Dynamical TAP equations for non-equilibrium Ising spin glasses

Yasser Roudi\textsuperscript{1,2} and John Hertz\textsuperscript{1,3}

\textsuperscript{1} Nordita, SE-106 91 Stockholm, Sweden
\textsuperscript{2} Kavli Institute for Systems Neuroscience, NTNU, N-7010 Trondheim, Norway
\textsuperscript{3} The Niels Bohr Institute, DK-2100 Copenhagen, Denmark
E-mail: yasser@nordita.org and hertz@nordita.org

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Abstract. We derive and study dynamical TAP equations for Ising spin glasses obeying both synchronous and asynchronous dynamics using a generating functional approach. The system can have an asymmetric coupling matrix and the external fields can be time-dependent. In the synchronously updated model, the TAP equations take the form of self-consistent equations for magnetizations at time $t+1$, given the magnetizations at time $t$. In the asynchronously updated model, the TAP equations determine the time derivatives of the magnetizations at each time, again via self-consistent equations, given the current values of the magnetizations.

Keywords: disordered systems (theory), spin glasses (theory), stochastic processes (theory)
1. Introduction

Within the mean-field approximation, spin models with quenched disorder can be studied by analyzing their quenched averaged behavior or, alternatively, for a specific realization of the quenched disorder [1]. In the equilibrium case, the former type of analysis includes the replica method, while the latter one is usually formulated as naive mean-field, TAP equations [2] or, more generally, a Plefka expansion [3]. These equations can be derived by calculating the free energy in a high temperature (weak coupling) expansion, with the first-order calculation giving the mean-field free energy, the second order the TAP free energy and so on. For non-equilibrium and kinetic spin glass models, soft spin systems were the first ones to be analyzed, using the Martin–Siggia–Rose generating functional formalism [4]. Spin glass models with hard spins were first treated in [5–7]. A powerful generating functional approach was then developed by Coolen and collaborators [8,9] and it forms the basis of our analysis here; see also [10,11] for reviews of the techniques used in both soft and hard spin models. However, dynamical TAP equations to describe the kinetics of order parameters for a specific realization of the disorder have only been derived for the spherical p-spin model [12] and the stationary state of the Ising spin model with asynchronous update dynamics [13].

In the same way that studying the quenched averaged kinetics of hard spin models usually involves a different approach compared to soft spin models, deriving the dynamical TAP equations for hard spin models is somewhat different from doing so for their soft spin counterparts. The aim of this paper is to develop a dynamical mean-field theory that
relates the dynamics of mean magnetizations, potentially time-varying external fields and the quenched couplings for two kinetic versions of the Sherrington–Kirkpatrick model, one with synchronous update, the other with asynchronous update. Using a generating functional approach, we derive the dynamical naive mean-field and TAP equations as first and second orders of a high temperature expansion, similar to the equilibrium case for these two kinetic models.

In addition to the technical issues, the recent use of hard spin models with discrete states, e.g. Potts and Ising models [14]–[17], in reconstructing the connectivity of biological networks encourages the study of the dynamics of these models in more detail. Once the forward dynamics is described, it is possible to use the results to construct approximations at the corresponding levels for the inverse problem: finding the couplings, given the magnetizations and correlation functions. In this way, one can develop effective approximate reconstruction techniques that exploit the temporal structure of data and significantly improve the quality of network reconstruction in biological systems. In fact, the results of this paper have been recently used in two other recent papers on the inverse problem [18,19].

This paper is organized as follows. After defining the dynamical models in the following section, we derive dynamical naive mean-field equations using the generating functional for the synchronous updated model. We report the TAP equations, for which the details of the derivations are reported in the appendices. We then numerically calculate the errors for these kinetic equations as a function of the strength of the couplings for the synchronous dynamics.

2. Dynamical model

We consider a system of $N$ Ising spins $s_i = \pm 1, i = 1, \cdots, N$ and assume that its state at time $t$, $s(t) = \{s_1(t), \ldots, s_N(t)\}$, follows one of the following dynamics:

(i) Synchronous dynamics. In this case time is discretized and the probability of being in state $s$ at time step $t$, $p_t(s)$, is given by

$$p_t(s) = \sum_{s'} W_t[s; s'] p_{t-1}(s')$$

(1a)

$$W_t[s; s'] = \prod_i \frac{\exp(s_i \theta_i(t-1))}{2 \cosh(\theta_i(t-1))}$$

(1b)

$$\theta_i(t) = h_i(t) + \sum_j J_{ij} s_j(t).$$

(1c)

This is, in other words, a Markov chain with transition probability $W_t$.

(ii) Asynchronous dynamics. In this case time is continuous and, $p_t(s)$ satisfies the following equation:

$$\frac{d}{dt} p_t(s) = \sum_i [p_t(F_i s) w_i(F_i s; t) - p_t(s) w_i(s; t)]$$

(2a)

$$w_i(s; t) = \frac{1}{2} [1 - s_i \tanh(\theta_i(s; t))]$$

(2b)

where the operator $F_i$ acting on $s$ flips its $i$th spin.
For each of these processes one can define a generating functional. For the synchronous case it takes the form of

\[ Z[\psi, h] = \exp \left\{ \sum_{i,t} \psi_i(t)s_i(t) \right\}, \]  

(3)

where for any quantity \( A \) defined as a function of a path \((s(T), \ldots, s(0))\), \( \langle \cdots \rangle \) indicates averaging over the paths taken by \( s(t) \) under the stochastic dynamics of equations (1a)–(1c), i.e.

\[ \langle A \rangle = \text{Tr} \ W_{T-1}[s(T); s(T-1)] \cdots W_0[s(1); s(0)] \ p_0(s(0)) \ A(s(T), \ldots, s(0)), \] 

(4)

and

\[ \text{Tr} \equiv \sum_{s(T)} \sum_{s(T-1)} \cdots \sum_{s(0)}. \]  

(5)

The asynchronous case is similar except that the sum over \( t \) in equation (3) should be replaced by an integration; see appendix B.

