A message-passing scheme for non-equilibrium stationary states

Erik Aurell$^{1,2,3}$ and Hamed Mahmoudi$^2$

$^1$ Department of Computational Biology, AlbaNova University Centre, 106 91 Stockholm, Sweden
$^2$ Department of Information and Computer Science, Aalto University, Finland
$^3$ ACCESS Linnaeus Centre, KTH—Royal Institute of Technology, Stockholm, Sweden
E-mail: eaurell@kth.se and mahmoudi.hamed@gmail.com

Received 9 January 2011
Accepted 24 March 2011
Published 18 April 2011

Abstract. We study stationary states in a diluted asymmetric (kinetic) Ising model. We apply the recently introduced dynamic cavity method to compute magnetizations of these stationary states. Depending on the update rule, different versions of the dynamic cavity method apply. We here study synchronous updates and random sequential updates, and compare local properties computed by the dynamic cavity method to numerical simulations. Using both types of updates, the dynamic cavity method is highly accurate at high enough temperatures. At low enough temperatures, for sequential updates the dynamic cavity method tends to a fixed point, but this does not agree with numerical simulations, while for parallel updates, the dynamic cavity method may display oscillatory behavior. When it converges and is accurate, the dynamic cavity method offers a huge speed-up compared to Monte Carlo, particularly for large systems.

Keywords: cavity and replica method
A message-passing scheme for non-equilibrium stationary states

1. Introduction

Stationary states of classical equilibrium systems are described by the Boltzmann–Gibbs measure. In complex systems, the exact computation of even local properties (marginals) is not feasible, and perturbative methods or other approximations therefore have to be used. Much attention has over the last decade been given to the belief propagation (BP) or Bethe–Peierls ansatz class of approximations of the marginals, which are exact if the underlying graph of interactions is a tree, and generally expected to be accurate if the underlying graph is locally tree-like [16,30].

In contrast to equilibrium systems, non-equilibrium systems do not admit a similar, universal, description of their stationary states. We here take a small step in this direction. We show that the recently introduced dynamic cavity method, essentially a Bethe–Peierls ansatz on spin system histories, can be used effectively to compute local properties in stationary states when the underlying graph of interactions is sparse, and locally tree-like. A key technical step to make this a computationally feasible scheme is a stationarity assumption, here termed time factorization. With this step we find a message-passing scheme similar to belief propagation, but for dynamics, and for non-equilibrium systems. When these approximations work, at sufficiently high temperatures (weak interactions) they offer a huge speed-up compared to Monte Carlo.

We now give a synthetic overview of the dynamic cavity approach. A total history of a collection of spins, evolving in discrete time steps according to some dynamics, can be described by the total joint probability \( p(\vec{\sigma}(0) \cdots \vec{\sigma}(t)) \). From such a total joint probability one can construct the marginal probability over the history of one spin \( p_i(\sigma_i(0) \cdots \sigma_i(t)) \). If the underlying graph of interactions is locally tree-like, then this marginal probability can

doi:10.1088/1742-5468/2011/04/P04014
be expressed using ‘messages’ from the neighboring nodes of the type \( \mu_{j \rightarrow i}(\sigma_j(0) \cdots \sigma_j(t)) \), and these messages in turn obey update rules similar (in principle) to belief propagation. In contrast to the cavity method in equilibrium analysis, messages carry the whole information of spin histories over time. The difficulty arises when we want to marginalize further to the configuration of one spin at one time in its history. In general, the resulting equations are non-Markovian, and hard to solve. One level of approximation is to assume that the messages factorize in time, as \( \mu_{j \rightarrow i}(\sigma_j(0) \cdots \sigma_j(t)) = \prod_{s=0}^{t} \mu_{j \rightarrow i}^{(s)}(\sigma_j(s)) \), and in the stationary state we can further assume that the terms in the product \( \mu_{j \rightarrow i}^{(s)}(\sigma_j(s)) \) are all the same function, i.e. do not depend on \( s \). The terms in the factorized messages \( \mu_{j \rightarrow i}^{(s)}(\sigma_j) \) then obey a set of distributed equations analogous to (but more complex than) belief propagation. Depending on the dynamics of the spin system, the resulting equations will differ. We here investigate both parallel updates, as studied recently by Neri and Bollé [22], as well as random sequential updates.

A summary of our results is as follows. We study stationary states in a diluted asymmetric (kinetic) Ising model. This well-studied non-equilibrium model has (qualitatively) three parameters: the asymmetry degree (how much the system is out of equilibrium), the connectivity of the underlying interaction graph (how accurate a Bethe–Peierls ansatz can be expected to be), and the strength of the interactions, customarily denoted inverse ‘temperature’. Furthermore, the type of the dynamics influences the behavior. We here study parallel (synchronous) updates and sequential updates (one spin at a time). We compare dynamic cavity results to numerical simulations of the spin system dynamics, which we will refer to as Monte Carlo. The first result is that the more asymmetric the network, the better the dynamic cavity method agrees with Monte Carlo. This can be understood as an effect of lack of memory in the graph: messages go out, and rarely come back. The second result is that the sparser the underlying graph of interactions, the better the dynamic cavity method agrees with Monte Carlo. This can be understood as an effect of the Bethe–Peierls approximation in itself being more accurate for locally tree-like graphs. The third result is that the dynamic cavity agrees well with Monte Carlo at high temperature, but deviates from numerical simulations of the full dynamics at low enough temperatures. The way in which the dynamic cavity diverges from Monte Carlo at low temperature depends on the update rule. For random sequential dynamics we find that the dynamic cavity (in the time-factorized approximation for the stationary state) goes to a fixed point, but which does not agree with the stationary state estimated from Monte Carlo. For parallel updates, on the other hand, we find that the dynamic cavity method at low enough temperature does not go to a fixed point. As the system size increases, we find that the dynamic cavity matches Monte Carlo better, and that the fluctuations in parallel updates diminish. In summary, the parameter ranges where the dynamic cavity method as presented here will be a promising avenue to compute and explore stationary states of large non-equilibrium systems.

