_i^r are iid random variables drawn from a distribution P_u with zero mean and unit variance, and the v_μ^r are iid random variables drawn from a distribution P_v with zero mean and unit variance. Note that the scaling has been chosen such that, in the large γ limit, the pattern elements ξ_i^μ become iid Gaussian random variables with unit variance, and one finds back the standard Hopfield model.

We call the type of disorder generated by (73) a combinatorial disorder. A natural case where it occurs is the following: imagine that the patterns are built from a number γN of possible features, where the feature number r is described by the neural activity u_i^r . The variable v_μ^r encodes to what extent feature r belongs to pattern μ . For instance, using binary variables $v_\mu^r = \pm 1$, one can interpret $v_\mu^r = 1$ if and only if feature r belongs to feature μ . Then the pattern μ on site i is (up to an overall constant), by the sum of the features r belonging to μ .

In combinatorial disorder, the random patterns expressed as (73) can be seen as a kind of superposition of features. This is in contrast with usual types of correlations that were studied in previous years, like biased patterns, or gaussian-distributed patterns with a non-trivial correlation matrix. Obviously, the structure of combinatorial disorder can be elaborated further and the features could become themselves combination of subfeatures etc.

We shall now develop the mean-field equations for this modified model.

A. Representation with hidden variables

Using the representation (5), the partition function of the modified Hopfield model with combinatorial disorder can be written as:

$$Z = \sum_s \int \prod_\mu \frac{d\lambda_\mu e^{-\beta \lambda_\mu^2/2}}{\sqrt{2\pi\beta}} \exp \left[\frac{\beta}{\sqrt{\gamma}} \sum_{r=1}^{\gamma N} \left(\frac{\sum_i u_i^r s_i}{\sqrt{N}} \right) \left(\frac{\sum_\mu v_\mu^r \lambda_\mu}{\sqrt{N}} \right) \right]. \quad (74)$$

It is useful to introduce the auxiliary variables

$$U^r = \frac{1}{\sqrt{N}} \sum_i u_i^r s_i \quad (75)$$

and to use the representation

$$1 = \frac{\beta}{2\pi i} \int dU^r d\hat{U}^r \exp \left[\beta \hat{U}^r \left(\frac{1}{\sqrt{N}} \sum_i u_i^r s_i - U^r \right) \right] \quad (76)$$

where the auxiliary variable \hat{U}^r is integrated in the complex plane along the imaginary axis.

Similarly, we introduce the variable

$$V^r = \frac{1}{\sqrt{N}} \sum_\mu v_\mu^r \lambda_\mu \quad (77)$$

and write an integral representation in terms of an auxiliary variable \hat{V}^r .

This gives, up to some overall irrelevant constants:

$$Z = \sum_s \int \prod_\mu d\lambda_\mu \int \prod_r d\vec{t}^r e^{-\frac{\beta}{2} \sum_\mu \lambda_\mu^2 + \beta \sum_{r=1}^{\gamma N} \left(+\frac{U^r V^r}{\sqrt{\gamma}} - \hat{U}^r U^r - \hat{V}^r V^r \right)} \exp \left[\frac{\beta}{\sqrt{N}} \sum_{r=1}^{\gamma N} \sum_{i=1}^N \hat{U}^r u_i^r s_i + \frac{\beta}{\sqrt{N}} \sum_{r=1}^{\gamma N} \sum_{\mu=1}^{\alpha N} \hat{V}^r v_\mu^r \lambda_\mu + \frac{\beta}{\sqrt{\gamma}} \sum_{r=1}^{\gamma N} U^r V^r \right] \quad (78)$$

where the variable \vec{t}^r is: $\vec{t}^r = (\hat{U}^r, U^r, \hat{V}^r, V^r)$, the integration element is $d\vec{t}^r = d\hat{U}^r dU^r d\hat{V}^r dV^r$, and the integrals over \hat{U}^r and \hat{V}^r run along the imaginary axis, while those over U^r and V^r are along the real axis.

