

Improving Variational Methods via Pairwise Linear Response Identities

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Abstract

Inference methods are often formulated as variational approximations: these approximations allow easy evaluation of statistics by marginalization or linear response, but these estimates can be inconsistent. We show that by introducing constraints on covariance, one can ensure consistency of linear response with the variational parameters, and in so doing inference of marginal probability distributions is improved. For the Bethe approximation and its generalizations, improvements are achieved with simple choices of the constraints. The approximations are presented as variational frameworks; iterative procedures related to message passing are provided for finding the minima.

Keywords: variational inference, graphical models, message passing algorithms, statistical physics, linear response

1. Introduction

Given a probability distribution $p(x)$, estimation of marginal probability distributions such as $p(x_i)$ and $p(x_i; x_j)$ is one of the most important inference tasks addressed in graphical models, alongside estimation of the maximum probability state and the log partition function (see Wainwright and Jordan, 2008; Mezard and Montanari, 2009; MacKay, 2004). The challenge is addressed in many research fields by a variety of methods. In Boltzmann machine learning and probabilistic independent component analysis the expectation-maximization algorithm requires such estimates (see Wainwright and Jordan, 2008; Miskin and MacKay, 2000). In heuristic optimization, a branch and bound search (or decimation procedure) over a high dimensional space can be made more efficient, by branching on x_i (or some small set of variables) in an informed manner using approximate probabilities (see Montanari et al., 2007). In channel coding we wish to determine the likely state of a bit sent over a noisy channel, which can be inferred with a measure of certainty from the marginal probability (see Richardson and Urbanke, 2008). In statistical physics, marginal probability

distributions provide insight into phase transitions and thermodynamic phases (see Parisi, 1987).

Approximation of marginal probability distributions (called marginals henceforth) with high accuracy is NP-hard even in the case of Ising spins (binary variables) with pairwise interactions (see Dagum and Luby, 1993; Long and Servedio, 2010), but in practice, many schemes might be applied successfully. Approximate inference of marginal distributions is often performed by Markov chain Monte Carlo (MCMC) procedures (see Andrieu et al., 2003). These methods are a workhorse of inference, but have some disadvantages: the estimates are achieved with an accuracy that decays only slowly with time resources (exploiting the central limit theorem), the result is stochastic, and takes a non-parametric form. For these reasons variational approximations are often preferred, the price being a (difficult to quantify) bias in the approximations (see Wainwright and Jordan, 2008; Mezard and Montanari, 2009; MacKay, 2004).

In a basic variational approximation an intractable probability distribution $p(x)$ is approximated by a tractable one $q(x)$, the parameters of q are determined by minimizing the Kullback Leibler (KL) divergence $D_{KL}[p||q]$. The challenge of marginalization is thus replaced by two linked challenges: appropriate construction of q , and minimization of a KL-divergence. An example of a tractable distribution is a factorized one: $q(x) = \prod_i q(x_i)$, which leads to a mean-field variational approximation; KL-divergence could then typically be minimized by an iteration of fixed point equations (see Wainwright and Jordan, 2008; Mezard and Montanari, 2009). It is common for the estimates obtained by variational approximations to be over-confident, the uncertainty in some variables is reduced since the structure of the approximation q discounts some sources of variance.

A given variational framework may be minimized by several algorithms, and it is interesting that many famous heuristic algorithms developed independently of variational frameworks have been shown to be particular solutions to variational approximations. Most notably loopy belief propagation has been shown to be one method to solve the Bethe variational approximation, and expectation propagation was shown to be one method to solve the expectation consistent variational approximation. This connection to variational frameworks has allowed interesting insight into algorithm construction, proofs of solution existence and convergence (see Yedidia et al., 2005; Wainwright and Jordan, 2008; Yuille, 2002).

We have so far identified one mechanism by which to estimate marginals: we can directly marginalize our approximation $q(x)$, which is tractable by construction. These same estimates (when not extremal) can be found as first derivatives of the variational function (in the above description, the KL-divergence), as we later show. Second order derivatives of the KL-divergence are also possible and can give covariance estimates. These covariance estimates are called linear responses, since they measure the response of some expectation (the first derivative estimate) to an infinitesimal linear perturbation (the second derivative). Linear response and marginalization estimates are tractable for variational approximations; and for some statistics, we can use either method to obtain an estimate for the same quantity.

We will consider variational approximations applied to a model of N discrete variables x_i defined by probability ¹

$$p(x) = \frac{1}{Z} \prod_{a=1}^M \psi_a(x_a), \quad (1)$$

where ψ_a are the potentials (also called factors) and are non-negative functions of the variables indexed by subset a , $x_a = \{x_i : i \in a\}$, Z is the partition function. Probabilities of this kind can be represented as a factor graph (see Wainwright and Jordan, 2008; Mezard and Montanari, 2009), as shown in Figure 1. Our aim is to demonstrate a mechanism whereby existing variational schemes can be leveraged for improved inference of marginals.

This paper considers a new self-consistent approximation to improve variational methods, with an emphasis on the Bethe approximation and its generalizations (called region-based, or cluster-variational, approximations). We propose the addition of constraints requiring the consistency of estimates obtained via direct marginalization and linear response. We minimize the variational function subject to an agreement of these estimates and show that the resulting unique estimate is an improvement on the two estimates that are obtained without the constraints.

1.1 Literature Review

The linear response has been leveraged to improve estimates of marginals in a variety of problems, the idea originating in statistical physics (see Parisi, 1987; Opper and Winther, 2003; Welling and Teh, 2004).

Physics approaches often aim to improve understanding of phase transitions for problem classes in the limit of a large number of variables (see Parisi, 1987), rather than in development of algorithmic approaches to solve particular finite instances. An early application of linear response was the self-consistent Ornstein-Zernike approximation (SCOZA), proposed by Høye and Stell (1977), which was later applied by Dickman and Stell (1996) to simple graphical models. The SCOZA has been applied to disordered models where marginals are not homogeneous, for example to the random field Ising model in Kierlik, Rosinberg, and Tarjus (1999), but in the service of estimating globally averaged and disorder averages quantities, and never in such a way as to understand particular single variable or pairwise marginals, which is the question we address.

Opper and Winther (2001) proposed the adaptive-TAP approach as an extension of the standard Thouless-Anderson-Palmer mean-field method; in the original formulation of this method, a self-consistency relation between the linear response and magnetizations of a mean-field approximation were reconciled to arrive at a more advanced mean-field theory. Opper and Winther (2005) and Winther and Opper (2005) later reinterpreted this method as a special case of expectation consistent approximate inference, that made a connection between moment-matching algorithms such as expectation propagation and variational frameworks, as well as expanding the range of applications. Expansions of the expectation consistent approximation to mitigate for errors on higher order cumulants have

1. For brevity in expressions we will use the notation x both for a random variable and its realization, relying on context for the distinction.

shown promise in Opper, Paquet, and Winther (2013) and Paquet, Winther, and Opper (2009), but at this point come with few theoretical guarantees.

In the context of machine learning, other related approaches for improving mean-field estimation have been successfully demonstrated in Kappen and Rodriguez (1998) and Giordano, Broderick, and Jordan (2015). Mean-field variational Bayes is an important application of variational approximations, but the absence of an accurate understanding of covariance in the model parameters had been a weakness. Recently it was shown by Giordano, Broderick, and Jordan (2015) that linear response could be used to more accurately estimate these quantities.

The Bethe variational approximation is also an important approximation in the context of sparse graphical models, for which loopy belief propagation (LBP) is the most famous algorithm. Linear response has also been used to improve this approximation, examples include Montanari and Rizzo (2005) and Mooij, Wemmenhove, Kappen, and Rizzo (2007). A large part of this development has been through loop-correction algorithms since the failure of the approximation is known to be related to loops in the graphical model representation. There also exist elegant loop correction methods not relying on the linear response: libDAI is a code repository that has collected some of the methods together (see Mooij, 2010), we developed our methods based on this library, in particular, the implementation of Heskes, Albers, and Kappen (2003). An expansion about the loop free approximation was developed by Chertkov and Chernyak (2006), but is cumbersome when many loops are present.

Several papers related to an extension of the Bethe approximation were published by Yasuda and Tanaka (2013), Raymond and Ricci-Tersenghi (2013b), Raymond and Ricci-Tersenghi (2013a) and Yasuda (2013). The idea was very similar to that of adaptive-TAP, to minimize the variational function subject to the constraint of statistical consistency. When applied to the mean-field approximation it was realized these methods were equivalent to adaptive-TAP, but in the context of Bethe and region-based free energies improved performance was identified. In Raymond and Ricci-Tersenghi (2013b) and Huang and Kabashima (2013) linear response frameworks were also leveraged in the reverse direction to solve the inverse-Ising problem (inferring parameters from statistics).

These variational frameworks were applied initially to Bethe and mean-field approximations on pairwise binary state models, in Yasuda (2013) an extension to general discrete states was provided, whereas Raymond and Ricci-Tersenghi (2013b) applied the technique to region-based variational frameworks and a broader range of constraint types. In this paper, we consider generic discrete alphabets, region-based free energies (inclusive of the Bethe approximation) and both single-variable and pairwise variable consistency constraints. Building on a belief propagation approach we derive tools for minimizing constrained variational free energies.

1.2 Outline

In Section 2, we define a set of variational approximations and motivate the inclusion of additional constraints. In Section 3, we describe methods to minimize the free energy subject to these constraints. In Section 4, we compare the performance of constrained approximations against exact results on some standard models, demonstrating a significant advantage in many cases. In Section 5, we discuss our findings in the context of all experimental results

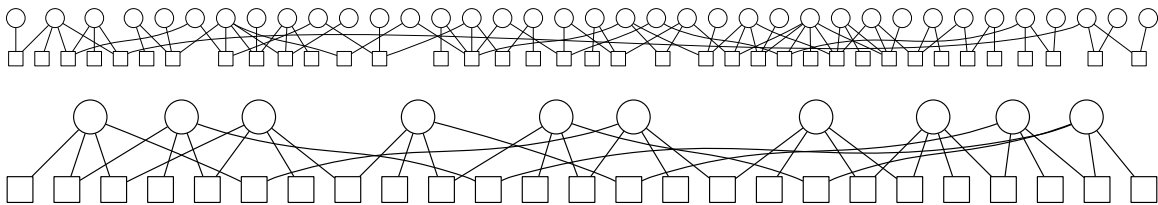


Figure 1: The constrained variational approximations we present can be applied to models with multi-variable interactions, as represented by factor graphs. Two examples are shown. Top: the alarm network is a well-known toy example of a Bayesian net, here represented as a factor graph. Squares denote factors $\psi_a(x_a)$, which act over subsets of variables x_a , each variable represented by a circle. Bottom: $N = 10$ variables interacting according to a random cubic graph is represented, each coupling (J) is represented by a factor with two connections, each field (h) by a singly connected factor.

and other insights gained, before concluding in Section 6. Appendices include exact expressions for the fully connected ferromagnet example, pseudocode and algorithmic details, proofs of convergence for some methods, discussion of solution existence and convergence, and how to select constraints for inclusion.

2. Constrained Variational Approximations

Variational free energy approximations are powerful tools for approximate inference (see Yedidia et al., 2005; Opper and Winther, 2005; Wainwright and Jordan, 2008; Mezard and Montanari, 2009). We introduce in this section the mean-field, Bethe, and region-based (also called Kikuchi) approximations. A set of simplified expressions appropriate to the Bethe approximation for an Ising model is given alongside the general expressions. We first introduce a generalization of the probability over the N variables x , introducing auxiliary parameters ν ,

$$p_\nu(x) = \frac{1}{Z(\nu)} \prod_{a=1}^M \psi_a(x_a) \prod_{i=1}^N \left[\prod_y \exp(\nu_{i,y} \delta_{x_i,y}) \right]. \quad (2)$$

This coincides with (1) in the limit $\nu \rightarrow 0$. The product on y is over all possible states of x_i . For our method to apply the probability needs to be differentiable with respect to the parameters ν , though modifications allow for the more general case². The choice of statistics $\{\delta_{x_i,y}\}$ simplifies our presentation, but more generally we might consider a set of single variable functions $\{\phi_y(x_i)\}$, this is discussed in Appendix B.2.

A Boltzmann machine will be presented as a running example. The model³ has Ising spin variables $x \in \{-1, 1\}^N$, fields h and pairwise couplings J . A connected graphical model will be assumed for notational simplicity, so each variable has connectivity $k_i \geq 1$, and a unique connected component exists. If an edge set $E = \{(i, j)\}$ specifies the interacting

2. Special care should be taken in cases where $\psi_a(x_a) = 0$ for some x_a , in such cases it may not be meaningful to perturb by ν . Furthermore, we note that ν are a redundant set of parameters since variation of $\sum_y \nu_{i,y}$ leaves the probability unchanged.