The paper is organized as follows. In section 2 we briefly describe the model, introduce the macroscopic observables and study the dynamic update rules. Section 3 summarizes previous studies using ‘naive’ mean-field theory for the kinetic Ising model. In section 4 we introduce the dynamic cavity method for parallel and sequential updates, and in section 5 we compare the dynamic cavity to direct numerical simulation (Monte Carlo). Section 6 contains concluding remarks.
2. The diluted asymmetric (kinetic) spin glass

Kinetic Ising models were originally motivated by neural networks, to extend the Hopfield model to asymmetric interactions [12]. These non-equilibrium systems with random interactions have formal similarities to the equilibrium and especially out-of-equilibrium (relaxation) dynamics of spin glasses, and therefore have a long history of study using methods from that field. Sompolinsky and Zippelius [28] introduced a formalism based on the Langevin equations of spherical spin models. An analogous approach was then proposed by Sommers in [27] through a path integral analysis of the Glauber dynamics. More recently, the dynamic replica theory has been developed, partly with an application to this kind of systems in mind [4, 19, 20]. A general feature of dynamic replica theory is an average over disorder (average over a class of random graphs and random interactions); in addition technical assumptions may be needed such as considering the dynamics of some finite set of appropriate observables [4]. In [9] a combination of dynamic replica theory and the cavity method (equilibrium) concept was applied to finitely connected disordered spin systems. An alternative approach to dynamic replica theory is generating functional analysis (GFA). The GFA has a long history in analyzing non-equilibrium statistical mechanics of disordered systems [7]. In particular, it allows us to study systems with non-symmetric interacting couplings [5, 10]. More recently it has been developed to study the dynamics of spin glass systems with finite connectivity interactions [10]. In its general formalism, GFA aims at solving the dynamics of a spin system exactly; however, due to the complicated nature of the problem, one needs either to use a perturbative approach [15] or to restrict the analysis of GFA up to some approximation levels [10, 21]. For ferromagnetic systems with regular connectivity, which are much simpler than spin glasses, a recursive set of dynamical equations can be derived for some finite macroscopic observations [26].

The dynamic cavity method shares some of the features of the dynamic replica theory and generating functional analysis. In equilibrium analysis, the Ising spin glass systems in the Bethe lattice model have been solved by the cavity method on the level of replica symmetry breaking. However, in contrast to the replica method, cavity applies to one single graph instance (one single set of interactions). Neri and Bollé [22] and Kanoria and Montanari [13] considered the dynamic cavity method in parallel updates under respectively Glauber dynamics and majority rule dynamics. In the present work we extend the dynamic cavity method to random sequential updates, and investigate stationary states of the diluted asymmetric spin glass over a wide range of parameters, for both parallel updates and random sequential updates.

The asymmetric diluted Ising model is defined over a set of $N$ binary variables $\vec{\sigma} = \{\sigma_1, \ldots, \sigma_N\}$, and an asymmetric graph $G = (V, E)$, where $V$ is a set of $N$ vertices, and $E$ is a set of directed edges. To each vertex $v_i$ is associated a binary variable $\sigma_i$. The graphs $G$ are taken from random graph ensembles with bounded average connectivity. Following the parameterization of [10] we introduce a connectivity matrix $c_{ij}$, where $c_{ij} = 1$ if there is a link from vertex $i$ to vertex $j$, $c_{ij} = 0$ otherwise, and the matrix elements $c_{ij}$ and $c_{kl}$ are independent unless $\{kl\} = \{ji\}$. The random graph is specified by marginal (one-link) distributions

$$p(c_{ij}) = \frac{c}{N} \delta_{1, c_{ij}} + \left(1 - \frac{c}{N}\right) \delta_{0, c_{ij}}$$

(1)
and the conditional distributions

$$p(c_{ij}|c_{ji}) = \epsilon \delta_{c_{ij},c_{ji}} + (1 - \epsilon)p(c_{ij}).$$

(2)

In this model the average degree distribution is given by $c$, and the asymmetry is controlled by $\epsilon \in [0, 1]$. The two extreme values of $\epsilon$ give respectively an asymmetric network ($\epsilon = 0$), where the probabilities of having two directed links between pairs of variables are uncorrelated, and the fully symmetric network ($\epsilon = 1$) where the two links $i \rightarrow j$ and $j \rightarrow i$ are present or absent together. The parameter set is completed by a (real-valued) interaction matrix $J_{ij}/c$. We will always take $J_{ij}$ to be independent identically distributed random variables with zero mean and unit variance (Gaussian or binary) such that for the fully connected networks ($c = N$), the interactions scale as the Sherrington–Kirkpatrick model.

The definition of the kinetic Ising model is completed by a dynamics, or a spin update rule. In the synchronous update rules, which will be considered here, at each (discrete) time, a set of candidate spins is selected, and then updated according to the rule

$$\sigma_i(t + \Delta t) = \begin{cases} +1 & \text{with probability } \{1 + \exp(-2\beta h_i(t + \Delta t))\}^{-1} \\ -1 & \text{with probability } \{1 + \exp(2\beta h_i(t + \Delta t))\}^{-1} \end{cases}$$

(3)

where $\Delta t$ is the time interval in which the update procedure takes place and $h_i(t)$ is the effective field on spin $i$ at time step $t$,

$$h_i(t) = \sum_{j \in \partial i} \frac{J_{ij}}{c} \sigma_j(t - \Delta t) + \theta_i(t),$$

(4)

and the parameter $\beta$, analogous to inverse temperature, is a measure of the overall strength of the interactions. The notation $j \in \partial i$ in (3) and (4) indicates all vertices having a direct link to node $i$ (defined by $c_{ji} = 1$) and $\theta_i$ is the (possibly time dependent) external field acting on spin $i$.

We will consider two cases of synchronous updates: either all spins are selected and updated at each time step, or only one spin is randomly selected and updated in each time step. We refer to the first update rule as parallel, and the second as sequential. The time interval between updates is taken as $\Delta t = 1$ in parallel updates, and $\Delta t = 1/N$ in sequential updates, such that in both cases $\mathcal{O}(N)$ spins are updated per unit time.

