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Replicated Bethe Free Energy: A Variational Principle behind Survey Propagation

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A scheme to provide various mean-field-type approximation algorithms is presented by employing the Bethe free energy formalism to a family of replicated systems in conjunction with analytical continuation with respect to the number of replicas. In the scheme, survey propagation (SP), which is an efficient algorithm developed recently for analyzing the microscopic properties of glassy states for a fixed sample of disordered systems, can be reproduced by assuming the simplest replica symmetry on stationary points of the replicated Bethe free energy. Belief propagation and generalized SP can also be offered in the identical framework under assumptions of the highest and broken replica symmetries, respectively.

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Recent research in cross-disciplinary fields involving statistical mechanics and information sciences has shown that methods and concepts from physics can be useful in the development and analysis of efficient algorithms for computing probabilities or solving combinational problems.[1)] One of the most prominent examples in such research is the development of survey propagation (SP).[2)] This algorithm approximately evaluates the microscopic averages of dynamical variables in a feasible amount of time for a fixed sample of disordered systems utilizing the concept of replica symmetry breaking (RSB), which was discovered in the study of spin glasses.[3)] SP has been reported to give excellent results in studies on spin glass models[4)] and in various combinatorial problems,[2,5)] promoting further extension of the applicable range.[6)] It has also been shown that SP reproduces the one-step RSB (1RSB) solution of replica theory[3)] when applied to the mean-field-type spin glass models.[7)] This clarity of behavior is an important feature of the SP algorithm. However, the nature of solutions found by SP for general systems remains poorly understood, which may restrict the range of possible applications.

The aim of the present Letter is to partially resolve this problem. More precisely, a family of approximation algorithms employing the Bethe free energy formalism[8,9)] is proposed for replicated systems. Analytically extending the proposed algorithms with respect to the number of replicas $x = 1, 2, \ldots$ to $x \in \mathbf{R}$ under the simplest replica symmetric ansatz turns out to provide a general expression of SP, in which x plays the role of a parameter specifying the size of a subgroup of replicas in the conventional 1RSB scheme.[3)] In this way, SP can only converge to a point offered by the analytical continuity of stationary points of the x-replicated Bethe free energy.

As a basis for proposed algorithms, consider a joint distribution of N dimensional state variables $\boldsymbol{S} = (S_1, S_2, \ldots, S_N)$, as given by

$$P(\boldsymbol{S}) = Z^{-1} \prod_{\mu=1}^{M} \psi_\mu(\boldsymbol{S}_\mu) \prod_{l=1}^{N} \psi_l(S_l), \tag{1}$$

where $\psi_\mu(\boldsymbol{S}_\mu)$ and $\psi_l(S_l)$ are termed the clique and local evidences, which are dependent on a certain subset of multiple components (clique) $\boldsymbol{S}_\mu$ and a single component S_l, respectively, and $Z = \sum_{\boldsymbol{S}} \prod_{\mu=1}^{M} \psi_\mu(\boldsymbol{S}_\mu) \prod_{l=1}^{N} \psi_l(S_l)$ is the partition function. For simplicity, only the Ising spin systems $\boldsymbol{S} = \{+1, -1\}^N$ are considered here, but extension to other cases is straightforward. In such systems, evaluation of the marginal probabilities,

$$P(S_l) = \sum_{\boldsymbol{S} \backslash S_l} P(\boldsymbol{S}), \tag{2}$$

is in general computationally difficult, where $X \backslash Y$ denotes a subset of X from which Y is excluded. The development of computationally tractable algorithms achieving an accurate approximation of eq. (2) is therefore of great importance.

The Kullback–Leibler divergence (KLD), as given by

$$\mathrm{KL}(Q \mid P) = \sum_{\boldsymbol{S}} Q(\boldsymbol{S}) \ln \tfrac{Q(\boldsymbol{S})}{P(\boldsymbol{S})}, \tag{3}$$

where $Q(\boldsymbol{S})$ is an arbitrary test distribution of $\boldsymbol{S}$, offers a useful guideline for developing such an algorithm. As $\mathrm{KL}(Q \mid P)$ is always nonnegative and minimized to zero if and only if $Q(\boldsymbol{S}) = P(\boldsymbol{S})$, the minimization of $\mathrm{KL}(Q \mid P)$ with respect to $Q(\boldsymbol{S})$ generally yields the correct distribution $Q(\boldsymbol{S}) = P(\boldsymbol{S})$. Direct application of this algorithm, however, is not particularly useful for computing eq. (2) because $P(\boldsymbol{S})$ itself is in general not computationally tractable. Instead, applying this variational (minimization) principle of KLD or its approximation to a family of tractable test distributions systematically leads to a number of potentially effective approximation algorithms.