It is useful to rewrite the generating functional by considering \( \theta_i(t) \) for each spin and each time step as a free parameter, integrate over it and make sure that the definition equation (1c) is satisfied by inserting an appropriate delta function. This yields

\[ Z[\psi, h] = \int D\theta \exp \left\{ \sum_{i,t} \theta_i(t) s_i(t) \right\} \prod_{i,t} \delta \left( \theta_i(t) - h_i(t) - \sum_j J_{ij} s_j(t) \right) \left\{ \theta_i(t) - h_i(t) - \sum_j J_{ij} s_j(t) \right\} \]  

(6)

where \( D\theta = \prod_{i,t} d\theta_i(t) \) and \( D\theta \hat{\theta} = \prod_{i,t}(1/2\pi) d\theta_i(t) d\hat{\theta}_i(t) \). Using equation (4) in equation (6), we get

\[ Z_\alpha[\psi, h] = \int D\theta \hat{\theta} \ \text{Tr} \exp[L_\alpha] \]  

(7a)

\[ L_\alpha = \sum_{i,t} \left\{ i\hat{\theta}_i(t) \left( \theta_i(t) - \alpha \sum_j J_{ij} s_j(t) \right) + s_i(t+1)h_i(t) - \log \cosh \theta_i(t) \right\} \]  

(7b)

where the parameter \( \alpha \) is introduced to control the magnitude of the couplings, as will become clear later.

The generating functional has the property that its derivatives with respect to \( \psi \) and \( h \) give the averages of the correlators involving the spins and auxiliary fields. In particular, defining

\[ \langle A \rangle_\alpha = \frac{\int D\theta \hat{\theta} \ \text{Tr} \ A \exp[L_\alpha]}{\int D\theta \hat{\theta} \ \text{Tr} \exp[L_\alpha]}, \] 

(8)

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and using equations (7a) and (7b), we can define \( m_i(t) \) and \( \dot{m}_i(t) \) as

\[
-i\dot{m}_i(t) \equiv \frac{\partial \log Z}{\partial h_i(t)} = -i\langle \dot{\theta}_i(t) \rangle_\alpha \quad (9a)
\]

\[
m_i(t) \equiv \frac{\partial \log Z}{\partial \psi_i(t)} = \langle s_i(t) \rangle_\alpha. \quad (9b)
\]

From equation (6), we can see that the \( \psi \to 0 \) limit of \( \dot{m}_i(t) \) is the expected value of the auxiliary field \( \dot{\theta}_i(t) \) under the measure inside the integral of equation (6). It is easy to show that this average, similar to the soft spin case, is zero. The same limit for \( m_i(t) \) give us the mean magnetizations. We therefore have

\[
\langle \dot{\theta}_i(t) \rangle = \lim_{\psi \to 0} \dot{m}_i(t) = 0 \quad (10)
\]

\[
\langle s_i(t) \rangle = \lim_{\psi \to 0} m_i(t). \quad (11)
\]

For a detailed discussion about these and other dynamical processes on Ising spin models see [11].

To derive the dynamical mean-field and TAP equations, one first calculates the Legendre transform of the logarithm of the generating functional of the process defined by equations (1a)–(1c). In this dynamical case, the logarithm of the generating functional plays the role of the Helmholtz free energy in the equilibrium statistical mechanics while its Legendre transform corresponds to the Gibbs free energy. One then expands this dynamical Gibbs free energy around the zero coupling limit, similarly to the equilibrium case [3] and the soft spin model [12]. In the following, we do this for Ising spins up to linear order in the couplings for the synchronous update and use it to derive the dynamical mean-field equations. The details of how to proceed to the TAP for the synchronous and asynchronous dynamics are provided in the appendices.

3. Outline of the derivation of the dynamical equations

The Legendre transform of the logarithm of the generating functional with respect to the real fields, \( h_i \), and the auxiliary fields, \( \psi_i \), is

\[
\Gamma[\hat{m}, m] \equiv \log Z[\psi[\hat{m}, m], h[\hat{m}, m]] - \sum_{i,t} \psi_i[\hat{m}, m](t) m_i(t) + i \sum_{i,t} h_i[\hat{m}, m](t) \dot{m}_i(t), \quad (12)
\]

where \( \psi \) and \( h \) are now treated as functions of \( \hat{m} \) and \( m \) through the following equalities:

\[
\frac{\partial \Gamma}{\partial m_i(t)} = -\psi_i[\hat{m}, m](t) \quad (13a)
\]

\[
\frac{\partial \Gamma}{\partial \dot{m}_i(t)} = ih_i[\hat{m}, m](t). \quad (13b)
\]
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Equations (13a) and (13b) together with the definition of $\Gamma_\alpha$ in equation (12) imply equations (9a) and (9b). Using equation (12) in equation (7), $\Gamma_\alpha$ can also be written as

$$
\Gamma_\alpha[\hat{m}, m] = \log \int D\theta \text{Tr} e^{\Omega_\alpha}
$$

(14a)

$$
\Omega_\alpha = \sum_{i,t} \left\{ i\dot{\theta}_i(t) \left[ \theta_i(t) - \alpha \sum_j J_{ij} s_j(t) \right] + s_i(t+1)\theta_i(t) - \log \cosh(\theta_i(t)) 
- i\dot{\theta}_i(t)[\hat{\theta}_i(t) - \hat{m}_i(t)] + \psi_i(t)[s_i(t) - m_i(s)] \right\}.
$$

(14b)

The idea now is that for $\alpha = 0$ the generating functional and its Legendre transform can be easily calculated, as the spins will be independent of each other. For the generating functional we have

$$
Z_0[\psi, h] = \prod_i \prod_{t=1}^T \frac{2 \cosh[h_i(t-1) + \psi_i(t)]}{2 \cosh(h_i(t-1))},
$$

and for the Legendre transform of $\log Z_0$ we have

$$
\Gamma_0[\hat{m}, m] = \sum_{i,t} \left[ \log(2 \cosh(h_i^0(t) + \psi_i^0(t+1)) - \log 2 \cosh(h_i^0(t)) 
- \psi_i^0(t)m_i(t) + i\dot{h}_i^0(t)\hat{m}_i(t) \right],
$$

(16)

where $h^0$ and $\psi^0$ are the real and auxiliary fields for which equations (9a) and (9b) are satisfied for given $m$ and $\hat{m}$ at zero coupling ($\alpha = 0$), i.e.

$$
m_i(t) = \tanh[h_i^0(t-1) + \psi_i^0(t)]
$$

(17a)

$$
-\dot{m}_i(t) = \tanh[h_i^0(t) + \psi_i^0(t+1)] - \tanh[h_i^0(t)].
$$

(17b)

This can be used to express $h^0$ and $\psi^0$ in terms of $m$ and $\hat{m}$ as

$$
h_i^0(t) = \tanh^{-1} M_i(t)
$$

(18a)

$$
\psi_i^0(t) = \tanh^{-1} m_i(t) - \tanh^{-1} M_i(t-1),
$$

(18b)

where $M_i(t) = m_i(t+1) + i\dot{m}_i(t)$.