3. For binary variables, we will use Ising spins $s = \pm 1$ in place of binary states $b \in \{0, 1\}$. The transformation $s = 1 - 2b$ allows conversion between these two conventions.

variables, then

$$p_\nu(x) = \frac{1}{Z(\nu)} \prod_{(i,j) \in E} \exp(J_{ij}x_i x_j) \prod_i \exp[(h_i + \nu_i)x_i], \quad (3)$$

where we use a non-redundant set of auxiliary parameters $\nu_i = \nu_{i,1} - \nu_{i,-1}$.

In a variational approximation a trial probability distribution $q(x)$ is related to the log-partition function of the full model, derived from the Kullback-Leibler divergence

$$D_{KL}[q||p_\nu] = \sum_x q(x) \left[\log q(x) - \sum_{i,y} \nu_{i,y} \delta_{x_i,y} - \sum_a \log \psi_a(x_a) \right] + \log Z(\nu). \quad (4)$$

The variational free energy (VFE) is defined

$$F_\nu(q) = D_{KL}[q||p_\nu] - \log Z(\nu), \quad (5)$$

which is the tractable part of (4). The optimal variational parameters q^* are those minimizing (5).

In the simplest mean-field approximation a factorized variational form is considered $q(x) = \prod_{i=1}^N q_i(x_i)$. The parameters $\{q_i\}$ are precisely marginal distributions on single variables. Iterative methods are often successful in minimizing the VFE.

In another class of approximations the entropy term in the VFE, $-\sum_x q(x) \log q(x)$, is decomposed as a truncated sum of marginal entropies. In the Bethe approximation a redundant set of marginal probability distributions $\{q_a(x_a); q_i(x_i)\}$ ⁴ are introduced in one-to-one correspondence with the model factors and variables, and the entropy is approximated as

$$-\sum_x q(x) \log q(x) \approx -\sum_a \sum_{x_a} q_a(x_a) \log q_a(x_a) - \sum_i (1 - k_i) \sum_{x_i} q_i(x_i) \log q_i(x_i), \quad (6)$$

with k_i equal to the variable connectivity (the number of factors in which variable i participates). The reason this approximation may improve upon mean-field is that through $q_a(x_a)$ some correlations amongst variables may be explicitly represented, which are absent in the factorial form of mean-field. The variational parameters, q_a and q_i , are referred to as beliefs.

The Bethe approximation is a special case of the more general region-based approximation (see Yedidia et al., 2005), where the entropy approximation is implied by a choice of outer regions. Each outer region is defined by a set of variables x_α , and a generalized factor $\psi_\alpha(x_\alpha)$ that describes the interactions between those variables. The outer regions must be chosen to span all variables, and the factors (as well as auxiliary parameters ν) can be distributed amongst the generalized factors such that $\prod_\alpha \psi_\alpha(x) \propto p_\nu(x)$. Some examples of region selections discussed in this paper are shown in Figure 2.

The entropy approximation is implied by the choice of outer regions: it is the sum of the entropy on the outer regions α corrected by a weighted sum of entropies on region

4. $q_A(x_A)$ denotes a variational parameter, that can be interpreted as an approximation to the marginal probability $p(x_A)$.

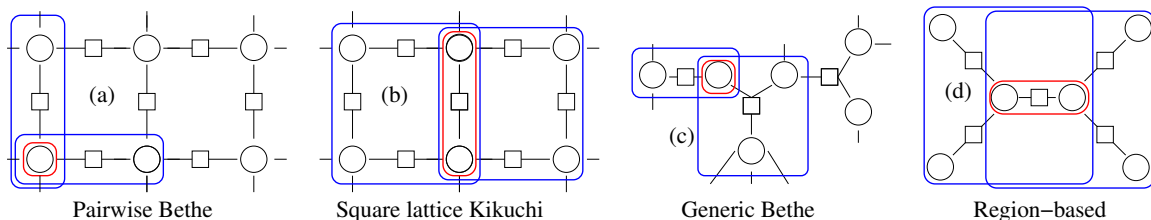


Figure 2: In a region-based approximation (Bethe is a special case), the assignment of outer regions determines the entropy approximation. Sensible choices collect nearby sets of strongly dependent variables. A region graph has outer regions (blue) and intersection regions (red), such that every factor is associated to exactly one outer region; the set of factors in a region α define an auxiliary interaction (8). Selection (a) is a Bethe approximation, the outer regions are pairs of variables, that intersect on single variables. (b) Alternatively, for a square lattice, we might consider outer regions of 4 variables (the central interaction could be assigned to either the right or left region), that intersect on pairs of variables, which in turn intersect on single variables. This approximation is powerful for square lattice models (see Raymond and Ricci-Tersenghi, 2013b; Domínguez et al., 2011; Lage-Castellanos et al., 2013). (c) The Bethe approximation on a factor graph with mixed (multi-variable) interaction types has outer regions containing exactly one factor and its variables, the intersections are single variables. (d) On a locally tree-like graph, we can also make an interesting approximation: outer regions are stars that intersect on edge regions. This approximation relates to the loop-correction algorithm of Montanari and Rizzo (2005).

intersections (β). The region based free energy is defined

$$F_\nu(q) = \sum_{\alpha} \sum_{x_{\alpha}} q_{\alpha}(x_{\alpha}) \log \left(\frac{q_{\alpha}(x_{\alpha})}{\psi_{\alpha}(x_{\alpha})} \right) + \sum_{\beta} c_{\beta} \sum_{x_{\beta}} q_{\beta}(x_{\beta}) \log q_{\beta}(x_{\beta}), \quad (7)$$

where c_{β} take integer values according to a simple rule (see Yedidia et al., 2005; Heskes et al., 2003). Larger regions are capable of capturing more correlations between variables explicitly, but at a computational cost that scales (in the absence of further approximations) exponentially with region size. This trade-off determines the choice of regions.

In the Bethe approximation, the outer regions (α) are in one-to-one correspondence with the factors (a) of the model, and intersection regions are single variables. In our running example of the Boltzmann machine (3), a Bethe approximation has edges as regions. Generalized factors can be chosen as

$$\psi_{(i,j)}(x_i, x_j) = \exp \left(J_{ij} x_i x_j + \frac{h_i + \nu_i}{k_i} + \frac{h_j + \nu_j}{k_j} \right). \quad (8)$$

We can define marginal variational parameters for each marginal probability in the free energy and then minimize (7) subject to local consistency constraints

$$\sum_{x_{\alpha}} q_{\alpha}(x_{\alpha}) = 1; \quad \forall \alpha, \quad (9)$$

$$\sum_{x_{\alpha} \setminus x_{\beta}} q_{\alpha}(x_{\alpha}) = q_{\beta}(x_{\beta}); \quad \forall \alpha, \forall \beta \subset \alpha. \quad (10)$$

Minimization of this free energy is a well-studied problem. Heuristic approaches normally lead to message passing algorithms, which are often convergent to good solutions even where guarantees of convergence are lacking. It is always possible to find minima of the region based free energy using a convex-concave procedure, which is guaranteed to converge to a local minima (see Yuille, 2002; Heskes et al., 2003).

Having found a minimum of the free energy at $q = q^*$, we can define the linear response in the beliefs to a perturbation in $\nu_{i,y}$, as

$$q_{\alpha,(i,y)}^*(x_\alpha) = \left. \frac{\partial q_\alpha(x_\alpha)}{\partial \nu_{i,y}} \right|_{q=q^*} .$$

Whereas the variational parameters q have an interpretation away from the fixed point, the linear response is only defined about a global (or heuristically, local) minima. Notation $*$ will be used to denote an evaluation at such a fixed point.

The entropy approximations (6-7) can be interpreted as truncated series (see Pelizzola, 2005; Wainwright and Jordan, 2008), that can be made good either by considering sufficiently large regions (those defining a junction tree, see Wainwright and Jordan, 2008), or including loop corrections (see Chertkov and Chernyak, 2006). The made-good approaches are not tractable in many interesting models of modest scale. The region based methods most often lead to improvements over mean-field, but entropy expansion can also lead to counterintuitive features. For example, the entropy estimate can be negative under such an approximation.

2.1 Inconsistency of Covariance Approximations

The covariance of a pair of statistics ϕ_1 and ϕ_2 , under probability distribution p is defined as

$$\begin{aligned} \mathbb{V}_p(\phi_1, \phi_2) &= \mathbb{E}_p(\phi_1 \phi_2) - \mathbb{E}_p(\phi_1) \mathbb{E}_p(\phi_2) , \\ \text{with } \mathbb{E}_p(\phi) &= \sum_x p(x) \phi(x) . \end{aligned}$$

For the case $\phi_1(x_\alpha) = \delta_{x_{i_1}, y_1}$ and $\phi_2(x_\alpha) = \delta_{x_{i_2}, y_2}$, we can replace the probability of interest p by q_α to obtain

$$\mathbb{V}_p(\delta_{x_{i_1}, y_1}, \delta_{x_{i_2}, y_2}) \approx C_{(i_1, y_1), (i_2, y_2)} := \mathbb{V}_{q_\alpha}[\delta_{x_{i_1}, y_1}, \delta_{x_{i_2}, y_2}] .$$

C will be called the marginal approximation to the covariance, and is a function of the variational parameter q_α . The optimal value $C^* = C(q^*)$ is independent of the region α , owing to the consistency constraints (9)-(10).

Alternatively, we can begin with a second derivative identity. By introducing parameters ν conjugate to each statistics (2), we have

$$\mathbb{V}_p(\delta_{x_{i_1}, y_1}, \delta_{x_{i_2}, y_2}) = \frac{\partial^2 \log Z(\nu)}{\partial \nu_{i_1, y_1} \partial \nu_{i_2, y_2}} .$$

We obtain a tractable approximation replacing $\log Z(\nu)$ by $-F_\nu(q^*)$

$$\mathbb{V}_p(\delta_{x_{i_1}, y_1}, \delta_{x_{i_2}, y_2}) \approx \chi_{(i_1, y_1), (i_2, y_2)} := \sum_{x_\alpha} q_{\alpha, (i_1, y_1)}^*(x_\alpha) \delta_{x_{i_2}, y_2} , \quad (11)$$

for any α containing i_2 , which is called the linear response estimate. χ will be called the linear response approximation to the covariance, it is defined only at the minima q^* , and is a symmetric matrix. We do not need to make explicit reference to the region α used in Eq. (11) since the linear response χ does not depend on that choice.

The name ‘linear response’ for the quantity χ comes from the fact it can be interpreted as

$$\chi_{(i_1, y_1), (i_2, y_2)} \approx \left. \frac{\partial \mathbb{E}_p[\delta_{x_{i_1}, y_1}]}{\partial \nu_{i_2, y_2}} \right|_{\nu=0} = \left. \frac{\partial \mathbb{E}_p[\delta_{x_{i_2}, y_2}]}{\partial \nu_{i_1, y_1}} \right|_{\nu=0}, \quad (12)$$

that is the linear variation of the mean value of a single variable statistic to a small perturbation in the parameter ν conjugated to another single variable statistic.

We denote the difference of these estimates for two statistics on variables (i_1, i_2) contained in region α as

$$\Delta_{(i_1, y_1), (i_2, y_2), \alpha}(q_\alpha, q_{\alpha, (i_1, y_1)}^*) = C_{(i_1, y_1), (i_2, y_2)} - \chi_{(i_1, y_1), (i_2, y_2)}. \quad (13)$$

Except for some simple models $C^* - \chi$ is non-zero, exposing an inconsistency in the variational method. The best marginal approximation does not match the best linear response estimate. To decide which estimate to use, either connected correlations or linear responses, we might consider the distance of these two different estimates from the correct value:

$$\Delta_{(i_1, y_1), (i_2, y_2)}^{(1)} = C_{(i_1, y_1), (i_2, y_2)}^* - \mathbb{V}_p(\delta_{x_{i_1}, y_1}, \delta_{x_{i_2}, y_2}), \quad (14)$$

$$\Delta_{(i_1, y_1), (i_2, y_2)}^{(2)} = \chi_{(i_1, y_1), (i_2, y_2)} - \mathbb{V}_p(\delta_{x_{i_1}, y_1}, \delta_{x_{i_2}, y_2}). \quad (15)$$

Graphical models in which the Bethe approximation is most successful have relatively weak correlations and/or few short loops. In these cases it is known that the linear response estimate (15) improves significantly upon (14) for $i_1 \neq i_2$ (see Welling and Teh, 2004; Raymond and Ricci-Tersenghi, 2013a). However, as the approximation breaks down (due to poor approximations of loops in the graphical model), the response estimate can be much worse, even giving infinite values for bounded statistics. For pairs with $i_1 = i_2$ (called diagonal), bounds can be violated even in regimes where the approximation is good. A simple example is the model of Section 4.1 with zero field ($h = 0$): whilst it is true that $\mathbb{V}_p(x_i, x_i) \leq 1$ for any model, $\chi_{i,i} > 1$ for in the weakly coupled (high temperature) regime.

2.2 Covariance Constraints

We would like to use the linear response information, in a safe manner to select the best covariance estimate, but also to make the approximation self-consistent. Rather than simply minimizing the free energy to determine q^* , we do this in the subspace where $\{\Delta_{(i_1, y_1), (i_2, y_2), \alpha} = 0\}$ for a subset of the covariances.