The central idea of the present treatment is the application of this principle not to the original system but to a family of replicated systems, as follows:

$$P_x(\{\boldsymbol{S}^a\}) = \prod_{a=1}^{x} P(\boldsymbol{S}^a), \tag{4}$$

where $\{\boldsymbol{S}^a\}$ is an abbreviation of the set of replicated systems $\{\boldsymbol{S}^1, \boldsymbol{S}^2, \ldots, \boldsymbol{S}^x\}$. The abbreviations $\{S_l^a\}$ and $\{\boldsymbol{S}_\mu^a\}$ are also used to represent $\{S_l^1, S_l^2, \ldots, S_l^x\}$ and $\{\boldsymbol{S}_\mu^1, \boldsymbol{S}_\mu^2, \ldots, \boldsymbol{S}_\mu^x\}$, respectively. Equation (4) yields the following equality regarding free energy:

$$-\ln Z = \mathcal{F}_x(Q) - \frac{1}{x} \mathrm{KL}(Q \mid P_x), \tag{5}$$

which holds for arbitrary $x = 1, 2, \ldots$ and the test distribution $Q(\{\boldsymbol{S}^a\})$, where

$$\mathcal{F}_x(Q) = \frac{1}{x}\sum_{\{S^a\}} Q(\{S^a\}) \ln \frac{Q(\{S^a\})}{\prod_{a=1}^{x}\left(\prod_{\mu=1}^{M}\psi_\mu(S_\mu^a)\prod_{l=1}^{N}\psi_l(S_l^a)\right)}. \quad (6)$$

As the true free energy $-\ln Z$ is constant, this implies that the minimization of $\mathrm{KL}(Q \mid P_x)$ is equivalent to that of $\mathcal{F}_x(Q)$. This yields the correct distribution $Q(\{S^a\}) = P_x(\{S^a\}) = \prod_{a=1}^{x} P(S^a)$. Since $\prod_{a=1}^{x} P(S^a)$ is simply a product of duplications of eq. (1), the minimization of eq. (3) for the original system and $\mathcal{F}_x(Q)$ for the replicated system are equivalent. The introduction of the family of replicas therefore provides no benefits as long as the search for the optimal test distribution covers all feasible functional spaces. However, the replicated formalism can potentially provide better approximation accuracy than the original algorithm when the test distributions are limited to a tractable family or when the cost functions are somewhat approximated, as the tractable family or characteristics of the approximated function depend on the number of replicas x.

To show this, we approximate $\mathcal{F}_x(Q)$ by the Bethe free energy[8,9] of the x-replicated system, as follows:

$$\begin{aligned}\mathcal{F}_x(Q) &\simeq \mathcal{F}_x^{\mathrm{Bethe}}(\{b_\mu\},\{b_l\}) \\ &= \frac{1}{x}\sum_{\mu=1}^{M}\sum_{\{S_\mu^a\}} b_\mu(\{S_\mu^a\}) \ln \frac{b_\mu(\{S_\mu^a\})}{\prod_{a=1}^{x}(\psi_\mu(S_\mu^a)\prod_{l\in\mathcal{L}(\mu)}\psi_l(S_l^a))} \\ &\quad + \frac{1}{x}\sum_{l=1}^{N}(1-C_l)\sum_{\{S_l^a\}} b_l(\{S_l^a\}) \ln \frac{b_l(\{S_l^a\})}{\prod_{a=1}^{x}\psi_l(S_l^a)}, \end{aligned} \quad (7)$$

