Mean Field Inference in a General Probabilistic Setting

M. Haft, R. Hofmann and V. Tresp

Corporate Technology, Department: Information and Communications Siemens AG, 81730 München, Germany E-mail: [Michael.Haft,Reimar.Hofmann,Volker.Tresp]@mchp.siemens.de

Abstract

We present a systematic, model-independent formulation of mean field theory (MFT) as an inference method in probabilistic mod-"Model-independent" means that we do not assume a particular type of dependency among the variables of a domain but instead work in a general probabilistic setting. In a Bayesian network, for example, you may use arbitrary tables to specify conditional dependencies and thus run MFT in any Bayesian network. Furthermore, the general mean field equations derived here shed a light on the essence of MFT. MFT can be interpreted as a *local* iteration scheme which relaxes in a consistent state (a solution of the mean field equations). Iterating the mean field equations means propagating information through the network. In general, however, there are multiple solutions to the mean field equations. We show that improved approximations can be obtained by forming a weighted mixture of the multiple mean field solutions. Simple approximate expressions for the mixture weights are given. The benefits of taking into account multiple solutions are demonstrated by using MFT for inference in a small Bayesian network representing a medical domain. Thereby it turns out that every solution of the mean field equations can be interpreted as a 'disease scenario'.

1 Introduction

The benefits of using a probabilistic setting in many applied fields where uncertainty plays a prominent role—such as image processing, neural networks and artificial intelligence—have become increasingly apparent [1]. Unfortunately, probabilistic solutions often re-

quire involved computation [2] and further progress is closely related to the development of methods for the efficient handling of probability distributions. The goal of this paper is to extend the concept of using mean field theory (MFT) as a systematic approach for approximating probability distributions. MFT is widely used in physics, in particular, in statistical mechanics [3, 4] and has found a number of applications in other areas as well [5, 6, 7, 8]. We present MFT in a generic way in the context of graphical models, which are a general framework for dealing with uncertainty in dependency models [1, 9, 10, 11]. The use of MFT in the context of graphical models was pioneered by Jordan, Saul and Jaakola [12, 13]. In our paper we develop this approach in two new directions. First, in contrast to previous work we develop a systematic approach to MFT without reference to a particular model but instead work in a general probabilistic setting*. The mean field equations based on our rigorous formalism are new in their general form. They can be applied for example to arbitrary graphical models, which include Boltzmann machines as a special case. The main advantage of our mean field equations is that they provide *local* inference rules. No global operations are needed when using MFT for propagating information in large systems of interacting modules.

The second contribution of this paper is to address the problem of multiple solutions of the mean field equations. This problem has been originally discussed in [14] and simultaneously in [15, 16, 17]. We show that in the case of multiple solutions, a weighted mixture of these solutions leads to reasonable estimates of expected values. Approximate and very plausible

^{*}In [12, 13] Jordan et al. use 'sigmoid belief nets', a network of binary variables with a particular kind of dependencies. The Boltzmann machines used in [6] are completely connected networks of binary variables with 'two-way interactions'. Here, we do not assume any particular kind of variables or a particular type of dependencies. As a consequence we may run mean field inference in any Bayesian network. At the moment we have implemented an interface to the Hugin net-file format.

mixing parameters are derived. The general formalism presented so far is applied to the special case of Bayesian networks. In this case the mixing parameters can be obtained in a consistent framework, that is, by means of only *local* computations. The benefits of taking into account multiple solutions of the mean field equations are demonstrated by using MFT for inference in a small illustration network representing a medical domain.

Finally, we comment on the relevance of MFT for human reasoning. Consistent propagation of information in large networks of interacting modules is in general a demanding task and requires global operations [1]. MFT, on the other hand, suggests itself as a local and very simple prescription for communication of autonomous processors.

2 Mean Field Theory in a Probabilistic Setting

2.1 The Cross Entropy as a Measure of Distance

In the following, a set of N variables \mathbf{X} = $\{X_1,\ldots,X_N\}$ with a finite number of discrete states $x_i \in \mathcal{H}_i$ is assumed. $P(\mathbf{X})$ denotes a probability distribution on the domain $\mathcal{H} = \mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_N$. We further assume that any distribution is strictly positive. $P(\mathbf{x})$ resp. $P(x_i)$ is the probability of the event $\mathbf{X} = \mathbf{x}$ resp. $X_i = x_i$. That is, $P(x_i)$ is a real number, $P(x_i) \in]0,1[$. In many interesting domains, $P(\mathbf{X})$ is computationally intractable. For this reason we introduce a distribution $Q(\mathbf{X})$ which is defined on the same domain of variables and which incorporates some simplifying constraints. The goal is to determine $Q(\mathbf{X})$ such that -obeying these constraints- it is 'as close as possible' to the given untractable distribution $P(\mathbf{X})$. As a measure of distance between $P(\mathbf{X})$ and $Q(\mathbf{X})$ we use the cross entropy (Kullback-Leibler distance) [18]