The representation (78) contains three types of variables:

- The N visible neuron-variables s_i .
- The αN pattern-variables λ_μ , which are hidden variables.
- The γN “feature-variables” \vec{t}^r , which build a new layer of hidden variables, interacting with the other two layers.

Figure 4 shows the factor graph for this problem.

B. Belief propagation

Writing the BP equations for the model (78) is a standard (but lengthy) exercise that goes along exactly the same lines as before. It involves 8 types of messages running along

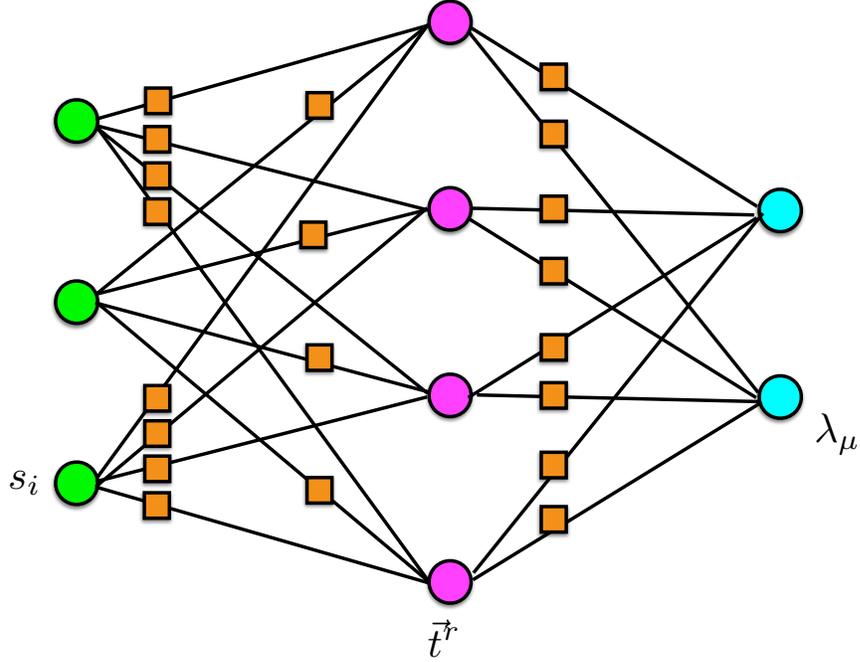


FIG. 4. Factor graph of the Hopfield model with combinatorial patterns, in the representation using visible spin-variables (s_i , left-layer green circles), hidden pattern-variables (λ_μ , right-layer blue circles) and hidden feature-variables (middle-layer purple circles). There exist interaction factors (squares) between each pair of variables belonging to two consecutive layers.

the edges of the factor graph shown in Fig. 4. These messages are:

$$m_{i \rightarrow r}(s_i), \hat{m}_{r \rightarrow i}(s_i), m_{\mu \rightarrow r}(\lambda_\mu), \hat{m}_{r \rightarrow \mu}(\lambda_\mu) \quad (79)$$

$$\hat{m}_{i \rightarrow r}(\vec{t}^r), m_{r \rightarrow i}(\vec{t}^r), m_{r \rightarrow \mu}(\vec{t}^r), \hat{m}_{\mu \rightarrow r}(\vec{t}^r) \quad (80)$$

Here and in the following, the letters i, j are indices of the neuron-variables running from 1 to N , the letters r, s are indices of the feature-variables running from 1 to γN , and the letters μ, ν are indices of the pattern-variables running from 1 to αN . Each message is a function of the argument which is written in parenthesis.