where $\mathcal{L}(\mu)$ is the set of elements that directly relate to clique μ and C_l is the number of cliques to which element S_l is directly related. The test distributions $b_\mu(\{S_\mu^a\})$ and $b_l(\{S_l^a\})$ are termed beliefs which approximate the marginals $\sum_{\{S^a\}\setminus\{S_\mu^a\}} P_x(\{S^a\})$ and $\sum_{\{S^a\}\setminus\{S_l^a\}} P_x(\{S^a\})$, respectively, when $\mathcal{F}_x^{\mathrm{Bethe}}$ is extremized. Note that since both of these marginals are reduced from the identical distribution $P_x(\{S^a\})$, the reducibility condition

$$\sum_{\{S_\mu^a\}\setminus\{S_l^a\}} b_\mu(\{S_\mu^a\}) = b_l(\{S_l^a\}), \quad (8)$$

must hold when S_l is an element of S_μ.

If the variable dependence in eq. (1) is represented by a cycle-free graph, eq. (7) under this constraint agrees exactly with $\mathcal{F}_x(Q)$ for the test distribution

$$Q(\{S^a\}) = \frac{\prod_{\mu=1}^{M} b_\mu(\{S_\mu^a\})}{\prod_{l=1}^{N} b_l^{C_l-1}(\{S_l^a\})},$$

in which case extremizing eq. (7) leads to the exact assessment of eq. (2).[9,10] Unfortunately, $\mathcal{F}_x(Q)$ and $\mathcal{F}_x^{\mathrm{Bethe}}(\{b_\mu\},\{b_l\})$ do not accord in general. However, this indicates that the stationary point of eq. (7) may provide a good approximation when the influence of the cycles can be regarded as weak.

Extremizing eq. (7) with respect to the beliefs, adding the terms $\sum_{\{S_l^a\}} \lambda_{\mu l}(\{S_l^a\})(\sum_{\{S_\mu^a\}\setminus\{S_l^a\}} b_\mu(\{S_\mu^a\}) - b_l(\{S_l^a\}))$, where $\lambda_{\mu l}(\{S_l^a\})$ are the Lagrange multipliers imposing constraint (8), yields

$$b_\mu(\{S_\mu^a\}) = \frac{\prod_{a=1}^{x}\psi_\mu(S_\mu^a)\prod_{l\in\mathcal{L}(\mu)}(\mathrm{e}^{-\lambda_{\mu l}(\{S_l^a\})}\prod_{a=1}^{x}\psi_l(S_l^a))}{\sum_{\{S_\mu^a\}}\prod_{a=1}^{x}\psi_\mu(S_\mu^a)\prod_{l\in\mathcal{L}(\mu)}(\mathrm{e}^{-\lambda_{\mu l}(\{S_l^a\})}\prod_{a=1}^{x}\psi_l(S_l^a))}, \quad (9)$$

$$b_l(\{S_l^a\}) = \frac{\prod_{a=1}^{x}\psi_l(S_l^a)\prod_{\mu\in\mathcal{M}(l)}\mathrm{e}^{-\lambda_{\mu l}(\{S_l^a\})/(C_l-1)}}{\sum_{\{S_l^a\}}\prod_{a=1}^{x}\psi_l(S_l^a)\prod_{\mu\in\mathcal{M}(l)}\mathrm{e}^{-\lambda_{\mu l}(\{S_l^a\})/(C_l-1)}}. \quad (10)$$

Then, inserting eqs. (9) and (10) into eq. (8) affords the stationary point condition of the Lagrange multipliers, which can be read as

$$\begin{aligned}\mathrm{e}^{-\hat{\lambda}_{\mu l}(\{S_l^a\})} &\propto \sum_{\{S_\mu^a\}\setminus\{S_l^a\}}\prod_{a=1}^{x}\psi_\mu(S_\mu^a) \\ &\quad\times \prod_{j\in\mathcal{L}(\mu)\setminus l}\left(\mathrm{e}^{-\lambda_{\mu j}(\{S_j^a\})}\prod_{a=1}^{x}\psi_j(S_j^a)\right), \end{aligned} \quad (11)$$

$$\mathrm{e}^{-\lambda_{\mu l}(\{S_l^a\})} \propto \prod_{\nu\in\mathcal{M}(l)\setminus\mu}\mathrm{e}^{-\hat{\lambda}_{\nu l}(\{S_l^a\})}, \quad (12)$$

where $\mathcal{M}(l)$ denotes the sets of cliques that directly relate to clique elements l and $\hat{\lambda}_{\mu l}(\{S_l^a\}) = \frac{1}{C_l-1}\sum_{\nu\in\mathcal{M}(l)}\lambda_{\nu l}(\{S_l^a\}) - \lambda_{\mu l}(\{S_l^a\})$.

