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Jonathan S. Yedidia

Message-passing Algorithms for Inference and Optimization:

"Belief Propagation" and "Divide and Concur"

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Abstract Message-passing algorithms can solve a wide variety of optimization, inference, and constraint satisfaction problems. The algorithms operate on factor graphs that visually represent the problems. After describing some of their applications, I survey the family of belief propagation (BP) algorithms, beginning with a detailed description of the min-sum algorithm and its exactness on tree factor graphs, and then turning to a variety of more sophisticated BP algorithms, including free-energy based BP algorithms, "splitting" BP algorithms that generalize "tree-reweighted" BP, and the various BP algorithms that have been proposed to deal with problems with continuous variables.

The Divide and Concur (DC) algorithm is a projection-based constraint satisfaction algorithm that deals naturally with continuous variables, and converges to exact answers for problems where the solution sets of the constraints are convex. I show how it exploits the "difference-map" dynamics to avoid traps that cause more naive alternating projection algorithms to fail for non-convex problems, and explain that it is a message-passing algorithm that can also be applied to optimization problems. The BP and DC algorithms are compared, both in terms of their fundamental justifications and their strengths and weaknesses.

Keywords message-passing algorithms · factor graphs · belief propagation · divide and concur · difference-map · optimization · inference · constraint satisfaction

J.S. Yedidia
Disney Research Boston
222 3rd Street, Suite 1101
Cambridge, MA 02142 USA
E-mail: yedidia@disneyresearch.com

1 Introduction

This paper is a tutorial introduction to the important "Belief Propagation" (BP) and "Divide and Concur" (DC) algorithms. The tutorial will be informal, and my main goal is to explain the fundamental ideas clearly.

Iterative message-passing algorithms like BP and DC have an amazing range of applications, and it turns out that their theory is deeply connected to concepts from statistical physics. BP algorithms are already very well-known, and have been discussed in depth in some excellent reviews [1–3]. The DC algorithm [4] has important advantages compared with BP, but is so far much less known and used.

I have a couple target audiences in mind. One target reader is learning about message-passing algorithms for the first time; this paper can serve as a gentle introduction to the field. Another target reader might already have an knowledge of at least some aspects of BP, but may not be familiar with recent advances in our understanding of BP, or with projection-based algorithms like DC, which are not usually described as message-passing algorithms. For such readers, I will present an overview of different BP algorithms, and show that DC can be interpreted as a message-passing algorithm that can be easily compared and contrasted with other BP algorithms.

2 Inference and Optimization Problems

No algorithm can be discussed in isolation from the problem it is solving. BP and DC Message-passing algorithms are used to solve *inference* problems, *optimization* problems, and *constraint satisfaction* problems.

In an inference problem, one takes as input some noisy or ambiguous measurements, and tries to infer from those measurements the likely state of some hidden part of the world. In general, it is impossible to make those inferences with complete certainty, but one can at least try to obtain, within a model of the world and the measurements, the most *probable* state of the hidden part of the world [5,6].

As an example, consider the "channel coding" problem which is fundamental to information theory [7–9]. We want to transmit a message consisting of some sequence of bits across a noisy channel that might corrupt those bits. To deal with that noise, additional bits that depend on the message are appended to it by an encoder before it is transmitted. The task of the decoder is one of probabilistic inference: it tries to compute, from all the possibly noisy received bits, the most probable message that might have been transmitted.

Computer vision is another example of a field where probabilistic inference problems are ubiquitous [10–12]. In a typical scenario, one obtains images or videos from one or more cameras, and wants to infer something about the scene being captured. For a computer, photographic images are simply two-dimensional matrices of color intensities, and the scene is a hidden three-dimensional world of objects that must somehow be inferred from those inherently ambiguous measurements. A computer vision probabilistic inference system uses a statistical model that connects the camera measurements to the scene quantities of interest (e.g. the depth or the identity of objects), and tries to find the most probable interpretation of the scene quantities given the measurements.

Speech recognition [13–15] and language understanding [16,17] systems are similar. Here one obtains measurements of a sound signal, and tries to infer the most probable sequence of words, or meanings, consistent with those sounds.

In statistical physics, one deals with mathematically analogous problems [18,19]. If one is given the energy function for some magnetic system or some macromolecule, the most probable configuration of the system is the one that has the lowest energy. Of course, as physicists are well aware, the lowest energy configuration may be the most probable, while not being a *typical* configuration. To obtain probabilities about typical configurations, one must also take into account the entropy of the system. In probabilistic inference, this distinction corresponds to the difference between two tasks the system might be asked to perform. First, it might be asked to obtain the one most probable state of the entire system, or second, one might ask for the marginal probabilities of particular hidden variables, after summing over the probabilities of all possible configurations.

A probabilistic inference problem can be converted into a statistical physics problem by defining an energy function using Boltzmann's Law:

$$p(X) \propto \exp(-E(X)). \tag{1}$$

That is, if we are given a statistical model (say for coding, or vision, or speech recognition) that assigns probabilities $p(X)$ to states X, we can completely equivalently think of it as assigning energies $E(X)$, and proceed using any method of our choice from statistical physics. Or, if we are given a physical system with an energy function $E(X)$, we can fruitfully apply the probabilistic inference algorithms that have been invented by computer scientists and electrical engineers. Mathematically, many of the problems studied by statistical physicists and computer scientists are completely equivalent [19].

3 Factor Graphs

The task of inferring the most probable state of a system is actually the optimization problem of finding the minimum energy of that system. I will now describe a very convenient data structure called a *factor graph* [20,21] which can be used to visualize and precisely define such optimization problems. A variety of other "graphical models" exist (e.g. Bayesian networks [22], Markov random fields [23], normal factor graphs [24,21]), and have their advantages, but all these models can be easily converted into the standard factor graphs I will discuss [25].

Factor graphs are bipartite graphs containing two types of nodes: *variable* nodes and *factor* nodes. See figure 1 for our first example of a toy factor graph.

The variable nodes, usually denoted using circles, represent the variables in the optimization problem. A variable might be discrete—that is, it can only take on a finite number of states, like an Ising spin, which can only be

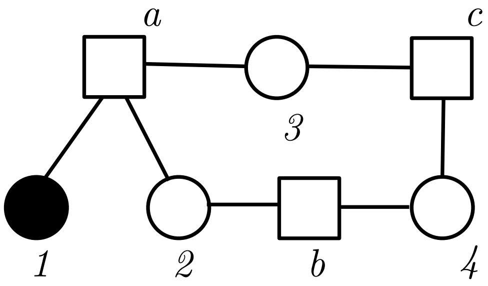


Fig. 1 A toy factor graph with one observed variable node (variable 1), three hidden variable nodes, and three factor nodes.

in the two states that we might call "up" and "down"—or it might have a continuous range of possible states.

If a variable's state is known (or "observed"), we fill in the corresponding circle in the factor graph; otherwise we use an open circle to denote a so-called "hidden" variable. The factor graph of figure 1 has three hidden variables and one observed variable.

