Unifying Message Passing Algorithms Under the Framework of Constrained Bethe Free Energy Minimization

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Abstract—Variational message passing (VMP), belief propagation (BP) and expectation propagation (EP) have found their wide uses in complex statistical signal processing problems. In addition to view them as a class of algorithms operating on graphical models, this paper unifies them under an optimization framework, namely, Bethe free energy minimization with differently and appropriately imposed constraints. This new perspective in terms of constraint manipulation can offer additional insights on the connection between message passing algorithms and it is valid for a generic statistical model. It also founds a theoretical framework to systematically derive message passing variants. Taking the sparse Bayesian learning (SBL) problem as an example, a lowcomplexity EP variant can be obtained by simple constraint reformulation, delivering better estimation performance with lower complexity than the standard EP algorithm. Furthermore, we can resort to the framework for systematic derivation of hybrid message passing for complex inference tasks. A hybrid message passing algorithm is exemplarily derived for joint sparse signal reconstruction and statistical model learning. It achieves near-ideal inference performance with manageable complexity.

Index Terms—Statistical inference, Bethe free energy, message passing algorithms, constrained optimization.

I. INTRODUCTION

Many signal processing problems can be formulated as the following: One aims at an estimate of a latent random variable x given the realization of a statistically related observable random variable y. It is a statistical inference task. If one has the access to the likelihood function p(y|x)and the prior density p(x) of x, the inference task can be theoretically performed under the Bayesian framework. Namely, the a-posteriori density $p(x|y) \propto p(y|x)p(x)$, from the Bayesian viewpoint, provides a complete summary of the uncertainty of x given the knowledge of y, permitting inference under various criteria, e.g., minimum mean square error (MMSE) $\hat{x} = E[x|y]$, or maximum a-posteriori (MAP) $\hat{x} = \arg \max_{x} p(x|y)$. Considering x and y as the input and output of a system, the a-posteriori density effectively represents a mathematical model that describes the inputoutput statistical dependence. The MMSE and MAP estimate are then statistical properties of x derived from this model.

In many applications, it will be too complex to evaluate $p(\boldsymbol{x}|\boldsymbol{y})$ or to derive statistical properties with respect to it. The reason could be a too large feasible space of \boldsymbol{x} , or the form of $p(\boldsymbol{x}|\boldsymbol{y})$ is analytically intractable. In such cases, we have to resort to some form of approximations. They generally fall into

two classes, i.e., deterministic and stochastic approximations. As mentioned in [1], [2], stochastic approximations, e.g., the Markov Chain Monte Carlo (MCMC) technique, tend to be more computationally demanding. Aiming at large-scale systems, here we consider a family of deterministic approximations termed variational Bayesian inference.

Briefly, variational Bayesian inference attempts to approximate p(x|y) by an alternative density $\hat{b}(x)$. By constraining the form of $\hat{b}(x)$, one can ensure the mathematical tractability of deriving statistical properties on top of it. On the other hand, one shall ensure sufficient approximation accuracy to generate right inference. To this end, the Kullback-Leibler divergence (a.k.a. relative entropy), quantifying the difference between a given density pair, is used here. Limiting to a family \mathcal{Q} of densities in the desired form, $\hat{b}(x)$ is chosen to yield the minimal Kullback-Leibler divergence with respect to p(x|y) [3]. In the context of physics, such an optimization problem is also known as variational free energy minimization (a.k.a. Gibbs free energy minimization) [4].

A. Overview of message passing algorithms

There are two well-accepted approaches to construct the specialized density family Q. Firstly, the mean field approach defines it as a set of fully factorisable densities. For solving the problem, variational message passing (VMP) [5] (a.k.a. mean field algorithm) is an iterative solution. Here, we note that the expectation maximization (EM) algorithm initially introduced to solve the maximum likelihood (ML) estimation problem [6] can be viewed as a special case of VMP. It additionally forces the densities to be Dirac-delta functions which are parameterizable by a single parameter.

The second approach constructs \mathcal{Q} by exploiting the factorization of $p(\boldsymbol{x}|\boldsymbol{y})$ or $p(\boldsymbol{x},\boldsymbol{y}).^2$ The variational free energy is then approximated by the so-called Bethe free energy [4], which can be minimized by belief propagation (BP) [7]. However, BP is not well suited to accomplish tasks that involve continuous random variables, e.g., synchronization and channel estimation in communications systems. To tackle this issue, expectation propagation (EP) adds one step to BP,

¹Here we note that no single approximation technique, neither deterministic nor stochastic, outperforms all others on all problems. In fact, both types of approximations are broad enough research topics to be studied on their own.

²Here, the density p(y) of y involved in p(x, y) = p(x|y)p(y) can be treated as a constant as it is not a function of the latent variable x.

i.e., projecting the beliefs onto a specific function family for analytical tractability [8].

In short, the above mentioned message passing algorithms are approximate solutions to variational free energy minimization. They have been widely applied in solving challenging signal processing problems that are in systems of large dimensions. In the following, we list a number of application examples.

In the context of large-scale estimation and detection, BP and its variants were applied for large-scale multiuser detection when non-orthogonal multiple access techniques are in use, e.g., [9], [10], and also for large-scale multiple-input multiple-output (MIMO) detection, e.g., [11], [12]. As a classic technique for multiuser detection, MMSE with iterative cancellation can be systematically derived from the EP framework [13]. In [14], an EP based iterative receiver was developed for joint channel estimation and decoding for massive MIMO systems using the orthogonal frequency division multiplexing (OFDM) waveform. We applied EP for jointly equalizing the inter-symbol, inter-carrier and interantenna interferences that are experienced by a non-orthogonal multicarrier waveform termed generalized frequency division multiplexing (GFDM) in a MIMO setup [15].

Approximate message passing (AMP) was developed in [16] and generalized by [17] (thereby termed GAMP) for recovering sparse input signal of a linear under-determined system. They exhibit intrinsic connections to EP in the large system limit, e.g., circumventing matrix inversion of EP with the aid of the self-averaging method [18] or neglecting high-order terms while computing EP messages [19].³ Due to the low complexity, they have become pragmatic alternatives to BP and EP for large-scale estimation and detection, e.g., [20]–[24]. Under an i.i.d. MIMO Gaussian channel, the optimality of GAMP for large-scale MIMO detection was assessed in [25].

Large-scale sparse signal reconstruction is relevant to communication systems that are under-determined, e.g., the active user detection problem in massive machine-type communication (mMTC) and channel estimation problem in mmWave broadband communication. Among different kinds of techniques, one class based on the Bayesian framework is termed sparse Bayesian learning (SBL). Both VMP (including its special case EM) and GAMP are applicable [21], [26], [27]. Therefore, they have been applied in the literature for estimating sparse channels, e.g., [28]–[30], and also for active user detection on random access channels [31].

Apart from practical applications of message passing algorithms for signal processing problems, theoretical understanding on them has also been an important research problem in different fields. The convergence of BP is not guaranteed. To understand its convergence behavior, one class of works interprets it as an instance of fixed-point iteration. Its fixed points correspond to the stationary points of the constrained Bethe free energy, e.g., [32]. Another class of works is devoted to rephrase it as an iterative information projection algorithm using information geometry, e.g., [33]. Furthermore,

there are two analytical tools developed for tracking the iterative process of BP. One is to model it as a discretetime nonlinear dynamical system, e.g., [34]. The other is a statistical approached called density evolution, e.g., [35]. Extrinsic information transfer (EXIT) charts developed by ten Brink in [36] attempt to track the density evolution by a onedimensional parameter. Similar to BP, EP converges in many practical cases, but not always. Given their tight connection, the convergence analysis of EP can be analogously treated, e.g., [37], [38]. Different to BP and EP, VMP is guaranteed to converge, but it may terminate on a local optimum [5]. GAMP recently has attracted considerable research interest due to its good performance and low complexity in estimating a random vector based on the observation of its large-scale linear transformation. The convergence behavior of GAMP is well studied for large i.i.d. linear transformation matrices [39]. However, the extension to a general linear transformation matrix under arbitrary statistical models is not trivial. In [40] sufficient conditions are derived for the convergence of a damped version of GAMP in the case of Gaussian distributions.

B. Motivation and contribution of this work

From the above state-of-the-art overview, we notice that most existing theoretical works investigated message passing algorithms individually, even though their heuristic combinations have already found its applications, e.g., [41]–[45].

With a joint use of the mean field and Bethe approaches for approximating the variational free energy, VMP and BP were merged in [46]. Apart from that, to our best knowledge, little results have been reported on unifying message passing algorithms in a single mathematical framework. This motivates our work, aiming at an optimization framework that can link them with a generic statistical model.

In this paper, we construct the framework based on constrained Bethe free energy minimization. Namely, the Bethe free energy, as an approximation to the variational free energy, is used as the objective function. On top of it, we introduce a set of constraint formulation methods such that BP, EP, and VMP can be analytically attributed to corresponding constrained Bethe free energy minimization. From this novel perspective of constraint manipulation, we can systematically derive new message passing variants, in particular hybrid ones for complex statistical inference problems. It is noted that under our framework BP and VMP can be combined in a more generalized manner than that in [46]. To further ease the understanding and implementation of hybrid message passing, the conventional factor graph is adapted accordingly for visualization.

Furthermore, we exemplarily address a classic SBL problem under the developed framework. Through constraint reformulation, we successfully derive an EP variant that outperforms the standard EP algorithm in both performance and complexity. Interestingly, it exhibits high similarity to AMP. Without the assumption of knowing the statistical model, a hybrid message passing algorithm is obtained for joint sparse signal reconstruction and statistical model learning. Such algorithm can approach the performance that is only accessible with perfect knowledge of the statistical model.

³The EP algorithms considered by the work [18] and [19] are with respect to two different types of factorization on the same objective function.

C. Structure of the paper

The remainder of this paper is organized as follows: Section II lists some notes on measure, probability and exponential family that are the relevant background information of the paper. Section III introduces the message passing algorithms, i.e., BP, EP and VMP, for variational free energy minimization, respectively. The key part of the paper is given in Section IV. It describes the optimization framework that can unify BP, EP and VMP. In Section V, a SBL problem is considered as an example for practicing the developed framework. Finally, a conclusion and outlook are presented in Section VI.

II. SOME NOTES ON MEASURE, PROBABILITY AND EXPONENTIAL FAMILY

A. Measure space

An ordered pair (\mathcal{X},Ω) , where \mathcal{X} is a set and Ω is a σ -algebra over \mathcal{X} , is called a measurable space. On (\mathcal{X},Ω) , a measure μ is defined as a certain type of functions from the σ -algebra Ω to $[0,\infty]$ (In the extended real system, ∞ is considered to be attainable.). With $\mu(\Omega) < \infty$, the measure μ is finite; otherwise, it is σ -finite. The triplet (\mathcal{X},Ω,μ) forms a measure space. Let ν also be a measure on (\mathcal{X},Ω) . It is absolutely continuous with respect to μ if $\mu(\omega) = 0$ implies $\nu(\omega) = 0$ for any $\omega \in \Omega$. We compactly denote such relation as $\nu \ll \mu$ and state that ν is dominated by μ .