A remarkable property of these replicated systems is the invariance of stationary conditions (11) and (12) under the permutation of replica indices $a = 1, 2, \ldots, x$. This naturally leads to the assumption that the stationary point possesses the same symmetry. In the case of Ising spin systems $S = \{+1, -1\}^N$, this can be represented as the simplest replica symmetric (RS) ansatz on the Lagrange multipliers,

$$\mathrm{e}^{-\lambda_{\mu l}(\{S_l^a\})}\prod_{a=1}^{x}\psi_l(S_l^a) \propto \int \mathrm{d}h\, \pi_{l\to\mu}(h)\frac{\exp\left(h\sum_{a=1}^{x}S_l^a\right)}{(2\cosh(h))^x}, \quad (13)$$

$$\mathrm{e}^{-\hat{\lambda}_{\mu l}(\{S_l^a\})} \propto \int \mathrm{d}\hat{h}\, \hat{\pi}_{\mu\to l}(\hat{h})\frac{\exp\left(\hat{h}\sum_{a=1}^{x}S_l^a\right)}{(2\cosh(\hat{h}))^x}, \quad (14)$$

without a loss of generality,[11] where $\pi_{l\to\mu}(h)$ and $\hat{\pi}_{\mu\to l}(\hat{h})$ are distributions that absorb the degree of freedom of the Lagrange multipliers. Inserting these multipliers into eqs. (11) and (12) provides a couple of saddle point equations in which $\hat{\pi}_{\mu\to l}(\hat{h})$ and $\pi_{l\to\mu}(h)$ are solved explicitly for given $\pi_{l\to\mu}(h)$ and $\hat{\pi}_{\mu\to l}(\hat{h})$, respectively. The natural iteration of the resultant equations yields a family of algorithms that are parameterized by the number of replicas $x = 1, 2, \ldots,$

$$\hat{\pi}_{\mu\to l}^{t+1}(\hat{h}) \propto \int \prod_{j\in\mathcal{L}(\mu)\setminus l}\mathrm{d}h_j\,\pi_{j\to\mu}^{t}(h_j)\left(\sum_{S_\mu}\psi_\mu(S_\mu)\prod_{j\in\mathcal{L}(\mu)\setminus l}\left(\frac{\mathrm{e}^{h_jS_j}}{2\cosh(h_j)}\right)\right)^x \delta(\hat{h} - \hat{h}(\{h_{j\in\mathcal{L}(\mu)\setminus l}\})), \quad (15)$$

$$\pi_{l\to\mu}^{t}(h) \propto (2\cosh(h))^x \int \prod_{\nu\in\mathcal{M}(l)\setminus\mu}\frac{\mathrm{d}\hat{h}_\nu\,\hat{\pi}_{\nu\to l}^{t}(\hat{h}_\nu)}{(2\cosh(\hat{h}_\nu))^x}\delta\left(h - h_l^0 - \sum_{\nu\in\mathcal{M}(l)\setminus\mu}\hat{h}_\nu\right), \quad (16)$$

where t represents the number of iterations,

$$\hat{h}(\{h_{j\in\mathcal{L}(\mu)\backslash l}\}) = \tanh^{-1}\left(\frac{\sum_{\boldsymbol{S}_\mu} S_l\psi_\mu(\boldsymbol{S}_\mu)\prod_{j\in\mathcal{L}(\mu)\backslash l}\left(\frac{e^{h_jS_j}}{2\cosh(h_j)}\right)}{\sum_{\boldsymbol{S}_\mu}\psi_\mu(\boldsymbol{S}_\mu)\prod_{j\in\mathcal{L}(\mu)\backslash l}\left(\frac{e^{h_jS_j}}{2\cosh(h_j)}\right)}\right)$$

and

$$h_l^0 = \tanh^{-1}\left(\frac{\sum_{S_l} S_l\psi_l(S_l)}{\sum_{S_l}\psi_l(S_l)}\right).$$