To calculate the integral on the right-hand side of equation (14a) for $\alpha = 1$, we can expand $\Gamma_\alpha$ around $\alpha = 0$ and eventually set $\alpha = 1$. Using the fact that

$$
\frac{\int D\theta \text{Tr} A \exp[\Omega_\alpha]}{\int D\theta \text{Tr} \exp[\Omega_\alpha]} = \frac{\int D\theta \text{Tr} A \exp[L_\alpha]}{\int D\theta \text{Tr} \exp[L_\alpha]} = \langle A \rangle_\alpha,
$$

(19)

for the first derivative of $\Gamma_\alpha$ with respect to $\alpha$ we have

$$
\frac{\partial \Gamma_\alpha}{\partial \alpha} = \left\langle \frac{\partial \Omega_\alpha}{\partial \alpha} \right\rangle_\alpha.
$$

(20)

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yielding
\[ \frac{\partial \Gamma_\alpha}{\partial \alpha} = -i \sum_{ij,t} J_{ij} \langle \hat{\psi}_i(t)s_j(t) \rangle_\alpha - i \sum_{i,t} \frac{\partial h_i^\alpha(t)}{\partial \alpha} \langle [\hat{\theta}_i(t) - \hat{m}_i(t)] \rangle_\alpha \]
\[ + \sum_{i,t} \frac{\partial \psi_i^\alpha(t)}{\partial \alpha} \langle [s_i(t) - m_i(t)] \rangle_\alpha. \]  
(21)

The last two terms in equation (21) are zero because of equations (9a) and (9b); hence
\[ \frac{\partial \Gamma_\alpha}{\partial \alpha} = -i \sum_{ij,t} J_{ij} \langle \hat{\psi}_i(t)s_j(t) \rangle_\alpha. \]  
(22)

The correlation function \( \langle \hat{\psi}_i(t)s_j(t) \rangle_\alpha \) can also be easily calculated at \( \alpha = 0 \) yielding
\[ -i\langle \hat{\psi}_i(t)s_j(t) \rangle_0 = \frac{1}{Z_0} \frac{\partial^2 Z_0}{\partial h_i(t) \partial \psi_j(t)} = (\tanh[h_i^0(t) + \psi_j^0(t + 1)] - \tanh[h_i^0(t)]) \tanh[h_i^0(t - 1) + \psi_j^0(t)], = -i\hat{m}_i(t)m_j(t) \]  
(23)

where the last equality follows from equations (17a) and (17b). Consequently, to first order in \( \alpha \), we have
\[ \Gamma_\alpha[\hat{m}, m] = \sum_{i,t} [\log 2 \cosh(h_i^0(t - 1) + \psi_j^0(t))] - 2 \cosh(h_i^0(t))] \]
\[ - \sum_{i,t} \psi_i^0(t)m_i(t) + \sum_{i,t} i h_i^0(t)\hat{m}_i(t) - i\alpha \sum_{i,j,t} J_{ij}\hat{m}_i(t)m_j(t) \]  
(24)

which, combined with equations (18a) and (18b), gives
\[ \Gamma_\alpha[\hat{m}, m] = -\frac{1}{2} \sum_{i,t} \left\{ \log \left[ \frac{1 + m_i(t)}{2} \right] + \log \left[ \frac{1 - m_i(t)}{2} \right] \right\} \]
\[ + \frac{1}{2} \sum_{i,t} \left\{ \log \left[ \frac{1 + M_i(t)}{2} \right] + \log \left[ \frac{1 - M_i(t)}{2} \right] \right\} \]
\[ - \sum_{i,t} m_i(t) \tanh^{-1}[m_i(t)] + \sum_{i,t} M_i(t) \tanh^{-1}[M_i(t)] - i\alpha \sum_{i,j,t} J_{ij}\hat{m}_i(t)m_j(t) \]
\[ + O(\alpha^2). \]  
(25)

Using equation (13b) yields
\[ \tanh^{-1} M_i(t) = h_i(t - 1) + \sum_{j} J_{ij} m_j(t - 1). \]  
(26)

In the limit \( \psi \to 0 \) for which equation (11) is satisfied, we have
\[ m_i(t + 1) = \tanh \left( h_i(t) + \sum_{j} J_{ij}m_j(t) \right). \]  
(27)

This is the dynamical (naive) mean-field equation for the evolution of the mean magnetization. The TAP equations can be derived in a similar way by expanding \( \Gamma_\alpha \).
to second order in $\alpha$, as shown in appendix A. This yields the dynamical TAP equations

$$m_i(t + 1) = \tanh \left[ h_i(t) + \sum_j J_{ij} m_j(t) - m_i(t + 1) \sum_j J_{ij}^2 [1 - m_j(t)^2] \right].$$

(28)

To find the time-evolving magnetizations for a given external field and coupling within the TAP approximation, the above equation should be solved self-consistently for $m_i(t + 1)$ at each time step. Note the form of the Onsager correction (the last term in equation (28)). The $(1 - m_j^2)$ term is evaluated at time step $t_0$, but $m_i$ is evaluated at time step $t + 1$. Thus (28) is a set of equations to be solved for $m_i(t + 1)$, not just a simple expression for $m_i(t + 1)$ in terms of the $m_j(t)$, as in naive mean-field theory.