We shall not write explicitly the BP equations, but proceed directly to the rBP ones,

which can be expressed in terms of the messages $h_{i \rightarrow r}, a_{\mu \rightarrow r}, c_{\mu \rightarrow r}$ defined from:

$$m_{i \rightarrow r}(s_i) \cong e^{h_{i \rightarrow r} s_i} \quad (81)$$

$$\int d\lambda_\mu m_{\mu \rightarrow r}(\lambda_\mu) \lambda_\mu = a_{\mu \rightarrow r} \quad (82)$$

$$\int d\lambda_\mu m_{\mu \rightarrow r}(\lambda_\mu) \lambda_\mu^2 = c_{\mu \rightarrow r} + a_{\mu \rightarrow r}^2 \quad (83)$$

They are related through the following set of equations:

$$h_{i \rightarrow r} = \frac{1}{\sqrt{N}} \sum_{s(\neq r)} u_i^s f(p_{s \rightarrow i}, d_{s \rightarrow i}, \pi_s, \delta_s) \quad (84)$$

$$c_{\nu \rightarrow r} = \frac{1}{\beta} \left[1 - \frac{1}{N} \sum_{s(\neq r)} (v_\nu^s)^2 \phi'(p_s, d_s, \pi_{s \rightarrow \nu}, \delta_{s \rightarrow \nu}) \right]^{-1} \quad (85)$$

$$a_{\nu \rightarrow r} = \beta c_{\nu \rightarrow r} \frac{1}{N} \sum_{s(\neq r)} v_\nu^s \phi(p_s, d_s, \pi_{s \rightarrow \nu}, \delta_{s \rightarrow \nu}) \quad (86)$$

where:

$$p_r = \frac{1}{\sqrt{N}} \sum_i u_i^r \tanh(\beta h_{i \rightarrow r}) \quad (87)$$

$$d_r = \frac{1}{N} \sum_i (u_i^r)^2 (1 - \tanh^2(\beta h_{i \rightarrow r})) \quad (88)$$

$$\pi_r = \frac{1}{\sqrt{N}} \sum_\nu v_\nu^r a_{\nu \rightarrow r} \quad (89)$$

$$\delta_r = \frac{1}{N} \sum_\nu (v_\nu^r)^2 c_{\nu \rightarrow r} \quad (90)$$

and

$$p_{r \rightarrow j} = \frac{1}{\sqrt{N}} \sum_{i(\neq j)} u_i^r \tanh(\beta h_{i \rightarrow r}) \quad (91)$$

$$d_{r \rightarrow j} = \frac{1}{N} \sum_{i(\neq j)} (u_i^r)^2 (1 - \tanh^2(\beta h_{i \rightarrow r})) \quad (92)$$

$$\pi_{r \rightarrow \mu} = \frac{1}{\sqrt{N}} \sum_{\nu(\neq \mu)} v_\nu^r a_{\nu \rightarrow r} \quad (93)$$

$$\delta_{r \rightarrow \mu} = \frac{1}{N} \sum_{\nu(\neq \mu)} (v_\nu^r)^2 c_{\nu \rightarrow r} \quad (94)$$

The functions f, ϕ, ϕ' are functions of four variables defined as:

$$f(p, d, \pi, \delta) = \langle \hat{U} \rangle \quad (95)$$

$$\phi(p, d, \pi, \delta) = \langle \hat{U}^2 \rangle - \langle \hat{U} \rangle^2 \quad (96)$$

$$\phi'(p, d, \pi, \delta) = \frac{\partial}{\partial \pi} \phi(p, d, \pi, \delta) \quad (97)$$

where the expectations are taken with the following measure over $\vec{t} = (U, V, \hat{U}, \hat{V})$:

$$\exp \left[\beta \left(-\hat{U}U - \hat{V}V + \frac{1}{\sqrt{\gamma}}UV + p\hat{U} + \pi\hat{V} \right) + \frac{\beta^2}{2} (d\hat{U}^2 + \delta\hat{V}^2) \right] \quad (98)$$