The "factor" nodes in a factor graph show how the overall objective ("energy" or "cost") function of our optimization problem breaks up—factorizes—into local terms. We draw an edge between each factor node representing a local cost function, and the variables that are involved in that local cost function. For example, for the factor graph of figure 1, the overall "cost" $C(x_1, x_2, x_3, x_4)$ for a configuration (x_1, x_2, x_3, x_4) will be

$$C(x_1, x_2, x_3, x_4) = C_a(x_1, x_2, x_3) + C_b(x_2, x_4) + C_c(x_3, x_4). \tag{2}$$

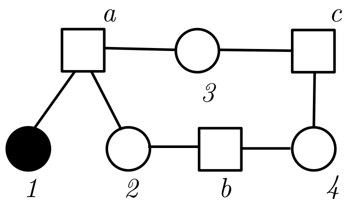
More generally, if there are M local cost functions, we can write the overall cost function $C(X)$ as

$$C(X) = \sum_{a=1}^{M} C_a(X_a) \tag{3}$$

where X_a is the set of variables involved in the ath local cost function.

By itself, a factor graph just lets one visualize the relationships between the variables and local functions in the problem; but it does not give the full information one needs to compute the cost associated with a configuration. To fill out that information, we would need to provide a table or explicit function for each factor node. For example, in figure 2, we supplement the factor graph from figure 1 with lookup tables that specify the local costs associated with each factor. Notice that in this example some of the local costs for factor a are infinite; this means that the corresponding configurations are forbidden and represents a "hard" constraint. For factors b and c, all the costs are finite, so these factors represent "soft" preferences.

x_1	x_2	x_3	C_a
0	0	0	∞
0	0	1	0
0	1	0	0
0	1	1	∞
1	0	0	0
1	0	1	∞
1	1	0	∞
1	1	1	0



x_2	x_4	C_b
0	0	1.2
0	1	1.7
0	2	3.2
1	0	1.9
1	1	0.6
1	2	1.4

x_3	x_4	C_c
0	0	0.4
0	1	1.9
0	2	0.2
1	0	4.9
1	1	0.3
1	2	2.4

Fig. 2 A factor graph, along with the lookup tables associated with each local cost function. Note that for this factor graph the four variables are all discrete. Factor a is a "hard" constraint, that either allows or disallows different local configurations, while factors b and c are "soft" factors.

The factor graph we have been looking at is just a toy example; we normally are interested in problems where there are a large number of hidden variables—at least hundreds, maybe thousands or millions. In that case, there will be an exponentially huge number of possible states of the system, so while it is always easy to compute the energy of one configuration, finding the lowest energy state, or summing over all the states, can be a very hard problem.

In fact, it should be obvious that our formulation is so general that many NP-hard optimization problems can be described in this way. Thus, we certainly are not going to be able to specify here an algorithm that is guaranteed to find the lowest cost state of an arbitrary factor graph, while using computational resources that only grows polynomially with the size of a factor graph. Nevertheless, it turns out that the BP and DC message-passing algorithms are often successfully used on problems that are NP-hard, and can in fact often efficiently find the global optimum for those problems. The point is that a problem might be NP-hard, and yet specific instances of it that we care about may be in an easier regime than the worst case, and often be solved by a clever algorithm. For example, the problem of finding the optimal decoding of a low-density parity-check (LDPC) code is NP-hard, and yet efficient state-of-the-art BP decoders succeed sufficiently often that they

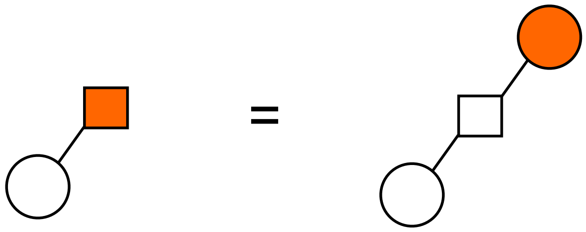


Fig. 3 Any observed variable nodes in a factor graph can be absorbed as parameters in the factor nodes that they are connected to, leaving only "hidden" variable nodes, and factor nodes that depend on the observations.

closely approach the Shannon limit of possible channel coding performance [8,9].

4 Example Factor Graphs and Applications

Let's take a look at just a few examples of how factor graphs can represent interesting problems. To simplify the factor graphs in the following examples, we take advantage of the fact that we can absorb any observed variable nodes as parameters in the factors they are attached to, leaving only hidden variables in the factor graph (see figure 3).

In the following examples, we will also describe some properties of message-passing algorithms, anticipating our more extensive discussion in future sections.

4.1 Error Correcting Codes

Our first example is a factor graph for an error correcting code—the simple $(N = 7, k = 4)$ Hamming code shown in figure 4. In this code, there are seven "hidden" variable nodes that represent the seven unknown transmitted bits. The first four of those bits are information bits that encode the original message, the other three are additional parity bits that can be computed from the information bits using the parity check factor nodes. The three parity check factor nodes are hard constraints that force the sum of the bits connected to them to equal 0 modulo 2. There are also seven "soft" channel evidence factor nodes that give the *a priori* probability that each of the hidden codeword bits is equal to a one or zero, given the observed received bits.

The goal will be to find the most likely values of the seven hidden transmitted bits, given the channel evidence and the fact that they must be consistent with the parity check constraints.

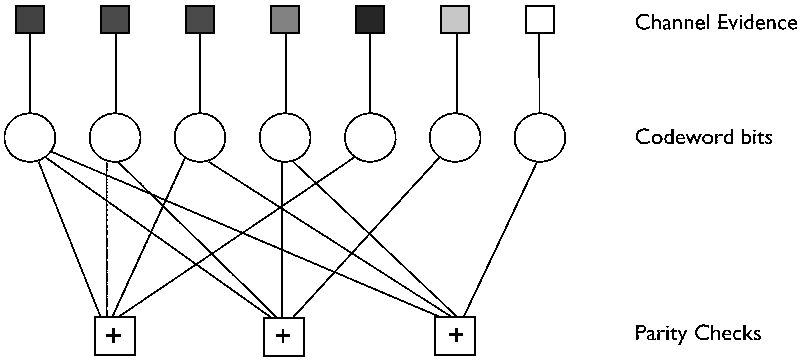


Fig. 4 A factor graph for the $(N = 7, k = 4)$ Hamming code, which has seven codeword bits, of which the left-most four are information bits, and the last three are parity bits.

Such factor graphs were introduced into coding theory in 1981 by Tanner [26], to describe and visualize the low-density parity-check (LDPC) codes and the BP decoder for LDPC codes that had been introduced earlier by Gallager in 1963 [27]. LDPC codes were given their name because each parity check is only connected to a small number of codeword bits. LDPC codes and their factor graphs are similar to the Hamming code in figure 4, except that the number of codeword bits is usually on the order of a few thousand in practical LDPC codes, and the codeword bits are not simply divided into information bits and extra parity check bits. BP decoders of LDPC codes are very practically significant, because if they are properly designed, their performance can closely approach the Shannon limit, and they can be implemented in modern hardware [8,9].

4.2 Diagnosis

Our next example (see figure 5) is a toy factor graph representing a medical diagnosis problem. The hidden variable nodes in this factor graph labeled "T," "L," and "B" represent different possible diagnoses of some patient (e.g. Tuberculosis, Lung Cancer or Bronchitis). The other variables may represent some information about the patient (e.g. "S" represents how much the patient smokes). The factor nodes encode the known statistical relationships between diseases and other variables.