The derivations of dynamical naive mean-field and TAP equations for the case of asynchronous dynamics defined in equations (2a) and (2b) are given in appendix B. As shown there, these equations are

$$m_i(t) + \frac{dm_i(t)}{dt} = \tanh \left[ h_i(t) + \sum_j J_{ij} m_j(t) \right]$$

(29)

$$m_i(t) + \frac{dm_i(t)}{dt} = \tanh \left[ h_i(t) + \sum_j J_{ij} m_j(t) - \left( m_i(t) + \frac{dm_i(t)}{dt} \right) \sum_j J_{ij}^2 (1 - m_j^2(t)) \right].$$

(30)

4. Numerical results

To test the dynamical naive mean-field (hereafter: nMF) and TAP equations (27) and (28), we ran simulations in which we simulated the process defined by (1a) and (1c) for $L$ time steps, for couplings drawn from a zero mean Gaussian distribution with variance $g^2/N$ ($J_{ij}$ drawn independent of $J_{ji}$) and subjected to two alternative types of external field. One was a temporally constant field with a magnitude drawn independently for each spin from a zero mean, unit variance Gaussian distribution. The other was a sinusoidally varying external field. For each sample of $J$s and the fields, we generated data from the system for $r$ repeats, calculated $m_i(t)$ from these repeats and used it in (27) and (28) to predict $m_i(t + 1)$. Finally, we calculated the mean squared errors of these predicted values:

$$\text{MSE}^{\text{nMF/TAP}} = \frac{1}{LN} \sum_{i=1}^N \sum_{t=1}^L [m_i^{\text{nMF/TAP}}(t + 1) - m_i(t)]^2.$$  

(31)

The results for the two external fields used are shown below.

4.1. Uniform field

Figure 1(A) shows the dependence of the error for predicting the magnetizations at time $t + 1$, given the measured magnetizations at $t$. Both TAP and nMF errors increase as $g$ increases, but the error of nMF is always larger than that of TAP. Furthermore, how close to the true ($r \to \infty$) values the measured magnetizations are systematically affects the
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Figure 1. (A) The effect of magnitude of the couplings, $g$, on the error of TAP and nMF in predicting the magnetization at $t + 1$ given the measured magnetizations at $t$ using $r$ runs. (B) The effect of the number of runs, $r$, on the error of TAP (red) and nMF (blue), for $N = 10$ (full curve) and $N = 50$ (dashed), and $g = 0.3$. All errors are averages over 25 samples of the system. The error bars show the standard deviation of these samples. (C) and (D) The same as (A) and (B) but for a sinusoidal field.

nMF and TAP predictions: increasing $r$ decreases the errors for all $g$. This can also be seen in figure 1(B), where the errors at $g = 0.3$ are shown as functions of $r$, also for two different values of $N$.

4.2. Sinusoidal field

Figures 1(C) and (D) show the same thing as figures 1(A) and (B), but now the system is subjected to a sinusoidal external field with a peak amplitude of 0.1 and a period of 20 time steps. The results are qualitatively the same. For this case, we also look at the time dependence of the errors in TAP and nMF equations.

Figure 2 shows the time-dependent error (i.e. the right-hand side of equation (31) without averaging over time) versus time. For weak coupling, the errors of both nMF and
TAP are very small. At intermediate values of $g$, the error of nMF is still comparable to TAP, but fluctuating. At yet stronger couplings, the nMF prediction very rapidly becomes different from the actual measured values of the magnetizations.

5. Discussion

The TAP approach, formulated as a high temperature Taylor series expansion of the equilibrium Gibbs free energy [3], is a powerful method for studying equilibrium spin glass models. Similarly, dynamical TAP equations allow analyzing the dynamics of a single sample of a disordered system away from equilibrium. In this paper, we derived these equations for Ising spin glasses with both synchronous and asynchronous updates. The main idea behind the derivation is similar to the one used by Biroli [12] for the soft p-spin model obeying a Langevin equation, with the difference that, instead of an MSR formalism, we had to use the generating functional approach of Coolen. For the p-spin model the spherical condition results in the appearance of the autocorrelation, $\langle s_i(t)s_i(t') \rangle$, and response functions as order parameters in dynamical TAP. For the hard spin Ising model, this is not the case. The response function can, of course, be directly calculated from its definition and the TAP equations, but calculating a correlation, $\langle s_i(t)s_j(t') \rangle$, function requires a different approach.

The derivation does not rely on the symmetry of the couplings and can, therefore, be applied to systems without detailed balance. For the stationary case, the TAP equations are identical to those derived for the equilibrium model with symmetric connections. This has been previously shown by Kappen and Spanjer [13] using an information geometric
derivation for the stationary state of the asynchronously updated model. Numerical simulations with both a constant external field and a rapidly evolving one show that the TAP equations, at high temperature, predict the dynamics of the individual site magnetizations very well. This may not be surprising given the fact that the model we studied here was a kinetic variant of the SK model for which the equilibrium TAP equations provide the exact picture.

It is intriguing that the Onsager term in equations (28) and (30) does not get the form $J_{ij}J_{ji}(1 - m_j^2)$, as would be expected from a simple reaction argument. This observation has also been made earlier by Kappen and Spanjers [13]. A naive argument showing that the true correction to the mean-field equations is of the type $J_{ij}^2(1 - m_j^2)$ follows.

Starting from the exact equation

$$m_i(t + 1) = \left\langle \tanh \left[ h_i(t) + \sum_j J_{ij} s_j(t) \right] \right\rangle,$$

we expand tanh around $b_i(t) = h_i(t) + \sum_j J_{ij} m_j(t)$ to quadratic order in $\sum_j J_{ij} \delta s_j(t)$, where $\delta s_j(t) = s_i(t) - m_i(t)$. The linear term vanishes, and using $\langle [\delta s_j(t)]^2 \rangle = 1 - m_j^2(t)$ we have

$$m_i(t + 1) = \tanh[b_i(t)] - (1 - \tanh^2[b_i(t)]) \tanh[b_i(t)] \left\langle \left[ \sum_j J_{ij} \delta s_j(t) \right]^2 \right\rangle$$

$$= \tanh[b_i(t)] - (1 - \tanh^2[b_i(t)]) m_i(t + 1) \sum_j J_{ij}^2(1 - m_j^2(t))$$

$$= \tanh \left[ h_i(t) + \sum_j J_{ij} m_j(t) - m_i(t + 1) \sum_j J_{ij}^2(1 - m_j^2(t)) \right]$$

where in the second line we have used the mean-field equation $m_i(t + 1) \approx \tanh(b_i(t))$.