Radon-Nikodym (RN) theorem: Let $(\mathcal{X}, \Omega, \mu)$ be a σ -finite measure space and ν is a measure with $\nu \ll \mu$. Then, there exists a non-negative function f subject to

$$\nu(\omega) = \int_{\Omega} p(\boldsymbol{x})\mu(\mathrm{d}\boldsymbol{x}) \quad \forall \, \omega \in \Omega. \tag{1}$$

Here, p(x) is called the density of ν with respect to the measure μ . It is also the RN derivative of ν with respect to μ .

B. Probability

A measure space (\mathcal{X},Ω,ν) is a probability space if $\nu(\mathcal{X})=1$. In this case ν is termed a probability measure. On (\mathcal{X},Ω,ν) , a measurable function $g:\mathcal{X}\mapsto\mathbb{R}^s$ yields a random variable. With $\nu\ll\mu$, the expectation of g with respect to the probability measure ν , i.e., $\mathrm{E}_{\nu}[g]=\int g(x)\nu(\mathrm{d}x)$, can then be computed from the integral of the product g(x)p(x) with respect to the underlying dominating measure μ

$$E_{\nu}[\mathbf{g}] = \int \mathbf{g}(\mathbf{x}) p(\mathbf{x}) \mu(\mathrm{d}\mathbf{x}). \tag{2}$$

For two probability measures ν , ν' on the same space and $\nu' \ll \nu$, the relative entropy between ν and ν' with respect to the common dominating measure μ is defined as

$$D\left[\nu\|\nu'\right] = E_{\nu}\left[\ln\frac{\nu(\mathrm{d}\boldsymbol{x})}{\nu'(\mathrm{d}\boldsymbol{x})}\right] = \int\left[\ln\frac{p(\boldsymbol{x})}{p'(\boldsymbol{x})}\right]p(\boldsymbol{x})\mu(\mathrm{d}\boldsymbol{x}) \quad (3)$$

where p(x) and p'(x) are the densities of ν and ν' with respect to the measure μ , respectively.

Very often μ will be either the Lebesgue measure in which case $\mu(dx)$ reduces to dx and the integrals in above can

⁴In the literature, random variables quite often are complex-valued. We can view the target space \mathbb{C}^s as \mathbb{R}^{2s} .

be handled using standard calculus, or counting measure in which case the integrals reduce to summations. When it is clear from the context, in this work we will interchangeably use the notations for the probability measure and its density, e.g., $D[\nu||\nu'|] = D[p||p'|]$ and $E_{\nu}[\cdot] = E_{p}[\cdot]$.

C. Exponential family

Exponential families are classes of probability measures constructed from a dominating measure μ and a sufficient statistic. For instance, normal and Poisson distributions are typical exponential families. The former is with respect to the Lebesgue measure, while the measure of the latter is the outcome of modulating the counting measure with h(x) = 1/x!.

Formally, let $(\mathcal{X}, \Omega, \mu)$ be a measure space and $t : \mathcal{X} \mapsto \mathbb{R}^s$ be an s-dimensional statistic that does not satisfy any linear constraints. A collection of densities defined on the measure space is given by

$$Q = \left\{ p(\boldsymbol{x}; \boldsymbol{\eta}) = e^{\boldsymbol{\eta}^T \boldsymbol{t}(\boldsymbol{x}) - \Phi(\boldsymbol{\eta})} : \boldsymbol{\eta} \in \mathcal{H} \right\} \text{ with}$$

$$\Phi(\boldsymbol{\eta}) = \ln \int e^{\boldsymbol{\eta}^T \boldsymbol{t}(\boldsymbol{x})} \mu(\mathrm{d}\boldsymbol{x}), \quad \mathcal{H} = \{ \boldsymbol{\eta} : \Phi(\boldsymbol{\eta}) < \infty \}. \quad (4)$$

In above, η is the natural parameter in the natural parameter space \mathcal{H} and $\Phi(\eta)$ is its log-partition function. Each density $p(x;\eta)$ in the family defines a measure $\nu_{\eta} \ll \mu$ via $\nu_{\eta}(\omega) = \int_{\omega} p(x;\eta) \mu(\mathrm{d}x)$. Furthermore, $\theta = \mathrm{E}_{p_{\eta}}[t(x)]$ is the moment parameter in accordance with the density $p(x;\eta)$ parameterized by the natural parameter η .

If Q is an exponential family with minimal representation, then there is a bijective mapping ψ between the natural parameter η and the moment parameter θ , i.e.,

$$\eta = \psi(\theta) \quad \text{and} \quad \theta = \psi^{-1}(\eta).$$
(5)

Consider the m-projection of a density p' onto Q

$$\hat{p} = \arg\min_{p \in \mathcal{Q}} D[p'||p] = \operatorname{Proj}_{\mathcal{Q}}(p'). \tag{6}$$

The optimal solution \hat{p} as a member of the exponential family Q has the moment parameter $\hat{\theta} = \mathrm{E}_{p'}[t(x)]$. Relying on the bijective mapping $\psi(\cdot)$, one can eventually find the form of \hat{p} by moment matching to p' followed by computing the natural parameter from $\eta = \psi(\hat{\theta})$.

From the exponential family Q, one can construct a socalled *unnormalized* exponential family Q^u made of the set of functions

$$p^{\mathrm{u}}(\boldsymbol{x};\boldsymbol{\eta}) = e^{\boldsymbol{\eta}^T \boldsymbol{t}(\boldsymbol{x})}.$$
 (7)

The family Q^u is closed under multiplication and division. It is noted that its members are in general no densities and some of them may not be normalizable, i.e., its integral with respect to the measure μ diverges.

III. VARIATIONAL FREE ENERGY MINIMIZATION

Consider a target non-negative function f(x) with the following factorization

$$f(\boldsymbol{x}) = \prod_{a} f_a(\boldsymbol{x}_a), \tag{8}$$

⁵For compact notation, here we absorb h(x) into the measure μ .

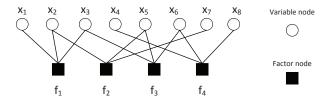


Figure 1: An illustration of a factor graph that depicts the function $f(\mathbf{x}) = f_1(x_1, x_2, x_3) f_2(x_2, x_5, x_7) f_3(x_3, x_5, x_6) f_4(x_4, x_6, x_8)$.

where the argument x_a of the factor function $f_a(x_a)$ is a subvector of the vector x. One graphical model to describe f(x) and its corresponding factorization is termed factor graph [47]. Namely, each entry of x is depicted as a variable node, while factor nodes are used for denoting the factor functions $\{f_a\}$. One factor node is connected to a set of variable nodes that are its arguments, e.g., Fig. 1.

The message passing algorithms, i.e., BP, EP and VMP, are usable for computing the marginals $\{f(x_i)\}$ of f(x). In many practical cases, however, only approximate marginals are attainable. In this section, we aim at linking them to one type of optimization problems termed variational free energy minimization [4]. Such link provides a theoretical understanding on their usability for approximate marginalization.

Consider a density p(x) that is constructed from f(x) as

$$p(\mathbf{x}) = \frac{1}{Z} f(\mathbf{x})$$
 with $Z = \int f(\mathbf{x}) \mu(\mathrm{d}\mathbf{x})$. (9)

The measure μ depends on the space that the whole system concerns. Using a trial density b(x), we define a new function

$$F(b) = \int b(\mathbf{x}) \ln b(\mathbf{x}) \mu(\mathrm{d}\mathbf{x}) - \int b(\mathbf{x}) \ln f(\mathbf{x}) \mu(\mathrm{d}\mathbf{x})$$
$$= -\ln Z + \mathrm{D}[b||p]. \tag{10}$$

In physics, it is known as the variational free energy of the system and $-\ln Z$ is termed Helmholtz free energy. By minimizing F(b) over all possibilities of the trial density $b(\boldsymbol{x})$, the solution is straightforward, i.e., $\hat{b}(\boldsymbol{x}) = p(\boldsymbol{x})$ and $F(\hat{b}) = -\ln Z$. Therefore, it is an exact procedure to compute $-\ln Z$ and recover $p(\boldsymbol{x})$ through F(b) minimization.

However, such a variational free energy minimization problem is not always tractable. One common approximate solution is to limit the feasible set of b(x) to a density family Q, i.e.,

$$\hat{b}(\boldsymbol{x}) = \arg\min_{b \in \mathcal{Q}} F(b). \tag{11}$$

Apparently, the choice of $\mathcal Q$ determines the fidelity and tractability of the resulting approximation $p(x) \approx \hat b(x)$ and $F(\hat b) \approx -\ln Z$. Solving (11), one can further derive approximations to the marginals $\{f(x_i)\}$ based on the knowledge of $\{\hat b(x_i)\}$ and $F(\hat b)$. In the following, we will show how to construct $\mathcal Q$ such that BP, EP and VMP are iterative solutions to the corresponding minimization problem.

A. Mean field approximation

The mean field approximation to the variational free energy minimization problem (11) constructs Q as a collection of

fully factorizable densities, i.e.,

$$b(\boldsymbol{x}) = \prod_{i} b_{i}(x_{i}) \quad \forall \ b(\boldsymbol{x}) \in \mathcal{Q}.$$
 (12)

With such a family, the primary problem (11) becomes

$$\{\hat{b}_i(x_i)\} = \arg\min_{\{b_i(x_i)\}} F\left(\prod_i b_i(x_i)\right). \tag{13}$$

The problem (13) is only convex with respect to an individual $b_i(x_i)$ while the others are considered to be fixed. This identification suggests to successively optimize one of $\{b_i(x_i)\}$ from solving a convex optimization problem while fixing the others. Such a process guarantees to reduce the objective function after each step until a local minimum or a saddle point is reached.

Solving the above-specified convex optimization problem, we obtain the following update equation for $b_i(x_i)$

$$b_i(x_i) \propto e^{\int \ln f_a(\boldsymbol{x}_a) \prod_{i' \in \mathcal{I}_a \setminus i} b_{i'}(x_{i'}) \mu(\mathrm{d}\boldsymbol{x}_{a \setminus i})},$$
 (14)

where \mathcal{I}_a stands for the index set of the entries of \boldsymbol{x}_a in the complete vector \boldsymbol{x} and the integral is with respect to \boldsymbol{x}_a except x_i . With proper initialization, $\{b_i(x_i)\}$ shall then be successively and iteratively updated as (14) until convergence.

We note that eq. (14) is identical to the message update rule of VMP [5], implying VMP as an iterative solution to (13). From the construction of \mathcal{Q} used in (13), one can infer that full factorization of the trial density b(x) is a good approximation when the target density p(x) indicates low statistical correlation among the variables $\{x_i\}$. In other words, VMP is expected to be a good approximate inference solution in such cases.