This factor graph is adapted from an example in [28] that originally used a Bayes network, a graphical model that uses directed edges and that has the advantage of explicitly encoding *conditional* probabilities. The name "Belief Propagation" was in fact introduced by Pearl [22] for a version of the BP algorithm working on Bayes networks. It is easy to convert between different graphical models [25], and one reason that I am focusing here on standard factor graphs is that BP algorithms are easier to describe on standard factor graphs because they are undirected.

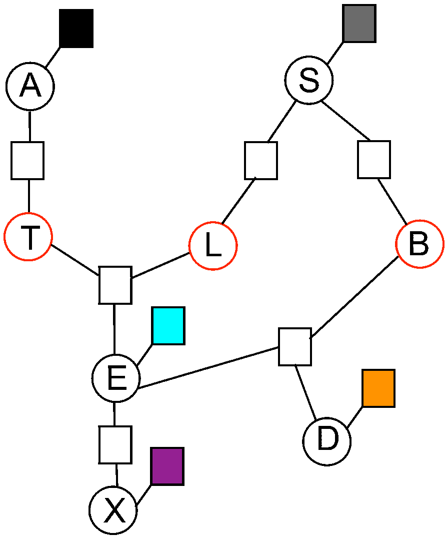


Fig. 5 A toy factor graph representing an "expert system" for a medical diagnosis problem. The hidden variables represent the unknown possible diseases (e.g. "L" represents lung cancer), or information about the patient such whether he is a smoker ("S") or test results. The factors represent known statistical relationships (e.g. a smoker is more likely to have lung cancer). The goal is to obtain the best estimate of the probabilities of possible diseases given the available information.

This example highlights an important point about probabilistic inference algorithms—one is often interested in more detailed information than the overall most probable configuration. For example, one might want an accurate estimate of the marginal probability that the patient has a particular disease. As we shall see, different BP algorithms are designed to give answers to different types of questions—for the kind of marginal probabilities we want here, we should use the "sum-product" version of BP, which we will describe in more detail later in this paper.

4.3 Computer Vision

Our next example (see figure 6) is a cartoon factor graph depicting the way factor graphs are used in low-level computer vision. The colored factor nodes in this example represent image intensity pixels that would be captured by a camera. The hidden variable nodes are some variables about the scene that we would like to infer (for example, the depth from the camera associated with each pixel). These hidden variables have some local probabilities given the observations, but there are also correlations between them—for example, if the depth has a certain value at one pixel, it is likely (but not guaranteed) to have similar values at neighboring pixels.

Our goal, as usual, will be to find the most probable values of the hidden scene variables given what our cameras observe.

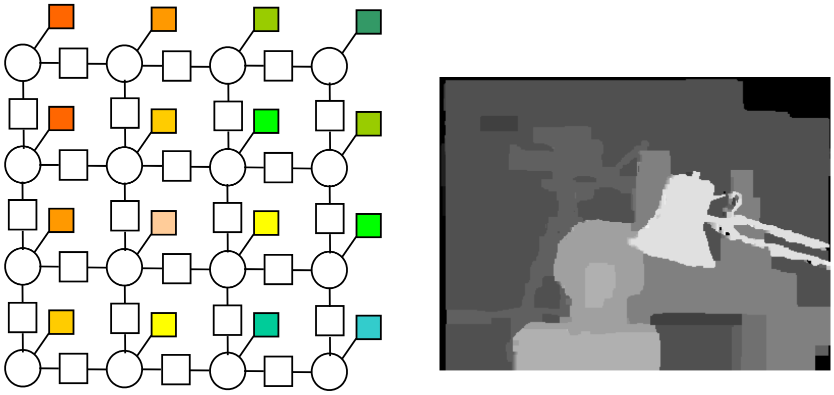


Fig. 6 An illustration of a factor graph equivalent to a pairwise Markov random field (left) as is often used to representing a computer vision problem, and a depth map returned by a BP algorithm [11] using stereo images (right). The variable nodes in the factor graph could represent unknown depth values, for which there exists some local evidence (the colored factor nodes), and which are statistically correlated (depths at particular pixels tend to be similar to nearby pixels).

Graphical models called "pairwise Markov random fields," which are equivalent to factor graphs like that shown in figure 6, were introduced into computer vision by Geman and Geman [23], and have become increasingly popular in the last 25 years [10–12], although the models used in practice are more complicated than the simplified cartoon shown in this figure. In a factor graph equivalent to a pairwise Markov random field, each factor node is connected to no more than two variable nodes.

One significant practical problem for BP algorithms is that the hidden variables of interest in computer vision are typically continuous, and are often severely quantized for the sake of efficiency when BP (or competing algorithms like "graph cuts" [29]) are run. This means that one often sees quantization artifacts in the results. The depth map on the right hand side of figure 6 is the result of running a BP algorithm on a pairwise Markov random field for stereo vision [11], and shows such artifacts.

Much recent research has focused on improving BP's performance or efficiency for problems with continuous variables (see section 10), but nevertheless the fact that the Divide and Concur algorithm works naturally with continuous quantities to any desired precision makes it an attractive potential alternative to BP for computer vision applications.

It should be emphasized that factor graphs only give a principled way of *representing* an optimization or probabilistic inference problem. You then need to separately choose an algorithm to *solve* it.

Many different variants of message-passing algorithms exist, and of course there are many other optimization algorithms (e.g. simulated annealing) that can be used once the problem is represented as a factor graph. I focus here on message-passing algorithms because they are often particularly powerful and efficient.

One should be careful to cleanly separate the model of an optimization or inference problem from the algorithm being used on that model. When a clean separation is made, one can determine whether it is the model or the optimization algorithm that needs improvement if one obtains an inadequate solution. For example, artifacts obtained using a particular stereo vision model (that was in principle NP-hard to optimize) were for a long time blamed on the inability of optimization algorithms to find the global optimum. Eventually though, it was found that even the *provably globally optima* found by BP-based algorithm were not completely adequate, demonstrating that it was the model that needed to be improved [30].

5 Message-Passing Algorithms

Let's turn now to the overall structure of message-passing algorithms, as they operate on factor graphs. This overall structure is shared by different classes of BP algorithms and by DC algorithms.

Figure 7 breaks the structure down into five steps. Message-passing algorithms get their name from the fact that in each step, messages are sent between nodes in the factor graph.

In the first step, the messages from variable nodes to factor nodes are initialized. The initial messages could be random, but more often, one uses non-informative messages from the hidden nodes, and messages that correspond to the observations from the observed nodes. Messages should be thought of as a variable telling its neighboring factors what it thinks its state is, or what it thinks would be the cost for it to be in each of its possible states. A non-informative message simply sets the costs of each possible state to be equal.

The factor nodes take in all the messages from their neighboring variable nodes, and in the second step, they compute messages that go back out to neighboring hidden variable nodes. These messages take into account what the variable nodes have told them, and the statistical relationships encoded by a factor node. The messages tell the neighboring variables what state they should be in, or what the costs will be for being in all their possible states.