There are two features to note here. First, the beliefs can be evaluated by inserting eq. (13) into eqs. (9) and (10) using the stationary solution of eqs. (15) and (16). Specifically, eq. (10) can be assessed as

$$b_l(\{S_l^a\}) = \int \mathrm{d}h\,\rho_l(h)\frac{\exp\left(h\sum_{a=1}^{x}S_l^a\right)}{(2\cosh(h))^x},$$

yielding the following approximation of eq. (2):

$$P(S_l) \simeq \int \mathrm{d}h\,\rho_l(h)\frac{e^{hS_l}}{2\cosh(h_l)},$$

where

$$\rho_l(h) = \frac{(2\cosh(h))^x\int\prod_{\mu\in\mathcal{M}(l)}\frac{\mathrm{d}\hat{h}_\mu\,\hat{\pi}_{\mu\to l}(\hat{h}_\mu)}{(2\cosh(\hat{h}_\mu))^x}\,\delta\left(h-h_l^0-\sum_{\mu\in\mathcal{M}(l)}\hat{h}_\mu\right)}{\int\prod_{\mu\in\mathcal{M}(l)}\frac{\mathrm{d}\hat{h}_\mu\,\hat{\pi}_{\mu\to l}(\hat{h}_\mu)}{(2\cosh(\hat{h}_\mu))^x}\left(2\cosh\left(h_l^0+\sum_{\mu\in\mathcal{M}(l)}\hat{h}_\mu\right)\right)^x}. \quad (17)$$

As the functional updates of eqs. (15) and (16) can be approximated by the Monte Carlo method on a practical time scale, these equations constitute a tractable algorithm for approximating the marginal probabilities (2).

Second, although $x = 1, 2, \ldots$ has been assumed, the expressions of eqs. (15)–(17) can be analytically continued to $x \in \mathbf{R}$. In addition, the extremized values of the replicated Bethe free energy $\Phi_x^{\mathrm{Bethe}} = \mathrm{Extr}_{\{\{b_\mu\},\{b_l\}\}}\{\mathcal{F}_x^{\mathrm{Bethe}}(\{b_\mu\},\{b_l\})\}$ can also be readily extended to $x \in \mathrm{R}$ as follows:

$$\begin{aligned}\Phi_x^{\mathrm{Bethe}} = &-\frac{1}{x}\sum_{\mu=1}^{M}\ln\left[\int\prod_{l\in\mathcal{L}(\mu)}\mathrm{d}h_l\,\pi_{l\to\mu}(h_l)\right.\\&\left.\times\left(\sum_{\boldsymbol{S}_\mu}\psi_\mu(\boldsymbol{S}_\mu)\prod_{l\in\mathcal{L}(\mu)}\left(\frac{e^{h_lS_l}}{2\cosh(h_l)}\right)\right)^x\right]\\&-\frac{1}{x}\sum_{l=1}^{N}(1-C_l)\ln\left[\int\prod_{\mu\in\mathcal{M}(l)}\mathrm{d}\hat{h}_\mu\,\hat{\pi}_{\mu\to l}(\hat{h}_\mu)\right.\\&\left.\times\left(\sum_{S_l}\psi_l(S_l)\prod_{\mu\in\mathcal{M}(l)}\left(\frac{e^{\hat{h}_\mu S_l}}{2\cosh(\hat{h}_\mu)}\right)\right)^x\right], \quad (18)\end{aligned}$$

where $\pi_{l\to\mu}(h)$ and $\hat{\pi}_{\mu\to l}(\hat{h})$ are the stationary solutions of eqs. (15) and (16). Analytical extension of the variational functional (7), however, is nontrivial. Nevertheless, the analytically continued expressions of eqs. (15) and (16) eventually lead to a general expression of SP in which $\pi_{l\to\mu}^t(h)$ and $\hat{\pi}_{\mu\to l}^t(\hat{h})$ are termed surveys, which is the main result of the present treatment. In this relation, x serves as the RSB parameter, which is introduced to represent the number of replicas in a subgroup in the conventional 1RSB formulation. For example, SP for the K-SAT problem of finite temperature, corresponding to eqs. (C1) and (C2) in ref. 12, can be derived from eqs. (16) and (15) by setting

$$x \to m, \quad \psi_\mu(\boldsymbol{S}_\mu) = \exp\left(-2\beta\prod_{l\in\mathcal{L}(\mu)}\frac{1-J_l^\mu S_l}{2}\right) \text{ and } \psi_l(S_l) = 1$$

in conjunction with rescaling fields as $h/\beta \to h$ and $\hat{h}/\beta \to \hat{h}$, where β is the inverse temperature and $J_l^\mu \in \{+1,-1\}$ are randomly predetermined constants. The derivation of SP for the famous Sherrington–Kirkpatrick (SK) model[13] is shown briefly in the appendix.