The joint probability distribution over all the spin histories $p(\vec{\sigma}(0), \ldots, \vec{\sigma}(t))$ has in principle the following simple Markovian form:

$$p(\vec{\sigma}(0), \ldots, \vec{\sigma}(t)) = \prod_{s=1}^{t} W[\vec{\sigma}(s)|\vec{h}(s)] p(\vec{\sigma}(0))$$

(5)

where $W$ is the appropriate transition matrix describing dynamics and updates. Solving equation (5) is in general infeasible for large system size, since it consists of $2^t 2^N$ equations corresponding to all possible spin history configurations. One therefore needs to restrict the analysis to some restricted set of observables. In this paper we are interested in approximations built on marginal probabilities. The evolution of a single spin is (trivially) defined by summing over the histories of all spins except one

$$p_i(\sigma_i(0), \ldots, \sigma_i(t)) = \sum_{\vec{\sigma}_{\backslash i}(0), \ldots, \vec{\sigma}_{\backslash i}(t)} p(\vec{\sigma}(0), \ldots, \vec{\sigma}(t))$$

(6)
and similarly for pairwise joint probability of the histories of two spins \((t > t')\)

\[
p_{ij}(\sigma_i(0), \ldots \sigma_i(t), \sigma_j(0), \ldots \sigma_j(t')) = \sum_{\bar{\sigma}_{\bar{\alpha},j}(0), \ldots \bar{\sigma}_{\bar{\alpha},j}(t)} p(\bar{\sigma}(0), \ldots, \bar{\sigma}(t)).
\]  

Consequently, the time evolution of single site magnetization and the pairwise correlations can be obtained from equations (6) and (7):

\[
p_i(\sigma_i(t)) = \frac{1 + m_i(t) s_i(t)}{2}
\]  
\[
p_{ij}(\sigma_i(t), \sigma_j(t')) = \frac{[1 + m_i(t)\sigma_i(t) + m_j(t')\sigma_j(t') + c_{ij}(t, t')\sigma_i(t)\sigma_j(t')]}{4}.
\]  

Computing the marginal probabilities directly is clearly an intractable problem for large system sizes, since the exact enumeration requires summation over an exponentially large number of states. The situation is even more involved for time dependent quantities since in addition the effect of past history must be taken into account.

3. Naive mean-field approximation

The dynamics of spin glass models has been widely studied using mean-field approximations; we follow recent practice in referring to this level of approximation as naive mean field \([23]\). In \([5,6]\) such a theory was proposed to describe the dynamics of the Little–Hopfield model in the case of fully asymmetric networks. Here we briefly summarize the naive mean-field theory for diluted asymmetric systems. The time evolution of magnetization and correlations for the parallel update defined in equation (5) can be explicitly written as

\[
m_i(t) = \langle \tanh(\beta \hat{h}_i(t)) \rangle
\]  

where \(\langle \cdot \cdot \cdot \rangle\) represents the average over the probability distribution at time \(t\). Similarly, for the sequential update we have

\[
m_i \left( t + \frac{1}{N} \right) = \left( 1 - \frac{1}{N} \right) m_i(t) + \frac{1}{N} \langle \tanh(\beta \hat{h}_i(t)) \rangle.
\]  

Equations (10) and (11) are exact. The right-hand side of the equations is, however, not easy to compute. The assumption in naive mean-field theory is to substitute the effective field \(\hat{h}_i(t)\) at time \(t\) with a time dependent random Gaussian noise which does not contain spin configurations \([5]\). The formula for the time evolution of the magnetization (expectation value of a single spin) is then

\[
m_i(t + 1) = \tanh(\beta \hat{h}_i(t)) \quad \text{parallel update}
\]  
\[
m_i \left( t + \frac{1}{N} \right) = m_i(t) + \frac{1}{N} (\tanh(\beta \hat{h}_i(t)) - m_i(t)) \quad \text{sequential update}
\]  

where \(\hat{h}_i(t)\) is given by the mean values of spins neighboring \(i\) and a Gaussian noise reflecting the effect of neighbors on the dynamics of spin \(i\) (see \([5]\) and \([27]\)). The fixed points of two dynamic updates coincide, but system size is important for the stability of the fixed point in the sequential update whereas it has no effect on the parallel
A message-passing scheme for non-equilibrium stationary states

Figure 1. Left figure: a directed network representation of the asymmetric Ising model. Interacting pairs are connected by directed edges where the arrows indicate the asymmetric nature of the model. Right figure: the cavity graph created by fixing the spin $i$ to have the value $s_i$. This affects other spins which were connected to vertex $i$ by an incoming edge from $i$ (shown by red color). In graphs with tree structure, this leads immediately to a factorized probability distribution for the set of spins in different branches outgoing from node $i$.

update scheme [2,29]. The naive mean-field approximation, although introduced quite some time ago, remains a main theoretical tool to analyze kinetic Ising models. More recently, these approximations have been used as the basis for ‘kinetic Ising’ reconstruction schemes [11,24,31].

4. The dynamic cavity method

In this paper we use the terms Bethe–Peierls approximation (BP) and cavity method interchangeably. Their modern use grew out of replica theory in spin glasses, but in a form which can be applied to a single instance [8,16,18]. We use the term dynamic cavity method for the use of the Bethe–Peierls approximation on spin histories.

The main idea of BP is to ignore long loop correlations, since BP is exact on trees. BP can then be described by a set of auxiliary graphs called cavity graphs, which are identical to the original graphs but with one of the vertices and its associated variable removed. The effects of removing a target node $i$ appear in the effective fields equation (4) acting on the set of variables neighboring node $i$ with direct interactions outgoing from spin $i$. Figure 1 illustrates the argument graphically. By the assumption that short loops are absent and long loops are ignored, the variables associated to the vertices which were connected to the removed vertex (denoted by $i$ in figure 1) are independent in the cavity graph. We can then consider the joint probability of the histories of all the other spins $p^{(i)}(\vec{\sigma}_i(0), \ldots, \vec{\sigma}_i(t) | \vec{\theta}_i(0), \ldots, \vec{\theta}_i(t))$ under the influence of the external fields modified by the action of spin $i$ i.e. $\theta_j^{(i)}(s) = \theta_j(s) + J_{ji} \sigma_i(s - \Delta t)$. Since the removed vertex only modifies the effective fields of its neighbors with an outgoing edge we can further marginalize the joint probability distribution to the set $\partial_i$ of spins ‘in the cavity’ which were directly connected to vertex $i$, $p^{(i)}(\sigma_{\partial_i}(0), \ldots, \sigma_{\partial_i}(t) | \theta_{\partial_i}^{(i)}(0), \ldots, \theta_{\partial_i}^{(i)}(t))$. The
assumption of no loops means that the set of spins neighboring vertex \( i \) ‘in the cavity’ produced by removing vertex \( i \) is independent, and that therefore this joint probability over these spin histories is factorized as

\[
p^{(i)}(\sigma_{\partial i}(0), \ldots, \sigma_{\partial i}(t) | \theta^{(i)}_{\partial i}(0), \ldots, \theta^{(i)}_{\partial i}(t)) = \prod_{j \in \partial i} \mu_{j \to i}(\sigma_j(0), \ldots, \sigma_j(t) | \theta^{(j)}_j(0), \ldots, \theta^{(j)}_j(t)). \tag{14}
\]