In the third step, the hidden variable nodes inspect all the incoming messages, and compute a "belief" about what their state should be. In BP algorithms, this belief takes the form of a cost, or a probability, associated with each possible state of a variable. In the example shown in figure 7, the three hidden variable nodes have respectively two, two, and three possible states, so the beliefs are similarly vectors (represented by the columns of red numbers) of the same lengths giving the costs of each state. Thus in a BP algorithm, if a variable is continuous valued, the belief associated with it must be a function of that continuous variable. In DC algorithms, the belief (and the messages) are just a single number, representing the current best guess for the state of that variable node.

The fourth step of a message passing algorithm is necessary for BP algorithms but not for DC, and involves thresholding the beliefs to obtain a

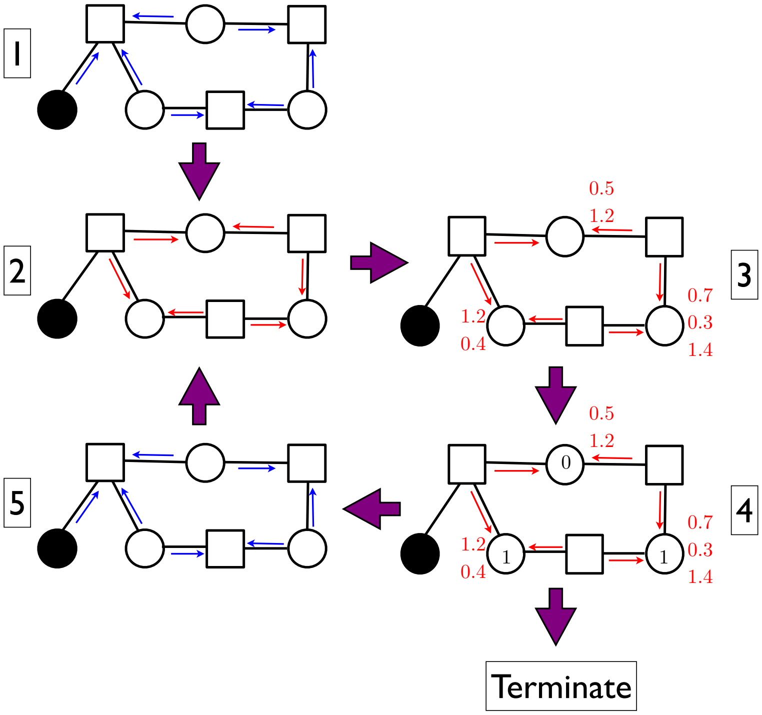


Fig. 7 The overall structure of message-passing algorithms. The algorithms iterate between steps, indicated by numbers in rectangles. In step 1, messages from variable nodes to factor nodes (in blue) are initialized to random or non-informative values. In step 2, the factor nodes compute from the incoming messages new outgoing messages (in red). In step 3, those messages are converted into beliefs, which in BP are generally represented as a cost for each possible state (the red numbers). In step 4, the beliefs are thresholded to their lowest cost state (represented by the number inside the variable node), and a termination condition is checked. In step 5, the beliefs and incoming messages are used to compute new outgoing messages from the variable nodes, and then one returns to step 2, and the cycle continues.

single best guess for a variable node. In our example, the beliefs represent costs, and the lowest cost state is chosen for each variable node (for example, the bottom right variable node has costs 0.7 for state 0, 0.3 for state 1, and 1.4 for state 2, so state 1 has the lowest cost for that variable).

After the fourth step is completed, one has obtained a guess for the overall configuration of the factor graph, and one can use that guess to check for a termination condition. For example, in BP-based decoders of LDPC codes, one can check whether the guess is a legal codeword that satisfies all the parity-check constraints. Or one can check whether the guess or the beliefs have changed from previous iterations, or whether a maximum number of iterations has been reached. If the termination condition is satisfied, one outputs the current guess.

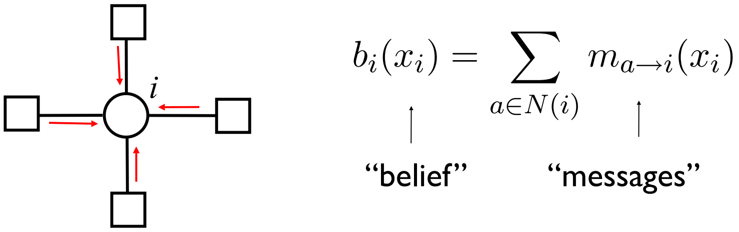


Fig. 8 The belief update rule for the min-sum BP algorithm says that the belief at a variable node is simply the sum of incoming messages from neighboring factor nodes.

Otherwise, in the fifth step, the variable nodes will compute new messages to send back to the factor nodes, based on their beliefs and the messages that they received. Then one goes back to the second step, and the cycle repeats.

Notice that all the factor nodes can compute their outgoing messages in step 2 in parallel, and similarly all the variable nodes can compute their outgoing messages in parallel in step 5. That makes these algorithms attractive for parallel implementation, either in hardware or software, and has contributed significantly to their popularity.

6 Message and Belief Update Rules

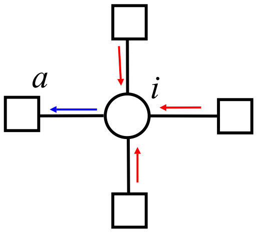
Message-passing algorithms differ in the details of and justifications for their message-update rules. I will begin by presenting one particular BP algorithm, the "min-sum" algorithm. This algorithm uses messages and beliefs that represent the costs for each variable to be in its different possible states. One sometimes sees the "min-sum" algorithm in a different guise, and referred to as the "max-product" BP algorithm. "Max-product" BP is equivalent to "min-sum" BP; the only (completely superficial) difference is that messages and beliefs are represented as probabilities rather than costs.

I begin with the belief update rules for min-sum BP, which relate the beliefs $b_i(x_i)$ at the variable node i to the messages $m_{a\to i}(x_i)$ coming into node i from neighboring factor nodes a (see figure 8). The rule is very simple: the belief is the sum of all the messages:

$$b_i(x_i) = \sum_{a \in N(i)} m_{a\to i}(x_i). \tag{4}$$

Here we use the notation x_i to represent the possible states of variable node i, and $N(i)$ to be the set of factor nodes neighboring node i.

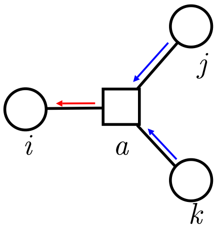
This rule is easy to understand if we think of the factor nodes as giving independent information about different parts of the graph. For example, if node i is a binary variable neighboring two factor nodes, and the first factor thinks it will cost A more for node i to be in state 1 than state 0, and the



$$m_{i\to a}(x_i) = \sum_{b\in N(i)\backslash a} m_{b\to i}(x_i)$$

$$m_{i\to a}(x_i) = b_i(x_i) - m_{a\to i}(x_i)$$

Fig. 9 The variable-to-factor message update rule in min-sum BP says that the outgoing (blue) message is the sum of all the incoming (red) messages on edges other than the edge of the outgoing message.



$$m_{a\to i}(x_i) = \min_{x_j,x_k} \left[C_a(x_i,x_j,x_k) + m_{j\to a}(x_j) + m_{k\to a}(x_k)\right]$$

Fig. 10 The factor-to-variable message update rule for a message from factor a to variable i depends on the local cost function C_a, and the incoming variable-to-factor messages on other edges.

second thinks it will cost B more to be in state 1, than it is natural to conclude that overall it will cost $A+B$ more to be in state 1, so long as the two factor nodes are using information from independent parts of the graph.