B. Bethe approximation

The key step of the Bethe approximation to (11) is to introduce the auxiliary densities $\{b_a(x_a)\}$ and $\{b_i(x_i)\}$ in accordance with the factor functions $\{f_a(x_a)\}$ and the variables $\{x_i\}$, respectively. If the factor graph of f(x) has a tree structure, we can define $\mathcal Q$ such that any $b(x) \in \mathcal Q$ follows

$$b(\boldsymbol{x}) = \frac{\prod_{a} b_{a}(\boldsymbol{x}_{a})}{\prod_{i} [b_{i}(\boldsymbol{x}_{i})]^{A_{i}-1}},$$
(15)

where A_i stands for the cardinality of the set A_i . It is noted that $\{b_a(\boldsymbol{x}_a), b_i(x_i)\}$ are marginals of $b(\boldsymbol{x})$. Therefore, they shall fulfill the marginalization consistency constraints⁶

$$\int b_a(\mathbf{x}_a)\mu(\mathrm{d}\mathbf{x}_{a\backslash i}) = b_i(x_i) \quad \forall i \,\forall a \in \mathcal{A}_i.$$
 (16)

Substituting (15) back into (10) and exploiting the fact that $\{b_a(\boldsymbol{x}_a), b_i(x_i)\}$ are marginals of $b(\boldsymbol{x})$, we obtain the Bethe free energy

$$F_{\mathrm{B}}(b_a, b_i) = \sum_{a} \int b_a(\boldsymbol{x}_a) \ln \frac{b_a(\boldsymbol{x}_a)}{f_a(\boldsymbol{x}_a)} \mu(\mathrm{d}\boldsymbol{x}_a)$$
$$-\sum_{i} (A_i - 1) \int b_i(x_i) \ln b_i(x_i) \mu(\mathrm{d}x_i). \quad (17)$$

⁶Since the normalization and non-negative constraints are default setting for any valid density, we will not list them explicitly for simplicity.

The optimal solution $\hat{b}_i(x_i)$ of

$$\min_{b_a,b_i} F_{\rm B}(b_a,b_i) \quad \text{s.t.} (16)$$

is exactly equal to $p(x_i)$ [4] and it can be found by BP.

If the factor graph contains cycles, we can still formulate and solve the constrained Bethe free energy minimization problem as given in (18). However, the obtained results are only approximations. The authors of [4] have proven the fixed points of BP satisfy the necessary conditions for being an interior optimum (local minimum or maximum) of (18) in the discrete case. In [32], stable fixed points of BP were shown to be local minima. Therefore, one can regard BP as an iterative solution to the problem (18).

On top of the factor graph, we can describe BP by specifying two rules for computing messages that are: i) from a factor node f_a to a variable node x_i and ii) in the reverse direction. In equations, they are respectively given as

$$m_{a \to i}(x_i) \propto \int f_a(\boldsymbol{x}_a) \prod_{i' \in \mathcal{I}_a \setminus i} n_{i' \to a}(x_{i'}) \mu(\mathrm{d}\boldsymbol{x}_{a \setminus i})$$
 (19)

$$n_{i \to a}(x_i) = \prod_{a' \in \mathcal{A}_i \setminus a} m_{a' \to i}(x_i), \tag{20}$$

where A_i collects the indices of the factor functions that have x_i as one of their arguments. The integral in (19) represents the local marginalization associated to the factor node f_a and with respect to x_i .

After proper initialization, the messages $\{m_{a\to i}(x_i)\}$ and $\{n_{i\to a}(x_i)\}$ can be iteratively and successively updated, representing a message passing flow on the factor graph [47]. After a termination condition is satisfied, the target $f(x_i)$ is approximated by

$$b(x_i) \propto m_{a \to i}(x_i) n_{i \to a}(x_i) \qquad \forall a \in \mathcal{A}_i$$

$$\propto \prod_{a' \in \mathcal{A}_i} m_{a' \to i}(x_i). \tag{21}$$

Here we omit the specification of the normalization terms in above as they can be case-dependent and often play a negligible role in computation.

Since the marginalization consistency constraint (16) can often be too complex to yield tractable messages $\{m_{a\to i}(x_i), n_{i\to a}(x_i)\}$, one natural solution is constraint relaxation, such as simplifying it to moment matching [37], i.e.,

$$\mathbf{E}_{b_a}[\boldsymbol{t}(x_i)] = \mathbf{E}_{b_i}[\boldsymbol{t}(x_i)],\tag{22}$$

where $t(x_i)$ stands for the sufficient statistics of x_i that are of concern. As shown in [37], the message update rule of EP can be derived from solving the stationary point equations of the Bethe free energy under the constraint (22). The messages belong to the (unnormalized) exponential family characterized by $t(x_i)$. Specifically, the message update rules in (20) and (21) also apply for EP except (19) changes to

$$m_{a \to i}(x_i) \propto \frac{\operatorname{Proj}_{\mathcal{Q}}\left(c \int f_a(\boldsymbol{x}_a) \prod_{i' \in \mathcal{I}_a} n_{i' \to a}(x_{i'}) \mu(\mathrm{d}\boldsymbol{x}_{a \setminus i})\right)}{n_{i \to a}(x_i)}.$$
(23)

In above, Q stands for the exponential family characterized by

 $t(x_i)$ and the parameter c is chosen to make the argument of $\operatorname{Proj}_{\mathcal{Q}}(\cdot)$ a density of x_i . We note that $m_{a \to i}(x_i), n_{i \to a}(x_i)$ are typically initialized as and thereby remain as members of the unnormalized family \mathcal{Q}^{u} . It may happen that normalization cannot make them members of \mathcal{Q} as they are not normalizable. In practical applications, empirical adjustments on the messages are often made whenever such situation takes place, e.g., [13], [43], [48].

The advantage of limiting the messages to an (unnormalized) exponential family is that the computational complexity of integration and multiplication becomes tractable all the time. Therefore, EP is often a pragmatic alternative to BP when the latter becomes intractable. On the other hand, this will degrade the result accuracy. In short, there exists a tradeoff in choosing the exponential family Q.

IV. BETHE APPROXIMATION BASED OPTIMIZATION FRAMEWORK

From the previous section, we have noticed that both BP and EP aim to minimize the same Bethe free energy but under differently formalized constraints. This inspires us to develop a mathematical framework that permits to systematically derive message passing variants through constraint manipulation. The Bethe free energy as the objective function is a natural choice. On top of it, we first show how to formulate the constraints such that VMP can be analytically attributed to the corresponding constrained Bethe free energy minimization. From this novel perspective of unifying BP, EP and VMP via constraint manipulation, we subsequently derive hybrid message passing variants in a structured manner. Finally, we introduce a modification onto the conventional factor graph for visualizing hybrid message passing.

A. VMP under constrained Bethe free energy minimization

Even though VMP is commonly interpreted as an iterative scheme to solve (13), the problem (13) is actually equivalent to adding the following constraint to the Bethe problem (18)

$$b_a(\mathbf{x}_a) = \prod_{i \in \mathcal{I}_a} b_a(x_i) \quad \forall \, a, \tag{24}$$

where $b_a(x_i)$ is a marginal of $b_a(x_a)$. The above equation effectively indicates $b_a(x_a)$ is fully factorizable. In doing so the marginalization consistency constraints become trivial to fulfill. Therefore, we can interpret (24) as one way of constraint manipulation to simplify the classic Bethe problem. On the other hand, it will degrade the accuracy for approximate marginalization as the correlation of variables is overlooked.

Specifically, the fulfillment of both constraint (16) and (24) implies $b_a(x_i) = b_i(x_i)$. Expressing $b_a(x_a)$ by means of $\{b_i(x_i)\}$, the optimization space of (18) can be reduced from (b_a,b_i) to b_i , namely replacing $b_a(x_a)$ by $\prod_{i\in\mathcal{I}_a}b_i(x_i)$. On this basis, the objective Bethe free energy then becomes

$$\sum_{i} \int b_{i}(x_{i}) \ln b_{i}(x_{i}) \mu(\mathrm{d}x_{i})$$
$$-\sum_{a} \int \prod_{i \in \mathcal{I}_{a}} b_{i}(x_{i}) \ln f_{a}(\boldsymbol{x}_{a}) \mu(\mathrm{d}\boldsymbol{x}_{a}), \qquad (25)$$

which is identical to the objective function in (13) under the factorization of f(x) in (8). In short, the optimization problem

$$\min_{b_a, b_i} F_{\mathcal{B}}(b_a, b_i) \quad \text{s.t.} (16), (24)$$

is equivalent to (13). Therefore, VMP is usable for solving it. Furthermore, instead of applying (24) for every possible a, we can select a subset, selectively ignoring the correlation of variables. This straightforwardly coincides with the optimization problem defined in [46]. However, different to our line of argumentation, the authors of [46] constructed the problem by partitioning the factor functions $\{f_a\}$ into two classes, and then applying the mean field and Bethe approximations respectively to approximate the variational free energy in (10). In [46] a combination of VMP and BP was then derived as an iterative solution. Namely, the beliefs originated from the factor node in the mean field (Bethe) class follow the rule of VMP (BP).

With our view of constraint manipulation, it is possible to further generalize such a hybrid BP-VMP by replacing (24) with the following factorization constraint

$$b_a(\mathbf{x}_a) = \prod_v b_{a,v}(\mathbf{x}_{a,v}), \tag{27}$$

where $x_{a,v}$ is a subvector of x_a and its entries in the complete vector x are recorded by the index set $\mathcal{I}_{a,v}\subseteq\mathcal{I}_a$. It is noted that $\{\mathcal{I}_{a,v}\}$ are mutually disjoint. Compared to (24), such formulated constraint imposes a partial rather than full factorization, thereby permitting to retain a part of correlation in $b_a(x_a)$. As this implies that the associated factor node f_a belongs to neither the mean field nor Bethe class in a general sense, the approach in [46] is not applicable for this case. On the other hand, we can readily form a Bethe problem by combining (27) with the marginalization consistency constraints (16). In the following, we will systematically derive an iterative solution and reveal its connection with BP and VMP. Under the framework of constrained Bethe free energy minimization, the obtained algorithm is not just an empirical combination of VMP and BP that operates on the factor graph.

B. Hybrid VMP-BP

Formally, the optimization problem is written as

$$\min_{b_a, b_i} F_{\rm B}(b_a, b_i)$$
 s.t. (16) and (27). (28)

In the sequel, we resort to five steps for solving it.

Firstly, we can get rid of the constraint (27) by interpreting it as a variable interchange, namely substituting $b_a(x_a)$ with $\prod_v b_{a,v}(x_{a,v})$ in the objective function $F_{\rm B}(b_a,b_i)$ and the other constraint (16). This yields

$$F_{\mathrm{B}}(b_{a,v}, b_{i})$$

$$= \sum_{a} \int \prod_{v} b_{a,v}(\boldsymbol{x}_{a,v}) \ln \frac{\prod_{v} b_{a,v}(\boldsymbol{x}_{a,v})}{f_{a}(\boldsymbol{x}_{a})} \mu(\mathrm{d}\boldsymbol{x}_{a})$$

$$- \sum_{i} (A_{i} - 1) \int b_{i}(x_{i}) \ln b_{i}(x_{i}) \mu(\mathrm{d}x_{i}), \tag{29}$$

while the marginalization constraint (16) becomes

$$b_{a,v(i)}(x_i) = b_i(x_i) \quad \forall i \, \forall a \in \mathcal{A}_i$$
 (30)

with v(i) giving $i \in \mathcal{I}_{a,v(i)}$.