An important issue that we have left out in this paper is the expected number of solutions to the TAP equations for arbitrary couplings. It has been known for a long time that, at low temperature, the expected number of solutions of the TAP equations for the SK model with symmetric couplings is exponential in $N$ [20]. It is also possible to calculate the number of metastable states for couplings with an antisymmetric component at zero temperature [7]. The TAP equations presented here allow extending the calculation in [20] to the type of couplings considered in [7] for non-zero temperatures. This calculation will be presented elsewhere.

The equilibrium TAP equations, derived for spin glass models with symmetric couplings, can be used in deriving efficient approximations for solving the inverse problem of reconstructing a spin glass model from samples of its states [21, 22]. As has been recently shown [18, 19], the dynamical equations derived here can be employed for taking the reconstruction to a more powerful level, allowing for the reconstruction of systems outside equilibrium.

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Appendix A. TAP equations for synchronous update

For deriving the TAP equations, we note that

\[
\frac{\partial^2 \Gamma_\alpha}{\partial \alpha^2} = \left\langle \left[ \frac{\partial^2 \Omega}{\partial \alpha^2} \right]_\alpha \right\rangle - \left\langle \left[ \frac{\partial \Omega}{\partial \alpha} \right]_\alpha \right\rangle^2. \quad (A.1)
\]

The first term on the right-hand side of the above equation is equal to zero. To calculate the next two terms, we use the Maxwell equations

\[
i \frac{\partial h_\alpha^\alpha(t)}{\partial \alpha} = -i \sum_j J_{ij} m_j(t) \quad (A.2a)
\]

\[
\frac{\partial \psi_\alpha^\alpha(t)}{\partial \alpha} = i \sum_j m_j(t) J_{ji} \quad (A.2b)
\]

to write

\[
\frac{\partial \Omega}{\partial \alpha} = -i \sum_{ij} J_{ij} \dot{\theta}_i(t) s_j(t) + i \sum_{ij} J_{ij} [\dot{\theta}_i(t) - \dot{m}_i(t)] m_j(t)
\]

\[
+ i \sum_{ij} J_{ji} [s_i(t) - m_i(t)] \dot{m}_j(t). \quad (A.3)
\]

We are therefore interested in calculating

\[
\frac{\partial^2 \Gamma_\alpha}{\partial \alpha^2} = \left\langle \left[ \delta \left( \frac{\partial \Omega}{\partial \alpha} \right) \right]^2 \right\rangle_\alpha = \left\langle \left( \frac{\partial \Omega}{\partial \alpha} - \left\langle \frac{\partial \Omega}{\partial \alpha} \right\rangle_\alpha \right)^2 \right\rangle_\alpha. \quad (A.4)
\]

where

\[
\delta \left( \frac{\partial \Omega}{\partial \alpha} \right) = -i \sum_{ij} \dot{\theta}_i(t) J_{ij} s_j(t) + i \sum_{ij} \delta \dot{\theta}_i(t) J_{ij} m_j(t)
\]

\[
+ i \sum_{ij} \dot{m}_i(t) J_{ij} \delta s_j(t) + i \sum_{ij} \dot{m}_i(t) J_{ji} m_j(t). \quad (A.5)
\]

Defining \( \delta s_j(t) = s_j(t) - m_j(t) \) and \( \delta \dot{\theta}_i(t) = \dot{\theta}_i(t) - \dot{m}_i(t) \), this can be rearranged into the following form:

\[
\delta \left( \frac{\partial \Omega}{\partial \alpha} \right) = -i \sum_{ij} \delta \dot{\theta}_i(t) J_{ij} \delta s_j(t). \quad (A.6)
\]

Now it is simple to evaluate equation (A.4):

\[
\left\langle \left[ \delta \left( \frac{\partial \Omega}{\partial \alpha} \right) \right]^2 \right\rangle_\alpha = - \sum_{ijj'j''} \langle \delta \dot{\theta}_i(t) J_{ij} \delta s_j(t) \delta \dot{\theta}_{i'}(t') J_{i'j'} \delta s_{j'}(t') \rangle_\alpha. \quad (A.7)
\]

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The factors have to be paired and for the pair averages we use

\[ \langle (-i \delta \hat{\theta}_i(t))^2 \rangle_\alpha = \frac{\partial \log Z_0}{\partial h_i(t)^2} = -\hat{m}_i^2(t) + 2i\hat{m}_i(t)m_i(t+1) \] (A.8a)

\[ \langle -i \delta \hat{\theta}_i(t-1)\delta s_i(t) \rangle_\alpha = \frac{\partial \log Z_0}{\partial h_i(t-1)\partial \psi_i(t)} = 1 - m_i^2(t) \] (A.8b)

\[ \langle \delta s_i(t)^2 \rangle_\alpha = \frac{\partial \log Z_0}{\partial \psi_i(t)^2} = 1 - m_i^2(t). \] (A.8c)

The terms containing products of two averages of the form \( \langle \delta \hat{\theta} \delta s \rangle \) vanish, because one pair factor has to have \( t' = t - 1 \) and the other has to have \( t = t' - 1 \), which cannot be satisfied simultaneously. This leaves

\[ \left\langle \left[ \delta \left( \frac{\partial \Omega}{\partial \alpha} \right) \right]^2 \right\rangle_0 = -\sum_{ijj't} \langle \langle \delta \hat{\theta}_i(t) \rangle \rangle_0 J_{ij} J_{i'j'} \langle \delta s_j(t) \delta s_{j'}(t) \rangle_0 \]

\[ = \sum_{ijt} [-\hat{m}_i^2(t) + 2i\hat{m}_i(t)m_i(t+1)]J_{ij}^2 [1 - m_j^2(t)]. \] (A.9)

Using this to calculate \( \Gamma_\alpha \) to the quadratic order in \( \alpha \), differentiating with respect to \( \hat{m}_j(t) \), and setting \( \hat{m}_j = 0 \) yields the dynamical TAP equations (28).