Turning next to the message update rule for a message $m_{i\to a}(x_i)$ from a variable i to a factor node a (see figure 9), we see that the message depends on all messages coming into variable node i from neighboring factor nodes b except for the one coming in from the target factor node a:

$$m_{i\to a}(x_i) = \sum_{b\in N(i)\backslash a} m_{b\to i}(x_i) \tag{5}$$

Again, the message out about the costs of the possible states of node i is just a sum of incoming messages from other parts of the graph. Note that if the belief has already been computed, we can use it to more efficiently compute the outgoing message:

$$m_{i\to a}(x_i) = b_i(x_i) - m_{a\to i}(x_i). \tag{6}$$

To complete our collection of update rules, we need the rule updating messages from factor to variable nodes. It's a little more complicated than the other rules, but still easy to understand. Let's look at the case when the factor node a is connected to three variable nodes i, j, and k (see figure 10). The message update rule

$$m_{a\to i}(x_i) = \min_{x_j,x_k} \left[C_a(x_i,x_j,x_k) + m_{j\to a}(x_j) + m_{k\to a}(x_k)\right]. \qquad (7)$$

The three terms in this equation can be understood as follows. The message $m_{a\to i}(x_i)$ should have node a tell node i what its costs would be for being in each of its possible states. For each choice of state for node i, we will arrange the other nodes attached to i to be in their best states given that choice (that is the explanation for the minimization over x_j and x_k). One part of the cost is the cost associated with a itself (the $C_a(x_i,x_j,x_k)$ term). The other parts of the cost are what it costs to place the x_j and x_k variables in the states that x_i would like them to be in, given by the incoming messages $m_{j\to a}(x_j)$ and $m_{k\to a}(x_k)$.

If X_a is the set of all variables attached to factor node a, and $X_a\backslash x_i$ is all those variables except for x_i, then the general update rule for messages from factor nodes to variable nodes, generalizing equation (7), is

$$m_{a\to i}(x_i) = \min_{X_a\backslash x_i} \left[C_a(X_a) + \sum_{j\in N(a)\backslash i} m_{j\to a}(x_j)\right] \qquad (8)$$

The form of equation (8) gives the min-sum algorithm its name. If the beliefs and messages represent probabilities instead of costs, we would obtain an equivalent message update rule with the sums replaced by products, and the minimization replaced by a maximization, so that equivalent algorithm is called the "max-product" algorithm.

We have written these rules as equations, but in fact they are normally used as iterative update rules. Only at a fixed point will they become equalities.

7 Exactness of BP for Tree Factor Graphs

We have already given some intuitive explanations for the form of the min-sum update rules, but a more rigorous justification for the rules is that on a graph with no cycles, applying the min-sum rules will provably give the lowest-cost configuration, using an amount of memory and time that only scales linearly with the number of nodes in the factor graph. I will not prove that fact here, and instead just give an example showing how that works.

Consider the tree factor graph shown in figure 11. Suppose that we want to compute the best state for variable node 1 in the optimal configuration. We can get that by computing $b_1(x_1)$, and thresholding it to the lowest cost state. By equation (4), that belief will be given by $b_1(x_1) = m_{A\to 1}(x_1)$. Now, we can replace $m_{A\to 1}(x_1)$ by using the min-sum update rule (8). If we continually replace messages with cost functions and other messages using the message update rules, we find:

$$b_1(x_1) = m_{A\to 1}(x_1)$$

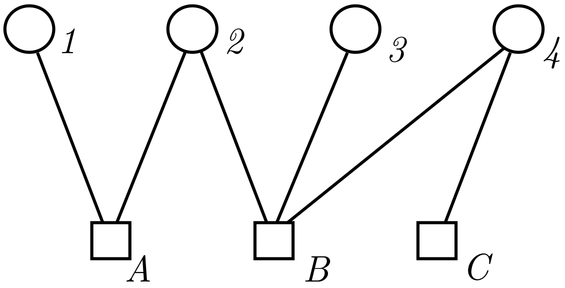


Fig. 11 A factor graph with no cycles used to illustrate the fact that min-sum BP finds an optimal configuration for such factor graphs.

$$
\begin{aligned}
&= \min_{x_2} \left[C_A(x_1, x_2) + m_{2\to A}(x_2)\right] \\
&= \min_{x_2} \left[C_A(x_1, x_2) + m_{B\to 2}(x_2)\right] \\
&= \min_{x_2,x_3,x_4} \left[C_A(x_1, x_2) + C_B(x_2, x_3, x_4) + m_{3\to B}(x_3) + m_{4\to B}(x_4)\right] \\
&= \min_{x_2,x_3,x_4} \left[C_A(x_1, x_2) + C_B(x_2, x_3, x_4) + m_{C\to 4}(x_4)\right] \\
&= \min_{x_2,x_3,x_4} \left[C_A(x_1, x_2) + C_B(x_2, x_3, x_4) + C_C(x_4)\right]
\end{aligned}
$$

In the end, we see that $b_1(x_1)$ gives the exact minimal overall cost for each possible state of the first node, and a similar result would hold starting with any other node.

It should be clear from this example that the min-sum algorithm is a "dynamic programming" algorithm [31] when run on trees, and only needs an amount of computation and memory that scales linearly with the number of nodes in the factor graph.

As we have seen, the min-sum or max-product algorithm finds, for a factor graph with no cycles, the lowest-cost or highest-probability configuration of the system. A small modification of the max-product algorithm can be used to obtain exact marginal probabilites $p_i(x_i)$ for the variable nodes being in each of their possible states, averaged over all possible configurations of the system. That modification, which simply replaces the "max" in the factor-to-variable message-update rule with a sum, gives the "sum-product" version of BP. The beliefs in sum-product BP are precisely equal to the desired marginal probabilities so long as the factor graph has no cycles.

The min-sum or max-product algorithm is also sometimes known as the "Viterbi" algorithm [32], and it has had enormous practical importance. Many problems, including decoding "convolutional" error-correcting codes, for which it was originally introduced, naturally can be represented using chain-like factor graphs, where the different variables in the chain represent states of the system at different times.

Forney [33] made clear the significance of the Viterbi algorithm as a efficient way of finding optimal state sequences for a wide range of such problems, and he also introduced an important graphical visualization of the algorithm,

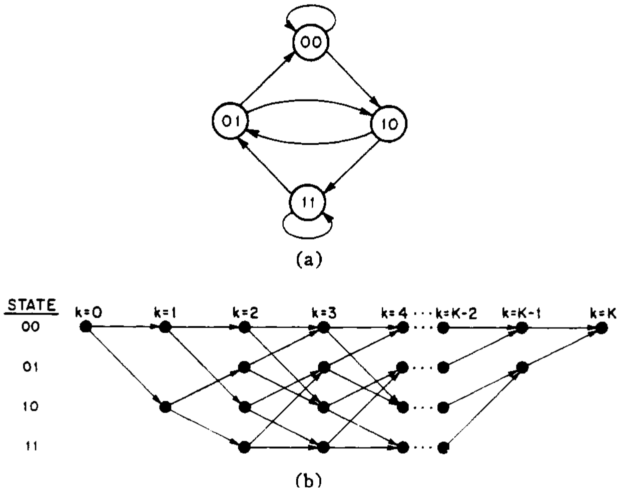


Fig. 12 An illustration from Forney's paper [33] on the Viterbi algorithm, showing a state diagram for a four-state shift-register process (a), and the corresponding trellis diagram given evidence for the state of the process from time 0 to time k (b).

the "trellis" diagram (see figure 12). Trellis diagrams can be used to effectively track the values of messages as a BP algorithm proceeds forward in time, or equivalently along the variables in a chain factor graph [24]. Each edge in the trellis corresponds to a choice for a value of a one or more variables in the factor graph. For sufficiently simple error-correcting codes, one can obtain optimal decoders from their trellis diagrams; and the important issue often becomes how to represent a code so as to obtain a minimal trellis diagram. [34].