$$\mathcal{D}(Q||P) = \sum_{\mathbf{x} \in \mathcal{H}} Q(\mathbf{x}) \log \frac{Q(\mathbf{x})}{P(\mathbf{x})} \equiv \left\langle \log \frac{Q(\mathbf{X})}{P(\mathbf{X})} \right\rangle_{Q(\mathbf{X})}.$$
(1)

Note, that this distance is not symmetric in P and Q and that, with even more justification, we might have used

$$\mathcal{D}(P||Q) = \sum_{\mathbf{x} \in \mathcal{H}} P(\mathbf{x}) \log \frac{P(\mathbf{x})}{Q(\mathbf{x})} \equiv \left\langle \log \frac{P(\mathbf{X})}{Q(\mathbf{X})} \right\rangle_{P(\mathbf{X})}.$$
(2)

as a distance measure since here the expectation is with respect to the 'true' distribution P. Any of the above two measures of distance is zero only if $Q(\mathbf{X}) = P(\mathbf{X})$. The reason to use the former measure (1), however, is that it can be calculated more easily

since the expectation is with respect to the less complex, approximate distribution Q. This finally leads to the *local* concept of MFT.

2.2 The Mean Field Assumption

MFT is a concept from theoretical physics and is used to describe systems of many interacting particles. Many different facets of MFT can be found in fields as different as relativistic nuclear physics [19, 20], statistical physics [3, 4, 21] and neural networks [22, 23, 24]. As a consequence, there exist a number of ways to derive mean field equations. Following the above discussion we define as mean field approximation the distribution $Q(\mathbf{X})$ which is closest to $P(\mathbf{X})$ using distance measure $\mathcal{D}(Q||P)$. Furthermore—and this is really the heart of the mean field approximation [3]—we assume that the variables in the Q-distribution are independent variables X_i . In this case we can write

$$Q(X_1, ..., X_N) = \prod_{i=1}^{N} Q(X_i).$$
 (3)

At first sight this ansatz seems to be much too simple, for obviously it is ignoring any interaction between the variables X_i . Nevertheless, one can take advantage of this approach for approximate propagation of information (evidence), as we will see later. To the best of our knowledge, Jordan et al. [12, 13] were the first ones to define MFT in a general way as the ansatz (3) together with $\mathcal{D}(Q||P)$ as a measure of distance.

2.3 General Mean Field Equations

Minimization of $\mathcal{D}(Q||P)$ can be done in an iterative way. Suppose $Q(X_k), \ k=1,\ldots,N$, are our current estimates of the Q-marginals. Our goal is to obtain an improved approximation to $P(\mathbf{X})$ by minimizing $\mathcal{D}(Q||P)$ with respect to $Q(X_i)$ thereby assuming fixed marginals $Q(X_j), \ j \neq i$. Let us denote the complement of X_i by $\overline{\mathbf{X}}_i$, that is $\overline{\mathbf{X}}_i \equiv \{X_j, j \neq i\} \equiv \mathbf{X} \setminus X_i$. When minimizing $\mathcal{D}(Q||P)$ with respect to $Q(X_i)$ we have to take into account the normalization constraint $\sum_{x_i \in \mathcal{H}_i} Q(x_i) = 1$. This can be done by using a Lagrange parameter λ , i.e., we have to solve the equations

$$\frac{\partial}{\partial Q(x_i)} \left[\mathcal{D}(Q||P) - \lambda \left(\sum_{x_i \in \mathcal{H}_i} Q(x_i) - 1 \right) \right] = 0 \quad (4)$$

with respect to the probabilities $Q(x_i)$, $x_i \in \mathcal{H}_i$. First, we split up $\mathcal{D}(Q||P)$ using the relations $P(\mathbf{X}) = P(\overline{\mathbf{X}}_i)P(X_i|\overline{\mathbf{X}}_i)$ and $Q(\mathbf{X}) = Q(\overline{\mathbf{X}}_i)Q(X_i)$. Inserting these relations in (1) we obtain

$$\mathcal{D}(Q||P) = \left\langle \log Q(\overline{\mathbf{X}}_i) \right\rangle_{Q(\overline{\mathbf{X}}_i)} - \left\langle \log P(\overline{\mathbf{X}}_i) \right\rangle_{Q(\overline{\mathbf{X}}_i)}$$
(5)
+ $\left\langle \log Q(X_i) \right\rangle_{Q(X_i)} - \left\langle \log P(X_i|\overline{\mathbf{X}}_i) \right\rangle_{Q(\mathbf{X})}$ (6)