An explicit computation shows that

$$f(p, d, \pi, \delta) = \frac{1}{1 - d\delta\beta^2/\gamma} \left(\frac{\beta\delta}{\gamma}p + \frac{1}{\sqrt{\gamma}}\pi \right) \quad (99)$$

$$\phi(p, d, \pi, \delta) = \frac{1}{1 - d\delta\beta^2/\gamma} \left(\frac{1}{\sqrt{\gamma}}p + \frac{\beta d}{\gamma}\pi \right) \quad (100)$$

$$\phi'(p, d, \pi, \delta) = \frac{1}{1 - d\delta\beta^2/\gamma} \left(\frac{\beta d}{\gamma} \right) \quad (101)$$

C. TAP equations

It turns out that the TAP equations can be written in terms of local quantities associated with each of the variable in the factor graph: starting from (84,85,86) we define

$$H_i = \frac{1}{\sqrt{N}} \sum_s u_i^s f(p_{s \rightarrow i}, d_{s \rightarrow i}, \pi_s, \delta_s) \quad (102)$$

$$C_\nu = \frac{1}{\beta} \left[1 - \frac{1}{N} \sum_s (v_\nu^s)^2 \phi'(p_s, d_s, \pi_{s \rightarrow \nu}, \delta_{s \rightarrow \nu}) \right]^{-1} \quad (103)$$

$$A_\nu = \beta c_{\nu \rightarrow r} \frac{1}{\sqrt{N}} \sum_s v_\nu^s \phi(p_s, d_s, \pi_{s \rightarrow \nu}, \delta_{s \rightarrow \nu}) \quad (104)$$

We first notice that, in the thermodynamic limit, $C_\nu = C$ becomes independent of ν , and we can also safely approximate $c_{\nu \rightarrow r} = C$, the correcting terms being irrelevant. Similarly, we notice that d_r becomes r -independent,

$$d_r = 1 - q = 1 - \frac{1}{N} \sum_i \tanh^2(\beta H_i) , \quad (105)$$

and δ_r becomes r -independent:

$$\delta_r = \alpha C . \quad (106)$$

The equation for C can be obtained from (85):

$$\frac{1}{C} = \beta - \frac{\beta^2(1 - q)}{1 - C\alpha\beta^2(1 - q)/\gamma} \quad (107)$$

and gives

$$C = \frac{\gamma}{2\alpha\beta^2(1 - q)} \left[1 - \beta(1 - q)(1 - \alpha/\gamma) - \sqrt{(1 - \beta(1 - q)(1 + \alpha/\gamma))^2 - 4\alpha\beta^2(1 - q)^2/\gamma} \right] \quad (108)$$

C is nothing but the variance of the local-fields A_ν for each pattern-variable. When $\gamma \rightarrow \infty$ one finds back that $C = (1/\beta)1/[1 - \beta(1 - q)]$, which is the expression found in the Hopfield model, as it should.

Defining:

$$\hat{f}(p, \pi) = f(p, 1 - q, \pi, \alpha C) = \frac{1}{1 - C \frac{\alpha}{\gamma} \beta^2 (1 - q)} \left[\frac{\alpha \beta C}{\gamma} p + \frac{1}{\sqrt{\gamma}} \pi \right] \quad (109)$$

$$\hat{\phi}(p, \pi) = \phi(p, 1 - q, \pi, \alpha C) = \frac{1}{1 - C \frac{\alpha}{\gamma} \beta^2 (1 - q)} \left[\frac{1}{\sqrt{\gamma}} p + \frac{\beta(1 - q)}{\gamma} \pi \right] \quad (110)$$