I will not pursue this important subject further, except to make some comments to connect threads from different fields. First, a physicist might recognize that the BP algorithm on chains operates very similarly to the transfer matrix approach used to exactly solve one-dimensional models in statistical physics. Second, I strongly recommend to the reader Knuth's remarkable recent tutorial [35] on binary decision diagrams [37] and zero-suppressed binary decision diagrams [38], which are generalizations of trellis diagrams that allow many different types of exact computations to be made for *general* factor graphs over discrete variables, using as little memory and time as possible. Knuth shows (among many other things) that there is a "sweeping generalization" to algorithms on binary decision diagrams that compute optimal configurations (min-sum), or marginal probabilities (sum-product), or the partition function (transfer matrix)—all these algorithms obey a general form which can be exploited to exactly compute other quantities of interest. Knuth's observation echoes and expands upon earlier work of Aji and

McEliece [36], which generalizes BP to a class of message-passing algorithms they call the "generalized distributive law."

8 Approaches Based on Free Energies

The min-sum and sum-product algorithms are perfectly well defined on factor graphs with cycles, but they are no longer necessarily exact. Nevertheless, they often give good approximate answers. Some insight into why this should be so was obtained when my colleagues Bill Freeman and Yair Weiss and I showed [25,39] that the fixed points obtained by sum-product BP were identical to the stationary points of a variational free energy, the so-called "Bethe free energy." If we use $b_a(X_a)$ to denote a multi-node belief over all the variable nodes attached to the factor node a (intended to approximate the multi-node marginal probability $p_a(X_a)$) then the Bethe free energy F_B is given by $F_B = U_B - S_B$, where the Bethe average energy U_B is

$$U_B = \sum_a \sum_{X_a} b_a(X_a) C_a(X_a) \tag{9}$$

and the Bethe entropy S_B is

$$S_B = -\sum_a \sum_{X_a} b_a(X_a) \ln b_a(X_a) + \sum_i (d_i - 1) \sum_{x_i} b_i(x_i) \ln b_i(x_i). \tag{10}$$

Here, d_i is the number of factor nodes neighboring variable node i.

The Bethe Free energy F_B is a functional of the beliefs $b_a(X_a)$ and $b_i(x_i)$, which must satisfy the normalization conditions (for all a and i):

$$\sum_{X_a} b_a(X_a) = \sum_{x_i} b_i(x_i) = 1 \tag{11}$$

and the marginalization conditions for variable nodes i neighboring factor nodes a:

$$b_i(x_i) = \sum_{X_a \backslash x_i} b_a(X_a). \tag{12}$$

where $X_a \backslash x_i$ denotes all variables attached to factor node a except x_i.

The marginalization condition turns out to be fundamental: the Lagrange multipliers that enforce it when minimizing the Bethe Free energy turn out to equal linear combinations of the fixed-point messages in sum-product BP.

The Bethe average energy U_B is actually exactly equal to the true average energy of the system given correct beliefs, but the Bethe entropy S_B is only an approximation. Improving that approximation, using larger regions of nodes to compute the entropy, gives better "Kikuchi" [40] or "region graph" free energies, and corresponding "generalized belief propagation" algorithms that gave more accurate marginal probabilities than the sum-product algorithm [39].

Building on these ideas, Chertkov and Chernyak developed another significant approach to improving BP, that begins with sum-product BP or the equivalent Bethe approximation as a zeroth order approximation, and obtains a “loop” series that systematically improves on that approximation [41].

Given the fact that spin glasses and related models can be described using factor graphs, it was perhaps unsurprising that the well developed statistical physics of disordered system, and in particular the “replica” and “cavity field” methods [42] would be related to BP message-passing algorithms [19]. From this perspective, it is clear that the sum-product BP equations only describe a single minimum of the free energy of the system, and ignore any fracturing of phase space such as often occurs in disordered systems. An important and surprising breakthrough exploiting this insight was the development of another improved message-passing algorithm called “survey propagation,” based on heuristic ideas that try to take phase-space fracturing into account [43]. Survey propagation has been shown to solve NP-hard random satisfiability problems very effectively, even very close to the satisfiability threshold where they are particularly difficult [44].

On the other hand, one can take the point of view that the Bethe free energy that underlies sum-product BP would be more convenient to work with if it was always convex as a function of the beliefs, as it is when the factor graph is a tree. Wainwright, Jaakkola, and Willsky [45] derived new message-passing algorithms by replacing the Bethe entropy approximation with concave entropies to obtain “convexified” free energies which are guaranteed to have a unique global minimum. They showed that their approach could be used to find upper bounds on the log partition function (or lower bounds on the Helmholz free energy) of the system.

9 Min-sum Algorithms Based on “Splitting”

Wainwright, Jaakkola, and Willsky also introduced related “tree-reweighted” BP algorithms, in both sum-product [46] and max-product [47] form, and proved several powerful theorems about them. These algorithms were originally introduced in the context of pairwise Markov random fields rather than standard factor graphs. I prefer therefore to consider instead the insightful recent formulation of Ruozzi and Tatikonda [48], which generalizes the tree-reweighted max-product algorithm in a way that directly connects to the min-sum BP algorithm on standard factor graphs.

Ruozzi and Tatikonda start from the idea that it is easy to create equivalent factor graphs for the same overall cost function by “splitting” either factor or variable nodes. For example, as illustrated in figure 13, we can split the factor node b into two factor nodes b_1 and b_2, each of which has the same neighboring nodes as b and gets exactly half of the cost associated with the original node b. Doing this gives us a factor graph that models exactly the same original cost function as the original cost function, but notice that the min-sum algorithm associated with new factor graph is different from the original one.