It has been reported that extremizing eq. (18) with respect to the RSB parameter x provides a reasonable description of equilibrium states in the conventional replica theory.[7] However, it may be difficult to deduce such a principle for the determination of x using only the framework presented here. The derivation is complicated by the dependence of the approximation accuracy on x, which is generally related to the specific characteristics of the target system in a nontrivial manner, although certain extra constraints related to the concept of thermodynamic limits (*e.g.*, homogeneity[14]) may be utilized for problems in the physics literature.

The formalism presented here is related to other algorithms as follows. Equations (15) and (16) always have special solutions of the forms $\pi_{l\to\mu}^t(h) = \delta(h-h_{l\to\mu}^t)$ and $\hat{\pi}_{\mu\to l}^t(\hat{h}) = \delta(\hat{h}-\hat{h}_{\mu\to l}^t)$, independently of x. The parameters $h_{l\to\mu}^t$ and $\hat{h}_{\mu\to l}^t$ are updated by $\hat{h}_{\mu\to l}^{t+1} = \hat{h}(\{h_{j\in\mathcal{L}(\mu)\backslash l}^t\})$, $h_{l\to\mu}^t = h_l^0 + \sum_{\nu\in\mathcal{M}(l)\backslash\mu}\hat{h}_{\nu\to l}^t$. Notice that these forms are an expression of the belief propagation (BP)[15,16] for eq. (1), the fixed point of which is usually linked to the variational condition of the conventional Bethe free energy $\mathcal{F}^{\mathrm{Bethe}} = \mathcal{F}_{x=1}^{\mathrm{Bethe}}$.[17] In the current formalism, on the other hand, BP can be characterized as the solution of the highest symmetry obtained assuming the Lagrange multipliers of the limited form

$$e^{-\lambda_{\mu l}(\{S_l^a\})}\prod_{a=1}^{x}\psi_l(S_l^a) \propto \frac{\exp\left(h_{l\to\mu}\sum_{a=1}^{x}S_l^a\right)}{(2\cosh(h_{l\to\mu}))^x},$$

$$e^{-\hat{\lambda}_{\mu l}(\{S_l^a\})} \propto \frac{\exp\left(\hat{h}_{\mu\to l}\sum_{a=1}^{x}S_l^a\right)}{(2\cosh(\hat{h}_{\mu\to l}))^x},$$

which exist for arbitrary RSB parameter $x \in \mathbf{R}$. This relationship between BP and the assumption of eqs. (13) and (14) is analogous to that for the RS solution under the 1RSB ansatz in the conventional replica theory employed in spin glass research.

The present algorithm can also be extended to the reduction of replica symmetry. For example, introducing the 1RSB ansatz[11] on the Lagrange multipliers, we obtain

$$e^{-\lambda_{\mu l}(\{S_l^a\})}\prod_{a=1}^{x}\psi_l(S_l^a) \propto \int\mathcal{D}\pi\,\Pi_{l\to\mu}[\pi] \times\prod_{\alpha=1}^{x/m}\left(\int\mathrm{d}h^\alpha\,\pi(h^\alpha)\frac{\exp\left(h^\alpha\sum_{a\in\mathcal{I}(\alpha)}S_l^a\right)}{(2\cosh(h^\alpha))^m}\right), \quad (19)$$

$$e^{-\hat{\lambda}_{\mu l}(\{S_l^a\})} \propto \int\mathcal{D}\hat{\pi}\,\hat{\Pi}_{\mu\to l}[\hat{\pi}] \times\prod_{\alpha=1}^{x/m}\left(\int\mathrm{d}\hat{h}^\alpha\,\hat{\pi}(\hat{h}^\alpha)\frac{\exp\left(\hat{h}^\alpha\sum_{\alpha\in\mathcal{I}(\alpha)}S_l^a\right)}{(2\cosh(\hat{h}^\alpha))^m}\right), \quad (20)$$