Secondly, we take the method of Lagrange multipliers to solve the problem

$$\min_{b_{a,v},b_i} F_{\mathcal{B}}(b_{a,v},b_i) \quad \text{s.t.} (30). \tag{31}$$

The Lagrange function is written as

$$L_{\rm B} = F_{\rm B}(b_{a,v}, b_i) + \sum_{(a,v)} \zeta_{a,v} [E_{b_{a,v}}(1) - 1] + \sum_{i} \zeta_{i} [E_{b_{i}}(1) - 1] + \sum_{i} \sum_{a \in A_{i}} \sum_{x_{i}} \lambda_{i \to a}(x_{i}) [b_{i}(x_{i}) - b_{a,v(i)}(x_{i})].$$
(32)

In above, we introduce the Lagrange multipliers $\{\zeta_i, \zeta_{a,v}\}$ for the implicit normalization constraints on the densities $\{b_{a,v}, b_i\}$, while the additional marginalization consistency constraint (30) is associated to the Lagrange multipliers $\{\lambda_{i\to a}(x_i)\}$. Here we omit the non-negative constraints on $\{b_{a,v}, b_i\}$ as later we will find that they are inherently satisfied by any interior stationary point of the Lagrange function.

Thirdly, let us now take the first-order derivatives of $L_{\rm B}$ with respect to $\{b_{a,v},b_i\}$ and $\{\lambda_{i\to a}(x_i),\zeta_i,\zeta_{a,v}\}$ equal to zeros. By solving the equations, we can express $\{b_{a,v},b_i\}$ as

$$b_{a,v}(\boldsymbol{x}_{a,v}) = e^{-1-\zeta_{a,v}} \prod_{i \in \mathcal{I}_{a,v}} e^{\lambda_{i \to a}(\boldsymbol{x}_i)}$$
$$\cdot e^{\int \prod_{v' \neq v} b_{a,v'}(\boldsymbol{x}_{a,v'}) \ln f_a(\boldsymbol{x}_a) \mu(\mathrm{d}\boldsymbol{x}_{a,\setminus v})} \qquad (33)$$

$$b_i(x_i) = e^{\frac{\zeta_i}{A_i - 1} - 1 + \frac{1}{A_i - 1} \sum_{a \in A_i} \lambda_{i \to a}(x_i)}, \tag{34}$$

where the Lagrange multipliers must be a solution of the following equations

$$e^{\zeta_{a,v}+1} = \int \mu(\mathrm{d}\boldsymbol{x}_{a,v}) \prod_{i \in \mathcal{I}_{a,v}} e^{\lambda_{i \to a}(x_{i})} \cdot \left[e^{\int \prod_{v' \neq v} b_{a,v'}(\boldsymbol{x}_{a,v'}) \ln f_{a}(\boldsymbol{x}_{a}) \mu(\mathrm{d}\boldsymbol{x}_{a,\setminus v})} \right]$$
(35)
$$e^{-\frac{\zeta_{i}}{A_{i}-1}+1} = \int e^{\frac{1}{A_{i}-1} \sum_{a \in A_{i}} \lambda_{i \to a}(x_{i})} \mu(\mathrm{d}x_{i})$$
(36)
$$e^{\frac{\zeta_{i}}{A_{i}-1} + \frac{1}{A_{i}-1} \sum_{a \in A_{i}} \lambda_{i \to a}(x_{i})}$$
(37)

$$= e^{-\zeta_{a,v}} \int \mu(\mathrm{d}\boldsymbol{x}_{a,v\setminus i}) \prod_{i\in\mathcal{I}_{a,v}} e^{\lambda_{i\to a}(x_i)} \cdot \left[e^{\int \prod_{v'\neq v} b_{a,v'}(\boldsymbol{x}_{a,v'}) \ln f_a(\boldsymbol{x}_a) \mu(\mathrm{d}\boldsymbol{x}_{a,\setminus v})} \right]. \tag{37}$$

As we can observe, $\{b_{a,v}, b_i\}$ in the form of (33) and (34) are non-negative functions.

Fourthly, attempting to solve the equations of the Lagrange multipliers, the key is to determine $\{\lambda_{i\to a}(x_i)\}$ from (37), while $\{\zeta_i, \zeta_{a,v}\}$ can be readily determined by them according to (35) and (36). Starting from simplifying the notations, we introduce a number of auxiliary variables given as

$$\lambda_{a \to i}(x_i) = \frac{1}{A_i - 1} \sum_{a' \in A_i} \lambda_{i \to a'}(x_i) - \lambda_{i \to a}(x_i)$$
 (38)

$$m_{a \to i}(x_i) = e^{\lambda_{a \to i}(x_i)} \tag{39}$$

$$n_{i \to a}(x_i) = e^{\lambda_{i \to a}(x_i)}. (40)$$

Using them, the equation (37) can be alternatively written as

$$m_{a \to i}(x_i) \propto \int \mu(\mathrm{d}\boldsymbol{x}_{a,v \setminus i}) \prod_{i' \in \mathcal{I}_{a,v \setminus i}} n_{i' \to a}(x_{i'}) \cdot \left[e^{\int \prod_{v' \neq v} b_{a,v'}(\boldsymbol{x}_{a,v'}) \ln f_a(\boldsymbol{x}_a) \mu(\mathrm{d}\boldsymbol{x}_{a \setminus v})} \right]$$
(41)

$$n_{i \to a}(x_i) = \sum_{a' \in \mathcal{A}_i \setminus a} m_{a' \to i}(x_i). \tag{42}$$

Its solutions yield

$$b_{a,v}(\boldsymbol{x}_{a,v}) \propto \prod_{i \in \mathcal{I}_{a,v}} n_{i \to a}(x_i)$$

$$\cdot e^{\int \prod_{v' \neq v} b_{a,v'}(\boldsymbol{x}_{a,v'}) \ln f_a(\boldsymbol{x}_a) \mu(\mathrm{d}\boldsymbol{x}_{a,\setminus v})} \qquad (43)$$

$$b_i(x_i) \propto \prod_{a \in \mathcal{A}_i} m_{a \to i}(x_i)$$

$$\propto n_{i \to a}(x_i) m_{a \to i}(x_i) \quad \forall a \in \mathcal{A}_i. \qquad (44)$$

After normalization, they correspond to local optima of the constrained Bethe free energy.

Finally, we present a message passing algorithm to solve the Bethe problem (28) by searching for the solutions of (41) and (42). Specifically, the equation (41) and (42) have an identical form to the message update rules of BP given in (19) and (20) if we treat

$$e^{\int \prod_{v'\neq v} b_{a,v'}(\boldsymbol{x}_{a,v'}) \ln f_a(\boldsymbol{x}_a) \mu(\mathrm{d}\boldsymbol{x}_{a \setminus v})}$$
(45)

as a factor function $f'_a(x_{a,v})$ of $x_{a,v}$, while the computation of the above term in (45) essentially follows the rule of VMP given in (14). This observation suggests a combination of VMP and BP for solving the problem. Specifically, with proper initialization of $\{b_{a,v}(\boldsymbol{x}_{a,v})\}\$, we can follow the rules of BP to update $\{m_{a\to i}(x_i), n_{i\to a}(x_i)\}$ followed by using the results to refine $\{b_{a,v}(\boldsymbol{x}_{a,v})\}$ according to (43). The VMPlike computation is a part of the refinement on $\{b_{a,v}(x_{a,v})\}\$ as given in (43).

C. Hybrid VMP-BP-EP

It is known that the marginalization consistency constraint, e.g., as given in (30), can often render the Bethe problem difficult to solve. Very often when the variables are continuous, the marginalization consistency constraints become intractable and this issue cannot be addressed by adding factorization constraints. As mentioned in the previous section, one pragmatic idea is to relax marginalization consistency into weaker moment matching constraints, yielding EP. In this part, we therefore aim at applying this constraint relaxation idea onto the problem (31). As a result, we combine the benefits of factorization and constraint relaxation for easing the classic Bethe problem solely targeted by BP.

Specifically, we choose a subset $\mathcal{I}^{[E]}$ of variables $\{x_i\}$ and relax the marginalization consistency constraints on them into

$$E_{b_{a,v(i)}}[\boldsymbol{t}_i(x_i)] = E_{b_i}[\boldsymbol{t}_i(x_i)] \quad \forall i \in \mathcal{I}^{[E]} \, \forall a \in \mathcal{A}_i.$$
 (46)

It is noted that the sufficient statistic $t_i(x_i)$ for each variable can be different, depending on real cases. The other variables with the index set $\mathcal{I}^{[B]}$ are still under the marginalization consistency constraints

$$b_{a,v(i)}(x_i) = b_i(x_i) \quad \forall i \in \mathcal{I}^{[B]} \, \forall a \in \mathcal{A}_i.$$
 (47)

The two index sets are disjoint and their union makes up the complete index set \mathcal{I} of the variables, i.e., $\mathcal{I}^{[E]} \cap \mathcal{I}^{[B]} = \hat{\emptyset}$ and $\mathcal{I}^{[E]} \cup \mathcal{I}^{[B]} = \mathcal{I}.$

Now, our target problem becomes

$$\min_{b_{a,v},b_i} F_{\rm B}(b_{a,v},b_i) \quad \text{s.t.} (46) \text{ and } (47).$$
 (48)

Analogously, we follow the method of Lagrange multipliers to solve the problem, starting from constructing the Lagrange function as

$$L_{\rm B} = F_{\rm B}(b_{a,v}, b_i) + \sum_{(a,v)} \zeta_{a,v} \left[E_{b_{a,v}}(1) - 1 \right] + \sum_{i} \zeta_i \left[E_{b_i}(1) - 1 \right] + \sum_{i \in \mathcal{I}^{\rm [B]}} \sum_{a \in \mathcal{A}_i} \sum_{x_i} \lambda_{i \to a}(x_i) \left[b_i(x_i) - b_{a,v(i)}(x_i) \right] + \sum_{i \in \mathcal{I}^{\rm [E]}} \sum_{a \in \mathcal{A}_i} \gamma_{i \to a}^T \left[E_{b_i}[t_i(x_i)] - E_{b_{a,v(i)}}[t_i(x_i)] \right].$$
(49)

In addition to $\{\zeta_{a,v}, \zeta_i, \lambda_{i \to a}(x_i)\}$, we associate the moment matching constraints with the Lagrange multipliers $\{\gamma_{i\rightarrow a}\}$. The dimension of each vector $\gamma_{i
ightarrow a}$ is identical to that of the corresponding sufficient statistic $t_i(x_i)$.