Only the terms in the last line (6) depend on $Q(x_i)$, those in the first line (5) do not. Differentiating the term $\langle \log Q(X_i) \rangle_{Q(X_i)}$ we find

$$\frac{\partial}{\partial Q(x_i)} \langle \log Q(X_i) \rangle_{Q(X_i)} =$$

$$= \frac{\partial}{\partial Q(x_i)} \sum_{x_i \in \mathcal{H}_i} Q(x_i) \log Q(x_i)$$

$$= \log Q(x_i) + 1.$$

After differentiating both the second term $\langle \log P(X_i|\overline{\mathbf{X}}_i)\rangle_{Q(\mathbf{X})}$ of line (6) and the constraint of Eq. (4) we obtain

$$Q(x_i) = \frac{1}{\exp(1-\lambda)} \exp\left\langle \log P\left(x_i | \overline{\mathbf{X}}_i\right) \right\rangle_{Q(\overline{\mathbf{X}}_i)}. \quad (7)$$

The Lagrange parameter λ or normalizing constant $\exp(1-\lambda)$ can be calculated easily,

$$\exp(1 - \lambda) = \sum_{x_i \in \mathcal{H}_i} \exp\left\langle \log P\left(x_i | \overline{\mathbf{X}}_i\right) \right\rangle_{Q(\overline{\mathbf{X}}_i)}. \quad (8)$$

This sum involves only $|\mathcal{H}_i|$ terms, i.e., for binary variables only two terms.

The result (7) is the unique solution to Eq. (4). It corresponds to a global minimum of $\mathcal{D}(Q||P)$ with respect to $Q(X_i)$ given our current estimates of $Q(X_j)$, $j \neq i$. That means, updating $Q(X_i)$ according to (7) decreases $\mathcal{D}(Q||P)$. Subsequently, we choose another variable out of \overline{X}_i and solve the mean field equations for this variable. Thus iterating repeatedly over all variables X_i we stepwise descend in $\mathcal{D}(Q||P)$. The cross entropy $\mathcal{D}(Q||P)$ is always positive, and, hence, this iteration ends up in a local minimum of $\mathcal{D}(Q||P)$.

The equations (7) may be viewed as mean field equations in their most general form since no model assumptions were made. As a special case we now assume that $P(\mathbf{X})$ is the Boltzmann distribution of a system of spins $x_i \in \{\pm 1\}$ defined by the Hamiltonian $H(\mathbf{x}) = -(1/2)\mathbf{x}^TJ\mathbf{x}$ with a symmetric interaction matrix J and diagonal elements $J_{ii} = 0$. For this system the conditional distribution $P(x_i|\overline{\mathbf{X}}_i)$ reads $P(x_i|\overline{\mathbf{X}}_i) \propto \exp\left(\beta x_i J_i \cdot \overline{\mathbf{X}}_i\right)$, where J_i is the ith row of the interaction matrix J and β is the inverse temperature. Hence, for the mean field equations (7) we obtain

$$Q(x_i) \propto \exp\left(\beta x_i J_i \cdot \left\langle \overline{\mathbf{X}}_i \right\rangle_{Q(\overline{\mathbf{X}}_i)}\right).$$
 (9)

For binary variables the mean values $\langle X_i \rangle$ completely determine the marginals $Q(X_i)$. In our case $x_i \in \{\pm 1\}$ we have $Q(x_i) = (1/2)(1 + x_i \langle X_i \rangle)$. Using this fact it can be shown easily that Eq. (9) leads to

$$\langle X_i \rangle_{Q(X_i)} = \tanh \left(\beta J_i \cdot \langle \overline{\mathbf{X}}_i \rangle_{Q(\overline{\mathbf{X}}_i)} \right), \quad (10)$$

which is the well-known mean field equation for a system of interacting spins [3], whereby the expected values $\langle X_i \rangle_{Q(X_i)}$ are usually denoted as magnetizations m_i .