We can write the TAP equations:

$$H_i = \frac{1}{\sqrt{N}} \sum_s u_i^s \hat{f}(p_s, \pi_s) - \frac{\alpha \beta C}{1 - C \frac{\alpha}{\gamma} \beta^2 (1 - q)} \tanh(\beta H_i) \quad (111)$$

$$A_\nu = \frac{1}{N} \sum_s v_\nu^s \hat{\phi}(p_s, \pi_s) \quad (112)$$

$$p_r = \frac{1}{\sqrt{N}} \sum_i u_i^r \tanh(\beta H_i) - \frac{\beta(1 - q)}{\sqrt{\gamma}} \frac{1}{\sqrt{N}} \sum_\nu v_\nu^r A_\nu \quad (113)$$

$$\pi_r = \frac{1}{\sqrt{N}} \sum_\nu v_\nu^r A_\nu - \frac{\alpha \beta C}{\sqrt{\gamma}} \frac{1}{\sqrt{N}} \sum_i u_i^r \tanh(\beta H_i) \quad (114)$$

Equations (111-114), together with the definitions (108,109,110) give the closed set of TAP equations relating the $N(1 + \alpha + 2\gamma)$ local fields H_i, A_ν, p_r, π_r .

It is interesting to notice that, due to the linear structure of these equations, the variables p_r, π_r can be eliminated explicitly, leading to a set of equations that relate only the fields on the site-variables, H_i , and those on the pattern-variables, A_μ :

$$H_i = \sum_\nu \frac{\xi_i^\nu}{\sqrt{N}} A_\nu - \frac{\alpha \beta C}{1 - C \frac{\alpha}{\gamma} \beta^2 (1 - q)} \tanh(\beta H_i) \quad (115)$$

$$A_\mu = \frac{1}{\sqrt{N}} \sum_j \xi_j^\mu \tanh(\beta H_j) \quad (116)$$

These TAP equations are similar to the ones of the Hopfield model, with a modified form of the Onsager reaction term. Again, because of their linear structure in A_μ , these variables can be eliminated, giving a set of TAP equation connecting only the local fields on the visible neuron-variables:

$$H_i = \frac{1}{N} \sum_j J_{ij} \tanh(\beta H_j) - \frac{\alpha \beta C}{1 - C \frac{\alpha}{\gamma} \beta^2 (1 - q)} \tanh(\beta H_i) \quad (117)$$

Again, the only modification due to the combinatorially correlated patterns is the value of the Onsager reaction term. Notice that, in the large γ limit, we get back the usual TAP equation of the Hopfield model.

We have derived four versions of the mean-field equations for this modified Hopfield: the rBP equations which relate messages that are propagated on the edges of the factor graph, and three versions of the TAP equations, one set of “expanded” equations which relate local quantities associated with each variable node of the factor graph, a second one, “intermediate”, which relates the local fields of the neuron-variables and the pattern-variables, and finally this last one that relates only the local fields on the neuron-variables. Which one is more useful remains to be investigated. The rBP equations should be studied statistically, and give the solution for the thermodynamic properties of this modified Hopfield model using the cavity method. The schedule of update of TAP equations is probably crucial, and working out the correct time indices for algorithmic purpose should go through the expanded version of the equations. It should also be kept in mind that, in general RBMs, the hidden variables are in general not Gaussian-distributed, and in such cases the simplification of TAP equations does not occur (see the next section). Therefore in general the correct form of TAP equations can be obtained only in their expanded form. This shows the importance of using multilayered networks.

VI. A FEW REMARKS ON MORE GENERAL RESTRICTED BOLTZMANN MACHINES

It is easy to generalize the Hopfield model in order to describe a general RBM. We shall give here the general form of BP, rBP and TAP equations. Similar results have been obtained recently in information-theoretic approaches to matrix factorization^{41,42}, but they generally address a form of “planted” problem where specific simplifications take place^{13,43}. We give here the general form of the equations.

Using the same notations as before, we consider a system of N spin-variables s_i and P pattern-variables λ_μ , described by a probability distribution:

$$P(\{s_i\}, \{\lambda_\mu\}) = \frac{1}{Z} \prod_i \tilde{\rho}(s_i) \prod_\mu \rho(\lambda_\mu) \exp \left[\beta \left(\sum_i \tilde{h}_i s_i + \sum_\mu h_\mu \lambda_\mu + \sum_{\mu,i} \frac{\xi_i^\mu}{\sqrt{N}} s_i \lambda_\mu \right) \right]. \quad (118)$$

With respect to the usual Hopfield model, three modifications have been introduced:

- The local measure on the spin variables is $\tilde{\rho}(s)$. In the Hopfield model one considers

$\tilde{\rho}(s) = (1/2)(\delta_{s,1} + \delta_{s,-1})$, but more general distributions can be studied as well.