An important question will be which covariances to constrain. Expansion methods indicate that adding all constraints is best when the approximation is very good (see Raymond and Ricci-Tersenghi, 2013a). More generally we wish to add important constraints in so far as it does not prevent solution existence and allows algorithmic stability as discussed in Appendices B.1-B.3.

Although general expressions are derived, experimental sections in this paper are restricted principally to the Bethe approximation, and with simple patterns of constraints

discussed in Appendix B.2. The Bethe approximation with the addition of all possible constraints (called *on and off diagonal*⁵) is considered, as well as the Bethe approximation with addition of only constraints for which $i_1 = i_2$ (*diagonal*). In Section 4.1 we also present results for the mean-field approximation with all possible constraints (since $i_1 = i_2$ in all cases, this is also called diagonal), as well as the Bethe approximation including only constraints for which $i_1 \neq i_2$ (*off-diagonal*). In other experiments, we do not present these latter two regimes since they performed consistently worse except in some narrow parameter ranges where all regimes were performing poorly.

2.3 Bethe Approximation to the Boltzmann Machine

In the case of our running example of the Boltzmann machine (3) we are considering a variation of $\nu_i = \nu_{i,1} - \nu_{i,-1}$, accordingly we can abbreviate notation everywhere (i, y) to i . In the diagonal constraint approximations, we will require consistency of $\mathbb{V}(x_i, x_i) \forall i$. In the on and off diagonal constrained approximations, we require in addition consistency of $\mathbb{V}(x_i, x_j)$ for all coupled pairs of variables.

The quantities made consistent are written more concisely as

$$\begin{aligned} \mathbb{V}_p(x_i, x_j) &\approx C_{i,j} := \mathbb{V}_{q_{(ij)}}(x_i, x_j), \\ \mathbb{V}_p(x_i, x_j) &\approx \chi_{i,j} := \sum_{x_i, x_j} q_{(ij),i}^*(x_i, x_j) x_j. \end{aligned}$$

When evaluated at minima of the free energy, both the approximation by marginalization C^* , and approximation by linear response χ , are symmetric.

3. Minimizing with Respect to the Constraints

We choose a Lagrangian formulation for minimizing the constrained free energy, introducing a Lagrange multiplier for each constraint connecting a linear response approximation to a marginalization approximation. Each statistic pair constraint will be associated with some unique outer region α , as this allows for a cavity heuristic that we later introduce. This association is not unique and may affect (to a limited extent) the convergence of the algorithms we will develop, but not the fixed points that might be achieved. This is discussed further in Appendix B.3. The set of constraints associated to region α are denoted $\omega_\alpha = \{(i_1, y_1), (i_2, y_2)\}$ with an associated set of Lagrange multipliers $\lambda_\alpha = \{\lambda_{(i_1, y_1), (i_2, y_2)}\}$. The constrained minimization is then achieved by minimizing the Lagrangian

$$F_\nu(q, \lambda, \chi) = F_\nu(q) + \sum_\alpha \left[\sum_{[(i_1, y_1), (i_2, y_2)] \in \omega_\alpha} \lambda_{(i_1, y_1), (i_2, y_2)} \Delta_{\alpha, (i_1, y_1), (i_2, y_2)}(q_\alpha, q_{\alpha, (i_1, y_1)}^*) \right], \quad (16)$$

with Lagrange multipliers set to meet the constraints. The global minima q^* for fixed λ can often be found. In cases where local minima can be avoided this is done either heuristically following a constrained loopy belief propagation (CLBP) approach, or in a more robust manner using a provably convergent method, as discussed in Appendix B. CLBP has the same (asymptotic) computational complexity as belief propagation, and is procedurally similar.

5. This terminology arises by considering which elements of the covariance matrix are constrained.

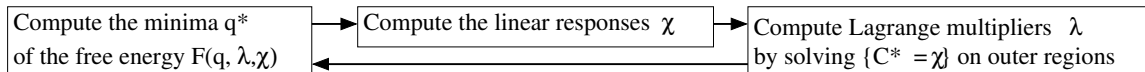


Figure 3: The basic scheme for minimizing our constrained variational free energy. The first stage is solved by a procedure closely related to belief propagation (that minimizes a convex-concave function), the second by a procedure related to susceptibility propagation (that solves a system of linear equations), and the final stage by a cavity approximation. In our experiments, we take $\lambda = 0$ as the initial condition. In the experiments presented we gradually increase or decrease T using the solution at $T \pm \delta T$ as an initial condition for the next experiment, this enables a solution to evolve continuously from a well-understood limit, but is not necessary for convergence in general.

It is shown in Appendix B.6 that given such a fixed point, whether a local or global minimum, it is subsequently relatively easy to calculate the linear response. The method we propose is procedurally similar to susceptibility propagation, originally introduced in Mezard and Mora (2008), which is a computational procedure that minimizes the variational parameters. If the number of constraints is linear in the size of the system the computational complexity is quadratic in system size. We call the linear response scheme constrained loop susceptibility propagation (CLSP). Yasuda and Tanaka (2013) proposed a closely related approach, specific to the case of diagonal constraints in the Bethe approximation.

Suppose we also have a method for iteratively determining λ , then we can approach the problem of finding a constrained local minima by a 3-stage iterative procedure (the same as proposed in Yasuda and Tanaka (2013)), and shown schematically in Figure 3. We also experimented with other minimization schemes, but found this to be algorithmically the most stable, and also pleasing in that we move all uncertainty in convergence of the method onto the two questions: (1) does there exist a fixed point at all and (2) does the iterative scheme for λ converge. These two questions are unfortunately very difficult to answer in general. To determine λ a heuristic *cavity* method is proposed in Section 3.1.

We found that in weakly correlated regimes the CLBP and CLSP, and iterative updating of λ quickly converges. However, in some other regimes where the variational approximation is less accurate, we found that the effect of non-zero λ could be either a help or a hindrance to the convergence of the CLBP. We also found that λ would sometimes not converge, even with strong damping (implementation of damping is discussed in Appendix C). Associated with regimes of non-convergence, we normally find a divergence of some λ values as discussed in the experimental section. This indicates that failure of the method is most likely related to non-existence (or criticality) of constrained solutions, the issue of solution existence is discussed in Appendix B.1.

3.0.1 BETHE APPROXIMATION TO THE BOLTZMANN MACHINE

For the on-and-off diagonal constrained case, the Lagrangian for the Boltzmann machine can be written in the form⁶.

$$\begin{aligned}
 F_\nu(\mathbf{q}, \boldsymbol{\lambda}, \chi) = & \sum_{(i,j) \in E} \sum_{x_i, x_j} q_{ij}(x_i, x_j) \log q_{ij}(x_i, x_j) + \sum_i (1 - k_i) \sum_{x_i} q_i(x_i) \log q_i(x_i) \\
 & + \frac{1}{2} \sum_i \lambda_{i,i} [(1 - M_i^2) - \chi_{i,i}] + \sum_{(i,j) \in E} \lambda_{(i,j)} \left[\sum_{x_i, x_j} q_{ij}(x_i, x_j) x_i x_j - M_i M_j - \chi_{i,j} \right], \quad (17)
 \end{aligned}$$

introducing abbreviations for single variable magnetization $M_i := \sum_{x_i} q_i(x_i) x_i$. We recover the diagonal constraint regime when $\lambda_{i,j} = 0 \quad \forall i, j$, and the unconstrained regime when all multipliers are zero. Constraints introduce quadratic functions of q , but terms are neither convex nor concave.

For given λ , a set of message passing equations can be written as a generalization of loopy belief propagation, a simplification of the general case in Appendix B.5 is presented here. At time t the edge-belief is approximated as the solution to the equation

$$\begin{aligned}
 q_{ij}^t(x_i, x_j) \propto & \mu_{i \rightarrow (i,j)}^t(x_i) \mu_{j \rightarrow (i,j)}^t(x_j) \\
 & \exp \left[(J_{ij} - \lambda_{ij}) x_i x_j + (h_i + \lambda_{ij} M_{ij,j}^t + \lambda_i M_{ij,i}^t) x_i + (h_j + \lambda_{ij} M_{ij,i}^t + \lambda_j M_{ij,j}^t) x_j \right],
 \end{aligned}$$

where we introduce two auxiliary magnetization parameters per edge⁷

$$M_{ij,i}^t = \sum_{x_i x_j} x_i q_{ij}^t(x_i, x_j). \quad (18)$$

Then we can define messages⁸ μ which are determined iteratively as

$$\begin{aligned}
 \mu_{(i,j) \rightarrow i}^t(x_i) & \propto \sum_{x_j} \mu_{j \rightarrow (i,j)}^t(x_j) \\
 & \exp \left[(J_{ij} - \lambda_{ij}) x_i x_j + (h_j + \lambda_j M_{ij,j}^t + \lambda_{ij} M_{ij,i}^t) x_j + \lambda_{ij} M_{ij,j}^t x_i \right], \\
 \mu_{i \rightarrow (i,j)}^{t+1}(x_i) & = \prod_{k \in \partial_i \setminus j} \mu_{(i,k) \rightarrow i}^t(x_i), \quad (19)
 \end{aligned}$$

where ∂_i are the variables interacting with i . Following message updates q^t and M^t must be made consistent, in the examples of this paper (and in general for small λ) this can be achieved simply by iterating Equations (18) and (19). For the experiments messages and beliefs are initialized as constants.

There are several methods by which linear response can be established. One standard approach is susceptibility propagation, which simply involves linearizing the above equations accounting for a small perturbation in some component of ν , this is the approach taken for the examples of this paper; for the general case, expressions are provided in Appendix B.6.

6. To maintain consistency with published research on Ising spin models a factor $1/2$ precedes the diagonal constraint term.

7. Note that at intermediate stages of the message passing, magnetizations for variable i on different beliefs (say $M_{ij,i}$, $M_{ik,i}$) may not agree, but will agree after convergence.

8. These differ by a simple transformation from the messages of the Appendix B.5, so that the limiting case ($\lambda = 0$) agrees with standard presentations for Ising models in the literature.

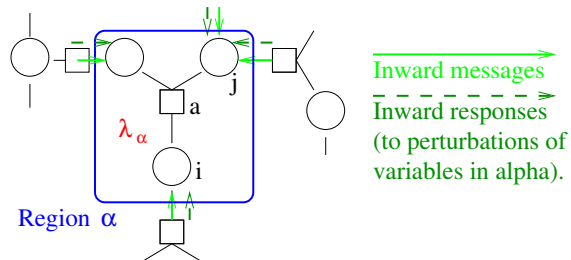


Figure 4: Given C^* and χ , determination of λ breaks into a set of independent problems on outer regions α . This can be understood as a cavity approximation. Assuming the incoming messages, and responses, to be fixed and approximately independent of the Lagrange multipliers to be set (λ_α), we can independently, on each region, solve the system of equations $\Delta_\alpha = 0$ for λ_α . A similar assumption often justifies message passing and mean-field iterative heuristics.

3.1 Determination of λ

To determine λ we propose the following scheme. We wish to solve at each α a set of non-linear equations $\{\Delta_\alpha(q_\alpha, q_{\alpha,(\cdot)}^*) = 0\}$, where q_α and $q_{\alpha,(\cdot)}^*$ are functions of all λ (through the system of message passing equations). One possibility is to linearize these equations about the current estimate (that is apply Newton's method), but this leads to an impractical $O(N^3)$ procedure, dominating other algorithmic time-scales for moderately sized systems.

Instead, we resort to a locally consistent and parallelizable approximation: For some λ we find a minimum defined by messages μ (Appendix B.5), and the linear response for these messages (Appendix B.6). If λ is approximately correct then the messages passing into the region α should be weakly dependent on any changes to λ_α in that region. Since we can define Δ_α in terms of the local parameters λ_α , and the incoming messages (which we argue are unchanged by an update of λ_α) the problem for determining λ is reduced to solving for λ_α independently on every region.

In this way, we arrive at a cavity-approximation style argument common in the motivation of message passing algorithms, see Figure 4. However, it is noteworthy that unlike LBP, incoming messages and responses depend on λ_α locally. There is a direct feedback that exists even in the absence of loops.

Unfortunately, $\Delta_\alpha = \mathbf{0}$ remains a (small) system of non-linear equations in λ_α , that does not allow a closed form solution in general. One exception is when only diagonal constraints are applied (see Yasuda, 2013; Yasuda and Tanaka, 2013), and the cavity argument is applied to single-variable regions. More generally we use Newton's method to solve these equations

$$\left[\frac{\partial \Delta_\alpha(q^*, q_{(\cdot)}^*)}{\partial \lambda_\alpha} \right]^{-1} \Delta_\alpha \Big|_{\lambda=\lambda^t} \delta \lambda_\alpha^{t+1} = - \Delta_\alpha(q^*, q_{(\cdot)}^*) \Big|_{\lambda=\lambda^t}, \quad (20)$$

where the dependence of q^* and $q_{(\cdot)}^*$ on λ follows from (??) and (28) with messages fixed.