where $\mathcal{I}(\alpha)$ $(\alpha = 1, 2, \ldots, m)$ denotes subsets of replica indices of an equal size m while $\mathcal{D}\pi\Pi_{l\to\mu}[\pi]$ and $\mathcal{D}\hat{\pi}\hat{\Pi}_{\mu\to l}[\hat{\pi}]$ represent the variational measures of distributions $\pi(h)$ and $\hat{\pi}(\hat{h})$, respectively. Analytically continuing this yields the conventional two-step RSB solution in the case of the SK model. This indicates that generalizing this provides an algorithm corresponding to the $r+1$-step RSB solution of conventional replica analysis under the assumption that the Lagrange multipliers are of the form of the r-step RSB.

In summary, a framework for the construction of a family of mean-field-type approximation algorithms was derived by introducing the Bethe free energy formalism for x-replicated systems. Analytically continuing the algorithm obtained for $x = 1, 2, \ldots$ to $x \in \mathbf{R}$ under the replica symmetric ansatz leads to a general expression of survey propagation for such systems [eq. (1)], in which x plays the role of a replica symmetry breaking parameter in the 1RSB solution of conventional replica analysis. Belief propagation and generalized survey propagation can be reproduced from an identical variational functional [eq. (7)] corresponding to various levels of RSB ansatz on the replica symmetry of the Lagrange multipliers. This may be useful for clarifying the relationships between solutions obtained using these various algorithms.

Although the focus here was on algorithms derived from natural iteration of eqs. (11) and (12), a range of schemes for the minimization of the Bethe free energy are available.[18,19] Furthermore, it is known that the Bethe free energy formalism itself can be generalized to a more advanced scheme as the cluster variation method.[9] Extending the present results to such schemes is a target of future work.

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Appendix: SP for the SK Model

The Sherrington–Kirkpatrick (SK) model is an Ising spin system characterized by the Hamiltonian $\mathcal{H}(\boldsymbol{S}) = -\sum_{l>k} J_{lk} S_l S_k - \sum_{l=1}^{N} H_l S_l$, where J_{lk} is sampled from an identical normal distribution $\mathcal{N}(J_0/N, J^2/N)$ independently of the unordered pair $\langle lk \rangle$, and H_l represents an external field. Identifying $\langle lk \rangle$ with μ leads to $\psi_\mu(\boldsymbol{S}_\mu) = \mathrm{e}^{\beta J_{lk} S_l S_k}$ and $\psi_l(S_l) = \mathrm{e}^{\beta H_l S_l}$.

Two distinct properties of this system are the denseness of connectivity and the weakness of each coupling constant. Let $\hat{\pi}^t_{\mu\to l}(\hat{h})$ be characterized by the two moments $\int \mathrm{d}\hat{h}\, \hat{\pi}^t_{\mu\to l}(\hat{h})\hat{h} = a^t_{\mu\to l}$ and $\int \mathrm{d}\hat{h}\, \hat{\pi}^t_{\mu\to l}(\hat{h})(\hat{h} - a^t_{\mu\to l})^2 = v^t_{\mu\to l}$. This representation allows eqs. (16) and (17) to be expressed in terms of the tth update as

$$\pi^t_{l\to\mu}(h) \simeq \frac{(2\cosh(h))^x \exp\left[-\frac{(h-\phi^t_{l\to\mu})^2}{2\Delta^t_{l\to\mu}}\right]}{\int \mathrm{d}h (2\cosh(h))^x \exp\left[-\frac{(h-\phi^t_{l\to\mu})^2}{2\Delta^t_{l\to\mu}}\right]}, \qquad \text{(A·1)}$$

and

$$\rho^t_l(h) \simeq \frac{(2\cosh(h))^x \exp\left[-\frac{(h-\phi^t_l)^2}{2\Delta^t_l}\right]}{\int \mathrm{d}h (2\cosh(h))^x \exp\left[-\frac{(h-\phi^t_l)^2}{2\Delta^t_l}\right]}, \qquad \text{(A·2)}$$