- The local measure on the pattern variables is $\rho(\lambda)$. In the Hopfield model one considers $\rho(\lambda) = (1/\sqrt{2\pi\beta}) \exp(-\beta\lambda^2/2)$, but more general distributions can be studied as well.
- We introduce local fields \tilde{h}_i and h_μ , which will make it possible to compute correlation functions through linear response, using for instance $\langle s_i s_j \rangle = \partial \langle s_i \rangle / \partial \tilde{h}_j$.

The BP equations are:

$$m_{i \rightarrow \mu}(s_i) \cong \tilde{\rho}(s_i) e^{\beta \tilde{h}_i s_i} \prod_{\nu(\neq \mu)} \hat{m}_{\nu \rightarrow i}(s_i) \quad (119)$$

$$\hat{m}_{\mu \rightarrow i}(s_i) \cong \int d\lambda_\mu m_{\mu \rightarrow i}(\lambda_\mu) \exp\left((\beta/\sqrt{N}) \xi_i^\mu s_i \lambda_\mu\right) \quad (120)$$

$$\hat{m}_{i \rightarrow \mu}(\lambda_\mu) = \int ds_i m_{i \rightarrow \mu}(s_i) e^{\beta \xi_i^\mu / \sqrt{N}} \quad (121)$$

$$m_{\mu \rightarrow i}(\lambda_\mu) \cong \rho(\lambda_\mu) e^{\beta h_\mu \lambda_\mu} \prod_{j(\neq i)} \hat{m}_{j \rightarrow \mu}(\lambda_\mu) \quad (122)$$

In order to write the rBP equations, we need to understand the scaling of the variables. In particular, we have seen in the Hopfield model that, in the retrieval phase, one of the variables λ_μ may become very large (of order \sqrt{N}), signalling a polarization towards this pattern. The possibility of such a phenomenon clearly depends on the measures $\tilde{\rho}(s)$ and $\rho(\lambda)$. In the Hopfield case, $\rho(\lambda)$ is a Gaussian. This means that the response of the pattern-variable λ to a local field h is a linear function of h . This allows the variable λ_μ to grow to very large values. In contrast, in many applications of RBMs, one uses variables with a bounded range of values. For instance, if $\rho(\lambda_\mu)$ vanishes outside an interval $[-C, C]$, then the response of the variable λ_μ is a non-linear, sigmoid-shaped function of the local field, and the condensation cannot occur.

One opposite case would be the one when both $\tilde{\rho}(s)$ and $\rho(\lambda)$ are Gaussian. It is then clear that, at low temperatures, the spins will acquire spontaneous polarization in the direction of the eigenvector of the J matrix (Eq.3) with largest eigenvalue. Both the spin-variables and the pattern-variables condense in this case.

We shall write here the rBP equations assuming that there is no condensation. As for the coupling variables ξ_i^μ , we suppose that they are iid variables with zero mean and a finite variance.

Following standard procedures like those used in¹⁴⁻¹⁸, the messages $m_{\mu \rightarrow i}(\lambda_\mu)$ and $m_{i \rightarrow \mu}(s_i)$ are parameterized in terms of their first two moments. Generalizing (17,18),

we define:

$$a_{\mu \rightarrow i} = \int d\lambda_\mu m_{\mu \rightarrow i}(\lambda_\mu) \lambda_\mu \quad (123)$$

$$c_{\mu \rightarrow i} = \int d\lambda_\mu m_{\mu \rightarrow i}(\lambda_\mu) \lambda_\mu^2 - a_{\mu \rightarrow i}^2 \quad (124)$$

$$\tilde{a}_{i \rightarrow \mu} = \int ds_i m_{i \rightarrow \mu}(s_i) s_i \quad (125)$$

$$\tilde{c}_{i \rightarrow \mu} = \int ds_i m_{i \rightarrow \mu}(s_i) s_i^2 - \tilde{a}_{i \rightarrow \mu}^2 \quad (126)$$

The rBP equations relating these four types of messages can be written in terms of the following four functions of two real variables.