An alternative expression based on a closed form for the covariance matrix approximation χ is discussed in Appendix C, alongside some other technical details on the determination of λ .

4. Results

In this section, we study the performance of our method on well-understood toy model frameworks. The scale and/or symmetries of these models mean they are exactly solvable, allowing precise statistical estimates to evaluate the method quality.

In Section 4.1 we study a fully connected ferromagnetic model (that is a model with a positive coupling between any pair of variables) with symmetry broken (that is with a non-zero mean value for each variable). This is a simple model for which we can present analytic results and understanding. There is either no mode (for weak coupling), or one dominating mode (for strong couplings). We expect the method to be weakest for intermediate coupling strength since the Bethe approximation becomes exact (with corrections $O(1/N)$) in the limit of strong (a single mode) or weak (no modes) coupling. In Section 4.2 we study a model with frustration (that is couplings have different signs and it is not possible to find a configuration satisfying them all at the same time) and a random distribution of optima and sub-optima. The problem is multi-modal in the limit of strong couplings and the Bethe approximation breaks down. In Section 4.3 we consider a simple model with an expanded discrete alphabet, where randomness is introduced through a random graphical structure. Like the ferromagnetic example, a single mode dominates for strong couplings. We anticipate the Bethe approximation to become exact in the limit of large problems, but for smaller problems the presence of short loops leads to inaccuracy. In the final example of Section 4.4 we consider a well-studied toy model involving both multi-variable interactions and multi-states, both the Bethe approximation and linear response perform poorly on this model. These examples cover a range of scenarios in which our method might be applied. Special cases of the variational approximation we present have previously been applied to lattice models commonly studied in statistical physics, and sparse prior models in Bayesian image modeling (see Raymond and Ricci-Tersenghi, 2013b,a; Yasuda and Tanaka, 2013; Yasuda, 2013).

We present behaviour of the Lagrange multipliers λ , the self-consistency error (13), errors on the pair statistics when using either marginals (14) or linear responses (15), and errors on the marginal estimates

$$\Delta_{(i,y)}^{(0)}(q^*) = q^*(x_i = y) - p(x_i = y) .$$

The maximum absolute deviation (MAD) on the marginals is defined as the largest error over all variables, or pairs of variables, depending on error type.

It is interesting to understand how the quality of approximation changes as a function of the goodness of the approximation, to do this we introduce a temperature parameter T in each model, that can sharpen or flatten the distribution.

$$p_T(x) \propto p(x)^{1/T} .$$

We can minimize with relative ease both the constrained and unconstrained free energies in the large T regime, and expect approximations to be correct at leading order in $1/T$ (see Raymond and Ricci-Tersenghi, 2013a). In some cases of small T , in which the probability is well described by a single mode, concentrated about some unique value $x_{GS} = \operatorname{argmax} p_T(x)$, the approximations we present are also exact up to $O(T)$ corrections.

We find that in many of the models, minimization of the constrained free energy is slow or impossible for T over some intermediate range, or below some threshold. To extend the range of T for which solutions could be found, an annealing procedure is employed: beginning at large (or small) T and proceeding through a sequence of models slowly changing T , and using the solution to the previous model as the initial condition for the subsequent minimization. Under this procedure, we find that $\lambda(T)$ and the variational parameters q evolve smoothly, but that there appears still to be a limit in the accessible temperature range. In the applications presented we did not find fixed points that appeared discontinuously. Solutions are reached by annealing from low temperature, from high temperature, or are absent.

Our motivation for introducing T is threefold: to study the breakdown of the approximation (absence of solutions), to mitigate for non-convergence, and to increase the speed of convergence. The annealing procedure introduces additional computational costs. We have not made timing comparisons against loopy belief propagation or other competitors, for either the simple or annealed procedure. Instead, we have prioritized an exploration of the nature of solutions that can be discovered, and we have sought very accurate estimates to the parameters describing those solutions. Compromises in the accuracy of constraint satisfaction, annealing rate (or absence of annealing), and damping can all have a significant impact on the speed of the method.

4.1 The Fully Connected Ferromagnet

We begin with a simple but informative case, that of a fully connected ferromagnetic Ising model in an external field.

$$p_T(x) = \frac{1}{Z} \exp \left[\frac{1}{2T} \left(h + \sum_{i=1}^N x_i \right)^2 \right]. \quad (21)$$

Variables are Ising spins $x_i = \pm 1$. The marginals for this model can be solved up to $O(1/N)$ by the mean-field approximation, and up to $O(1/N^2)$ by the Bethe approximation. Accuracy is a function of temperature; when this is large or small compared to $1/N$, the accuracy is correspondingly high. Under our method the equations to be solved and associated errors can be expressed concisely; this is done in Appendix A.

Three kinds of constraint are considered: diagonal $\{\Delta_{ii} = 0, \forall i\}$; off-diagonal $\{\Delta_{ij} = 0, \forall i \neq j\}$; and on-and-off diagonal applying both sets. Results for both the mean-field and Bethe approximations are presented. Only diagonal constraints can be applied in the mean-field case since the variational parameters are consistent only with zero off-diagonal covariances.

The left panel in Figure 5 shows the behavior of the magnetizations, $\mathbb{E}(x_i)$ for the case $N = 10$ and $h = 1$. The most accurate estimates are obtained with on and off-diagonal constraints applied at the Bethe approximation at high and low temperature. The unconstrained approximations overestimate the magnetization (bias in variables). The addition of constraints corrects this bias: in one constrained regime (off-diagonal constraints only) the suppression is clearly too strong at intermediate T , while in all other cases effective.

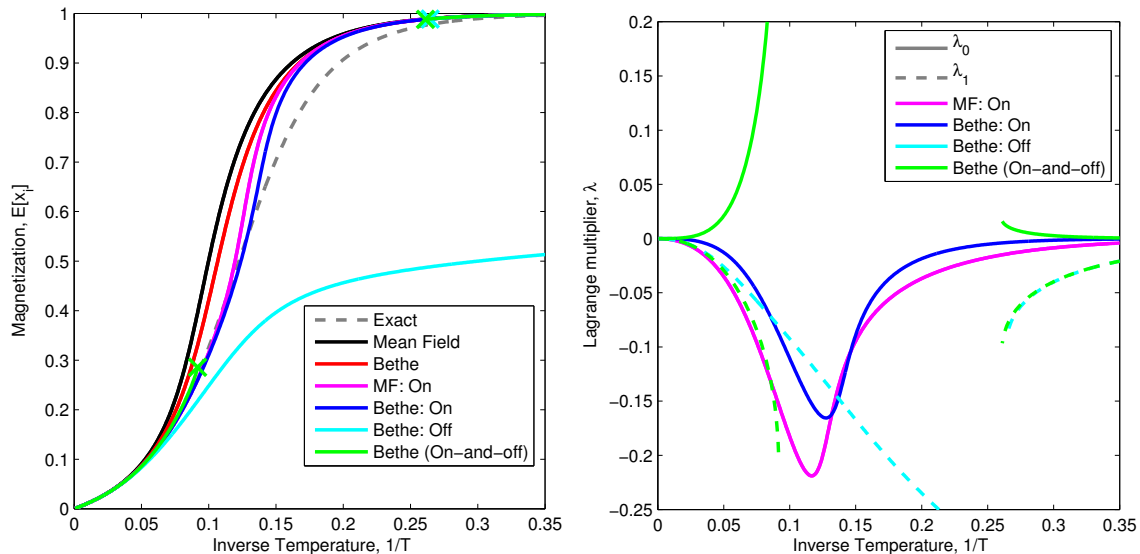


Figure 5: Results for the fully connected model (21) with $N = 10$ and $h = 1$. Results are presented for the mean-field and Bethe approximation schemes, with and without constraints. (left) The magnetization is overestimated in the Bethe and Mean-field approximations, the effect of the constraints is to suppress the magnetization. Certain solutions exist only in the high-temperature or low-temperature regimes, those solutions are demarcated by 'x'. One solution to the Bethe approximation with off-diagonal constraints only suppresses the magnetization too strongly, there is another solution that is present only at low temperature, where the estimate is more reasonable. Where it exists, the Bethe approximation with on and off-diagonal constraints is the most accurate. (right) There are at most two independent values for λ in this model: diagonal λ_0 and off-diagonal λ_1 . The Lagrange multipliers deviate most from zero at $T \sim 1/N$ (this is related to a ferromagnetic phase transition). λ diverge rapidly in some solutions demarcating regions where no solutions can be found.

In some constrained approximations there is a smooth evolution of the optimal beliefs with T , which reflects the behavior of the exact marginals. In others, the optimal beliefs for different T are not continuously related.

When off-diagonal constraints are applied in the Bethe approximation, either alongside or without diagonal constraints, we see a discontinuous emergence of the strongly magnetized solution. In the case of only off-diagonal constraints, there is a coexistence of two fixed points for small T . This means that as we vary the parameter T the q^* moves discontinuously from a relatively smooth approximation to one characterized by a single mode. As N increases the domain with coexistence shrinks, and all approximation approach the correct result for large N .

With on and off-diagonal constraints we find a range of T for which no solutions can be found by a continuous evolution of the low or high-temperature solutions. It seems highly likely that no solution exists, and empirically we were not able to find fixed points (for any model) that were not continuously related to either a high or low-temperature solution.

The behaviour of λ (see right panel in Figure 5) and indeed a careful examination of the fixed points indicate why solutions disappear in this simple case. The values of the Lagrange multipliers diverge, and this is related to marginals approaching their boundary values where variational inference breaks down due to the inflexibility of the parameters. By decreasing h or N we decrease the accuracy of the Bethe approximation at intermediate T , this can lead to discontinuity also for the diagonal constrained solution, and reduces the range of temperatures over which the low-temperature solution (the one with a large magnetization) can be found for constrained problems.

4.2 The Wainwright-Jordan Set-up

A common toy model on spin variables $x_i = \pm 1$ is the Wainwright-Jordan set-up where $N = L \times L$ Ising spins are arranged on a square grid (see Opper et al., 2009).

$$p_T(x) = \prod_{(i,j) \in E} \exp(J_{ij}x_i x_j / T) \prod_i \exp(h_i x_i / T).$$

Fields h_i are independent and identically distributed (iid) samples from $[-0.25, 0.25]$ and couplings J_{ij} are sampled i.i.d on $[-1, 1]$. The Bethe approximation fails on these models for smaller T owing to multi-modality of the distribution, but for larger T (where correlations are weaker) the approximation is a significant improvement upon the mean-field approximation.

Diagonal $\{\Delta_{i,i} = 0, \forall i\}$, or diagonal and off-diagonal $\{\Delta_{i,j} = 0, \forall (i, j) \in E\}$ constraint regimes are studied for the Bethe approximation.

We considered 20 instances for $L = 4$ and $L = 7$, and plot the MAD results in Figures 6 and 7. Shown are the quartiles, for cases where methods did not converge we assigned value $+\text{Inf}$ to the MAD so that the quartile values are truncated in cases where the fraction of non-convergent cases exceeded the quartile. For the smaller ($L = 4$) system, the Bethe approximation succeeds for typical cases to full scale ($T = 1$) either without constraints or with only diagonal constraints; the on-and-off diagonal scheme fails in a larger fraction of cases. For the larger ($L = 7$) system, LBP and CLBP fail at full scale: the model which prevails to lowest temperature is CLBP with diagonal constraints; the model failing soonest

is CLBP with on and off-diagonal constraints. The exact range of T for which methods were convergent was sensitive to the annealing procedure, the amount of damping used, and the convergence criteria; strong damping and slow annealing broaden the range for all methods.

Where the algorithm is convergent, there is significant improvement adding diagonal constraints, and more so with on and off-diagonal constraints. We find the improvement in the maximum deviation represents well the changes seen across the entire distribution of marginals in most models, almost all marginals are improved. The quartiles in figures 6 and 7 reflect model to model variations, and demonstrate that the MAD advantage is robust. For $N = 16$, we can compare the median behavior against that reported in Opper, Paquet, and Winther (2009); where the strongest method (tree-EP) also improves the MAD result for marginals by approximately one order of magnitude. Expansion methods offer some further, but modest gains (see Paquet et al., 2009; Opper et al., 2013).

On-diagonal constraints allow an increased range (in T) for convergence. Qualitatively, we offer the following explanation. In the constrained regimes (in the high-temperature regime, the only one for which we demonstrate solutions) the majority of Lagrange multipliers are negative. The effect is to suppress biases and decrease susceptibility (the sensitivity of biases to small changes in the parameters). We assume that reduced susceptibility also correlates with reduced sensitivity to small fluctuations in the messages, which should aid algorithmic stability. With on-and-off diagonal constraints the diagonal and off-diagonal Lagrange multipliers are strongly dependent where they constrain the same variable. The off-diagonal multipliers are typically negative, and suppressing biases; by contrast, the diagonal multipliers are positive and reinforce biases. The typical net effect is to reduce biases and susceptibility, as with the on-diagonal case. However, the strongly correlated nature of the parameters may be the source of convergence problems.