Let us subsequently set the first-order derivatives of the Lagrange function with respect to the densities to zeros. In doing so we obtain the density expressions that are in terms of the Lagrange multipliers, namely

$$b_{a,v}(\boldsymbol{x}_{a,v}) = e^{-1-\zeta_{a,v}} \prod_{i \in \mathcal{I}_{a,v}^{[B]}} e^{\lambda_{i \to a}(\boldsymbol{x}_{i})} \prod_{i \in \mathcal{I}_{a,v}^{[E]}} e^{\boldsymbol{\gamma}_{i \to a}^{T} \boldsymbol{t}_{i}(\boldsymbol{x}_{i})}$$
$$\cdot e^{\int \prod_{v' \neq v} b_{a,v'}(\boldsymbol{x}_{a,v'}) \ln f_{a}(\boldsymbol{x}_{a}) \mu(\mathrm{d}\boldsymbol{x}_{a,\setminus v})}$$
(50)

$$b_i(x_i) = e^{\frac{\zeta_i}{A_i - 1} - 1 + \frac{1}{A_i - 1} \sum_{a \in \mathcal{A}_i} \lambda_{i \to a}(x_i)}, \quad \forall i \in \mathcal{I}^{[B]}$$
 (51)

$$b_i(x_i) = e^{\frac{\zeta_i}{A_i - 1} - 1 + \frac{1}{A_i - 1} \sum_{a \in \mathcal{A}_i} \gamma_{i \to a}^T t_i(x_i)}, \quad \forall i \in \mathcal{I}^{[E]}, \quad (52)$$

with $\mathcal{I}_{a,v}^{[\mathrm{E}]} = \mathcal{I}_{a,v} \cap \mathcal{I}^{[\mathrm{E}]}$ and $\mathcal{I}_{a,v}^{[\mathrm{M}]} = \mathcal{I}_{a,v} \cap \mathcal{I}^{[\mathrm{M}]}$. In (52), it is noted that $b_i(x_i)$ is a member of the exponential family Q_i that is characterized by the sufficient statistic $t_i(x_i)$.

By also letting the first-order derivatives of $L_{\rm B}$ with respect to the Lagrange multipliers be zeros, the Lagrange multipliers are constrained to ensure that: 1) the above-expressed densities are normalized to one and 2) they fulfill the constraints (46) and (47). In addition to the variable interchanges introduced in (38), here we include the following three

$$\gamma_{a \to i} = \frac{1}{A_i - 1} \sum_{a' \in A_i} \gamma_{i \to a'} - \gamma_{i \to a}$$
 (53)

$$m_{a \to i}(x_i) = \begin{cases} e^{\lambda_{a \to i}(x_i)} & i \in \mathcal{I}^{[B]} \\ e^{\gamma_{a \to i}^T \mathbf{t}_i(x_i)} & i \in \mathcal{I}^{[E]} \end{cases}$$

$$n_{i \to a}(x_i) = \begin{cases} e^{\lambda_{i \to a}(x_i)} & i \in \mathcal{I}^{[B]} \\ e^{\gamma_{i \to a}^T \mathbf{t}_i(x_i)} & i \in \mathcal{I}^{[E]} \end{cases}$$

$$(54)$$

$$n_{i \to a}(x_i) = \begin{cases} e^{\lambda_{i \to a}(x_i)} & i \in \mathcal{I}^{[B]} \\ e^{\gamma_{i \to a}^T t_i(x_i)} & i \in \mathcal{I}^{[E]} \end{cases} .$$
 (55)

Using them, we can establish the following fixed-point equa-

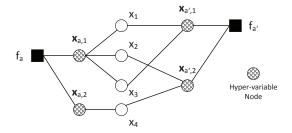


Figure 2: A modified factor graph to illustrate hybrid VMP-BP with $f(\mathbf{x}) = f_a(\mathbf{x}) f_{a'}(\mathbf{x}), \ b_a(\mathbf{x}) = b_{a,1}(x_1, x_2, x_3) b_{a,2}(x_4)$ and $b_{a'}(\mathbf{x}) = b_{a',1}(x_1, x_3) b_{a',2}(x_2, x_4)$.

tions of the Lagrange multipliers

$$m_{a \to i}(x_i) \propto \prod_{i' \in \mathcal{I}_{a,v} \setminus i} n_{i' \to a}(x_i) \cdot e^{\int \prod_{v' \neq v} b_{a,v'}(\boldsymbol{x}_{a,v'}) \ln f_a(\boldsymbol{x}_a) \mu(\mathrm{d}\boldsymbol{x}_{a,\setminus v})} \quad i \in \mathcal{I}^{[\mathrm{B}]}$$
(56)

$$m_{a\to i}(x_i) \propto \frac{1}{n_{i\to a}(x_i)} \operatorname{Proj}_{\mathcal{Q}_i} \left[c \prod_{i'\in\mathcal{I}_{a,v}} n_{i'\to a}(x_i) \right]$$

$$\cdot e^{\int \prod_{v'\neq v} b_{a,v'}(\boldsymbol{x}_{a,v'}) \ln f_a(\boldsymbol{x}_a) \mu(\mathrm{d}\boldsymbol{x}_{a,\setminus v})} \right] \quad i \in \mathcal{I}^{[\mathrm{E}]}$$
(57)

$$n_{i \to a}(x_i) = \prod_{a' \to A_i \setminus a} m_{a' \to i}(x_i). \tag{58}$$

Comparing with (41) and (42), we only have one additional case for the message $m_{a\to i}(x_i)$ if $i\in\mathcal{I}^{[E]}$, i.e., (57). This is mainly because for some variables the marginalization consistency constraints are relaxed to moment matching. In the previous part, we have identified the combination of BP and VMP to solve (41) and (42). The computation involved in (57) is identical to the message update rule of EP. Such identification indicates an iterative solution as a combination of VMP, BP and EP to solve the fixed-point equations. The obtained result shall yield us a local optimum of the Bethe problem (48) by taking the form given in (50), (51) and (52).

D. Visualization of hybrid message passing

To ease the understanding and implementation of the above-derived hybrid message passing, we propose a modification onto the factor graph, see an illustration in Fig. 2. Its key difference to the conventional factor graph, e.g., Fig. 1, is a new type of node termed hyper-variable node. They are associated to the subvectors $\{x_{a,v}\}$ that appear in the factorization constraints for $\{b_a(x_a)\}$, e.g., Fig. 2. Each of them is connected to one and only one factor node.

The message update rule for outgoing from a factor node to a hyper-variable node follows the rule of VMP, e.g.,

$$m'_{a\to(a,v)}(\boldsymbol{x}_{a,v}) \propto e^{\int \ln f_a(\boldsymbol{x}_a) \prod_{v'\neq v} q_{a,v'}(\boldsymbol{x}_{a,v'})\mu(\mathrm{d}\boldsymbol{x}_{a,\setminus v})}$$
 (59) with $\{q_{a,v'}\}$ given as

$$q_{a,v'}(\boldsymbol{x}_{a,v'}) = m'_{a \to (a,v')}(\boldsymbol{x}_{a,v'}) \prod_{i \in \mathcal{I}_{a,v'}} n'_{i \to (a,v')}(x_i). \quad (60)$$

We can interpret $q_{a,v}(x_{a,v})$ as the belief associated to the hyper-variable node $x_{a,v}$. It combines the inputs from all neighboring nodes. In the language of VMP, it is also the message going to the factor node from the hyper-variable node.

From a hyper-variable node to a normal variable node and its reverse direction, there are two cases of message updating. If the destination variable node is under the marginalization consistency constraint (i.e., x_i with $i \in \mathcal{I}^{[B]}$,), we take the message update rule of BP by treating the hyper-variable node as a factor node and taking the message $m'_{a\to(a,v)}(x_{a,v})$ from the uniquely connected factor node as the factor function

$$m'_{(a,v)\to i}(x_i) \propto \int m'_{a\to(a,v)}(\boldsymbol{x}_{a,v}) \cdot \prod_{i'\in\mathcal{I}_{a,v}\setminus i} n'_{i'\to(a,v)}(x_{i'})\mu(\mathrm{d}\boldsymbol{x}_{a,v\setminus i}), \quad (61)$$

where $n'_{i\rightarrow(a,v)}(x_i)$ given as

$$n'_{i\to(a,v)}(x_i) = \prod_{a'\in\mathcal{A}_i\setminus a} m'_{(a',v(i))\to i}(x_i)$$
 (62)

corresponds to the message from the variable node to the hyper-variable node following the BP rule. As compared to the previously derived hybrid VMP-BP, substituting (59) into (61) let $m'_{(a,v)\to i}(x_i)$ become equivalent to $m_{a\to i}(x_i)$ given in (41). Additionally, we have the associations $n'_{i\to(a,v)}(x_i)\leftrightarrow n_{i\to a}(x_i)$ and $b_{a,v}(\boldsymbol{x}_{a,v})\leftrightarrow q_{a,v}(\boldsymbol{x}_{a,v})$.

In the other case where the destination variable node is under the moment matching constraint (i.e., x_i with $i \in \mathcal{I}^{[E]}$,), we shall switch to the EP rule, namely

$$m'_{(a,v)\to i}(x_i) \propto \frac{1}{n'_{i\to(a,v)}(x_i)} \operatorname{Proj}_{\mathcal{Q}_i} \left[c \int m'_{a\to(a,v)}(\boldsymbol{x}_{a,v}) \cdot \prod_{i'\in\mathcal{I}_{a,v}} n'_{i'\to(a,v)}(x_{i'}) \mu(\mathrm{d}\boldsymbol{x}_{a,v\setminus i}) \right],$$
 (63)

where $n'_{i'\to(a,v)}(x_{i'})$ as the message in the reverse direction still follows (62). Comparing with the former case, the additional m-projection step is the only difference here. This coincides with the known difference between EP and BP.

In short, our framework specifies the message update rules between different types of nodes on this modified factor graph, namely, defining the algorithmic structure. On top of this structure, scheduling remains as a design freedom. In principle, the order of message updating and propagating on the modified factor graph can be arbitrary, depending on real applications, and may lead to different results and convergence behaviors.

E. Summary

Concluding this section, we base the framework of constrained Bethe free energy minimization to unify three widely used message passing algorithms for a generic model. Under the same objective function (i.e., the Bethe free energy), BP, EP and VMP are associated to the marginalization consistency, moment matching and partial factorization constraints, respectively. Moment matching is weaker than marginalization consistency, but beneficial to limit the form of messages. Partial factorization permits to ignore the variable dependences to

certain extent, easing local marginalization at the factor nodes $\{f_a(x_a)\}$. Therefore, we can interpret moment matching and partial factorization as constraint manipulation methods to trade inference fidelity for tractability.

On the other hand, if $f_a(x_a) = \prod_v f_a(x_{a,v})$ holds, then the partial factorization constraint (27) becomes redundant and thereby will not degrade inference performance. Analogously, moment matching becomes equivalent to marginalization consistency if the optimal solution $\{\hat{b}_i(x_i)\}$ under the latter one can be known beforehand as members of the exponential family specified by the former one. These identifications reveal relevant system properties that shall be considered for constraint manipulation.