Let’s assume that we initialize all messages from the same variable node but to different split copies of a factor node to be equal to each other, and similarly for messages from different split copies of a factor node. In that

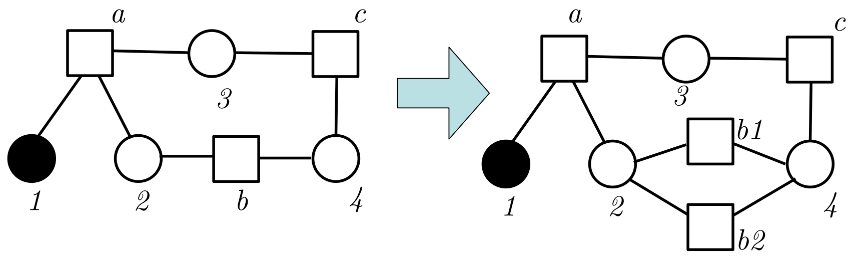


Fig. 13 One can obtain a new factor graph modeling exactly the same cost function by splitting a factor node into two identical factor nodes, each taking half the cost of the original, and connected to the same variable nodes.

case, the messages to and from split copies of a factor node will continue to maintain that symmetry, and can be identified with the messages to and from the factor node in the original factor graph. So in fact, we can translate the message-passing algorithm on the factor graph with split factor nodes into an induced message-passing algorithm on the original factor graph. If each variable node i is split k_i times, and each factor node a is split k_a times, it is easy to verify that the new induced message update rules are

$$m_{i\to a}(x_i) = (k_a - 1)m_{a\to i}(x_i) + \sum_{b\in N(i)\backslash a} k_b m_{b\to i}(x_i) \tag{13}$$

and

$$m_{a\to i}(x_i) = \min_{X_a\backslash x_i} \left[\frac{C_a(X_a)}{k_a} + (k_i - 1)m_{i\to a}(x_i) + \sum_{j\in N(a)\backslash i} k_j m_{j\to a(x_k)} \right]. \tag{14}$$

Notice that the message $m_{i\to a}(x_i)$ now depends directly on the message $m_{a\to i}(x_i)$ coming in the opposite direction on the same edge. This results from splitting: a message to one of the copies of a depends on the messages from the other copies of a.

Even though the message update rules (13) and (14) were originally derived using splitting factors k_a and k_i that were positive integers, they are also perfectly well-defined for any real values of k_a and k_i, including real values that are less than 1. Ruozzi and Tatikonda show that if k_a and k_i are chosen appropriately (e.g. for a regular graph where each variable node has degree d, choose $k_i = 1$, and k_a to be a positive real less than $1/d$), then one can prove some remarkable theorems about the resulting message-passing algorithm.

In particular, if a fixed point of the message-passing update rules is reached, and the resulting single node beliefs each have a unique lowest cost state for that node, then the overall state obtained by combining those single-node states is provably a *global* optimum! This is a surprising theorem, because it holds for arbitrary factor graphs, even those with cycles. Moreover, with the same choice of splitting constants, one can devise simple schedules that provably converge. Of course, the condition that each single-node belief must have a unique lowest cost state at the fixed point (no ties are allowed) is an important loophole that will often prevent a “splitting” message-passing algorithm from giving the globally optimal solution for an NP-hard problem in a difficult regime.

10 BP for Factor Graphs with Continuous Variables

Because BP messages and beliefs track the cost of every possible state of a variable, it is much easier in practice to apply BP to problems where the variables all have a small number of possible states. Nevertheless, the BP update rules are well-defined for continuous variables; it is just that the messages and beliefs must be full functions of the variables. There are certain circumstances when these functions can still be computed with efficiently.

First, suppose one tries to parameterize a message or belief function that represents a probability as a Gaussian (or equivalently as a quadratic if we use costs instead of probabilities); in this case one would only need to store its mean and variance. It turns out that there are a variety of important local cost functions such that locally, the max-product and sum-product BP algorithms preserve a Gaussian form [21]. The famous Kalman filtering problem is constructed from local cost functions that all have preserve Gaussians, and moreover the factor graph is a chain, so that a Gaussain BP algorithm parameterizing messages using means and variances is exact, and is equivalent to the Kalman smoothing algorithm [21,49].

For graphs with cycles, a BP algorithm may not converge, and in general its fixed points will no longer exact, even if the local cost functions preserve the Gaussian form of messages. However, in the important special case of a pairwise Markov random field that represents a Gaussian distribution of many variables, Weiss and Freeman [50] and Rusmevichientong and Van Roy [51] proved that if the BP algorithm converges, the calculated means (but not the variances) are exact. The conditions under which Gaussian BP converges [52], and how to fix its convergence properties [53], has been the subject of much recent work.

For certain problems, one can sometimes show that min-sum BP will preserve other functional forms. For example Gamarnik, Shah, and Wei recently showed that for the min-cost network flow problem, the messages preserve a piecewise linear form [54], and proved that min-sum BP converges to the optimal solution.

If one does not have local cost functions that preserve any nice form for the messages, dealing with continuous variables becomes very difficult. Nevertheless, one can begin with the assumption that messages have some nice form (for example Gaussians), then proceed by computing the outgoing messages using the sum-product or max-product BP update rules, and convert the results back into Gaussians by retaining only their means and variances. A systematic way to do this is provided by the popular “Expectation Propagation” algorithm [55].

“Non-parametric BP” is a similar but more accurate method that uses mixtures of Gaussians, and efficient sampling techniques [56]. Finally, the

"Particle Belief Propagation" approach [57] builds on the "Particle Filter" sampling technique [56] first developed for temporal processes. However, the drawback of relying on sampling is that it becomes increasingly computationally intensive to obtain more precise results.

As you can see, there are lots of options for dealing with continuous variables in the context of BP, which is not really surprising, because continuous variables are ubiquitous in inference and optimization problems that we care about. For an extensive review, with an emphasis on Gaussian BP for signal processing applications, see [58].

Consider however, the most simple and naive approach imaginable: instead of keeping track of the costs of every possible value of a variable, why don't we just use our single best current guess for the value as a message? It might seem unlikely that such an approach can give good results, but in fact with sufficient ingenuity it can; such an approach underlies the Divide and Concur algorithm, which we turn to now.

11 Divide and Concur

The DC algorithm was introduced by Gravel and Elser [4], and builds upon considerable earlier work done by Elser with his students on the use of "difference-map" dynamics in iterative projection algorithms [59]. As I did with the min-sum BP algorithms, I will begin by explaining how to implement DC, and then discuss its justifications.

Like BP, DC can be used to solve optimization and inference problems, but it is easier to begin by considering its application to *constraint satisfaction* problems. In a constraint satisfaction problem, we are looking for a configuration of variables such that all constraints are satisfied. In the language of factor graphs, all "cost" functions are "hard": their only possible values are zero (the constraint is satisfied) or infinite (the constraint is not satisfied).

To explain the DC algorithm it is standard to introduce "replicas" or "copies" of each variable; we introduce one replica of each variable for each constraint it is involved in. (These "replicas" have nothing to do with the "replica method" used for averaging over disorder in statistical physics [19], or the copies used in Ruozzi and Tatikonda's "splitting" method previously described [48].) Of course, the different replicas of the same variable eventually have to equal each other, but temporarily we can allow them to be unequal while they satisfy different constraints. Essentially we are lifting our original problem to a higher dimensional space where it is easier to solve.

In figure 14, I show a small example of a "constraint graph," which is useful for visualizing the DC algorithm. A constraint graph is like a factor graph, except that the factor nodes have been replaced with constraint nodes that represent hard constraints. These constraint nodes can represent arbitrary and possibly non-linear constraints on the neighboring variables.

Note that the variables in a constraint graph should always be thought of as real (continuous) numbers. However, problems with discrete variables can easily be handled by simply adding the appropriate constraints to the constraint graph.