**Appendix B. Asynchronous dynamics**

In the asynchronous case the generating functional takes the form

\[ Z_\alpha[\psi, h] = \int D\theta D\hat{\theta} \prod_i \left\langle \exp \left[ i \int dt \hat{\theta}_i(t) [\theta_i(t) - h_i(t) - \alpha \sum_j J_{ij} s_j(t)] \right. \right. \]

\[ \left. \left. + \int dt \psi_i(t) s_i(t) \right] \right\rangle \] (B.1)

and \( \langle \cdot \cdot \cdot \rangle \) now indicates averaging with respect to the distribution defined by the solution to the differential equation (2a). This solution can be written as

\[ p_t(s) = \prod_i \left[ \frac{1 + \mu_i(t)}{2} \delta_{s_i(t), 1} + \frac{1 + \mu_i(t)}{2} \delta_{s_i(t), -1} \right] \] (B.2a)

\[ \frac{d\mu_i}{dt} = -\mu_i + \tanh(\theta_i(t)), \quad \mu_i(0) = s_i(0). \] (B.2b)

The solution to equation (B.2b) can be written as

\[ \mu_i(t) = \int_0^t dt' e^{t' - t} \tanh(\theta_i(t')) + e^{-t} \mu_i(0). \] (B.3)
The dynamical Gibbs free energy (i.e. the Legendre transform of the log generating functional) is then
\[
\Gamma_\alpha[\hat{m}, m] = \log \int D\theta \prod_i \left< \exp \left[ i \int dt \hat{\theta}_i(t) [\theta_i(t) - h_i(t) \right] \right> - \alpha \sum_i J_{ij} s_j(t) + \int dt \psi_i(t) s_i(t) \right> + i \sum_i \int dt h_i(t) \hat{m}_i(t) - \sum_i \int dt \psi_i(t) m_i(t). \tag{B.4}
\]

**B.1. nMF for asynchronous update**

As we did for the synchronous case, we first calculate the non-interacting (\(\alpha = 0\)) generating functional:
\[
\log Z_0 = \sum_i \int dt \log[cosh(\psi_i(t)) + \mu_i^0(t) \sinh(\psi_i(t))] \tag{B.5a}
\]
\[
\mu_i^0(t) = \int_0^t dt' e^{t-t'} \tanh(h_i^0(t')) + e^{-t} \mu_i(0) \tag{B.5b}
\]
and
\[
\Gamma_0[\hat{m}, m] = \sum_i \int dt \left< \log[cosh(\psi_i^0(t)) + \mu_i^0(t) \sinh(\psi_i^0(t))] - \psi_i^0(t) m_i(t) + i h_i^0(t) \hat{m}_i(t) \right> \tag{B.6}
\]
where now \(\psi^0\) and \(h^0\) are functions of \(m\) and \(\hat{m}\) from the following equations:
\[
\frac{\delta \log Z_0}{\delta \psi_i^0(t)} = \frac{\sinh[\psi_i^0(t)] + \mu_i^0(t) \cosh[\psi_i(t)]}{\cosh[\psi_i(t)] + \mu_i^0(t) \sinh[\psi_i(t)]} = m_i(t) \tag{B.7a}
\]
\[
\frac{\delta \log Z_0}{\delta h_i(t)} = \int dt' \chi_i^0(t', t) \frac{\sinh[\psi_i^0(t')]}{\cosh[\psi_i^0(t')] + \mu_j^0(t') \sinh[\psi_j^0(t')]} = -i \hat{m}_i(t) \tag{B.7b}
\]
and
\[
\chi_i^0(t', t) = \frac{\delta \mu_i^0(t')}{\delta h_i(t)} = \Theta(t' - t) e^{t-t'} (1 - \tanh^2[h_i^0(t)]). \tag{B.8}
\]

For nMF, we need to calculate the linear term in \(\alpha\). This is
\[
\frac{\partial \Gamma_\alpha}{\partial \alpha} = -i \sum_{ij} J_{ij} \int dt \left< h_i(t) s_j(t) \right> = -i \sum_{ij} J_{ij} \int dt \hat{m}_i(t) m_j(t) \tag{B.9}
\]
where the last equality follows from
\[
\left< \theta_i(t) s_j(t) \right> = \frac{i}{Z_0} \frac{\delta^2 Z_0}{\delta h_i(t) \delta \psi_j(t)} = \hat{m}_i(t) m_j(t), \quad i \neq j. \tag{B.10}
\]
Consequently, up to the linear term in $\alpha$, we have
\[
\Gamma_\alpha[\hat{m}, m] = \Gamma_0[\hat{m}, m] - i\alpha \sum_{ij} J_{ij} \int dt \hat{m}_i(t)m_j(t). 
\] (B.11)

Using the fact that $\partial \Gamma_0/\partial \hat{m}_i(t) = i h_i^0(t)$, we find that
\[
 i h_i(t) = i h_i^0(t) - i \sum_j J_{ij} m_j(t). 
\] (B.12)

Together with the fact that, for $\psi^0 = 0$, we have $m_i(t) = \mu_i^0(t)$, the mean-field equation is
\[
\frac{d m_i(t)}{dt} + m_i(t) = \tanh[h_i(t) + \sum_j J_{ij} m_j(t)]. 
\] (B.13)