Combining three types of constraints in a general manner, systematic derivations lead us to hybrid VMP-BP-EP variants. We further map the corresponding message passing procedures onto the factor graph after proper modification, visualizing hybrid message passing to assist practical uses.

V. APPLICATION EXAMPLE: SPARSE BAYESIAN LEARNING

Under the developed framework, in this section, we aim at the sparse Bayesian learning (SBL) problem. First, assuming perfect knowledge of the statistical model, we systematically derive a low complexity variant of EP that is an outcome of constraint manipulation. Interestingly, it exhibits high similarity with AMP, thereby being implementation friendly for large-scale systems. Next, removing the assumption in the first step, we present a systematic derivation of hybrid message passing to efficiently solve a joint parameter estimation and model learning problem with low complexity.

Consider a generic linear model of SBL

$$y = Ax + w, (64)$$

where the matrix $A \in \mathbb{C}^{N \times M}$ consisting of N rows $\{a_n\}$ represents a linear transform on x and the noise vector w has i.i.d. entries following the Gaussian distribution $\mathcal{CN}(w_n; 0, \lambda^{-1})$. The general goal here is to estimate $x \in \mathbb{C}^M$ based on the observation vector $y \in \mathbb{C}^N$ and the knowledge of A. In the context of SBL, the unknown vector x represents a sparse signal only with a few non-zero entries. This prior knowledge is critical to reliably estimate x in particular when the linear system is large-scale and underdetermined $(N \ll M)$.

A. EP and its variant for sparse Bayesian learning (SBL)

In this part, we assume the a-priori density p(x) of x and the noise variance λ^{-1} are known. Our goal is to estimate $\{x_m\}$ by computing the marginals $\{p(x_m|y; A, \lambda)\}$ of $p(x|y; A, \lambda)$. BP is not a good choice in this continuous case. Alternatively, we consider EP under the first- and second-order moment matching constraints, yielding the messages in the Gaussian family with the sufficient statistic $t(x_i) = [\operatorname{Re}(x_i), \operatorname{Im}(x_i), |x_i|^2]^T$.

1) Inclusion of an auxiliary vector: If taking the straightforward factorization $p(\boldsymbol{x}|\boldsymbol{y};\boldsymbol{A},\lambda) \propto p(\boldsymbol{x})p(\boldsymbol{y}|\boldsymbol{x};\boldsymbol{A},\lambda)$, the resulting EP algorithm will require matrix inversion with complexity $O(N^2M)$.⁷ Considering the complexity issue of a

large-scale system, we introduce an auxiliary vector $z \in \mathbb{C}^N$ with the relation z = Ax. The target marginal $p(x_m|y;A,\lambda)$ is then alternatively proportional to the outcome of marginalizing

$$f(\boldsymbol{z}, \boldsymbol{x}) = p(\boldsymbol{y}|\boldsymbol{z}; \lambda)p(\boldsymbol{x}) \prod_{n=1}^{N} \delta(z_n - \boldsymbol{a}_n \boldsymbol{x})$$
 (65)

with respect to x_m . In the following, EP and its variant will be derived with respect to f(z, x).

Resorting to the constrained Bethe free energy minimization based approach, we introduce $b_{\mathbf{z}}(\mathbf{z})$, $b_{\mathbf{x}}(\mathbf{x})$, $\{b_{\mathbf{x},\mathbf{z},n}(\mathbf{x},z_n)\}$ and $\{b_{\mathbf{x},m}(x_m),b_{\mathbf{z},n}(z_n)\}$ in accordance with the above factorization. Using them, the Bethe free energy is defined by following the standard way [4]

$$F_{B}(b) = \sum_{m=1}^{M} NH(b_{x,m}) + \sum_{n=1}^{N} H(b_{z,n}) + D\left[b_{\mathbf{x}}(\boldsymbol{x}) \parallel p(\boldsymbol{x})\right]$$

$$+ \sum_{n=1}^{N} \int \int b_{\mathbf{x},z,n}(\boldsymbol{x},z_n) \ln \frac{b_{\mathbf{x},z,n}(\boldsymbol{x},z_n)}{\delta(z_n - \boldsymbol{a}_n \boldsymbol{x})} d\boldsymbol{x} dz_n$$

$$+ \int b_{\mathbf{z}}(\boldsymbol{z}) \ln \frac{b_{\mathbf{z}}(\boldsymbol{z})}{p(\boldsymbol{y}|\boldsymbol{z};\lambda)} d\boldsymbol{z},$$
(66)

where $H(\cdot)$ stands for the entropy function and the Lebesgue measure is considered in this case.

As the minimum of $F_{\rm B}(b)$ is of interest, we note the following property under the convention $0 \ln 0 = 0 \ln \frac{0}{0} = 0$ in probability theory

$$\int \int b_{\mathbf{x},\mathbf{z},n}(\boldsymbol{x},z_n) \ln \frac{b_{\mathbf{x},\mathbf{z},n}(\boldsymbol{x},z_n)}{\delta(z_n - \boldsymbol{a}_n \boldsymbol{x})} d\boldsymbol{x} dz_n$$

$$= \begin{cases}
\infty & \text{if } b_{\mathbf{x},\mathbf{z},n}(z_n | \boldsymbol{x}) \neq \delta(z_n - \boldsymbol{a}_n \boldsymbol{x}) \\
-H(b_{\mathbf{x},n}) & \text{else}
\end{cases} (67)$$

where the joint density $b_{\mathbf{x},\mathbf{z},n}(\boldsymbol{x},z_n)$ can be expressed as the product of $b_{\mathbf{x},n}(\boldsymbol{x}) \stackrel{\Delta}{=} \int b_{\mathbf{x},\mathbf{z},n}(\boldsymbol{x},z_n) \mathrm{d}z_n$ and $b_{\mathbf{x},\mathbf{z},n}(z_n|\boldsymbol{x})$ based on the Bayes rule. From the above, it is then evident to let $b_{\mathbf{x},\mathbf{z},n}(z_n,\boldsymbol{x}) = b_{\mathbf{x},n}(\boldsymbol{x})\delta(z_n-\boldsymbol{a}_n\boldsymbol{x})$ followed by reforming the Bethe free energy $F_{\mathrm{B}}(b)$ in (66) into

$$F_{\mathrm{B}}(b) = \mathrm{D}\left[b_{\mathbf{x}}(\boldsymbol{x}) \parallel p(\boldsymbol{x})\right] + \int b_{\mathbf{z}}(\boldsymbol{z}) \ln \frac{b_{\mathbf{z}}(\boldsymbol{z})}{p(\boldsymbol{y}|\boldsymbol{z};\lambda)} d\boldsymbol{z} + \sum_{m=1}^{M} N\mathrm{H}(b_{\mathbf{x},m}) + \sum_{n=1}^{N} \left[\mathrm{H}(b_{\mathbf{z},n}) - \mathrm{H}(b_{\mathbf{x},n})\right].$$
(68)

The classic Bethe problem implies $F_{\rm B}(b)$ minimization under the marginalization consistency constraints given as

$$\forall m \forall n \quad b_{\mathbf{x},m}(x_m) = \begin{cases} \int_{\boldsymbol{x}_{\backslash m}} b_{\mathbf{x},n}(\boldsymbol{x}) d\boldsymbol{x}_{\backslash m} & (\mathbf{a}) \\ \int_{\boldsymbol{x}_{\backslash m}} b_{\mathbf{x}}(\boldsymbol{x}) d\boldsymbol{x}_{\backslash m} & (\mathbf{b}) \end{cases}; \quad (69)$$

$$\forall n \quad b_{\mathbf{z},n}(z_n) = \begin{cases} \int_{\boldsymbol{x}} b_{\mathbf{x},n}(\boldsymbol{x}) \delta(z_n - \boldsymbol{a}_n \boldsymbol{x}) d\boldsymbol{x} \\ \int_{\boldsymbol{z}_{\backslash n}} b_{\mathbf{z}}(\boldsymbol{z}) d\boldsymbol{z}_{\backslash n} \end{cases}. \quad (70)$$

2) First- and second-order matching: With a continuous random vector x of large dimension, the above constraints are

⁷Since the factor graph of $p(x)p(y|x; A, \lambda)$ is a tree, the corresponding EP is convergent and exactly yields the MMSE estimate of x.

⁸By taking z as one argument of $f(\cdot)$, the following constrained Bethe free energy minimizations will yield estimates of $\{z_n\}$ as well, even though they are not our primary goal.

Algorithm 1 to minimize $F_{\rm B}(b)$ under (71) and (72)

1: Initialization:

$$b_{\mathbf{x}}(\mathbf{x}) = p(\mathbf{x}), \forall m \in \{1, 2, \dots, M\}, \ \alpha_{0,m} = \tau_{0,m} = 0$$

 $\forall n \in \{0, 1, \dots, N\} \forall m \in \{1, 2, \dots, M\}, \ \tilde{\alpha}_{n,m} = \tilde{\tau}_{n,m} = 0$

2: repeat

3:
$$\forall m,$$

$$\tilde{\alpha}_{0,m} = \frac{\mathbf{E}[x_m | b_{\mathbf{x}}]}{\mathbf{Var}[x_m | b_{\mathbf{x}}]} - \alpha_{0,m}$$

$$\tilde{\tau}_{0,m} = \frac{1}{\mathbf{Var}[x_m | b_{\mathbf{x}}]} - \tau_{0,m}$$

$$\begin{aligned} \text{4:} & \quad \text{For } n = 1, 2, \dots, N, \forall m, \\ & \quad \alpha_{n,m} = \sum_{n'=0, n' \neq n}^{N} \tilde{\alpha}_{n',m} \\ & \quad \tau_{n,m} = \sum_{n'=0, n' \neq n}^{N} \tilde{\tau}_{n',m} \\ \text{5:} & \quad \text{For } n = 1, 2, \dots, N, \ \gamma_{\mathbf{z},n} = \sum_{m} \frac{|a_{n,m}|^2}{\tau_{n,m}} \\ \text{6:} & \quad \text{For } n = 1, 2, \dots, N, \ \mu_{\mathbf{z},n} = \sum_{m} \frac{|a_{n,m}|^2}{\tau_{n,m}} \end{aligned}$$

5: For
$$n = 1, 2, ..., N$$
, $\gamma_{z,n} = \sum_{m} \frac{|a_{n,m}|^2}{\tau_{n,m}}$

6: For
$$n = 1, 2, ..., N$$
, $\mu_{z,n} = \sum_{m} \frac{a_{n,m} \alpha_{n,m}}{\tau_{n,m}}$

7: For
$$n = 1, 2, ..., N$$
, $\forall m$,
$$\tilde{\alpha}_{n,m} = \frac{a_{n,m}^* |y_n - \mu_{z,n}| + \alpha_{n,m} |a_{n,m}|^2 / \tau_{n,m}}{\lambda^{-1} + \gamma_{z,n} - |a_{n,m}|^2 / \tau_{n,m}}$$

$$\tilde{\tau}_{n,m} = \frac{|a_{n,m}|^2}{\lambda^{-1} + \gamma_{z,n} - |a_{n,m}|^2 / \tau_{n,m}}$$

8:
$$\forall m,$$

$$\alpha_{0,m} = \sum_{n'=1}^{N} \tilde{\alpha}_{n',m}$$

$$\tau_{0,m} = \sum_{n'=1}^{N} \tilde{\tau}_{n',m}$$

9:
$$b_{\mathbf{x}}(\boldsymbol{x}) \propto p(\boldsymbol{x}) \prod_{m} e^{-2\operatorname{Re}\left[\alpha_{0,m}^* x_m\right] + \tau_{0,m}|x_m|^2}$$

10: until the termination condition is fulfilled.