2.4 Locality of Mean Field Theory

The most appealing point of MFT is that only local operations are needed for iteration of the mean field equation (7). Given the Markov boundary[†] \mathbf{M}_i of the variable X_i the mean field equation (7) may be simplified to

$$Q(x_i) \propto \exp \langle \log P(x_i | \mathbf{M}_i) \rangle_{Q(\mathbf{M}_i)}$$
 (11)

Iterating these mean field equations means recursively estimating marginals $Q(X_i)$ based on the current marginals $Q(X_j)$ of only the 'neighboring' variables $X_j \in \mathbf{M}_i$ until the system relaxes into a consistent state. For updating $Q(X_i)$ we only need the conditional distribution $P(X_i|\mathbf{M}_i)$, which can be stored 'locally at node i', and the current estimates of the marginals $Q(X_j), X_j \in \mathbf{M}_i$, which can be stored at the corresponding 'neighboring nodes' of node i. All information which is needed for the renewed estimation of $Q(X_i)$ in equation (11) is thus available from node i and the neighboring nodes of node i (the Markov boundary \mathbf{M}_i of node i).

3 Mixing Mean Field Solutions

The iteration of the mean field equations (11) converges to one of typically many local minima of $\mathcal{D}(Q||P)$. In many physical model systems, these local solutions are of particular interest since they explain phase transitions and the phenomenon of spontaneous symmetry breaking [3]. The mean field dynamics in a Hopfield network converges to a local minimum of the 'free energy landscape' and thus restores one of many stored patterns. However, if we want to have a good approximation of a global distribution $P(\mathbf{X})$ and in particular if we are interested in expected values with respect to $P(\mathbf{X})$ we have to care about all solutions of the mean field equations (7). In the following we pursue the idea that instead of selecting one particular mean field solution, it might be more advantageous to form a weighted average (a mixture) of several mean field solutions. The mixture weights are derived in a principled way and are shown to be optimal under certain assumption. An additional benefit is that we can

[†]The Markov boundary \mathbf{M}_i of a variable X_i is the minimal set of variables $\mathbf{M}_i \subset \mathbf{X}$ which makes X_i independent of the 'rest' given \mathbf{M}_i , i.e., $P(X_i|\mathbf{M}_i,rest) = P(X_i|\mathbf{M}_i)$. In the above physical example the Markov boundary of X_i is the set of variables X_j with $J_{ij} \neq 0$.

relax the assumption of independent units since a mixture distribution can approximate a much larger class of distributions than the components of the mixture.

We enumerate the different mean field solutions by a 'hidden variable' a. That is, $Q(\mathbf{X}|a)$ now denotes a different mean field solutions for a different a. By assigning mixture weights Q(a) to every solution we form the mixture distribution

$$Q(\mathbf{X}) = \sum_{a} Q(\mathbf{X}|a)Q(a). \tag{12}$$

Again, the goal now is to determine the Q(a) under the constraint $\sum_a Q(a) = 1$, such that $\mathcal{D}(Q||P)$ is minimized. It is an easy exercise to perform this optimization via a Lagrange parameter λ analogous to the previous derivation. In a few lines we obtain for all a

$$\langle \log Q(\mathbf{X}) \rangle_{Q(\mathbf{X}|a)} = \langle \log P(\mathbf{X}) \rangle_{Q(\mathbf{X}|a)} - 1 + \lambda.$$
 (13)

We have to solve Eq. (13) for Q(a), which implicitly enters the above expression via $Q(\mathbf{X})$ and Eq. (12). However, the above Eq. (13) cannot be solved in a straightforward way for Q(a). With the aim of a simple expression we therefore use an additional approximation. The left hand side of (13) may be expressed as

$$\langle \log Q(\mathbf{X}) \rangle_{Q(\mathbf{X}|a)} = \left\{ \log \left[Q(a)Q(\mathbf{X}|a) + \sum_{a' \neq a} Q(a')Q(\mathbf{X}|a') \right] \right\}_{Q(\mathbf{X}|a)} \\ \approx \log Q(a) + \left\langle \log Q(\mathbf{X}|a) \right\rangle_{Q(\mathbf{X}|a)}, \tag{14}$$

where we have neglected the terms $Q(a')Q(\mathbf{X}|a')$ for $a' \neq a$ in the argument of the logarithm. We may do so if $Q(\mathbf{x}|a)Q(\mathbf{x}|a') \approx 0$ for all $a \neq a'$, that is, if there is no or sufficiently small overlap between different mean field solutions. By means of this 'small-overlap' approximation in (13) we obtain for the mixture weights

$$Q(a) \propto \exp \left[-\left\langle \log \frac{Q(\mathbf{X}|a)}{P(\mathbf{X})} \right\rangle_{Q(\mathbf{X}|a)} \right]$$

$$\propto \exp \left[-\mathcal{D}(Q(\mathbf{X}|a) || P(\mathbf{X})) \right]. \quad (15)$$