The failure of CLBP is most often due to non-convergence of λ , rather than a failure in the CLBP or CLSP iterative algorithms (at fixed λ). Figure 8 indicates why the iterative update is failing: some Lagrange multipliers are diverging in a strongly correlated manner and it seems likely there is a critical value of T close to the failure point beyond which no solutions exist, as found in Section 4.1.

The LBP implementation follows the same procedure as the constrained cases of Appendix B, with the difference that the innermost do-while loop is always convergent in one iteration, and $\lambda = 0$. Using a double loop procedure we might force convergence to a minimum of the Bethe approximation, but the convergence properties of LBP are still an interesting point of comparison.

We might seek to extend the range of convergence for CLBP by clever modifications. However, it seems that breakdown of convergence is closely related to breakdown of the underlying (Bethe) approximation. Algorithmic innovations would not extend significantly the range of problems for which the constrained approximation is useful in practice; just as the availability of double loop methods has not revolutionized the use of the Bethe approximation: where LBP fails the Bethe approximation is almost always a poor approximation.

For this type of problem a significant improvement to the Bethe approximation is made in moving to a plaquette-based Kikuchi approximations for the case of regular lattices (see Domínguez et al., 2011; Lage-Castellanos et al., 2013). Limited experiments on constrained

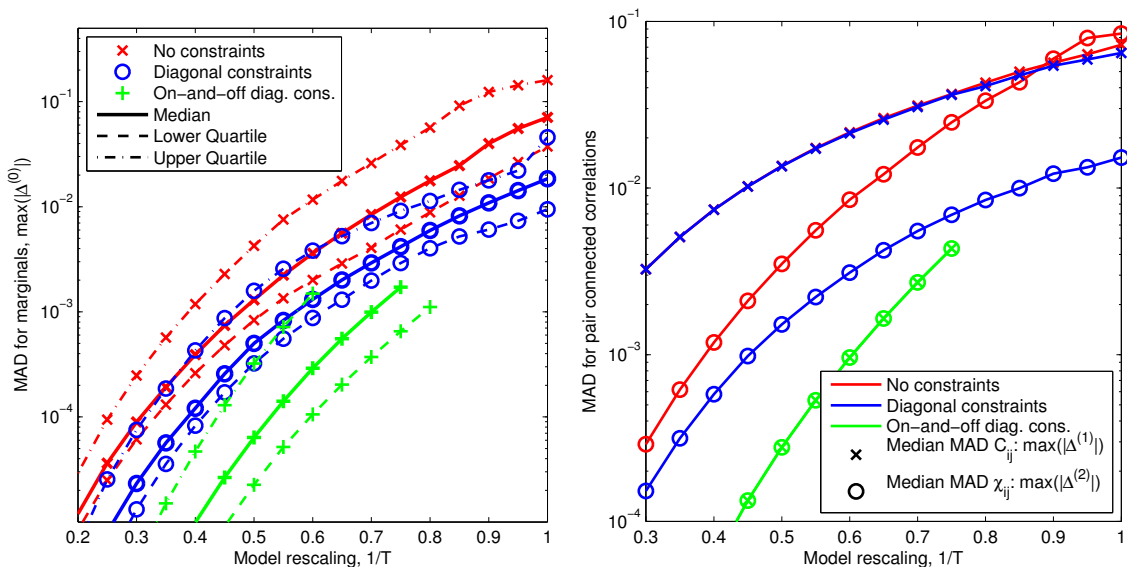


Figure 6: $L = 4$ Wainwright-Jordan set-up: The error on the marginals, and connected correlations (which together provide a sufficient description of pair probabilities) are improved everywhere by adding constraints, as long as the method converges. As discussed, the MAD for C_{ij} is worse than for χ_{ij} , although they are becoming comparable approaching $T = 1$. On the right the median over 20 models is shown, on the left the median and quartiles. The advantage is consistent across all models.

Kikuchi approximations also indicate a modest decrease in error on marginals with the application of constraints.

4.3 Potts Model in an External Field

Next we consider random 3-regular graphs $G = \{V, E\}$ of $N = |V|$ variables, where each variable is allowed 3 states: $x_i \in \{0, 1, 2\}$. The problems are defined by the probability

$$p(x) \propto \prod_{(ij) \in E} \exp(J_{ij} \delta_{x_i, x_j} / T) \prod_{i \in V} \exp(4 \delta_{x_i, 0} / T),$$

where couplings are i.i.d. random variables $J_{ij} \in \{-1, 1\}$. An example of a corresponding factor graph is shown in Figure 1 (lower panel). Like the fully connected Ising model, typical instances of this model are solved at leading order in N by the Bethe approximation, with finite size effects strongest at intermediate temperatures. At high temperature, the probability is relatively flat and disperse, whereas at low temperatures there is a single dominating mode concentrated about the value $\mathbf{0} = \operatorname{argmax}_x p(x)$.

We consider a diagonal constrained Bethe approximation: a set of 4 non-redundant statistic pairs are constrained per variable.

Figure 9 demonstrates that in graphs of size $N = 40$, the MAD on $p(x_i)$ is significantly improved with the addition of diagonal constraints. Furthermore, we see that as the Bethe approximation becomes accurate (high and low temperature, or large N) it becomes easier to enforce the constraints, as indicated by smaller values for the Lagrange multipliers.

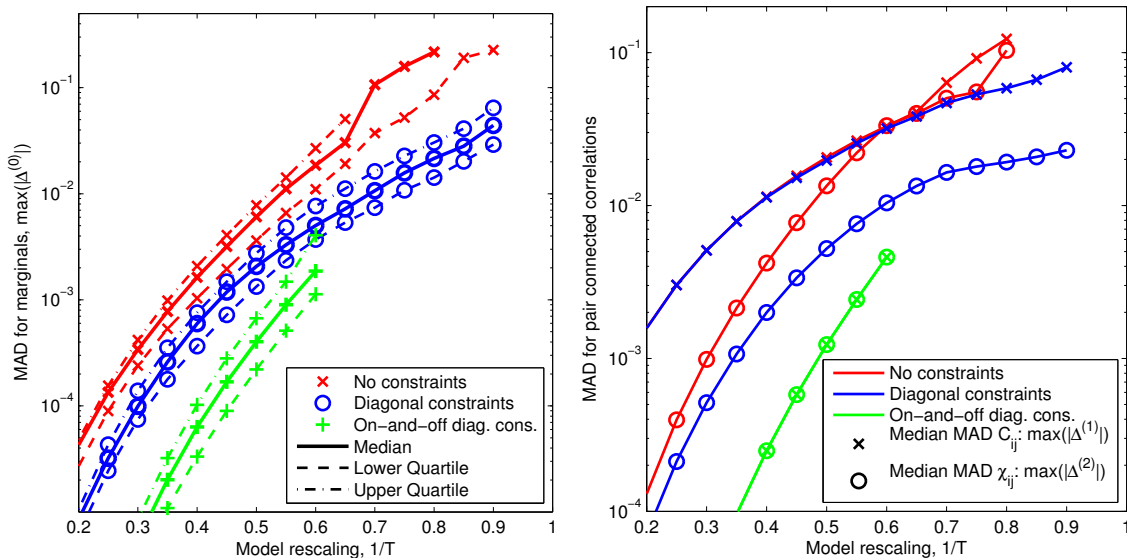


Figure 7: $L = 7$ Wainwright-Jordan set up: Trends are comparable to the smaller system in Figure 6. Where solutions exist, significant gains are made in all models with the addition of constraints. However, all approximations are now failing to reach full scale ($T = 1$). The method which is stable to lowest temperature is the model with diagonal constraints only, while the one with on-and-off constraints is the most accurate.

4.4 The Alarm Network

The alarm net is a pedagogical example of a graphical model that has been studied in the context of loop correction algorithms and is available in libDAI repository (see Mooij et al., 2007; Mooij, 2010). It has 37 variables, each variable takes either 2, 3 or 4 states (a mixture of Ising and Potts spins). Variables have biases, and participate in 2, 3 and 4 point interactions as shown in Figure 1 (upper graph). The model involves a mixture of factor types and variables. The Bethe approximation performs relatively poorly, due to short loops. We can again add a temperature and consider solutions up to the full scale $T = 1$ that defines the model.

Two constraint regimes were applied: in the first pure-diagonal constraints were applied: $\{(i, y), (i, y) : \forall i, y\}$, and in the second all block-diagonal constraints were applied $\{(i, y_1), (i, y_2) : \forall i, y_1, y_2\}$. The ability of both methods to improve local statistics were comparable and modest; for both the local diagonal and off-diagonal statistics as shown in Figure 10. Other schemes such as tree-EP and LCBP show improvements of one or two orders of magnitude on this problem (see Mooij et al., 2007; Oppen et al., 2009). However, the Bethe approximation and linear response estimates are known to be poor on this model, so it is not a surprise to see modest gains for our scheme.

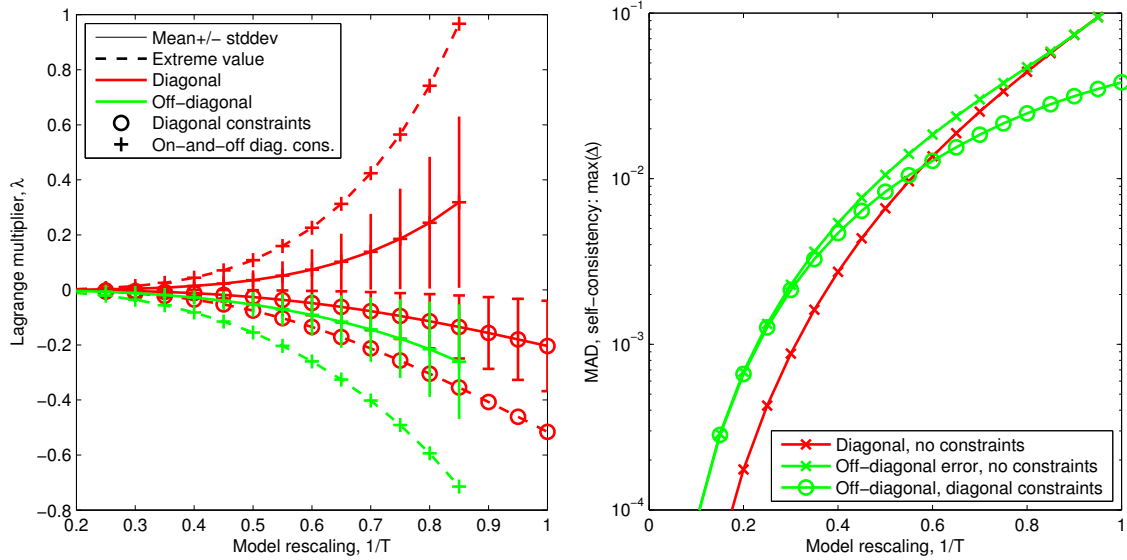


Figure 8: A typical problem in the Wainwright Jordan set up for $N = 16$. (left) Negative λ has the effect of effectively reducing the coupling strength; as with the fully connected ferromagnetic model, a mode of failure for the approximation is to over-estimate the bias in variables, and constraints appear to work by mitigating this effect. Bars indicate the 3 quartiles of the distribution, and the extremal values are also plotted. In the Bethe approximation with only diagonal constraints, most λ including the extremal value are negative. With on and off-diagonal constraints λ with a net effect of reducing interaction strength, values diverge approaching the point of algorithmic failure. (right) Adding diagonal constraints not only removes the diagonal self-consistency error, but also reduces the error in the unconstrained (off-diagonal) statistic. Adding both on and off diagonal constraints removes inconsistency for both types. The self consistency errors (13) grow with decreasing temperature.

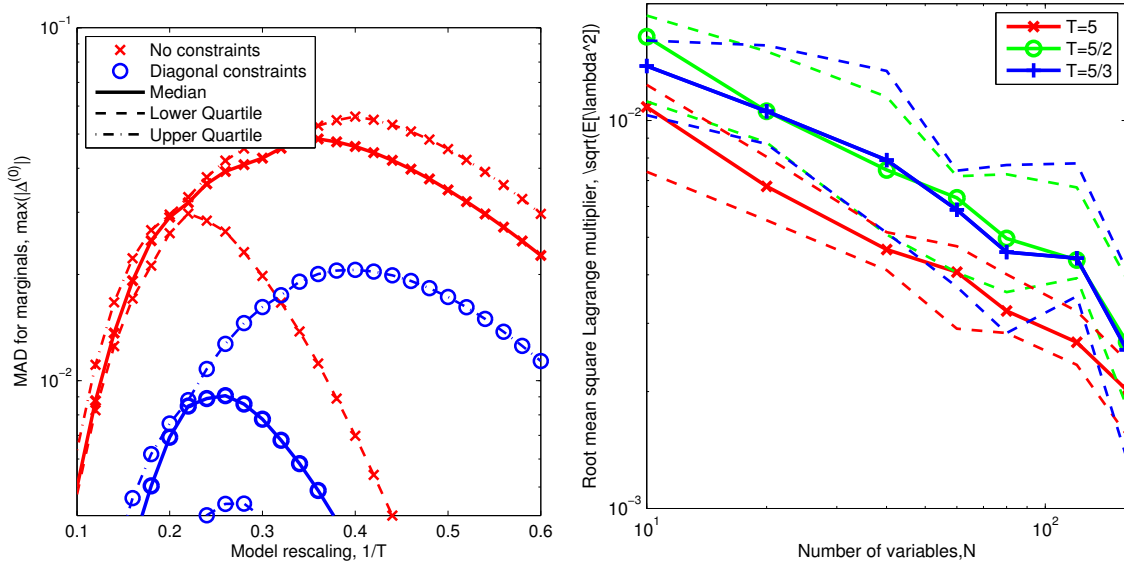


Figure 9: Errors and Lagrange multipliers are shown for the 3-states Potts model on 3-regular random graphs. (left) The diagonal constraint regime yields a significant improvement in maximum absolute deviation of $p(x_i)$ over the raw approximation on graphs with $N = 40$. (right) The Bethe approximation improves as $N \rightarrow \infty$ at all temperatures (due to the disappearance of many short loops). The Lagrange multipliers enforcing diagonal consistency typically decrease (in mean squared value) as system size increase. Quartiles are based on at least 20 samples per system size.