Considering a spin-variable s with local measure

$$\tilde{P}(s) = \frac{1}{\tilde{z}} \tilde{\rho}(s) e^{us + (v/2)s^2} \quad (127)$$

we define

$$\tilde{f}(u, v) = \int ds \tilde{P}(s) s \quad (128)$$

$$\tilde{f}'(u, v) = \frac{\partial}{\partial u} \tilde{f}(u, v) = \int ds \tilde{P}(s) s^2 - \tilde{f}_a(u, v)^2 \quad (129)$$

Considering a pattern-variable λ with local measure

$$P(\lambda) = \frac{1}{z} \rho(\lambda) e^{u\lambda + (v/2)\lambda^2} \quad (130)$$

we define

$$f(u, v) = \int d\lambda P(\lambda) \lambda \quad (131)$$

$$f'(u, v) = \frac{\partial}{\partial u} f(u, v) = \int d\lambda P(\lambda) \lambda^2 - f_a(u, v)^2 \quad (132)$$

The rBP equations can then be written as

$$a_{\mu \rightarrow i}^{t+1} = f \left(\beta h_\mu + \frac{\beta}{\sqrt{N}} \sum_{j(\neq i)} \xi_j^\mu \tilde{a}_{j \rightarrow \mu}^t, \frac{\beta^2}{N} \sum_{j(\neq i)} (\xi_j^\mu)^2 \tilde{c}_{j \rightarrow \mu}^t \right) \quad (133)$$

$$c_{\mu \rightarrow i}^{t+1} = f' \left(\beta h_\mu + \frac{\beta}{\sqrt{N}} \sum_{j(\neq i)} \xi_j^\mu \tilde{a}_{j \rightarrow \mu}^t, \frac{\beta^2}{N} \sum_{j(\neq i)} (\xi_j^\mu)^2 \tilde{c}_{j \rightarrow \mu}^t \right) \quad (134)$$

$$\tilde{a}_{i \rightarrow \mu}^{t+2} = \tilde{f} \left(\beta \tilde{h}_i + \frac{\beta}{\sqrt{N}} \sum_{\nu(\neq \mu)} \xi_i^\nu a_{\nu \rightarrow i}^{t+1}, \frac{\beta^2}{N} \sum_{\nu(\neq \mu)} (\xi_i^\nu)^2 c_{\nu \rightarrow i}^{t+1} \right) \quad (135)$$

$$\tilde{c}_{i \rightarrow \mu}^{t+2} = \tilde{f}' \left(\beta \tilde{h}_i + \frac{\beta}{\sqrt{N}} \sum_{\nu(\neq \mu)} \xi_i^\nu a_{\nu \rightarrow i}^{t+1}, \frac{\beta^2}{N} \sum_{\nu(\neq \mu)} (\xi_i^\nu)^2 c_{\nu \rightarrow i}^{t+1} \right) \quad (136)$$

where we have reintroduced the time indices corresponding to a parallel update of these equations.