This means, different mean field solutions $Q(\mathbf{X}|a)$ contribute to the global distribution $Q(\mathbf{X})$ according to their distance $\mathcal{D}\left(Q(\mathbf{X}|a)||P(\mathbf{X})\right)$ to $P(\mathbf{X})$. That is a plausible result which we might have guessed. Note, however, that this nice result relies on the small-overlap approximation, i.e., on the assumption that different minima of $\mathcal{D}(Q||P)$ are not 'close' to one another.

4 Mean Field Theory for Bayesian Networks

So far we did not make any assumptions about $P(\mathbf{X})$, and, hence, our results (the mean field equations (11) and the mixture weights (15)) are very general. We will now focus on a particular parameterization of a probability distribution, namely, on Bayesian networks [1, 25]. A Bayesian network has an expansion of the form

$$P(\mathbf{X}) = \prod_{i} P(X_i|X_1, \dots X_{i-1}) = \prod_{i} P(X_i|\mathbf{\Pi}_i),$$
(10)

where in a typical Bayesian network every variable X_i has only a small set of 'parents' $\Pi_i \subseteq \{X_1, \dots X_{i-1}\}$. The first equality is valid in general and follows by repeated application of the Bayes formula. For $\Pi_i \subset \{X_1, \dots X_{i-1}\}$ in Eq. (16) the second equality corresponds to the assertion of some conditional independencies. Usually the structure of a Bayesian network is depicted as an acyclic graph where arcs point from all parent Π_i to their corresponding children X_i (see Fig. 1 later in the text as an example). The 'tables' $P(X_i|\Pi_i)$ associated with the nodes X_i are the parameters of a Bayesian network.

For updating node X_i according to Eq. (11) we need to know the Markov boundary \mathbf{M}_i of X_i and the conditional distribution $P(X_i|\mathbf{M}_i)$. For a Bayesian network the Markov boundary of a node is given by its parents, its children and all 'coparents', that is, all parents of all children [1]. Let \mathcal{C}_i be the index set of all children of node X_i . For the conditional distribution $P(X_i|\mathbf{M}_i)$ we have

$$P(X_i|\mathbf{M}_i) \propto P(X_i|\mathbf{\Pi}_i) \prod_{k \in C_i} P(X_k|\mathbf{\Pi}_k)$$
 (17)

which can be easily derived from (16). Using this result in (11) we obtain

$$Q(x_i) \propto \exp\left[\langle \log P(x_i|\mathbf{\Pi}_i)\rangle_Q + \sum_{k \in \mathcal{C}_i} \langle \log P(X_k|\mathbf{\Pi}_k)\rangle_Q\right].$$
(18)

On the right hand side any instantiation of X_i is fixed to $X_i = x_i$, and the expected values are evaluated over the remaining variables. If compared to Eq. (11) this result greatly economizes the mean field updating rule. For evaluation of the expectation in (11) we have to perform a sum over the state space of the Markov boundary \mathbf{M}_i . In (18) we have to calculate different expectations which, however, are less expensive to evaluate for they only involve the table $P(x_i|\mathbf{\Pi}_i)$ and the tables $P(X_k|\mathbf{\Pi}_k)$, $k \in \mathcal{C}_i$.

Furthermore, note that given any table $P(x_i|\mathbf{\Pi}_i)$ we can exactly evaluate the expectation $\langle \log P(x_i|\mathbf{\Pi}_i) \rangle_Q$

by just performing the corresponding sum. Thus we may run mean field inference in any Bayesian network without further approximations. For nodes X_i with a large number of parents Π_i , however, the evaluation of the expectation $\langle \log P(x_i|\Pi_i)\rangle_Q$ is expensive. In practise large tables very often have a simple structure, e.g., by assuming a noisy-OR gate. Only rarely all degrees of freedom of a large table are needed. One should of course try to exploit the structure of a large table to calculate the expectation $\langle \log P(x_i|\Pi_i)\rangle_Q$ more efficiently. E.g. Saul et al. [12] use an additional approximation to evaluate corresponding terms in their case of a sigmoid belief network.