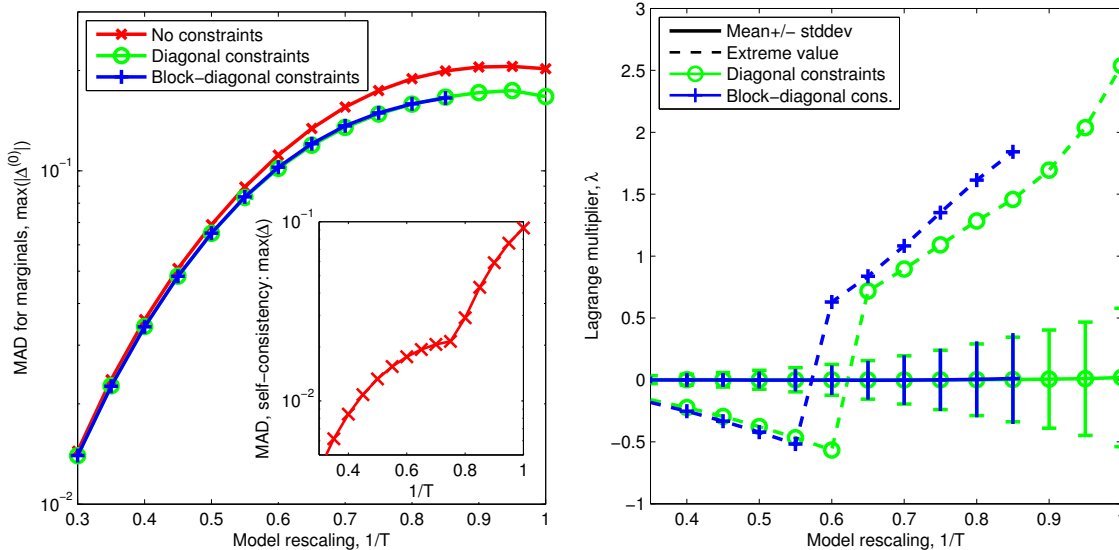


Figure 10: Results for the alarm network. (left) The diagonal and block-diagonal constraint regimes have indistinguishable performance in the MAD for $p(x_i)$, and improve modestly on the unconstrained problem. (inset) At intermediate T there is a qualitative change in the self-consistency error, as some variable subsets become strongly polarized. (right) The values for λ are for the most part small, with extreme values diverging as T approaches 1; a mixture of positive and negative Lagrange multipliers are required to enforce constraints.

5. Discussion

The aim of this paper is to show that for a range of models and variational methods we can have improved accuracy in marginal estimates by inclusion of a set of self-consistent constraints, and to propose this as a general mechanism by which to improve approximations with inconsistency between marginalization (first derivative) and linear response (second derivative) approximations.

We have expanded upon results for rather simple approximations, in easy to understand model frameworks: the marginals are improved in all cases, and in many scenarios by amounts measurable in orders of magnitude. The combination of a weak approximation method with constraints may result in there being no solutions and in marginal cases in a slow convergence of our proposed algorithm. On the other hand, if we are looking for a mechanism by which to leverage a good approximation this approach seems appropriate.

An interesting direction for investigation would be understanding whether partially reducing the violation, rather than eliminating it, might yield comparable results within a more robust algorithmic framework. There are two possibilities: (1) softening the constraint, introducing a penalty term that increases with $|\Delta|$ rather than requiring strict compliance; (2) expanding the range of solution existence by bounding λ . This would presumably maintain a large part of the method advantage by removing some pathologies. Further work could also relate to the choice of constraints, especially for non-Ising models

where the number of statistics available to constrain is large. Two directions are proposed in Appendix B.2.

Some powerful approximation methods are not variational and so the insight we provide cannot be leveraged. In other cases there is no inconsistency to exploit, this is true of adaptive-TAP and some moment matching methods. These have variational free energy frameworks, but by the Gaussian approximations therein used, there is a consistency of pairwise approximations, making redundant the constraints we suggest. This is in line with our thinking that good approximations should not violate these constraints.

We believe our method also sheds light on, or is inclusive of, previous attempts to leverage linear response. Consider the region-based free energy built on the set of regions indicated by Figure 2(d). Every outer region is a hub surrounded by leaves, and if we add constraints over the leaves within each region, a linear expansion in the Lagrange multipliers agrees with the linear expansion obtained in the scheme of Montanari and Rizzo (2005); however, outside of the linearized regime there are important differences.

There are three reasons one might not want to improve a variational approximation by adding self-consistency constraints: 1) The cost of the method which is dominated by a linear response evaluation (a cost that can be as large as $O(N^2)$ using susceptibility propagation), might be prohibitive in some applications. 2) Introducing such constraints may prevent the existence of any solutions (the method may reveal the uncomfortable truth that the approximation used is quite bad). 3) Even where a fixed point exists, it may be slow to reach it using a local iterative scheme for λ such as (20).

6. Conclusion

We have demonstrated that adding covariance constraints, which make the linear response and marginalization estimates consistent, improves the performance of the Bethe approximation for a variety of simple model types. We have argued this is true more generally of variational frameworks, and have provided an algorithmic framework for mean-field and region-based frameworks, generalizing previous results. The regimes of adding all possible constraints (on-and-off diagonal) and adding constraints only over single variable covariances (diagonal) were examined. The former tends to lead to better results, whilst the latter is simpler to implement and can yield solutions across a broader range of models.

The usefulness of this paper is not in the specific algorithm developed, but in the principle of statistical consistency. We hope it might be extended to other variational frameworks in which inconsistencies exist between first and second derivative estimates. We have presented and tested an algorithmic framework; the framework can solve the constrained free energy where solutions exist, but a rather expensive (annealed in T) procedure was exploited to obtain our results. Further work is required to make this reliable and competitive with state of the art marginal estimation.

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Appendix A. Exact Expressions for the Fully Connected Ising model

It is straightforward to calculate the exact marginal distributions for (21), for any pair of variables

$$p_T(x_i, x_j) \propto \sum_{n=0}^{N-2} \binom{N-2}{n} \exp \left[\frac{(h + [N-2-2n])^2}{2T} + \frac{1}{T} x_i x_j + \frac{h + [N-2-2n]}{T} (x_i + x_j) \right].$$

By contrast in the Bethe approximation

$$q_{ij}(x_i, x_j) \propto \exp \left[\frac{1}{T} x_i x_j + \frac{h_{\rightarrow}}{T} (x_i + x_j) \right], \quad (22)$$

where the log-ratio messages h_{\rightarrow} are defined as the solution to

$$h_{\rightarrow} = h + (N-1)T \operatorname{atanh} [\operatorname{tanh}(1/T) \operatorname{tanh}(h_{\rightarrow}/T)] ; \quad h_{\rightarrow} = \frac{1}{2} \log \left(\frac{\mu_{i \rightarrow (ij)}(1)}{\mu_{i \rightarrow (ij)}(-1)} \right).$$

Since we will place constraints on $\mathbb{V}_q(x_i, x_j)$ a convenient parameterization for the pair probability in our approximation will be

$$q_{ij}(x_i, x_j) = \frac{(1 + M_i x_i)(1 + M_j x_j) + C_{ij} x_i x_j}{4}. \quad (23)$$

We can restrict attention to symmetric solutions $M_i = M$ and $C_{ij} = C$, similarly at most two distinct Lagrange multiplier values need be considered: $\lambda_{i,i} = \lambda_0$, when diagonal constraints are applied, and $\lambda_{i,j} = \lambda_1$ when off-diagonal constraints are applied. Minimizing the variational free energy (17) with respect to M and C leads to the following pair of equations

$$0 = -[(n-1)M/T + \lambda_0 M] + \operatorname{atanh}(M) + (N-1) \sum_{x_1, x_2} \frac{x_1}{2} q_j(x_2) \log \left(\frac{q_{ij}(x_1, x_2)}{q_i(x_1)} \right), \quad (24)$$

$$0 = -[1/T - \lambda_1] + \sum_{x_1, x_2} \frac{x_1 x_2}{4} \log q_{ij}(x_1, x_2). \quad (25)$$

If we solve this pair of equations for $\lambda = 0$, we find an alternative representation of (22). Explicit expressions for the covariance matrix approximation χ are derived in Raymond and Ricci-Tersenghi (2013b) and Raymond and Ricci-Tersenghi (2013a), these can be concisely expressed in the inverse as

$$[\chi^{-1}]_{i,j} = \begin{cases} \frac{1}{1-M^2} \left[1 + (n-1) \frac{C^2}{(1-M^2)^2 - C^2} \right] - \lambda_0 & \text{if } i = j. \\ -1/T + \sum_{x_1, x_2} \left[\frac{x_1 x_2}{4} \log q_{ij}(x_1, x_2) \right] - \frac{C}{(1-M^2)^2 - C^2} & \text{otherwise.} \end{cases}$$

Abbreviating $\chi_{i,i}^{-1} = a$ and $\chi_{i,j(j \neq i)}^{-1} = b$ we can write the components of the covariance matrix approximation

$$\chi_{i,j} = \frac{1}{(a-b)(a+(N-1)b)} \begin{cases} a + (N-2)b & \text{if } i = j. \\ -b & \text{otherwise.} \end{cases}$$

Thus we have up to four parameters $\{M, C, \lambda_0, \lambda_1\}$, depending which constraints are applied. We solve (24) and (25) in combination with either, or both, $(1 - M^2 = \chi_{i,i})$ and $(C_{ij} = \chi_{i,j})$. These are non-linear equations in M, C and λ_0 ; we resort to local search to find solutions; solutions are possible by expansions at small or large T , or for large N . For the solution to be valid, we also check that the Hessian is positive definite, and that $p(x_i, x_j) \geq 0$.

Solutions for the equations are trivial for large or small T , and approach the solutions of the unconstrained approximation. By slowly varying T we can discover the solutions that evolve continuously from these two fixed points. We did not find any solutions appearing discontinuously, nor did we find any evidence for symmetry breaking (that is solutions in which the magnetizations, or correlations, differed by label index).

It is also straightforward to apply the same methodology for the mean-field approximation: there is one saddle-point equation, (24) with $C = 0$; and up to one type of covariance constraint ($\chi_{i,i} = 1 - M^2$), where the inverse covariance matrix elements become $[\chi^{-1}]_{i,j} = -1/T$, and $[\chi^{-1}]_{i,i} = 1/(1 - M^2) - \lambda_0$.

Appendix B. Algorithm for Finding Optimized Lagrangian Parameters, and the Linear Responses

Our approach to find solutions depends on their existence, this is discussed generically before we consider the impact of constraint selection strategies (and constraint representation) on solution existence and algorithmic stability. We then show that an exact method for minimizing the Lagrangian exists for some fixed values of the Lagrange parameters λ . The CLBP and CLSP algorithms are then presented in pseudocode. Finally, we discuss heuristics for the calculation of λ .

B.1 Existence

Certain models are known to be solved at leading order in some control parameter by region-based, Bethe or mean-field approximation. Examples are ferromagnetic random graphs or fully connected models in the limit of large number of variables (N), arbitrary models in the weakly interacting limit (also called high temperature T), finite models in the limit of strong biases on the variables (h). In these models, we find, of course, that the deviation between the linear response and marginal estimates are small in the corresponding control parameter. Expanding in this parameter (for example $1/T, 1/N$) it is straightforward to show the existence of solutions, and quantify the effectiveness of the constraints (see Raymond and Ricci-Tersenghi, 2013a). However, even outside the regime where expansions about the Bethe approximation are appropriate, we find solutions: this includes models where the covariance matrix has divergent terms, due to a mean-field phase transition as described in Raymond and Ricci-Tersenghi (2013b).