The above approximation is exact in trees, but in general it can be only considered as an approximation. For random graph ensembles with diluted interactions, the typical loop length diverges in the thermodynamic limit and BP is therefore expected to become inaccurate.

By the same argument we can marginalize the joint probability distribution over any single vertex in the neighborhood of \( i \) and consequently all individual spins. The cavity assumption causes the marginal probability \( \mu_{j \to i} \) to be dependent on the spins that are directly connected to the vertex \( j \). Therefore we can interpret marginal probabilities in the cavity graph as a set of ‘messages’ exchanged among interacting pairs. These messages themselves obey recursion equations (‘BP update equations’) which for parallel update are

\[
\mu_{j \to i}(\sigma_j(0), \ldots, \sigma_j(t) | \theta^{(j)}_j(0), \ldots, \theta^{(j)}_j(t)) = \sum_{\sigma_{\partial j \setminus i}(0), \ldots, \sigma_{\partial j \setminus i}(t-\Delta t)} \prod_{k \in \partial j \setminus i} \mu_{k \to j}(\sigma_k(0), \ldots, \sigma_k(t-\Delta t) | \theta^{(k)}_k(0), \ldots, \theta^{(k)}_k(t-\Delta t))
\]

\[
\times \prod_{s=1}^{t} w_j(\sigma_j(s) | h^{(j)}_j(s)) \mu_{j \to i}(\sigma_j(0)). \tag{15}
\]

Here \( h^{(j)}_j \) is the effective field on spin \( j \) in the cavity graph

\[
h^{(j)}_j(s) = \sum_{k \in \partial j \setminus i} \frac{J_{kj}}{\epsilon} \sigma_k(s-\Delta t) + \theta_j(t) \tag{16}
\]

and \( w_j(\sigma_j | h^{(j)}_j(s)) \) is the transition probability for the single spin \( j \) in the cavity graph. Similarly for the sequential update we have (see appendix for details)

\[
\mu_{j \to i}(\sigma_j(0), \ldots, \sigma_j(t) | \theta^{(j)}_j(0), \ldots, \theta^{(j)}_j(t)) = \sum_{\sigma_{\partial j \setminus i}(0), \ldots, \sigma_{\partial j \setminus i}(t-\Delta t)} \prod_{k \in \partial j \setminus i} \mu_{k \to j}(\sigma_k(0), \ldots, \sigma_k(t-\Delta t) | \theta^{(k)}_k(0), \ldots, \theta^{(k)}_k(t-\Delta t))
\]

\[
\times \prod_{s=1}^{t} \left[ \frac{1}{N} w_j(\sigma_j(s) | h^{(j)}_j(s)) + \left( 1 - \frac{1}{N} \right) \delta_{\sigma_j(s), \sigma_j(s-\Delta t)} \right] \mu_{j \to i}(\sigma_j(0)). \tag{17}
\]

Figure 2 illustrates how messages are distributed among interacting vertices: using the terminology of belief propagation (BP), the conditional probability \( \mu_{j \to i}(\sigma_j(0), \ldots, \sigma_j(t)) \) can be interpreted as a message sent from variable \( j \) to its neighbor \( i \) to indicate the probability of observing spin history \( \sigma_j(0) \ldots \sigma_j(t) \) when \( i \) is removed from the network.

doi:10.1088/1742-5468/2011/04/P04014
A message-passing scheme for non-equilibrium stationary states

Figure 2. Dynamic message-passing scheme for the diluted Ising systems. Each message contains information describing the evolution of marginal probability in the cavity graph. Messages are exchanged among the interacting pairs. The history of the target vertex may affect the incoming message.

The probability of the full history of one spin (‘BP output equation’) is on the same level of approximation

\[
p_i(\sigma_i(0), \ldots, \sigma_i(t)|\theta_i(0), \ldots, \theta_i(t)) = \sum_{\sigma_{\partial i}(0) \ldots \sigma_{\partial i}(t-\Delta t)} \prod_{k \in \partial i} \mu_{k \rightarrow i}(\sigma_k(0), \ldots, \sigma_k(t-\Delta t)|\theta_k^{(i)}(0), \ldots, \theta_k^{(i)}(t-\Delta t)) \times \prod_{s=1}^{t} W_i(\sigma_i(s)|h_i(s)) \ p_i(\sigma_i(0)). \tag{18}
\]

A peculiarity of this formula (shared with equations (15) and (17)) is that the probability distribution of \(i\) depends on the neighbors \(\partial i\) through the effective field \(h_i(s)\), but the messages sent from the neighbors to \(i\) also depend parametrically on the history of \(i\) through the modified external fields \(\theta_k^{(i)}\). This difficulty is absent for fully asymmetric networks, since then the messages sent to \(i\) do not depend on the history of \(i\), as we briefly review below in section 4.1. In the general case of partially or fully symmetric networks this difficulty is addressed in long time limit evolution by a stationary assumption and the time-factorization ansatz in section 4.2.