**B.2. TAP equations for asynchronous update**

To derive the TAP equations, we need to calculate the second derivative of $\Gamma$ with respect to $\alpha$. Similar to the synchronous update case, we have
\[
\frac{\partial^2 \Gamma_\alpha}{\partial \alpha^2} = - \sum_{ij,j'} J_{ij} J_{ij'} \int dt dt' \langle \delta \hat{h}_i(t) \delta s_j(t) \delta \hat{h}_j(t') \delta s_{j'}(t') \rangle_\alpha 
\] (B.14)
and the non-zero contributions come from pairing the terms inside the averages. Non-zero contributions come from $\langle \delta \hat{h}_i(t)^2 \rangle_\alpha$. A correlation function of the form $\langle \delta \hat{h}_i(t) \delta s_{j'}(t') \rangle_\alpha$ is non-zero for $t' < t$ but since it always appears multiplied by $\langle \delta s_j(t) \delta \hat{h}_j(t') \rangle_\alpha$, which is zero for $t' < t$, it does not contribute to the final results. We therefore have
\[
\frac{\partial^2 \Gamma_\alpha}{\partial \alpha^2} \bigg|_{\alpha=0} = - \sum_{ij} J_{ij} \int dt \langle [\delta \hat{h}_i(t)^2]_0 \langle \delta s_j(t)^2 \rangle_0 \rangle 
\] 
\[- \sum_{ij} J_{ij} J_{ji} \int dt \langle \delta \hat{h}_i(t) \delta s_i(t) \rangle_0 \langle \delta \hat{h}_j(t) \delta s_j(t) \rangle_0. 
\] (B.15)

To evaluate the above expression we first note that
\[
\langle [\delta s_j(t)^2]_0 \rangle = \frac{\delta^2 \log Z_0}{\delta \psi_j(t)^2} = 1 - m_j^2(t) 
\] (B.16a)
\[
\langle [\delta \hat{h}_i(t)^2]_0 \rangle = - \frac{\delta^2 \log Z_0}{\delta h_i(t)^2} = - \int dt' \frac{\delta \chi^0_i(t', t)}{\delta h_i(t)} \gamma_i(t') + \int dt' \chi_i(t', t) \gamma_i(t')^2 
\] (B.16b)
\[
\langle \delta \hat{h}_j(t) \delta s_j(t) \rangle_0 = \frac{\delta^2 \log Z_0}{\delta h_j(t) \delta \psi_j(t)} = 0 
\] (B.16c)
where the last equality follows from $\delta \mu_j^0(t)/\delta h_i(t) = 0$ and
\[
\gamma_i^0(t) \equiv \frac{\sinh[\psi_i^0(t)]}{\cosh[\psi_i^0(t)] + \mu_i^0(t) \sinh[\psi_i^0(t)]}
\tag{B.17a}
\]

\[
\frac{\delta \chi_i^0(t', t)}{\delta h_i(t)} = \frac{\delta^2 \mu_i^0(t')}{\delta h_i^2(t)} = -2 \tanh[h_i^0(t)][1 - \tanh^2[h_i^0(t)]]e^{t' - t} \Theta(t' - t) = -2 \tanh[h_i^0(t)]\chi_i^0(t', t).
\tag{B.17b}
\]

Using equation (B.17b) in equation (B.16b) gives
\[
\langle [\delta \hat{\theta}_i(t)]^2 \rangle_0 = -2i \tanh[h_i^0(t)] \hat{m}_i(t) + \int dt' \langle \chi_i^0(t', t) \gamma_i^0(t') \rangle^2.
\tag{B.18}
\]

The dynamical Gibbs free energy can then be written as
\[
\Gamma_\alpha[\hat{m}, m] = \Gamma_0[\hat{m}, m] - i\alpha \sum_{ij} J_{ij} \int \hat{m}_i(t)m_j(t)
\]
\[
- \frac{1}{2} \alpha^2 \sum_{ij} J_{ij}^2 \int dt \langle [\delta \hat{\theta}_i(t)]^2 \rangle_0 (1 - m_i^2(t)) \tag{B.19}
\]

where in the last sum $\langle [\delta \hat{\theta}_i(t)]^2 \rangle_0$ should be considered as a function of $m$ and $\hat{m}$.

**B.2.1. Stationary case.** For the stationary case we have $h_i^0(t) = h_i^{00}$ and we have to take $t \to \infty$. This gives
\[
\mu_j^0 = \tanh(h_j^{00}) \tag{B.20a}
\]
\[
m_i = \frac{\mu_i^0 + \tanh[\psi_i]}{1 + \mu_i^0 \tanh[\psi_i]} \tag{B.20b}
\]
\[
- i\hat{m}_i = (1 - [\mu_i^0]^2) \tanh[\psi_i] \left[ 1 + \mu_i^0 \tanh[\psi_i] \right] \tag{B.20c}
\]
\[
\int dt' \langle \chi_i^0(t', t) \gamma_i^0(t') \rangle^2 = (-i\hat{m}_i)^2. \tag{B.20d}
\]

Using equations (B.20a)–(B.20c) yields
\[
m_i + i\hat{m}_i = \tanh(h_i^{00}). \tag{B.21}
\]

Consequently, for the stationary case, equation (B.18) can be written as
\[
\langle [\delta \hat{\theta}_i(t)]^2 \rangle_0 = -2im_i\hat{m_i} + \mathcal{O}(\hat{m}_i^2) \tag{B.22}
\]

and therefore
\[
\frac{\partial^2 \Gamma_\alpha}{\partial \alpha^2} \bigg|_{\alpha=0} = 2i \sum_{ij} J_{ij}^2 \hat{m}_i m_j (1 - m_i^2) + \mathcal{O}(\hat{m}_i^2). \tag{B.23}
\]

Using this the TAP equations in the stationary case would be
\[
tanh^{-1} m_i = h_i + \sum_j J_{ij} m_j - m_i \sum_j J_{ij}^2 (1 - m_j^2) \tag{B.24}
\]

which is identical to the result of [13].

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B.2.2. General case. Under general conditions we cannot express $h$ and $\psi$ explicitly in terms of $m$ and $\hat{m}$. However, we can still calculate $\partial \Gamma / \partial \hat{m}_i(t)$ at $\hat{m} = 0$, which is what we need for deriving the TAP equations.

First note that the second term on the right-hand side of equation (B.18) is of quadratic order in $\psi$ in the limit $\psi \to 0$ (from equation (B.17a)). But $\hat{m}$ is linear in $\psi$ (from equation (B.7b)), so this term is of second order in $\hat{m}$ and its derivative with respect to $\hat{m}$ vanishes as $\hat{m} \to 0$. Thus we can discard it in finding the TAP equations.