One gets the TAP equations using the same method as before. In the large N limit the messages depend only weakly on the index of arrival. Writing

$$a_{\mu \rightarrow i} \simeq A_\mu \ ; \ c_{\mu \rightarrow i} \simeq C_\mu \ ; \ \tilde{a}_{i \rightarrow \mu} \simeq \tilde{A}_i \ ; \ \tilde{c}_{i \rightarrow \mu} \simeq C_i \quad (137)$$

and expanding the leading correction terms, one obtains:

$$A_\mu^{t+1} = f(U_\mu^t, V_\mu^t) \quad (138)$$

$$C_\mu^{t+1} = f'(U_\mu^t, V_\mu^t) \quad (139)$$

$$\tilde{A}_i^{t+2} = \tilde{f}(\tilde{U}_i^{t+1}, \tilde{V}_i^{t+1}) \quad (140)$$

$$\tilde{C}_i^{t+2} = \tilde{f}'(\tilde{U}_i^{t+1}, \tilde{V}_i^{t+1}) \quad (141)$$

where :

$$U_\mu^t = \beta h_\mu + \frac{\beta}{\sqrt{N}} \sum_i \xi_i^\mu \tilde{A}_i^t - A_\mu^{t-1} \frac{\beta^2}{N} \sum_i (\xi_i^\mu)^2 \frac{\partial \tilde{f}}{\partial \tilde{U}}(\tilde{U}_i^{t-1}, \tilde{V}_i^{t-1}) \quad (142)$$

$$V_\mu^t = \frac{\beta^2}{N} \sum_i (\xi_i^\mu)^2 \tilde{C}_i^t \quad (143)$$

$$\tilde{U}_i^{t+1} = \beta \tilde{h}_i + \frac{\beta}{\sqrt{N}} \sum_\mu \xi_i^\mu A_\mu^{t+1} - \tilde{A}_i^t \frac{\beta^2}{N} \sum_\mu (\xi_i^\mu)^2 \frac{\partial f}{\partial U}(U_\mu^t, V_\mu^t) \quad (144)$$

$$\tilde{V}_i^{t+1} = \frac{\beta^2}{N} \sum_\mu (\xi_i^\mu)^2 C_\mu^{t+1} \quad (145)$$

Notice that, in general, when $\tilde{\rho}(s)$ and $\rho(\lambda)$ are non-gaussian, the functions f and \tilde{f} are nonlinear functions of u , and therefore one cannot easily eliminate one of the variables, as was done in the Hopfield model. This means that the correct form of TAP equations require working on the bipartite graph with the two layers of variables, visible and hidden.

VII. CONCLUDING REMARKS

We have seen that the correct mean-field "TAP" equations in the Hopfield model can be written most easily by introducing a layer of hidden variables, the pattern-variables, which interact with the neuron-variables. In the Hopfield model, the local fields associated with the hidden variables can be eliminated and one remains with TAP equations that are similar to those of general spin glasses, differing only in the detailed form of the Onsager

reaction term. However, when one deals with RBMs which generalize the Hopfield model with non-Gaussian hidden variables, the representation with the hidden layer is necessary.

In the case where the patterns to be memorized have correlations based on a combinatorial structure, the TAP equations involve one extra layer of hidden variables, and with a deeper structure of correlations, extra hidden layers would be added.

We believe that combinatorial disorder is actually an essential ingredient that is likely to be present in real data. In this respect, it is striking that the correct treatment of mean-field theory in RBMs with combinatorial disorder leads naturally to the appearance of layers of hidden variables. The present study of the Hopfield model is a kind of first test of this idea, which we hope could lead to a better understanding of the role of multilayered structures in practical applications of neural networks.

The present work calls for some further developments in several directions:

- It will be interesting to study how the TAP estimates for the magnetizations (and those for the correlation functions that are inferred through linear response) can be turned into efficient algorithms for unsupervised learning, along the lines of^{6–10}. In this respect, it is interesting to be able to study controlled problems. We think that the Hopfield model with combinatorial-correlated patterns can be used as an interesting teacher to generate data, i.e. patterns of neural activity, that can be used in the training of a “student” Hopfield network.
- The modified Hopfield model with combinatorial-correlated patterns is interesting in itself. It would be interesting to study its thermodynamics both with replicas and with the cavity method, through a statistical analysis of the rBP equations.

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