Starting from suitable initial conditions for messages, the evolution of messages can be followed from equations (15) and (17). Each message contains \(2^t\) different states corresponding to the trajectory of vertices. Marginalizing equations (15) and (17) to the single time step \(t\) would provide us with the time dependent magnetization through equation (8)

\[
\mu_{j \rightarrow i}^{t}(\sigma_j(t)|\theta_j^{(i)}(t)) = \sum_{\sigma_j(0) \ldots \sigma_j(t-1)} \mu_{j \rightarrow i}(\sigma_j(0), \ldots, \sigma_j(t)|\theta_j^{(i)}(0), \ldots, \theta_j^{(i)}(t)). \tag{19}
\]

However due to the history of target vertex \(i\) the single-time message does not obey a Markovian process. Therefore one can only hope to proceed with this iterative procedure for a few initial time steps.
4.1. The dynamic cavity method in fully asymmetric networks

Fully asymmetric diluted Ising models where if spin $i$ connects to spin $j$ then spin $j$ does not connect back to spin $i$ have, as alluded to above, the simplifying property that influences (through interactions) do not return. Accordingly, the dynamic cavity models also simplify. In the model family considered here, $\epsilon = 0$ corresponds to the case where the probabilities of having two directed links between spin pairs are independent. For fixed connectivity, the possibility of having simultaneously two links between spin pairs can be neglected in the thermodynamic limit; this case can hence be assimilated to a fully asymmetric network. For the dynamic cavity messages we then have

$$
\mu_{k \rightarrow i}(\sigma_k(0), \ldots, \sigma_k(t) | \sigma_i(0), \ldots, \sigma_i(t)) = \mu_{k \rightarrow i}(\sigma_k(0), \ldots, \sigma_k(t)).
$$

(20)

In parallel update this property allows us to sum over all the history except the last time step from equations (15) and (19), resulting in

$$
\mu_t^{i \rightarrow j}(\sigma_i(t)) = \sum_{\sigma_{\partial j}(t-1)} \prod_{k \in \partial i} \mu_{k \rightarrow i}^{t-1}(\sigma_k(t-1)) w_i(\sigma_i(s) | h_i(s))
$$

(21)

where we have introduced $\mu_t^{i \rightarrow j}(\sigma_i(t))$ as the message sent from $i$ to $j$ at time step $t$. Despite the general non-Markovian dynamics of the marginalization to one time instance in the dynamic cavity, for parallel update the fully asymmetric case does follow a Markovian dynamics: at any time, the messages carry information from the incoming messages at only one time step before. Note that the resulting Markovian dynamics in this case is a consequence of update rule and asymmetry properties in the coupling interactions and is not necessarily restricted to the belief propagation approximation. The exact dynamics in the fully asymmetric case would follow a similar equation for the joint probability distribution in which at each time the information from one time step is required. However, computationally, this is unfeasible to study the evolution of a large set of coupled spins. The case of random sequential update is more delicate, and will be discussed separately [1].

We now consider the transition matrix to represent the Glauber dynamics

$$
w_i(\sigma_i(s) | h_i(s)) = \frac{e^{\beta h_i(s)} \sigma_i(s)}{2 \cosh(\beta h_i(s))}
$$

(22)

from which the single site magnetization under parallel updates follows:

$$
m_i(t) = \sum_{\sigma_{\partial i}(t-1)} \prod_{j \in \partial i} \mu_{j \rightarrow i}^{t-1}(\sigma_j(t-1)) \tanh \left[ \beta \left( \sum_{j \in \partial i} J_{ji} \sigma_j(t-1) + \theta_i \right) \right].
$$

(23)

Due to the particular form of the transition matrix in the Glauber dynamics (local normalization), the resulting dynamic BP equations in the fully asymmetric networks still require a summation over the whole configuration of neighboring vertices. Note that some more simplified transition matrices would provide us with an even more efficient BP approximation where the number of required summations scales linearly with the size of neighboring vertices [13].

As an interesting extension, the fully connected graphs with weak interactions can be realized by taking the limits $c \to N$ and $N \to \infty$. Since the interaction couplings are scaled with $1/c$ the variables become weakly connected in this limit and the graph statistically uncorrelated. Introducing $\delta h_i(t) = \sum_{j \in \partial i} (J_{ji}/c)(\sigma_j(t-1) - m_j(t-1))$ we can
expand the right-hand side around $\delta h_i$, considering the fluctuation of spins to be small with respect to their mean value at each time

$$m_i(t) = \tanh \left[ \beta \left( \sum_{j \in \partial i} \frac{J_{ji}}{c} m_j(t-1) + \theta_i \right) \right] + \mathcal{O}(c^{-2}). \quad (24)$$

To first order in $1/c$ we end up with the same equation for the naive mean-field approximation as the one introduced in [6] and to the second order in $1/c$ with the dynamic TAP approximation [14,25].

### 4.2. The dynamic cavity method and stationary states

In this subsection we introduce an approximation scheme for general (not fully asymmetric) networks assuming that the system is in a stationary state. The problem to be solved is the non-Markovian nature of the evolution of the single-spin single-time marginals (e.g. equation (19)) which follows from marginalization of the full dynamic cavity equations (15) and (17) over time. The approximation is that the dynamic cavity messages factorize over time:

$$\mu_{i \rightarrow j}(\sigma_i(0), \ldots, \sigma_i(t)|\sigma_j(0), \ldots, \sigma_j(t)) = \prod_{s=0}^{t} \mu_{i \rightarrow j}^t(\sigma_i(s)|\sigma_j(s-1)). \quad (25)$$

This time-factorization assumption is clearly not appropriate to describe transients, where we would expect both dependences between messages and that the functional form of the messages depends on time. However, in a stationary state it may be acceptable to take the messages independent in time, and it is reasonable to assume that the single-time messages do not depend explicitly on time. On the other hand, from the computational point of view, time factorization provides us with a closed set of equations for the single-time marginals, which makes the whole scheme computationally feasible:

$$\mu_{i \rightarrow j}^t(\sigma_i(t)) = \sum_{\sigma_i(t-2), \sigma_{i\setminus j}(t-1) \in \partial \vec{h}_i \setminus j} \prod_{k \in \partial \vec{h}_i \setminus j} \mu_{k \rightarrow i}^{t-1}(\sigma_k(t-1)|\sigma_i(t-2))$$

$$\times w_i(\sigma_i(s)|h_i^{(j)}(s)) \mu_{i \rightarrow j}^{t-2}(\sigma_i(t-2)). \quad (26)$$