It remains to be shown that in the case of a Bayesian network even the mixture weights (15) can be calculated in an efficient way by means of *only local computations*. If we use the expansion (16) we obtain

$$\mathcal{D}\left(Q(\mathbf{X}|a)||P(\mathbf{X})\right) = \sum_{i} \left\langle \log \frac{Q(X_{i}|a)}{P(X_{i}|\mathbf{\Pi}_{i})} \right\rangle_{Q(X_{i},\mathbf{\Pi}_{i}|a)}.$$
(19)

Every term in the sum on the right hand side requires only local information, i.e., only the conditional distribution $P(X_i|\Pi_i)$ and the distribution $Q(X_i,\Pi_i|a) = Q(X_i|a)Q(\Pi_i|a)$. $P(X_i|\Pi_i)$ and $Q(X_i|a)$ are properties of X_i , i.e., they can be stored locally at node i. $Q(X_j|a)$, $X_j \in \Pi_i$, describes neighboring nodes of node X_i .

Thus, for Bayesian networks, for instance, we find a very simple computational scheme. In many other cases it might be computationally more expensive to perform the expectation in the updating rule (11) and to compute the distance $\mathcal{D}(Q(\mathbf{X}|a)||P(\mathbf{X}))$ in (15) to obtain the mixture weights Q(a). Mean field inference as formulated in this section directly refers to the parameters of a Bayesian network (namely to the tables $P(X_i|\mathbf{\Pi}_i)$; see the update equation (18) and the distance (19)). There is no intermediate redundant representation of the Bayesian network, such as a junction tree [25].

5 Illustration of Mean Field Inference

Quite a bit of theory has been presented so far. It is now time to show how things work in practice. In particular, we want to demonstrate the benefits of mixing multiple mean field solutions. A simple Bayesian network for illustration purposes is depicted in Fig. 1. The goal of this network is to support medical diagnosis. In our simple example we just want to discern between measles, chickenpox and scarlet fever.

Suppose a patient complains about an eczema and a weakly sore throat. We enter that piece of knowledge into the corresponding nodes. Our goal is to obtain

probabilities for the remaining nodes, in particular, for the disease nodes. For that reason we use the discussed mean field ansatz for the remaining nodes, i.e., we iterate the mean field equations for the remaining nodes. For our illustration network we find two different solutions of the mean field equations. These two solutions, the corresponding mixture distribution and the exact probabilities are compared in table 1.

Roughly speaking the first solution is the 'measles scenario' the other solution is the 'scarlet scenario'. There is no 'chickenpox scenario' since chickenpox does not cause a sore throat. Thus, the mean field method supplies us not only with beliefs for the unknown nodes; we obtain additional information about the character of the exact distribution $P(\mathbf{X}|evidence)$ as well, namely that the joint distribution is approximately a composition of two modes. Based on these two modes we may easily calculate approximate joint probabilities for any set of nodes; see for example table 2. The two modes or disease scenarios mainly differ in the belief for the node 'red eyes'. To obtain a unique diagnosis a natural question therefore is: 'Does the patient have red eyes?' Suppose his eyes are red. Propagating that evidence by iterating the mean field equations for all jet unknown nodes we find that there is only one solution left, the measles scenario. Our final belief for measles is 0.99, that for chickenpox is 0.03.

6 Discussion

In this article we have discussed MFT in a modelindependent way as a method to approximate a given probability distribution. Furthermore, we have extended the conventional mean field approach by the idea of mixing different mean field solutions. As illustrated in our toy experiment, our approach can be used for approximate propagation of evidence (inference). Thereby, first, evidence is entered into the model, then the mean field approximation $P(\mathbf{X}|\text{evidence}) \approx$ $Q(\mathbf{X}|\text{evidence}) = \prod_{i} Q(X_{i}|\text{evidence})$ is calculated. The results clearly demonstrated that reasonable probabilistic approximations can only be achieved if we take into account multiple solutions of the mean field equations. In doing so, we may even obtain easy interpretable information about the joint distribution of several variables.

[‡]You can compare these two solutions with the two solutions 'all spins up' and 'all spins down' in a ferro magnet below the Curie temperature.