However, in experiments, we present it is shown that variation of the temperature (which controls the smoothness of the probability) can lead to models with no solutions, for some constraint sets. In the case of both on and off-diagonal constraints in Ising models defined on some graph $G = \{V, E\}$, with $|V|$ variables and $|E|$ edges, we have $|E| + |V|$ variational parameters but also $|E| + |V|$ constraints—solving a system of non-linear equations where the number of parameters matches the number of constraints seems optimistic; and perhaps it should not be surprising that as the Bethe approximation breaks down solutions fail to

exist; applying all constraints is certainly a marginal case unless some are redundant. If we move to alphabets with more than 2 states per variable the number of pair-statistics for on-and-off diagonal constraints exceeds the number of variables (with no obvious redundancy); certainly such a system can have no solutions. We must think carefully on which constraints to implement, and this is discussed in Appendix B.2.

In the experiments of this paper we have introduced for all models the control parameter T , with all models being well approximated by Bethe (and Mean-field) approximations in the weak coupling limit ($T \rightarrow \infty$), and some models also being well approximated in the strong coupling limit ($T \rightarrow 0$). To extend the regime in which our algorithms are convergent, an annealing approach was taken—slowly increasing $1/T$ (or T) and following a solution which evolved continuously in the marginals and Lagrange multipliers from the exactly solved regime. In many cases, solutions were found to reach a critical point T^* beyond which they could not be continuously evolved to new solutions. At these points we invariably found no new solutions emerging discontinuously by simply iterating our procedures. By undertaking annealing, it would in principle be possible to miss some solution that emerges discontinuously; the example of Section 4.1 shows this is possible (there is coexistence of two solutions at low temperature for the case of off-diagonal constraints only), but in the other examples of this paper we found no evidence for this. We expect in most practical applications, and for good choices of the constraints, coexistence will be absent.

A common feature in solution discontinuity during annealing is the divergence of some Lagrange multiplier(s); this indicates that the failure was due to inviability of solutions rather than a breakdown of algorithmic dynamics. Unlike the Bethe approximation, which can be forced to converge to a local minimum at any T , replacing LBP by a convex-concave procedure. We speculate that the constrained free energy has no solutions in strongly coupled regimes and that where practical solutions do exist the cavity based algorithms will be sufficient if combined with appropriate damping and/or annealing.

B.2 Selection of Constraints for Best Solutions

In this section we consider reasonable choices for the constraints, assuming a solution exists, and algorithmic convergence is possible.

Since we are applying constraints to discrete models it is clear that the a priori constraints selection should be independent of the labeling convention. Furthermore, we note that we made the rather arbitrary choice in (2) of perturbations in the set of statistics $\{\delta_{x_i,y} : y = 1 \dots Y\}$, Y being the number of states. Whilst this is invariant under relabeling, and spans all possible perturbation directions (and one redundant direction $\sum_y \delta_{x_i,y}$), we might get different covariances according to our choice. It would seem sensible to choose our constraint regime so that any set of statistics that spans the set of perturbations yields the same result. To achieve this we must pick a complete basis $\{\phi\}$, and apply constraints on all-covariance pairs.

The consideration of bases motivates the regimes we have explored: diagonal, off-diagonal, on-and-off diagonal. These schemes are basis-independent. If the condition $C_{(i,\cdot),(j,\cdot)} = \chi_{(i,\cdot),(j,\cdot)}$ is met in one basis for all elements, then a change between two (orthonormal) basis is a rotation, and the identities remain intact.

We found that off-diagonal typically performed worse than on-diagonal, as well as being computationally more challenging. In the final experiment of Section 4.4 we also tried one basis dependent set of constraints, the so-called *pure-diagonal* regime. Despite breaking the paradigm of basis independence, it performed just as well as the *block-diagonal* regime that is basis independent, so this indicates that basis independence is not an essential feature in constraint selection.

Topological distinctions amongst constraints can also be made. In a region-based approximation, we can distinguish the “2-core” from the rest of the graph. The 2-core is the set of variables that are found by recursively removing variables that are involved in at most one “outer region” (generalized interaction). We advise constraining variables on the 2-core only. The reason for this is that the set of variables that are not in the 2-core form a forest—a set of disconnected trees for which the approximation is conditionally exact even without constraints. If we have the core correct, then other constraints will be redundant. It is only in the case of the alarm net (Figure 1, Section 4.4) that the 2-core is distinguished from the full graph and we make this approximation. Other topological distinctions could be applied, distinguishing constraints by the distance between variables might be one possibility (in Figure 2(b) for example there are nearest, and next nearest neighbors within the regions); however, in the Bethe approximation (all experiments we present) only nearest neighbors might be constrained so the example is mute.

Beyond these considerations, we did not attempt to further restrict the set of constraints in a model specific manner, but several options might be worth exploring, in particular: (1) Consider the covariance matrix restricted to a single variable “block”, $\chi_{(i,\cdot),(i,\cdot)}$. For a given approximation (for example Bethe) there is a unique orthonormal basis $\{\phi_i\}$ that diagonalizes the covariance matrix. This would provide a natural choice for the statistic basis. The eigenvalue-vector pairs determine which direction is most susceptible to a change in parameters, and so (loosely speaking) most sensitive to approximation errors. We might, therefore, rank constraints by this eigenvalues for inclusion. (2) If we can solve the problem to obtain q_i^* , then we can consider defining only one perturbation statistic per variable as $\phi(x_i) \propto \log(Yq^*(x_i))$. Since we know approximations tend to be overconfident, it would seem a natural choice to constrain in line with the belief, rather than wasting resources on unimportant directions in parameter space.

B.3 Assignment of Constraints to Regions, and Basis selection, for Best Convergence

For our constraint regimes (diagonal, on-diagonal and on-and-off diagonal), the allocation of constraints to specific regions, the choice of statistical basis, the initial condition of the algorithm and the damping, leave the algorithmic fixed points unchanged. Owing to our slow annealing approach (increasing or decreasing T) our results were not very sensitive to the other implementation details. However, these choices do impact convergence significantly.

We find that a non-redundant orthonormal set of statistics leads to faster convergence. Orthonormality ensures that, at leading order, the Lagrange multipliers are independent of one another, which is the criterion that guarantees the success of our method. A redundant statistic is $\phi(x_i) = \sum_{y=0}^{Y-1} \delta_{x_i,y}$, where x_i has Y states, and so only $Y - 1$ orthonormal

statistics need be implemented. A nice approach to the selection of an orthonormal basis is discussed in Yasuda (2013), for Ising spins, a unique choice per variable is x_i .

We allocated constraints in a naive manner, assigning each constraint to the first available “outer region”. For diagonal constraints an approach where constraints are allocated to single-variable regions was proposed by Yasuda et al., and this allows some simplifications as well as implying a unique allocation (see Yasuda, 2013). Approaches that do not allocate constraints to regions, such as iteration by linear expansion of the covariance matrix have been attempted (29), but those were slower to converge.

As a general rule, we wish to group Lagrange multipliers together as much as possible. In this way, correlations amongst the Lagrange multipliers are accounted for locally. A potentially better approach than our fixed assignment suggestion might be to update all Lagrange within some outer region. Where a constraint could be allocated to more than one region, the results could be averaged, or regions could be selected differently on each cycle to avoid conflicting assignments.

A damping factor that begins as 1 and decreases during the annealing procedure (as required to enable convergence) is applied in the experiments. In simulations without an annealing scheme, a rate $\lesssim 0.5$ could be essential to prevent oscillations that arise from correlated updating of Lagrange multipliers. In particular, off-diagonal values λ_{ij} and diagonal values λ_{ii} can be anti-correlated. If they are not updated on the same region undamped iteration can lead to slow convergence or oscillations.

Initial conditions are chosen as $\lambda = 0$; so that the first iteration is equivalent to an unconstrained approximation. One advantage of the annealing approach (where we first solve the trivial model $T = 0$ or $+\infty$, and then increase or decrease T , initializing by the current solution), is that we do not require the convergence of the unconstrained approximation to find a solution in the constrained regime.

B.4 Convex Concave Procedure

We prove that it is possible to minimize (16) in q by a convex-concave decomposition. In Heskes, Albers, and Kappen (2003) by introducing auxiliary parameters q' over the inner regions, a pair of convex optimization procedures were developed that led to minima of the region based free energy. With the addition of our constraints, we only need to make a minor modification to their argument. Consider an auxiliary free energy $F(q, q')$, where q' are additional parameters in one to one correspondence with the original variational parameters. Heskes et al. outline three requirements of this free energy

- 1 Convexity of $F(q, q')$ with respect to q .
- 2 $F(q, q' = q) = F(q)$
- 3 $F(q, q') \geq F(q)$

that guarantee that the iterative procedure

$$q'_{t+1} = \operatorname{argmin}_q F(q, q'_t) , \quad (26)$$

converges to values that are minimizing arguments of $F(q)$.

Since the violation term (13) is a quadratic function of the variational parameters $q(x_\alpha)$, it can be expressed by a constant A_0 , a vector of linear coefficients A_1 and quadratic coefficients A_2 that define a symmetric matrix. A_2 can be decomposed as a positive definite and negative semi-definite part (A_2^+ and A_2^-). It is then easy to define a function in vector notation

$$\Delta^+(q, q', q_{(\cdot)}^*) = A_0(q_{(\cdot)}^*) + q^T A_1 + (q')^T A_2 q' + (q - q')^T A_2^+ (q - q'). \quad (27)$$

To minimize our region-based free energy with constraints (16) we substitute (27) for (13) and follow the procedure in Heskes, Albers, and Kappen (2003) for the remaining terms. The free energy meets the criteria for convergence under the iterative scheme (26).

The double loop procedure, despite not changing the asymptotic complexity of message passing $O(N)$ is often considered impractical, but, in the framework we are proposing, the largest cost is the evaluation of the linear response, implementing a double loop procedure may be sensible. In practice we have used the variation on loopy belief propagation, rather than the double-loop procedure, to extremize the Lagrangian. Despite the absence of theoretical guarantees, the 3-fold scheme proves to be reliable: solving for variational parameters (by CLBP); solving for the linear response (by CLSP); and update of the Lagrange multipliers.

B.5 Pseudocode for Determining the Fixed Point of q Given λ

We determine q by the constrained loopy belief propagation (CLBP) algorithm, described in Algorithm 1, which is a modified form of the Heskes, Albers, and Kappen (2003) loopy belief propagation algorithm, that uses the convex-concave procedure with guaranteed convergence.

In Algorithm 1 we consider an auxiliary region interaction including both interactions and the Lagrange multiplier terms

$$\psi_\alpha(x_\alpha; \lambda_\alpha, q_\alpha) = \psi_\alpha(x_\alpha) \prod_{[(i,s_1),(j,s_2)] \in \omega_\alpha} \exp \left\{ -\lambda_{(i_1,y_1),(i_2,y_2)} \hat{\phi}_{(i_1,y_1),(i_2,y_2)}(x_\alpha; q_\alpha) \right\},$$

and

$$\begin{aligned} \hat{\phi}_{(i_1,y_1),(i_2,y_2)}(x_\alpha; q_\alpha) = & \left(\delta_{x_{i_1,y_1}} - \mathbb{E}_{q_\alpha}(\delta_{x_{i_1,y_1}}) \right) \left(\delta_{x_{i_2,y_2}} - \mathbb{E}_{q_\alpha}(\delta_{x_{i_2,y_2}}) \right) \\ & + \mathbb{E}_{q_\alpha}(\delta_{x_{i_2,y_2}}) \mathbb{E}_{q_\alpha}(\delta_{x_{i_1,y_1}}). \end{aligned}$$

Simplified expressions for the Ising model are presented in the main text. Terms here have an interpretation compatible with Heskes, Albers, and Kappen (2003), with U are the set of *outer regions*, and V are the set of intersection regions (see Figure 2). In the case of a Bethe approximation U are the set of edges, and V are the set of variables.

Algorithm 1 λ compatible Heskes-Albers-Kappen algorithm

while \neg converged **do**
for all $\beta \in V$ **do**
for all $\alpha \in U, \alpha \supset \beta$ **do**

$$q_\alpha(x_\beta) = \sum_{x_\alpha \setminus \beta} q_\alpha(x_\alpha)$$

$$\mu_{\alpha \rightarrow \beta}(x_\beta) = \frac{q_\alpha(x_\beta)}{\mu_{\beta \rightarrow \alpha}(x_\beta)}$$

end for

$$q_\beta^{(num)}(x_\beta) = \prod_{\alpha \supset \beta} \mu_{\alpha \rightarrow \beta}(x_\beta)$$

$$q_\beta(x_\beta) = \frac{q_\beta^{(num)}(x_\beta)}{\sum_{x'_\beta} q_\beta^{(num)}(x'_\beta)}$$

for all $\alpha \in U, \alpha \supset \beta$ **do**

$$\mu_{\beta \rightarrow \alpha}(x_\beta) = \frac{q_\beta(x_\beta)}{\mu_{\alpha \rightarrow \beta}(x_\beta)}$$

while \neg converged (solve self-consistently) **do**

$$q_\alpha^{(num)}(x_\alpha) = \psi_\alpha(x_\alpha; \lambda, q_\alpha) \prod_{\beta \subset \alpha} \mu_{\beta \rightarrow \alpha}(x_\beta)$$

$$q_\alpha(x_\alpha) = \frac{q_\alpha^{(num)}(x_\alpha)}{\sum_{x'_\alpha} q_\alpha^{(num)}(x'_\alpha)}$$

end while
end for
end for
end while

B.6 Linear Response about the Fixed Point

By linearizing the CLBP method, we obtain a constrained loopy susceptibility propagation (CLSP) method. Qualitatively similar is the I-SUSP algorithm of Yasuda and Tanaka (2013), which applies only to the case of diagonal constraints and the Bethe approximation.