In the above, for parallel updates, as treated in [22], the summation over time history results in $\mu_{i \rightarrow j}^{t-2}(\sigma_i(t-2))$. We refer to the appendix for the corresponding equations for sequential updates. Note that in this approximation the single-time dynamic cavity messages at time $t$ depend on messages sent at most two time steps earlier. For Ising spins, we can write the single-time dynamic cavity messages using cavity biases $\mu_{i \rightarrow j}^t(\sigma_i(t)) = (\beta u_{i \rightarrow j}(t) \sigma_i(t))/(2 \cosh(u_{i \rightarrow j}(t)))$, and inserting this equation into (26) we get an evolution equation for the cavity biases

$$u_{i \rightarrow j}(t) = \frac{1}{2\beta} \sum_{\sigma_i(t)} \frac{\sigma_i(t) \log \left( \sum_{\sigma_{i\setminus j}(t-1), \sigma_{i\setminus j}(t-2)} e^{\beta \left( \sum_{k \in \partial \vec{h}_i \setminus j} u_{k \rightarrow i} + J_{ik} \sigma_i(t-2) \right) \sigma_k(t-1)} \right)}{2 \cosh(\beta \sigma_i(t)) \cosh(\beta u_{i \rightarrow j}(t-2))}$$

$$\times \frac{e^{\beta h_i^{(j)}(t)} \sigma_i(t)}{2 \cosh(\beta h_i^{(j)}(t)) \cosh(\beta u_{i \rightarrow j}(t-2))}. \quad (27)$$

doi:10.1088/1742-5468/2011/04/P04014
supplemented by equation (16), i.e. \( h^{(i)}_j(t) = \sum_{k \in \partial_j \backslash i} (J_{kj}/c) \sigma_k(t - 1) + \theta_j(t) \) for the cavity fields. Solving for the stationary state of the kinetic Ising model using dynamic cavity equations in the time-factorized approximation hence means finding a fixed point of (27) and (16) when the external fields \( \vec{\theta} \) are independent in time. Note that \( \sigma_i(t - 2) \) contributes only when the edges from \( i \) to \( j \) and from \( j \) to \( i \) are both present. Therefore, in the fully asymmetric network this term disappears and we get back to equation (21).

On the other hand, for fully symmetric networks, as has been already pointed out in [22] and also in GFA analysis in [4], the ordinary belief propagation equation is a solution of the dynamic cavity equation in the time-factorized approximation. Indeed, it can be verified that equation (27) for \( c_{ij} J_{ij} = c_{ji} J_{ji} \) admits a solution of the form

\[
\begin{align*}
    u_{i \rightarrow j}(t) &= \theta_i + 1/\beta \sum_{k \in \partial_i \backslash j} \tanh(\beta J_{ki} \tanh(u_{k \rightarrow i}(t))) \\
    \sigma_i(t - 2) &= 2 \cosh(\beta u_{i \rightarrow j}(t - 2))
\end{align*}
\]

This is not expected to be accurate unless we are already in a stationary state, but will be used below in section 5 to monitor the approach to the stationary state.

5. Results

In this section we investigate the stationary states of diluted spin glass by the dynamic cavity approach in both parallel and sequential update. We show how the total magnetization of diluted Ising systems as computed by the dynamic cavity method evolves with time. In order to verify the results, we perform a numerical simulation (Monte Carlo) based on the appropriate dynamics.

5.1. BP versus Glauber dynamics

We first generate diluted graphs from random ensembles of sizes \( 10^3 \) and \( 10^4 \) using asymmetry and connectivity parameters as in equations (1) and (2). For each graph instance we iterate the dynamic cavity equations and simulate Monte Carlo analysis to test the accuracy of the dynamic cavity method. The system is initialized to a random configuration with small external fields acting on each individual variable. In Monte Carlo simulations, we generate up to 10,000 samples to estimate the time evolution of the magnetization at short time steps. We focus on the high-temperature regime to avoid the spin glass phase (for networks with symmetric interaction couplings, and presumably also for weakly asymmetric networks). Typical results for the time evolution of total magnetization \( m(t) = 1/N \sum_{i=1}^{N} m_i(t) \) under sequential updates are illustrated in figure 3. For short times, the dynamic cavity method differs significantly from Monte Carlo.
A message-passing scheme for non-equilibrium stationary states

Figure 3. Time evolution of the magnetization in a diluted network under the sequential update. The interactions are random variables from normal distribution, the connectivity parameter is fixed to $c = 3$ and simulations are performed for $\epsilon = 0, 0.5, 1$ and $\beta = 0.7, 2, 3$. A non-zero static external field $\theta_i = 0.01$ acts on each individual spin. Left panel: fully asymmetric network, middle panel: partially asymmetric with $\epsilon = 0.5$, right panel: a fully symmetric network. The symbols show the dynamic cavity method and the solid lines show the numerical simulations by Monte Carlo averaged over $10^4$ samples of the size $N = 1000$.

Figure 4. Left panel: the time evolution of the total magnetization at $\beta = 1$ for networks of size $N = 10^4$ with asymmetric and fully symmetric interactions. In all cases, a stationary solution according to dynamic BP exists which is consistent with numerical simulations. Right panel: the comparison between the fixed point of ordinary BP and the time evolution of the magnetization obtained by the dynamic cavity method for fully symmetric networks. The inverse temperature $\beta$ is chosen to be 1 and 2. In both cases, ordinary BP converges and the limit $D(t) \to 0$ exists. For lower $\beta$ a faster convergence of the dynamic cavity method is found.

Carlo, and also displays its own (unrelated) dynamics. For long times, however, the dynamic cavity reaches a fixed point, and this stationary state agrees well with Monte Carlo (for the magnetizations). The time needed for Monte Carlo to reach the stationary state grows with $\beta$ as can be seen from figure 3, while for the dynamic cavity in sequential update there is no such noticeable dependence except for the fully symmetric networks (right panel).

For parallel dynamics, the situation is more involved. For low enough $\beta$, again we have consistent results for the dynamic cavity and Monte Carlo simulations (figure 4, left panel). Note that the dynamic cavity method for a diluted fully asymmetric network in
A message-passing scheme for non-equilibrium stationary states

Figure 5. Dynamic cavity results for diluted spin glass systems in parallel update at low temperature. The interactions are random variables from the normal distribution, the system size is $N = 1000$ with an average connectivity $c = 3$. Left panel: the time evolution of the magnetization for $\epsilon = 0.5$ and $\beta = 4.5$ in the absence of external fields. It shows an oscillatory behavior even at long limit time (for non-fully asymmetric networks and low temperature). Right panel: the evolution of $\delta$ for a system size of $N = 1000$ after $t = 10^4$ steps and for $\epsilon = 0.2, 0.5, 1$. For fully asymmetric networks $\delta = 0$, showing the existence of a stable stationary state.