11:
$$\hat{x}_m = E[x_m | b_{x,m}]$$

often intractable. For the sake of complexity, here we relax them into the first- and second-order moment matching ones

$$\forall m \forall n \ \mathrm{E}[x_m | b_{\mathbf{x},m}] = \mathrm{E}[x_m | b_{\mathbf{x},n}] = \mathrm{E}[x_m | b_{\mathbf{x}}]$$

$$\forall n \ \mathrm{E}[z_n | b_{\mathbf{z},n}] = \mathrm{E}[\boldsymbol{a}_n \boldsymbol{x} | b_{\mathbf{x},n}] = \mathrm{E}[z_n | b_{\mathbf{z}}]$$

$$; \tag{71}$$

$$\forall m \forall n \ \mathrm{E}[|x_m|^2|b_{\mathbf{x},m}] = \mathrm{E}[|x_m|^2|b_{\mathbf{x},n}] = \mathrm{E}[|x_m|^2|b_{\mathbf{x}}]$$
$$\forall n \ \mathrm{E}[|z_n|^2|b_{\mathbf{z},n}] = \mathrm{E}[|a_n \mathbf{x}|^2|b_{\mathbf{x},n}] = \mathrm{E}[|z_n|^2|b_{\mathbf{z}}]$$
(72)

Following the method of Lagrange multipliers to minimize $F_{\rm B}(b)$ under the constraints (71) and (72), this yields Alg. 1.

Two remarks on Alg. 1 are made as follows: First, it follows the message update rules of EP, but appears differently in comparison with the general EP presentation in terms of $\{m_{a\to i}(x_i), n_{i\to a}(x_i)\}$. This is an outcome of applying proper simplification with respect to the specific system model. For instance, as our ultimate goal is to estimate x the message updates for the auxiliary variable z are absorbed into the messages for x in the presentation of Alg. 1. Second, we note that from step 4 to 7, the computations for n = 1, 2, ..., N are simultaneously executed. Such parallel scheduling is beneficial to limit the processing latency when N tends to be large. In principle, other scheduling schemes are applicable as well. The developed framework permits to define the structure of the algorithm. Scheduling on top of it remains as a design freedom, which is beyond the scope of this work.

3) Mean and variance consistency: In the sequel, we illustrate how to derive a low complexity EP variant by simple constraint reformulation. Namely, under the first-order moment (mean) matching, we can equivalently and alternatively turn the second-order moment matching into the variance consis-

Algorithm 2 to minimize $F_{\rm B}(b)$ under (71) and (73)

1: Initialization:

$$b_{\mathbf{x}}(\mathbf{x}) = p(\mathbf{x}), \ \forall m \in \{1, 2, \dots, M\}, \ \tau_{0,m} = 0$$

 $\forall n \in \{0, 1, \dots, N\}, \beta_n = 0$
 $\forall n \in \{0, 1, \dots, N\} \forall m \in \{1, 2, \dots, M\}, \ \tilde{\tau}_{n,m} = 0$
2: **repeat**

3:
$$\forall m, \ \tilde{\tau}_{0,m} = \frac{1}{\text{Var}[x_m | b_x]} - \tau_{0,m}$$

3:
$$\forall m, \ \tilde{\tau}_{0,m} = \frac{1}{\text{Var}[x_m|b_x]} - \tau_{0,m}$$

4: For $n = 1, 2, \dots, N \forall m, \ \tau_{n,m} = \sum_{n'=0, n' \neq n}^{N} \tilde{\tau}_{n',m}$
5: For $n = 1, 2, \dots, N, \ \gamma_{z,n} = \sum_{m'=1}^{M} \frac{|a_{n,m'}|^2}{\tau_{n,m'}}$

5: For
$$n = 1, 2, ..., N$$
, $\gamma_{z,n} = \sum_{m'=1}^{M} \frac{|a_{n,m'}|^2}{\tau_{n,m'}}$

6: For
$$n = 1, 2, \dots, N$$
, $\mu_{\mathbf{z},n} = \boldsymbol{a}_n \mathbf{E}[\boldsymbol{x}|b_{\mathbf{x}}] - \beta_n \gamma_{\mathbf{z},n}$

7: For
$$n = 1, 2, ..., N$$
, $\beta_n = (y_n - \mu_{z,n}) / (\lambda^{-1} + \gamma_{z,n})$

8: For
$$n = 1, 2, ..., N \forall m$$
, $\tilde{\tau}_{n,m} = \frac{|a_{n,m}|^2}{\gamma_{z,n} + \lambda^{-1} - |a_{n,m}|^2 / \tau_{n,m}}$

9:
$$\forall m, \ \tau_{0,m} = \sum_{n'=1}^{N} \tilde{\tau}_{n',m}$$

10:
$$\forall m, \ \mu_{\mathbf{x},m} = \mathbf{E}[x_m | b_{\mathbf{x}}] + \tau_{0,m}^{-1} \sum_{n=1}^{N} a_{n,m}^* \beta_n$$

11:
$$b_{\mathbf{x}}(\mathbf{x}) \propto p(\mathbf{x}) \prod_{m=1}^{M} \mathcal{CN}(x_m; \mu_{\mathbf{x},m}, \tau_{0,m}^{-1})$$

12: until the termination condition is fulfilled.

13:
$$\hat{x}_m \leftarrow \mathrm{E}[x_m|b_{\mathbf{x}}]$$

tency constraint, i.e., replacing (72) by

$$\forall m \forall n \ \operatorname{Var}[x_m | b_{\mathbf{x},m}] = \operatorname{Var}[x_m | b_{\mathbf{x},n}] = \operatorname{Var}[x_m | b_{\mathbf{x}}]$$

$$\forall n \ \operatorname{Var}[z_n | b_{\mathbf{x},n}] = \operatorname{Var}[a_n \boldsymbol{x} | b_{\mathbf{x},n}] = \operatorname{Var}[z_n | b_{\mathbf{z}}]$$

$$(73)$$

By analogy, we apply the method of Lagrange multipliers for minimizing $F_{\rm B}(b)$ under (71) and (73). This leads to Alg. 2. Comparing it with Alg. 1, the updates for $\{\tilde{\alpha}_{n,m}, \alpha_{n,m}\}$ are avoided, thereby requiring less computation efforts. Both algorithms aim at the same optimization problem as the constraints (71) and (73) are equivalent to those in (71) and (72).

4) Performance comparison: In this part, we compare the performance of Alg. 1 and Alg. 2 for SBL in a 250×500 linear system, see Fig. 3. For a comparison purpose, we evaluate the performance of AMP as well. It is noted that AMP attempts to approximate EP (i.e., Alg. 1) in the large system limit, where the high-order terms in the message update equations are ignored [19]. Alg. 2 on the other hand is an outcome of systematic derivation from an equivalent formulation of the constrained Bethe free energy minimization problem targeted by Alg. 1, being independent of the system dimension.

In the present case, AMP is sketched in Alg. 3. The key difference between Alg. 2 and Alg. 3 lies in the computation of $\{\tilde{\tau}_{n,m}\}$. Apart from that, they are nearly identical to each other, being composed of basic arithmetic operations.

As expected, Fig. 3 shows both AMP and our proposed EP variant, i.e., Alg. 2, achieve the best performance. On the contrary, the performance of Alg. 1 degrades severely when the sparsity ratio ρ is beyond 0.25. From our analysis, such performance degradation mainly arises from the iteration divergence under parallel message updating. This is an interesting observation, indicating that the form of constraints not only impacts the complexity and performance, but also the convergence behavior of message passing. Therefore, it

⁹In this case, AMP is also equivalent to S-AMP presented in [18], which is an EP variant in the large system limit aiming at the factorization $p(\mathbf{x})p(\mathbf{y}|\mathbf{x};\mathbf{A},\lambda)$ in a tree structure.

Algorithm 3 AMP for sparse Bayesian learning

1: Initialization : $b_{\mathbf{x}}(\mathbf{x}) = p(\mathbf{x}), \forall n, \beta_n = 0$

2: repeat

3: $\forall m, \ \tilde{\tau}_{0,m} = \frac{1}{\operatorname{Var}[x_m|b_x]}$

4: For n = 1, 2, ..., N, $\gamma_{\mathbf{z},n} = \sum_{m=1}^{M} |a_{n,m}|^2 / \tilde{\tau}_{0,m}$

5: For n = 1, 2, ..., N, $\mu_{\mathbf{z},n} = \boldsymbol{a}_n \mathbb{E}[\boldsymbol{x}|b_{\mathbf{x}}] - \beta_n \gamma_{\mathbf{z},n}$

6: For n = 1, 2, ..., N, $\beta_n = (y_n - \mu_{z,n})/(\lambda^{-1} + \gamma_{z,n})$

7: For $n = 1, 2, ..., N \forall m, \ \tilde{\tau}_{n,m} = \frac{|a_{n,m}|^2}{\gamma_{z,n} + \lambda^{-1}}$

8: $\forall m, \ \tau_{0,m} = \sum_{n'=1}^{N} \tilde{\tau}_{n',m}$

9: $\forall m, \ \mu_{\mathbf{x},m} = \mathbf{E}[x_m | b_{\mathbf{x}}] + \tau_{0,m}^{-1} \sum_n a_{n,m}^* \beta_n$

10: $b_{\mathbf{x}}(\mathbf{x}) \propto p(\mathbf{x}) \prod_{m=1}^{M} \mathcal{CN}(x_m; \mu_{\mathbf{x},m}, \tau_{0,m}^{-1})$

11: until the termination condition is fulfilled.

12:
$$\hat{x}_m = E[x_m | b_{\mathbf{x}}]$$

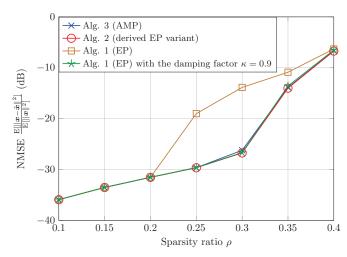


Figure 3: Normalized mean square error (NMSE) performance versus the sparsity ratio ρ . In this example, the matrix ${\bf A}$ of dimension 250×500 is drawn with i.i.d. $\mathcal{CN}(a_{n,m};0,N^{-1})$ entries and the signal-to-noise ratio (SNR) is set to $30\,\mathrm{dB}$. The vector ${\bf x}$ of interest follows a Bernoulli-Gaussian distribution, i.e., $p({\bf x}) = \prod_m (1-\rho)\delta(x_m) + \rho\mathcal{CN}(x_m;0,1)$. Its sparsity reduces as ρ increases. The maximum limit on the number of iterations equals M.

is worth to treat constraint manipulation as an important design freedom in the optimization framework when developing practical and effective message passing algorithms for various applications.