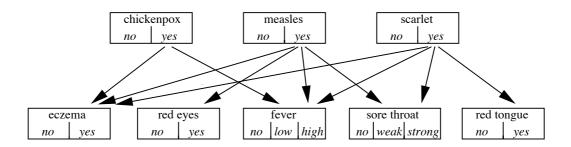


Figure 1: Our Bayesian network example for illustration of mean field inference. The network is modeling three children's diseases (chickenpox, measles and scarlet). The arcs are pointing from diseases to symptoms (eczema, red eyes, fever, sore throat and red tongue), that is, from cause to effect. Note, that the variables are not just binary. Plausible values for the conditional probabilities tables P(symptom|diseases) of that network have been estimated by consulting a text book on children's diseases.

	first MF-solution 'measles scenario' Q(a) = 0.68	second MF-solution 'scarlet scenario' Q(a) = 0.32	marginals of the MF-mixture distribution	marginals of the exact distribution
measles	0.996	0.008	0.679	0.641
scarlet	0.008	0.985	0.322	0.301
chickenpox	0.030	0.031	0.030	0.054
red eyes	0.903	0.052	0.630	0.598
red tongue	0.031	0.695	0.244	0.240
low fever	0.257	0.257	0.257	0.258
high fever	0.551	0.547	0.550	0.527

Table 1: Marginal probabilities of MFT as compared to the exact results. The first two columns show that any single mean field solution on its own results in a very poor approximation of the exact marginals. Furthermore, note that the two solutions have nearly no overlap, which can be seen from the first two rows 'measles' and 'scarlet'.

		scarlet		
		no	yes	
measles	no	P: 0.067 Q: 0.008	P: 0.292 Q: 0.313	
medicies	yes	P: 0.623 Q: 0.671	P: 0.017 Q: 0.008	

Table 2: Joint probability table of the mean field mixture distribution (Q) as compared to the exact results (P). Plain MFT is based on the assumption of independent variables (3) and, hence, cannot easily explain joint tables. This example shows, however, that the mixture distribution Q may give reasonable approximations to joint tables as well.

The presented procedure (finding solutions of the mean field equations (7) and mixing them) does not optimize the parameters Q(a) and $Q(\mathbf{X}|a)$ of the approximating distribution $Q(\mathbf{X})$ simultaneously since the different solutions $Q(\mathbf{X}|a)$ of the mean field equations (7) for different a are determined independently and prior to determining the mixture weights Q(a). It might be possible to derive a more refined simultaneous optimization of the parameters Q(a) and $Q(\mathbf{X}|a)$. However, the resulting equations will not be as simple as (11) and (15). Their simplicity and locality (!) justifies the above step by step procedure and the introduced small-overlap approximation. When used for inference in graphical models, MFT exploits the structure of a graphical model even in non tree-like graphs since, as discussed previously, only 'neighboring nodes' have to communicate. This locality is the appealing point of MFT. There is no necessity to compile the original graph to a tree-like cover model as it is done by the junction tree algorithm by means of moralization and triangulation [9, 10]. In particular in the case of Bayesian networks, mean field inference exhibits further simplifications. An additional advantage is that in many cases the existence of several mean field solutions sheds a light on the structure of the exact distribution. In our example the exact distribution could be interpreted as being composed of two 'scenarios'. Thus, MFT represents an interesting complement to other inference methods.

Finally, a few words on human reasoning are appropriate. In his book "Probabilistic Reasoning in Intelligent Systems" Pearl argues that '... any viable model of human reasoning should be able to perform this task (consistent propagation of information) with a self-activated propagation mechanism, i.e., with an array of simple autonomous processors, communication locally via the links provided by the network itself. The impact of each new piece of evidence is viewed as a perturbation that propagates through the network via message-passing between neighbouring variables, with a minimal external supervision.' Mean field inference exactly meets these demands. As a consequence mean field inference permits a significant amount unsupervized parallelism, which is ascribed to the human way of information processing. Furthermore, arguing in terms of 'scenarios' is much closer to the human way of reasoning then global probabilistic calculations. Mean field inference even reflects this way of arguing.

References

[1] J. Pearl. Probabilistic Reasoning in Intelligent Systems. Morgan Kaufmann, San Francisco, 2 edition, 1988.