Parallel update is exact, and the lower curve of figure 4, left panel, gives a measure of the numerical fluctuations. In figure 4, right panel, we verify that for symmetric interactions and in low enough $\beta$, the solution for the dynamic cavity is also a solution of ordinary BP. Introducing $D(t) = 1/N \sum_{i=1}^{N} (m_i(t) - m_i^{(BP)})^2$, where $m_i^{(BP)}$ is the single magnetization obtained from output belief propagation (equilibrium), we expect to get a zero value for $D(t)$ by evolving the dynamic cavity during time. Figure 4, right panel, shows the evolution of $D(t)$ for $\beta = 1$ and 2. For both cases, ordinary BP converges to a fixed point and the dynamic cavity method predicts a stationary solution to the time dependent magnetization. For $\beta = 1$ a fast convergence for the dynamic cavity solution is observed to the total magnetization predicted by ordinary BP. Increasing $\beta$ (still in the phase where ordinary BP converges) would require longer relaxation time for constant results.

In the large $\beta$ limit, however, the system may fall into limit cycles with no stable stationary state. This can be observed by computing the total magnetization over long periods of time. In figure 5 the time evolution of the total magnetization in a fully symmetric network computed by the dynamic cavity is illustrated for $\beta = 4$ and 5. We observe that, even in the long time limit, the dynamics according to the cavity method does not approach a fixed solution but roughly oscillates between two states. Interestingly, for fully asymmetric networks we do not observe such cyclic behavior.

5.2. Cyclic stationary states

In order to study the cyclic behavior of stationary states in parallel update we introduce a time dependent quantity which measures the difference of total magnetizations in two successive time steps

$$\delta(t) = \frac{1}{N} \sum_{i=1}^{N} (m_i(t) - m_i(t-1))^2.$$  (29)
A zero value for $\delta(t)$ indicates the existence of a stationary state. On the other hand, non-zero $\delta(t)$, even after long times, means that either a stationary state does not exist, or is not reachable in finite time. Our results (from figure 5 and data not shown) are that cyclic behavior (of this type) is observed for parallel updates at sufficiently low temperature if the network is not fully asymmetric, but not for sequential updates. The strongest cyclic behavior belongs to fully symmetric networks. At fixed connectivity the amplitude of the oscillations tends to decrease with system size (data not shown).

6. Conclusion and discussion

In this paper we have studied stationary states of diluted asymmetric (kinetic) Ising models by the dynamic cavity method, both for parallel updates (as in [22] and [13]) and for sequential updates (new). We find that for many such systems with different asymmetry, sparseness and interaction strengths, the total magnetization computed by the dynamic cavity method matches direct numerical simulation (Monte Carlo)—at many orders of magnitude less computational effort.

Nothing, however, comes for free, and for all cases except a fully asymmetric network in parallel update, the dynamic cavity method presumably fails at low enough temperature. We observe (for the cases we have studied) different failure modes for different update rules, where for parallel updates the method simply no longer converges (no longer finds a stationary state), while for sequential updates the method converges to a fixed point, but which does not correspond to the stationary state found by direct simulation.

The full phase diagram of these models remains to be determined; we have, e.g., not verified that the dynamic cavity fails at low temperature for all models except fully asymmetric ones (although we expect that to be true). The comparison should also be made in a more detailed spin-by-spin manner, and extended at least to pairwise correlations. We intend to return to these topics in a future contribution.

The sequential update model is close to an asynchronous update model (continuous time), i.e. the master equation, as simulated, e.g., by the Gillespie algorithm. But at least for finite $N$, the two models are not identical, and the analysis carried out here should be extended to the master equation (if this is possible).

Finally, since kinetic Ising models have recently been used for inference and dynamic network reconstruction [23,24], and since ordinary BP has been used for inference in equilibrium systems [17], it would be interesting if the two strands could be combined.

Acknowledgments

We thank Dr Izaak Neri for interesting discussions and Institute of Theoretical Physics—Chinese Academy of Sciences (Beijing, China) for hospitality. The work was supported by the Academy of Finland as part of its Finland Distinguished Professor program, project 129024/Aurell.

Appendix

The dynamic cavity approach to the parallel update was first derived by Neri and Bolle in [22]. Here we show how it can be extended to sequential update. In the sequential

doi:10.1088/1742-5468/2011/04/P04014
A message-passing scheme for non-equilibrium stationary states

update we assume that at each time step, one single variable is selected randomly and will be updated according to equation (3). The time evolution of the probability distribution of all variables follows:

\[
p(\vec{\sigma}(0), \ldots, \vec{\sigma}(t)) = \prod_{s=1}^{t} W(\vec{\sigma}(s)|\vec{h}(s)) p(\vec{\sigma}(0))
\] (A.1)

where the transition probability contains the sequential update. The appropriate choice for the single variable update is the uniform probability distribution over all spins (see [3]):

\[
W(\vec{\sigma}(t)|\vec{h}(t)) = \frac{1}{N} \sum_{i=1}^{N} \left\{ \prod_{j \neq i} \delta_{\sigma_{j}(t),\sigma_{j}(t-\Delta t)} w_{i}(\sigma_{i}(t)|h_{i}(t)) \right\}.
\] (A.2)

Following the cavity graph argument discussed in section 4, the evolution of marginal probability follows:

\[
p_{i}(\sigma_{i}(0), \ldots, \sigma_{i}(t))
= \frac{1}{N} \sum_{\vec{\sigma}_{\setminus i}} \prod_{k \in \partial i} \mu_{k \rightarrow i}(\sigma_{k}(0), \ldots, \sigma_{k}(t-\Delta t)|\theta_{k}^{(i)}(0), \ldots, \theta_{k}^{(i)}(t-\Delta t)) \times \prod_{s=\Delta t}^{t} \sum_{j=1}^{N} \left\{ \prod_{k \neq j} \delta_{\sigma_{k}(s),\sigma_{k}(s-\Delta t)} w_{i}(\sigma_{j}(s)|h_{j}(s)) \right\} p_{i}(\sigma_{i}(0)).
\] (A.3)