To alleviate this issue of Alg. 1, here we empirically introduce damping onto the step 7 of Alg. 1, i.e.,

$$\tilde{\alpha}_{n,m} = (1 - \kappa)\tilde{\alpha}_{n,m} + \kappa \frac{a_{n,m}^*(y_n - \mu_{z,n}) + \alpha_{n,m}|a_{n,m}|^2 / \tau_{n,m}}{\lambda^{-1} + \gamma_{z,n} - |a_{n,m}|^2 / \tau_{n,m}},$$

$$\tilde{\tau}_{n,m} = (1 - \kappa)\tilde{\tau}_{n,m} + \kappa \frac{|a_{n,m}|^2}{\lambda^{-1} + \gamma_{z,n} - |a_{n,m}|^2 / \tau_{n,m}},$$
(74)

where $\kappa \in (0, 1]$ is the damping factor. In doing so the damped Alg. 1 is able to deliver similar performance as the others.

B. Hybrid message passing for joint parameter and statistical model estimation

Without assuming any prior knowledge of λ and the a-priori density p(x), the above-mentioned algorithms are not straight-

forwardly usable to estimate $\{x_m\}$. Alternatively, we include hierarchical prior models of λ and x into the construction of the Bethe problem. Based on the results in the work [49] that compares different prior models for SBL, the following ones are chosen for an illustration

$$p(\boldsymbol{x}; \boldsymbol{\alpha}) = \prod_{m=1}^{M} \mathcal{CN}(x_m; 0, \alpha_m) \text{ with } p(\alpha_m) = \text{Ga}(\alpha_m | \epsilon, \eta);$$
$$p(\lambda) = \text{Ga}(\lambda | c = 0, d = 0),$$

where (ϵ, η) and (c, d) are the pre-selected shape and rate parameters of the two Gamma distributions, respectively.

From the above statistical modeling, our target function of marginalization becomes

$$f(\boldsymbol{x}, \boldsymbol{z}, \lambda, \boldsymbol{\alpha}) = p(\boldsymbol{y}|\boldsymbol{z}; \lambda)p(\lambda; c, d)p(\boldsymbol{x}; \boldsymbol{\alpha})$$

$$\cdot \prod_{m=1}^{M} p(\alpha_m; \epsilon, \eta) \prod_{n=1}^{N} \delta(z_n - \boldsymbol{a}_n \boldsymbol{x}).$$
 (75)

The statistical modeling parameters $\{\lambda, \alpha\}$ in addition to $\{x, z\}$ are included into the space of variational Bayesian inference. As the parameters $\{\epsilon, \eta, c, d\}$ are considered to be pre-selected, they are not taken as the arguments of $f(\cdot)$.

Following the standard way, the Bethe free energy can be written as a function of a set of densities, i.e., $b_{\mathbf{z},\lambda}(\mathbf{z},\lambda), b_{\lambda}(\lambda), b_{\mathbf{x},\alpha}(\mathbf{x},\alpha), \{b_{\alpha_m}(\alpha_m)\}, b_{\mathbf{x},\mathbf{z},n}(\mathbf{x},z_n)$ plus $\{b_{\mathbf{x},m}(x_m), b_{\mathbf{z},n}(z_n)\}$. For the sake of problem tractability, the constraints on these densities are designed to be

$$b_{\mathbf{z},\lambda}(\mathbf{z},\lambda) = b_{\mathbf{z}}(\mathbf{z})b_{\lambda}(\lambda);$$
 (a)

$$b_{\mathbf{x},\lambda}(\mathbf{x},\alpha) = b_{\mathbf{x}}(\mathbf{x}) \prod_{m=1}^{M} b_{\alpha_m}(\alpha_m);$$
 (b)

$$b_{\alpha_m}(\alpha_m) = \delta(\alpha_m - \hat{\alpha}_m) \tag{c}$$

together with the mean and variance consistency constraints (71) and (73) for the factor densities $\{b_{\mathbf{z}}(\mathbf{z}), b_{\mathbf{x}}(\mathbf{x})\}$ in relation to $\{b_{\mathbf{x},m}(x_m), b_{\mathbf{z},n}(z_n)\}$. In particular, the factorization constraints in (76)-(a) and -(b) follow the idea for VMP in (27). By doing so we can decouple the correlation between the model parameters $\{\alpha, \lambda\}$ and the latent variables $\{x_m, z_n\}$. The third one, additionally letting the factor density of α_m be a Dirac delta-function, reduces VMP to expectation maximization (EM) [50]. Such a single-parameter model reduces the complexity for estimating the model parameter α_m at the cost of accuracy.

Applying the method of Lagrangian multipliers to minimize the Bethe free energy under the above-formulated constraints, we reach to Alg. 4 that combines EM, VMP and Alg. 2 (as the EP variant). In particular, the initialization c=d=0 ensures a non-informative prior for λ . The pair (ϵ,η) on the other hand reflects the sparsity-inducing property of the prior model on x [49]. In particular, ϵ plays a dominant role. A smaller ϵ encourages a more sparse estimate. Without any prior knowledge of the sparsity of x, we empirically propose in Alg. 4 to adaptively reduce ϵ over iterations. The rationale behind the proposal follows the general idea of compressed sensing. Namely, we aim at approximating y by $A\hat{x}$ where the support of the estimate \hat{x} shall be as small as possible.

Fig. 4 shows that Alg. 4 can approach the performance of Alg. 2 with exact knowledge of λ and p(x) when x exhibits

Algorithm 4 Hybird EM-VMP-Alg. 2 for SBL

1: Initialization:

$$\forall m \in \{1, 2, \dots, M\}, \ \tau_{0,m} = 0$$

$$\forall n \in \{0, 1, \dots, N\}, \ \beta_n = 0$$

$$\forall n \in \{0, 1, \dots, N\} \forall m \in \{1, 2, \dots, M\}, \ \tilde{\tau}_{n,m} = 0$$

$$\lambda = \frac{100}{\text{Var}(\boldsymbol{y})}, \ \forall m, \ \alpha_m = 1/M$$

$$b_{\mathbf{x}}(\boldsymbol{x}) = \prod_m \mathcal{CN}(x_m; 0, \alpha_m)$$

$$c = d = 0, \ \epsilon = 1.5, \ \eta = 1, \ e^{\text{old}} = 0$$

2: repeat

3:
$$p(\boldsymbol{x}) \leftarrow \prod_{m=1}^{M} \mathcal{CN}(x_m; 0, \hat{\alpha}_m)$$

4: step
$$3 \sim 11$$
 of Alg. 2

5:
$$e^{\text{new}} \leftarrow \frac{1}{N} \| \boldsymbol{y} - \boldsymbol{A} \hat{\boldsymbol{x}} \|^2$$

6:
$$\lambda \leftarrow \left[e^{\text{new}} + \frac{1}{N} \sum_{n=1}^{N} \frac{\gamma_{z,n}}{1 + \lambda \gamma_{z,n}} \right]^{-1}$$

6:
$$\lambda \leftarrow \left[e^{\text{new}} + \frac{1}{N} \sum_{n=1}^{N} \frac{\gamma_{z,n}}{1 + \lambda \gamma_{z,n}}\right]^{-1}$$
7:
$$\alpha_m \leftarrow \left\{\epsilon - 2 + \sqrt{(\epsilon - 2)^2 + 4\eta \mathbb{E}[|x_m|^2 | b_{\mathbf{x}}]}\right\} / (2\eta)$$

8: If
$$|e^{\rm new} - e^{\rm old}| < 10^{-6}$$
 and the support of ${\rm E}[{\pmb x}|b_{\bf x}]$ is not reducing, $\epsilon \leftarrow 0.95\epsilon$

 $e^{\text{old}} \leftarrow e^{\text{new}}$

10: **until** the termination condition is fulfilled.

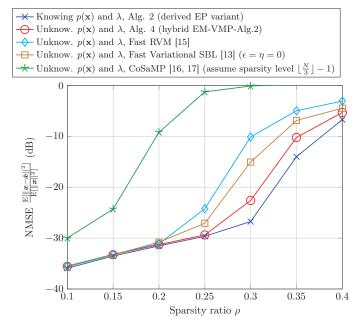


Figure 4: Normalized mean square error (NMSE) performance versus the sparsity ratio ρ . This figure is based on the same system configuration as Fig. 3.

low and medium levels of sparsity, i.e., $\rho<0.3.$ With the sparsity beyond 0.4, the measurement ratio $\frac{N}{M}=0.5$ is too low to yield reliable estimate \hat{x} . For comparison, we also include the results from the fast implementation of the relevance vector machine (RVM) [51] and variational SBL (i.e., VMP) [49] together with a non-Bayesian approach CoSaMP [52], [53]. Besides the performance gain, Alg. 4 also avoids complex matrix inversion and factorization required by them.

VI. CONCLUSION

This paper unified the message passing algorithms termed BP, EP and VMP under the optimization framework of

constrained Bethe free energy minimization. With the same objective function, the key difference of these algorithms simply lies in the way of formulating the constraints. With this identification, it becomes natural to apply proper constraint manipulation for systematically deriving message passing variants from the same framework. In other words, one can treat constraint manipulation as a design freedom, enabling tradeoffs between tractability and fidelity of approximate inference.

In particular, we shown that a structured rather than an adhoc combination of BP, EP and VMP can be obtained under a set of partial factorization, marginalization consistency and moment matching constraints. Taking a classic SBL problem as an example, we subsequently derived an EP variant for SBL through constraint reformulation. It is able to outperform the standard EP algorithm with lower computational complexity. Last but not least, hybrid message passing was derived and applied for SBL when the statistical model of the system is unknown. It can deliver the performance that is close to the one attained with perfect knowledge of the statistical model. It can also outperform state-of-the-art solutions in the literature.

In short, constrained Bethe free energy minimization serves as a theoretical framework to perform joint investigation on different message passing algorithms for an improved performance. We focused on constraint manipulation in this work, illustrating its impact on the performance and complexity of message passing. For future works under this framework, it would be interesting to examine other design freedoms, such as the non-convex objective function Bethe free energy. Its construction can be influenced by, but not limited to, factorization of the target function f(x), design of auxiliary variables (e.g., z in the examined SBL application), and inclusion of a temperature parameter¹⁰. It is worth to note that all theses design freedoms are mutually orthogonal, implying the possibility of exploiting them in a combined manner.

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¹⁰The original definition of Bethe free energy in physics already contains a temperature, but it is commonly set to one for variational Bayesian inference.

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