We are now interested in the following quantity:

$$
\frac{\delta}{\delta \hat{m}_i(t)} \int dt' (\langle \delta \hat{h}_j(t') \rangle_0 (1 - m_k^2(t'))
= -2i x_i(t) (1 - m_k^2(t)) \delta_{ij} - 2i \int dt' \frac{\delta x_i(t')}{\delta \hat{m}_i(t)} \hat{m}_j(t') (1 - m_k^2(t')) \tag{B.25a}
$$

where $x_i(t) = \tanh(h^0_i(t))$. For $\hat{m}_j(t) \to 0$, the only term that will be non-zero on the right-hand side of equation (B.25a) is the first, as long as $\delta x_i(t')/\delta \hat{m}_i(t)$ does not diverge as fast as or faster than $1/\hat{m}$ as $\hat{m} \to 0$. Whether $\delta x_i(t')/\delta \hat{m}_i(t)$ is regular in the limit $\hat{m} \to 0$ or not depends on whether the functional matrix $\delta(m, \hat{m})/\delta (h, \psi)$ is regular in this limit. The latter is not singular when the generating functional is regular unless the system is at a phase transition. Assuming that this is not the case, we can ignore the last term in equation (B.25a).

Now we can proceed the way we did in the naive mean-field case, but evaluating $\Gamma_\alpha$ to second order in $\alpha$. The functional derivative of $\Gamma_\alpha$ with respect to $\hat{m}$, evaluated at $\alpha = 1$, gives $ih$:

$$ih_i(t) = ih^0_i(t) - i \sum_j J_{ij} m_j(t) + i \tanh(h^0_i(t)) \sum_j J_{ij}^2 [1 - m_j^2(t)], \tag{B.26}
$$

tanh$h^0_i(t)$ can be related to $\mu_i^0(t)$ through

$$
\frac{d\mu_i^0}{dt} = -\mu_i^0 + \tanh h^0_i(t), \tag{B.27}
$$

and $\mu_i^0 \to m_i$ when $\psi$ and $\hat{m} \to 0$, yielding the TAP equations

$$
\frac{dm_i(t)}{dt} + m_i(t) = \tanh \left[ h_i(t) + \sum_j J_{ij} m_j(t) - \left( \frac{dm_i(t)}{dt} + m_i(t) \right) \sum_j J_{ij}^2 [1 - m_j^2(t)] \right]. \tag{B.28}
$$

Note that these are of the same form as those for the synchronous-update model with $m_i(t + 1)$ replaced by $m_i + dm_i/dt$.

References

[1] Mezard M, Parisi G and Virasoro M A, 1987 Spin Glass Theory and Beyond (Singapore: World Scientific)
[2] Thouless D J, Anderson P W and Palmer R G, Solution of solvable model of a spin glass, 1977 Phil. Mag. 35 593
[3] Plefka T, Convergence condition of the tap equation for the infinite-ranged Ising spin glass model, 1981 J. Phys. A: Math. Gen. 15 1971
[4] Sompolinsky H and Zippelius A, Dynamic theory of the spin-glass phase, 1981 Phys. Rev. Lett. 47 359
[5] Sommers H J, Path-integral approach to Ising spin-glass dynamics, 1987 Phys. Rev. Lett. 58 1268
doi:10.1088/1742-5468/2011/03/P03031
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[6] Rieger H, Schreckenberg M and Zittartz J, Glauber dynamics of neural network models, 1988 J. Phys. A: Math. Gen. 21 L263
[7] Crisanti A and Sompolinsky H, Dynamics of spin systems with randomly asymmetric bonds: Ising spins and glauber dynamics, 1988 Phys. Rev. A 37 4865
[8] Coolen A C C and Sherrington D, Dynamics of fully connected attractor neural networks near saturation, 1993 Phys. Rev. Lett. 71 3886
[9] Coolen A C C and Sherrington D, Order-parameter flow in the sk spin glass. i. Replica symmetry, 1994 J. Phys. A: Math. Gen. 27 7687
[10] Fischer K H and Hertz J A, 1991 Spin Glasses (Cambridge: Cambridge University Press)
[11] Coolen A C C, Statistical mechanics of recurrent neural networks ii. Dynamics, 2000 arXiv:cond-mat/0006011
[12] Biroli G, Dynamical tap approach to mean field glassy systems, 1999 J. Phys. A: Math. Gen. 32 8365
[13] Kappen H J and Spanjers J J, Mean field theory for asymmetric neural networks, 2000 Phys. Rev. E 61 5658
[14] Lezon T R, Banavar J R, Cieplak M, Maritan A and Fedoroff N, Using the principle of entropy maximization to infer genetic interaction networks from gene expression patterns, 2006 Proc. Nat. Acad. Sci. 103 19033
[15] Weigt M, White R A, Szurmant H, Hoch J A and Hwa T, Identification of direct residue contacts in protein–protein interaction by message passing, 2009 Proc. Nat. Acad. Sci. 106 67
[16] Cocco S, Leibler S and Monasson R, Neuronal couplings between retinal ganglion cells inferred by efficient inverse statistical physics methods, 2009 Proc. Nat. Acad. Sci. 106 14058
[17] Roudi Y, Tyrcha J and Hertz J, Ising model for neural data: model quality and approximate methods for extracting functional connectivity, 2009 Phys. Rev. E 79 051915
[18] Roudi Y and Hertz J, Mean field theory for nonequilibrium network reconstruction, 2011 Phys. Rev. Lett. 106 048702
[19] Zeng H-L, Alava M, Mahmoudi H and Aurell E, Network inference using asynchronously updated kinetic Ising model, 2010 arXiv:1011.6216v1
[20] Bray A J and Moore M A, Metastable states in spin glasses, 1980 J. Phys. C: Solid State Phys. 13 L469
[21] Kappen H J and Rodriguez F B, Efficient learning in boltzmann machines using linear response theory, 1998 Neural Comput. 10 1137
[22] Tanaka T, Mean-field theory of Boltzmann machine learning, 1998 Phys. Rev. E 58 2302

doi:10.1088/1742-5468/2011/03/P03031