where $\phi^t_{l\to\mu} = \beta H_l + \sum_{\nu\in\mathcal{M}(l)\backslash\mu} a^t_{\nu\to l}$, $\Delta^t_{l\to\mu} = \sum_{\nu\in\mathcal{M}(l)\backslash\mu} v^t_{\nu\to l}$, $\phi^t_l = \beta H_l + \sum_{\mu\in\mathcal{M}(l)} a^t_{\mu\to l}$ and $\Delta^t_l = \sum_{\mu\in\mathcal{M}(l)} v^t_{\mu\to l}$.[20] In turn, let us introduce $\int \mathrm{d}h\, \pi^t_{l\to\mu}(h)\tanh(h) = m^t_{l\to\mu}$, $\int \mathrm{d}h\, \pi^t_{l\to\mu}(h)\tanh^2(h) = M^t_{l\to\mu}$, $\int \mathrm{d}h\, \rho^t_l(h)\tanh(h) = m^t_l$ and $\int \mathrm{d}h\, \rho^t_l(h)\tanh^2(h) = M^t_l$. Here, m^t_l is the estimated local magnetization at the tth update. The weakness of each coupling constant in conjunction with eq. (15) indicates that $a^t_{\mu\to l}$ and $v^t_{\mu\to l}$ are updated as $a^{t+1}_{\mu\to l} \simeq \beta J_\mu m^t_{k\to\mu}$, $v^{t+1}_{\mu\to l} \simeq \beta^2 J^2_\mu (M^t_{k\to\mu} - (m^t_{k\to\mu})^2)$. Employing the law of large numbers, this implies that variances $\Delta^t_{l\to\mu}$ and Δ^t_l are updated independently of the pairs of indices $(l\mu)$ as $\Delta^{t+1}_{l\to\mu} \simeq N^{-1}\beta^2 J^2 \sum_{\nu\in\mathcal{M}(l)\backslash\mu} (M^t_{l\to\nu} - (m^t_{l\to\nu})^2) \simeq N^{-1}\beta^2 J^2 \sum_{\mu\in\mathcal{M}(l)} (M^t_l - (m^t_l)^2) \simeq \Delta^{t+1}_l \simeq \beta^2 J^2 (Q^t_1 - Q^t_0)$, where $Q^t_1 = N^{-1}\sum_{l=1}^N M^t_l$ and $Q^t_0 = N^{-1}\sum_{l=1}^N (m^t_l)^2$. This also indicates that $m^t_{l\to\mu}$ and m^t_l are related by $m^t_{l\to\mu} \simeq m^t_l - \beta J_\mu (1 - Q^t_1 + x(Q^t_1 - Q^t_0)) m^{t-1}_k$ via the Taylor expansion. Inserting these results into eqs. (A·1) and (A·2) leads to the following expression of SP for the SK model:

$$\phi^{t+1}_l = \beta H_l + \sum_{k\neq l} \beta J_{lk} m^t_k - \Gamma^t m^{t-1}_l, \qquad \text{(A·3)}$$

$$m^t_l = \frac{\int \mathrm{d}h (2\cosh(h))^x \exp\left[-\frac{(h-\phi^t_l)^2}{2\beta^2 J^2 (Q^t_1 - Q^t_0)}\right]\tanh(h)}{\int \mathrm{d}h (2\cosh(h))^x \exp\left[-\frac{(h-\phi^t_l)^2}{2\beta^2 J^2 (Q^t_1 - Q^t_0)}\right]}, \qquad \text{(A·4)}$$

where $\Gamma^t = \beta^2 J^2 (1 - Q^t_1 + x(Q^t_1 - Q^t_0))$, and $\sum_{\mu\in\mathcal{M}(l)} J^2_\mu = \sum_{k\neq l} J^2_{lk}$ is replaced with its expectation $(N-1)N^{-1}J^2 \simeq J^2$ using the law of large numbers.

Notice that the fixed point condition of eqs. (A·3) and (A·4) is in agreement with the 1RSB analogue to the Thouless–Anderson–Palmer equation of the SK model.[3,21] This demonstrates the consistency of SP with the 1RSB solution in conventional replica theory.

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