The summation over variable update inside the formula will contribute in two terms: either the index \( j \) is equal to the cavity variable \( i \) or it is different. We can now introduce messages among neighboring variables carrying the marginal probability in the cavity graph. They fulfil the same recursive equation as parallel update:

\[
\mu_{i \rightarrow j}(\sigma_{i}(0), \ldots, \sigma_{i}(t)|\theta_{i}^{(j)}(0), \ldots, \theta_{i}^{(j)}(t))
= \sum_{\vec{\sigma}_{\setminus \setminus i,j}} \prod_{k \in \partial i \setminus j} \mu_{k \rightarrow i}(\sigma_{k}(0), \ldots, \sigma_{k}(t-\delta t)|\theta_{k}^{(i)}(0), \ldots, \theta_{k}^{(i)}(t-\Delta t)) \times \prod_{s=\Delta t}^{t} \frac{1}{N} \left[ w_{i}(\sigma_{i}(s)|h_{i}(s)) + (1 - \frac{1}{N}) \delta_{\sigma_{i}(s),\sigma_{i}(s-\Delta t)} \right] \mu_{i \rightarrow j}(\sigma_{i}(0))
\] (A.4)

which is equation (17) used in section 4 for the dynamic cavity in the sequential update. In the stationary state where the initial condition is assumed to be irrelevant we can perform the time-factorized approximation over the time evolution of messages. The time evolution of messages at each time \( t \) then simplifies following a Markovian dynamics of length two:

\[
\mu_{i \rightarrow j}^{t}(\sigma_{i}(t)|\theta_{i}^{(j)}(t)) = \frac{1}{N} \mu_{i \rightarrow j}^{t-\Delta t}(\sigma_{i}(t)|\theta_{i}^{(j)}(t-\Delta t)) + \left( 1 - \frac{1}{N} \right) \times \sum_{\sigma_{i}(t-2\Delta t),\vec{\sigma}_{\setminus \setminus i,j}(t-\Delta t)} \prod_{k \in \partial i \setminus j} \mu_{k \rightarrow i}^{t-\Delta t}(\sigma_{k}(t-\Delta t)|\theta_{i}^{(j)}(t-2\Delta t)) \times w_{i}(\sigma_{i}(t)|h_{i}(t)) \mu_{i \rightarrow j}^{t-2\Delta t}(\sigma_{i}(t-2\Delta t)).
\] (A.5)

doi:10.1088/1742-5468/2011/04/P04014
A message-passing scheme for non-equilibrium stationary states

References

[1] Aurell E and Mahmoudi H, 2011 arXiv:1104.0649
[2] Brunetti R, Parisi G and Ritort F, 1992 Phys. Rev. B 46 5339
[3] Coolen A C C, 2001 Statistical Mechanics of Recurrent Neural Networks II: Dynamics (Amsterdam: Elsevier) pp 597–662
[4] Coolen A C C, Laughton S N and Sherrington D, 1996 Phys. Rev. B 53 8184
[5] Crisanti A and Sompolinsky H, 1988 Phys. Rev. A 37 4865
[6] Derrida B, Gardner E and Zippelius A, 1987 Europhys. Lett. 4 167
[7] De Dominicis C, 1989 Phys. Rev. B 18 4913
[8] Hartmann A and Weigt M, 2005 Phase Transitions in Combinatorial Optimization Problems (Berlin: Wiley–VCH)
[9] Hatchett J P L, Castillo I P, Coolen A C C and Skantzos N S, 2005 Phys. Rev. Lett. 95 117204
[10] Hatchett J P L, Wemmenhove B, Pérez Castillo I, Nikoletopoulos T, Skantzos N S and Coolen A C C, 2004 J. Phys. A: Math. Gen. 37 6201
[11] Hertz J A, Roudi Y, Thorning A, Tyrcha J, Aurell E and Zeng H-Li, 2010 BMC Neurosci. 11 P51
[12] Hopfield J J, 1982 Proc. Nat. Acad. Sci. 79 2554
[13] Kanoria Y and Montanari A, 2009 arXiv:0907.0449
[14] Kappen H J and Spanjers J J, 2000 Phys. Rev. E 61 5658
[15] Kiemes M and Horner H, 2008 J. Phys. A: Math. Theor. 41 324017
[16] Mezard M and Montanari A, 2009 Information, Physics, and Computation (Oxford: Oxford University Press)
[17] Mezard M and Mora T, 2009 J. Physiol. Paris 103 107
[18] Mézard M and Parisi G, 2001 Eur. Phys. J. B 20 217
[19] Mozeika A and Coolen A C C, 2008 J. Phys. A: Math. Theor. 41 115003
[20] Mozeika A and Coolen A C C, 2009 J. Phys. A: Math. Theor. 42 195006
[21] Mimura K and Coolen A C C, 2009 J. Phys. A: Math. Theor. 42 415001
[22] Neri I and Bollé D, 2009 J. Stat. Mech. P08009
[23] Roudi Y, Aurell E and Hertz J A, 2009 Front. Comput. Neurosci. 3 22
[24] Roudi Y and Hertz J A, 2010 Phys. Rev. Lett. 106 048702
[25] Roudi Y and Hertz J A, 2010 arXiv:1103.1044
[26] Semerjian G and Weigt M, 2004 J. Phys. A: Math. Gen. 37 5525
[27] Sommers H J, 1987 Phys. Rev. Lett. 58 1268
[28] Sompolinsky H and Zippelius A, 1982 Phys. Rev. B 25 6860
[29] Wang L P, Pichler E E and Ross J, 1990 Proc. Nat. Acad. Sci. 87 9467
[30] Yedidia J S, Freeman W T and Weiss Y, 2001 Advances in Neural Information Processing Systems (Cambridge, MA: MIT Press) p 689
[31] Zeng H-Li, Aurell E, Alava M and Mahmoudi H, 2010 arXiv:1011.6216

doi:10.1088/1742-5468/2011/04/P04014