The implementation we use follows Algorithm 1, but with the following replacements for each equation (in order):

$$\begin{aligned}
 \delta \hat{q}_\alpha(x_\beta) &= \sum_{x_{\alpha \setminus \beta}} \frac{q_\alpha(x_\alpha)}{q_\beta(x_\beta)} \delta \hat{q}_\alpha(x_\alpha) ; \\
 \delta \hat{\mu}_{\alpha \rightarrow \beta}(x_\beta) &= \delta \hat{q}_\alpha(x_\beta) - \delta \hat{\mu}_{\beta \rightarrow \alpha}(x_\beta) ; \\
 \delta \hat{q}_\beta^{(num)}(x_\beta) &= \sum_{\alpha \supset \beta} \delta \hat{\mu}_{\alpha \rightarrow \beta}(x_\beta) ; \\
 \delta \hat{q}_\beta(x_\beta) &= \delta \hat{q}_\beta^{(num)}(x_\beta) - \sum_{x_\beta} q_\beta(x_\beta) \delta \hat{q}_\beta^{(num)}(x_\beta) ; \\
 \delta \hat{\mu}_{\beta \rightarrow \alpha}(x_\beta) &= \delta \hat{q}_\beta(x_\beta) - \delta \hat{\mu}_{\alpha \rightarrow \beta}(x_\beta) ; \\
 \delta \hat{q}_\alpha^{(num)}(x_\alpha) &= \frac{\delta_{x_i, y} \mathbb{I}(i \in \alpha)}{k_i} + \sum_{\beta \subset \alpha} \delta \hat{\mu}_{\beta \rightarrow \alpha}(x_\beta) \\
 &\quad + \sum_{x'_\alpha} q_\alpha(x'_\alpha) \delta \hat{q}_\alpha(x'_\alpha) \frac{\partial \log \psi(x_\alpha; \boldsymbol{\lambda}_\alpha, q_\alpha)}{\partial q_\alpha(x'_\alpha)} ; \\
 \delta \hat{q}_\alpha(x_\alpha) &= \delta \hat{q}_\alpha^{(num)}(x_\alpha) - \sum_{x'_\alpha} q_\alpha(x'_\alpha) \delta \hat{q}_\alpha^{(num)}(x'_\alpha) ;
 \end{aligned}$$

where $\mathbb{I}(i \in \alpha)$ is an indicator function evaluating to one if i is contained in α , and k_i is the number of outer regions containing i . From the converged quantities we can identify

$$q_{\alpha, (i, y)}^*(x_\alpha) = q_\alpha(x_\alpha) \delta \hat{q}_\alpha(x_\alpha) . \quad (28)$$

Since the linear response is a linearized method, the innermost do-while loop of Algorithm 1 could be replaced by a method for solving linear equations. Both have been tried with similar outcomes.

Appendix C. Solving for λ , Explicit Expressions and Simplification

The diagonal update scheme of I-SUSP relies on a similar reasoning as that undertaken in Yasuda and Tanaka (2013) and Yasuda (2013). The difference between the two approaches is that in the works by Yasuda et al. only diagonal constraints (restricted to single variable consistency relations) are considered. As such it is possible to choose in general a single variable cavity i , rather than a region cavity α (see Figure 4). To consider statistics not restricted to single variables our scheme is required. The I-SUSP method has an advantage over our method in that there is a simplification of the expressions on a single variable region that allows a closed form for updating the Lagrange multipliers. One advantage of our scheme is that we may fix several Lagrange multipliers on a region simultaneously, thus accounting for correlations in their values, and perhaps reducing the number of updates to convergence.

In practice, damping within the 3-cycle of Figure 3 can be necessary for convergence. In practice, we replace $\lambda^{t+1} = d\lambda^t + (1-d)\lambda^*$, where λ^* is the cavity approximation. As $1/T$ was increased (or decreased) at a constant rate we increased d whenever the solution failed to converge, and this modification extended the region of convergence.

An exact expression for the correlation matrix χ as a function of the variational parameters was derived in Raymond and Ricci-Tersenghi (2013b) and Raymond and Ricci-Tersenghi (2013a), the special case for homogeneous graphs is made explicit (Appendix A). The inverse covariance matrix χ^{-1} is, in the basis where variational parameters are beliefs q , a linear function of λ . Updating a single λ can be achieved by the Sherman-Morrison formula, which in its linearized form becomes

$$\chi_{i,i} \delta\lambda_{i,j} \chi_{j,j} = (C_{i,j}^* - \chi_{i,j}) . \quad (29)$$

It is also possible to write a similar expression blockwise (over λ_α). This scheme and variations were considered, but were found to require more iterations or stronger damping (for convergence) than the linearized cavity formula (20).

In our approach we associate each constraint to a unique region, but some statistics such as $\mathbb{V}_p(x_i, x_i)$ may be approximated by different α for the same variational approach (for example by q_{ij} or q_{ik} if i participates in two interactions). Though these estimates agree finally at the solution point, they disagree at intermediate stages of CLBP. Since updates for λ may be correlated (consider Figure 8 where diagonal and off-diagonal are strongly anti-correlated), the grouping of λ may be very important. Updating non-disjoint sets and averaging over results may be more stable than our scheme where closely correlated λ (for example $\lambda_{i,i}$ and $\lambda_{i,j}$) may be updated on different regions.

References

- C. Andrieu, N. de Freitas, A. Doucet, and M. I. Jordan. An introduction to MCMC for machine learning. *Machine Learning*, 50(1):5–43, 2003.
- M. Chertkov and V.Y. Chernyak. Loop calculus in statistical physics and information science. *Phys. Rev. E*, 73:065102, 2006.
- P. Dagum and M. Luby. Approximating probabilistic inference in Bayesian belief networks is NP-hard. *Artif. Intell.*, 60(1):141–153, March 1993.
- R. Dickman and G. Stell. Self-consistent Ornstein-Zernike approximation for lattice gases. *Physical review letters*, 77(6):996, 1996.
- E. Domínguez, A. Lage-Castellanos, R. Mulet, F. Ricci-Tersenghi, and T. Rizzo. Characterizing and improving generalized belief propagation algorithms on the 2d Edwards–Anderson model. *Journal of Statistical Mechanics: Theory and Experiment*, 2011(12):P12007, 2011.
- R.J. Giordano, T. Broderick, and M.I. Jordan. Linear response methods for accurate covariance estimates from mean field variational Bayes. In *Advances in Neural Information Processing Systems 28*, pages 1441–1449. Curran Associates, Inc., Red Hook, NY, 2015.
- T. Heskes, K. Albers, and B. Kappen. Approximate inference and constrained optimization. In *Uncertainty in Artificial Intelligence: Proceedings of the Nineteenth Conference (UAI-2003)*, pages 313–320, San Francisco, CA, 2003. Morgan Kaufmann Publishers.

- J. S. Høye and G. Stell. Thermodynamics of the MSA for simple fluids. *J. Chem. Phys.*, 67:439–445, July 1977. doi: 10.1063/1.434887.
- H. Huang and Y. Kabashima. Adaptive Thouless-Anderson-Palmer approach to inverse Ising problems with quenched random fields. *Phys. Rev. E*, 87:062129, Jun 2013.
- H.J. Kappen and F.B. Rodriguez. Efficient learning in Boltzmann machines using linear response theory. *Neural Comput.*, 20:1137, 1998.
- E. Kierlik, M.L. Rosinberg, and G. Tarjus. A self-consistent Ornstein–Zernike approximation for the random field Ising model. *Journal of Statistical Physics*, 94(5-6):805–836, 1999.
- A. Lage-Castellanos, R. Mulet, F. Ricci-Tersenghi, and T. Rizzo. Replica cluster variational method: the replica symmetric solution for the 2d random bond Ising model. *Journal of Physics A: Mathematical and Theoretical*, 46(13):135001, 2013.
- P.M. Long and R.A. Servedio. Restricted Boltzmann machines are hard to approximately evaluate or simulate. In *Proceedings of the 27th International Conference on Machine Learning*, pages 703–710. Omnipress, 2010.
- D.J. MacKay. *Information Theory, Inference and Learning Algorithms*. Cambridge University Press, Cambridge, UK, 2004.
- M. Mezard and A. Montanari. *Information, Physics, and Computation*. Oxford University Press, Inc., New York, NY, USA, 2009.
- M. Mezard and T. Mora. Constraint satisfaction problems and neural networks: a statistical physics perspective. arXiv:0803.3061, 2008.
- J. Miskin and D. J. C. MacKay. *Ensemble Learning for Blind Image Separation and Deconvolution*, pages 123–141. Springer London, London, 2000.
- A. Montanari and T. Rizzo. How to compute loop corrections to the Bethe approximation. *J. Stat. Mech.*, page P10011, 2005.
- A. Montanari, F. Ricci-Tersenghi, and G. Semerjian. Solving constraint satisfaction problems through belief propagation-guided decimation. In *45th Annual Allerton Conference on Communication, Control and Computing*, Red Hook, NY, USA, 2007. Curran Associates, Inc.
- J.M. Mooij. libDAI: A free and open source c++ library for discrete approximate inference in graphical models. *Journal of Machine Learning Research*, 11:2169–2173, August 2010.
- J.M. Mooij, B. Wemmenhove, B. Kappen, and T. Rizzo. Loop corrected belief propagation. In *International Conference on Artificial Intelligence and Statistics*, pages 331–338, 2007.
- M. Opper and O. Winther. Tractable approximations for probabilistic models: The adaptive Thouless-Anderson-Palmer mean field approach. *Phys. Rev. Lett.*, 86:3695–3699, 2001.

- M. Opper and O. Winther. Variational linear response. In *Advances in Neural Information Processing Systems 16*. MIT Press, Cambridge, MA, 2003.
- M. Opper and O. Winther. Expectation consistent free energies for approximate inference. In *Advances in Neural Information Processing Systems 17*. MIT Press, Cambridge, MA, 2005.
- M. Opper, U. Paquet, and O. Winther. Improving on expectation propagation. In *Advances in Neural Information Processing Systems 21*. MIT Press, Cambridge, MA, 2009.
- M. Opper, U. Paquet, and O. Winther. Perturbative corrections for approximate inference in Gaussian latent variable models. *Journal of Machine Learning Research*, 14:2857–2898, 2013.
- U. Paquet, O. Winther, and M. Opper. Perturbation corrections in approximate inference: Mixture model applications. *Journal of Machine Learning Research*, 10:1263–1304, 2009.
- G. Parisi. *Statistical Field Theory*. Addison-Wesley, Boston, MA, USA, 1987.
- A. Pelizzola. Cluster variation method in statistical physics and probabilistic graphical models. *J. Phys. A*, 38(33):R309, 2005.
- J. Raymond and F. Ricci-Tersenghi. Correcting beliefs in the mean-field and Bethe approximations using linear response. In *Communications Workshops (ICC), 2013 IEEE International Conference on*, pages 1429–1433, 2013a.
- J. Raymond and F. Ricci-Tersenghi. Mean-field method with correlations determined by linear response. *Phys. Rev. E*, 87:052111, 2013b.
- T. Richardson and R. Urbanke. *Modern Coding Theory*. Cambridge University Press, Cambridge, UK, 2008.
- M.J. Wainwright and M.I. Jordan. Graphical models, exponential families, and variational inference. *Found. Trends Mach. Learn.*, 1(1-2):1–305, 2008.
- M. Welling and Y.W. Teh. Linear response algorithms for approximate inference in graphical models. *Neural Comput.*, 16:197–221, 2004.
- O. Winther and M. Opper. Expectation consistent approximate inference. *Journal of Machine Learning Research*, 6:2177–2204, 2005.
- M. Yasuda. An generalization of improved susceptibility propagation. In *Inference, Computation, and Spin Glasses (ICSG2013)*, 2013.
- M. Yasuda and K. Tanaka. Susceptibility propagation by using diagonal consistency. *Phys. Rev. E*, 87:012134, Jan 2013.
- J.S. Yedidia, W.T. Freeman, and Y. Weiss. Constructing free-energy approximations and generalized belief propagation algorithms. *Information Theory, IEEE Transactions on*, 51(7):2282–2312, 2005.

A. L. Yuille. CCCP algorithms to minimize the Bethe and Kikuchi free energies: Convergent alternatives to belief propagation. *Neural Computation*, 14:2002, 2002.