- [2] G. Cooper. Computational complexity of probabilistic inference using bayesian belief networks. *Artificial Intelligence*, 42:393–405, 1990.
- [3] J. J. Binney, N. J. Dowrick, A. J. Fisher, and M. E. J. Newman. The Theory of Critical Phenomena. Oxford University Press, New York, 3 edition, 1995.
- [4] G. Parisi. Statistical Field Theory. Addison-Wesley, Reading, MA, 1988.
- [5] C. Peterson and J. R. Anderson. A mean field theory learning algorithm for neural networks. *Com*plex Systems, 1:995–1019, 1987.
- [6] C. Peterson and E. Hartman. Explorations of the mean field theory learning algorithm. *Neural Networks*, 2:475–494, 1989.
- [7] T. Hofmann and J. Buhmann. Pairwise data clustering by deterministic annealing. *IEEE Trans. Pattern Analysis and Machine Intelligence*, 19(1):1–14, 1997.
- [8] M. Haft. Robust 'topological' codes by keeping control of internal redundancy. *Phys. Rev. Letters*, 81(18):4016–4019, 1998.
- [9] S. L. Lauritzen and D. J. Spiegelhalter. Local computations with probabilities on graphical structures and their applicatin to expert systems. J. Roy. Statist. Soc. B, 50:154–227, 1988.
- [10] F. V. Jensen, S. L. Lauritzen, and K. G. Olsen. Bayesian updating in causal probabilistic networks by local computations. *Computational Statistics Quaterly*, 4:296–282, 1990.
- [11] J. Wittaker. Graphical Models in Applied Multivariate Statistics. Wiley, New York, 1990.
- [12] L. K. Saul and M. I. Jordan. Exploiting tractrable substructures in untractable networks. In D. Touretzky, M. Moser, and M. Hasselmo, editors, Advances in Neural Information Processing Systems: Proceedings of the 1995 Conference, pages 486–492, Cambridge MA, 1995. MIT Press.
- [13] K. L. Saul, T. Jaakkola, and M. I. Jordan. Mean field theory for signoide belief networks. *Journal* of Artificial Intelligence Research, 4:61–76, 1996.
- [14] M. Haft, R. Hofmann, and V. Tresp. Modelindependent mean field theory as a local method for approximate propagation of information. *Technical Report*, http://www7.informatik.tumuenchen.de/ hofmann/mf_abstr.html, 1997.

- [15] C. M. Bishop, T. Lawrence, N. D.and Jaakkola, and M. I. Jordan. Approximating posterior distributions in belief networks using mixtures. In M. I. Jordan, M. J. Kearns, and S. A. Solla, editors, Advances in Neural Information Processing Systems 10, Proceedings of the 1997 Conference, pages 416–422. MIT Press, Cambridge MA, 1998.
- [16] N. D. Lawrence, C. M. Bishop, and M. I. Jordan. Mixture representations for inference and learning in boltzmann machines. In G. F. Cooper and S. Moral, editors, *Uncertainty in Artificial Intelligence: Proceedings of the Fourteenth Conference*, pages 320–327. Morgan Kaufmann, San Francisco, CA, 1998.
- [17] T. S. Jaakkola and M. I. Jordan. Improving the mean field approximation via the use of mixture distributions. In M. I. Jordan, editor, *Learning in Graphical Models*, pages 163–173. Kulwer, 1998.
- [18] T. M. Cover and J. A. Thomas. Elements of Information Theory. Wiley, New York, 1991.
- [19] B. D. Serot and J. D. Walecka. Advances in Nuclear Physics Vol. 16: The Relativistic Nuclear Many Body Problem. Plenum Press, New York, 1986.
- [20] N. K. Glendenning, D. von-Eiff, M. Haft, H. Lenske, and M. K. Weigel. Relativistic mean field calculations of Λ- and Σ-hypernuclei. *Phys. Rev.* C, 48:889–895, 1993.
- [21] K. H. Fischer and J. A. Hertz. *Spin Glasses*. Cambridge University Press, 1991.
- [22] J. L. van Hemmen and R. Kühn. Nonlinear neural networks. *Phys. Rev. Letters*, 57(7):913–916, 1986
- [23] J. L. van Hemmen and R. Kühn. Collective phenomena in neural networks. In E. Domany, J. L. van Hemmen, and K. Schulten, editors, *Models of Neural Networks I*, pages 1–113. Springer, New York, 1991.
- [24] J. A. Hertz, A. Krogh, and R. G. Palmer. *Introduction to the theory of neural computation*. Addison-Wesley, 1991.
- [25] V. J. Jensen. An Introduction to Bayesian Networks. UCL Press, London, 1996.