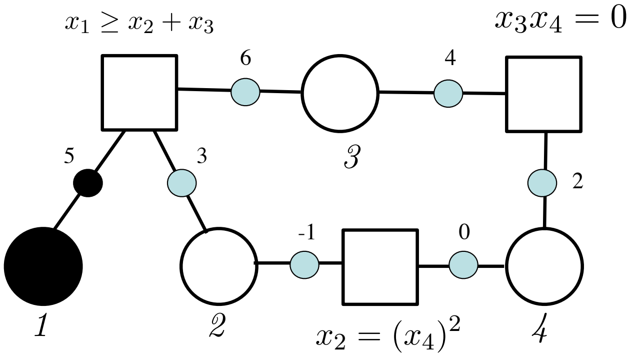


Fig. 14 A constraint graph with three hidden variables, one observed variable, and three hard constraints. The little blue "beads" placed on the edges represent replicas of the neighboring variable node, which can temporarily take different values, but must be equal at a solution.

Our example constraint graph explicitly represents the replicas of variable as little "beads" on the edges between constraint and variable nodes. Next to each replica bead there is a real number that is the current value of the replica. Notice that the replicas are associated with the edges of the constraint graph, just as BP messages are associated with the edges of factor graphs.

The DC algorithm is built from two "projections" on the replica values. The "Divide" projection does the most natural thing imaginable to satisfy the constraints: it moves the replica values from their current values to the nearest values that satisfy all the constraints. The "Concur" projection also is completely natural: it averages the replica values that belong to the same variable.

Let us use our example constraint graph, with its replica values, to illustrate how a "Divide projection" works. In the top left, we have a constraint $x_1 \geq x_2 + x_3$, and the current replica values are 5 for the replica of x_1, 3 for the replica of x_2, and 6 for the replica of x_3. We know that x_1 is an observed variable, so we leave it fixed, but otherwise we want to move the replicas of x_2 and x_3 as little as possible, but make them satisfy the constraint $x_1 \geq x_2 + x_3$.

When I say "move as little as possible," of course I must specify a metric. The choice of metric is a crucial issue, but for the moment, let's just use a standard Euclidean metric.

Using this metric, the Divide projection would satisfy its constraint by moving the replicas of x_2 and x_3 to the values 1 and 4 respectively. At the same time, and in parallel, we can project the replicas around the other constraints ($x_3 x_4 = 0$ and $x_2 = (x_4)^2$) to their nearest values which satisfy those constraints. Note that each replica is connected to only one constraint, so that all these local Divide projections can be done fully in parallel. The overall Divide projection of all the replicas is simply the concatenation of all the local projections.

Figure 15 shows the results of applying the Divide projection to the constraint graph from figure 14. It is usually easy to write a subroutine to com-

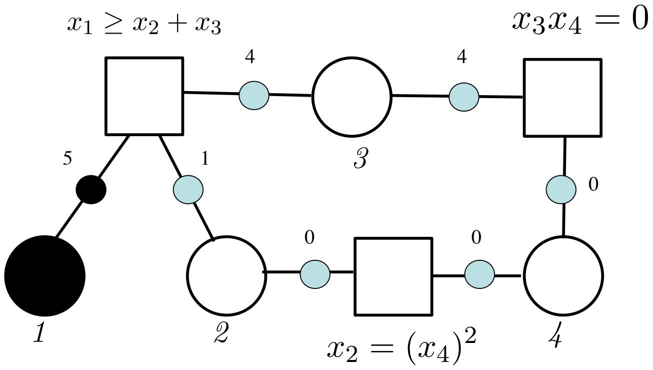


Fig. 15 State of the replicas of the constraint graph in figure 14 after applying a Divide projection.

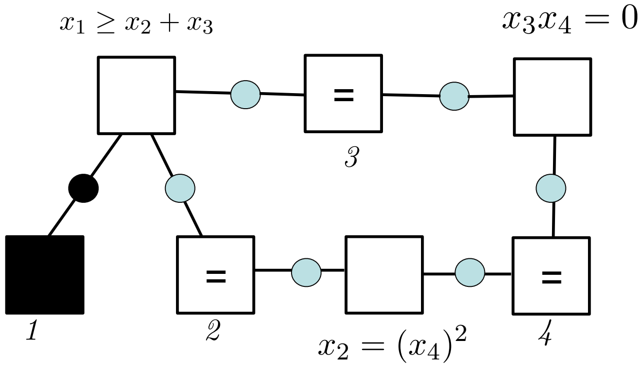


Fig. 16 A "normal" version of the constraint graph from figure 14, where the variable nodes are replaced with constraint nodes that impose equality on neighboring replicas.

pute each local divide projection at a particular constraint node, so the DC algorithm divides the overall problem of simultaneously satisfying all the constraints into a lot of small problems of projecting to the nearest solution of a single constraint.

The Concur projection can also be thought of as making the smallest move that satisfies a constraint; now the constraint is that different replicas of the same variable must be equal, and the smallest move is to move all the replicas to the average. Thus we could as well have drawn our constraint graph in the form shown in figure 16, where we have replaced the hidden variable nodes with constraints that impose equality on the neighboring replicas, and now the Divide and Concur projections would work in exactly the same way.

Forney introduced such so-called "normal" versions of standard factor graphs [24], which, while being equivalent to the standard version, have sev-

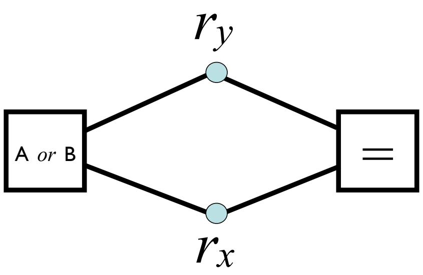


Fig. 17 A toy "normal" constraint graph used to illustrate replica dynamics.

eral advantages compared with standard factor graphs in terms of the insight they give. For example, using normal factor graphs, one sees that BP in fact has only one message update rule, just applied to different types of factors. Normal factor graphs are also well-suited for hierarchical modeling (it is easy to create a super-factor by enclosing a group of factors in a box), and they are compatible with standard block diagrams [21].

Returning to the DC algorithm, the simplest way to combine the Divide and Concur projections would be just to alternate between them—the so-called "alternating projections" algorithm. However, that is often a bad idea, as explained in the next section.

12 Traps in Alternating Projections

Let us denote the vector of all the values of the replicas in a constraint graph at iteration t by $\mathbf{r}_t$, and the replica values obtained by applying the Divide projection to $\mathbf{r}_t$ to be $P_D(\mathbf{r}_t)$. Then the alternating-projections algorithm would iteratively apply the Divide projection P_D and the Concur projection P_C; that is it would obtain $\mathbf{r}_{t+1}$ using the rule

$$\mathbf{r}_{t+1} = P_C(P_D(\mathbf{r}_t)). \tag{15}$$

The problem with alternating projections is that the algorithm can be trapped in a simple cycle, where the replica vector first satisfies the Divide constraints but not the Concur constraints, and then satisfies the Concur constraints but not the Divide constraints, and then goes right back to where it was before satisfying the Divide constraints.

Consider the somewhat contrived "normal" constraint graph [60] shown in figure 17. This constraint graph has two replicas, denoted r_x and r_y, and two constraints: an equality constraint on the right corresponding to a variable node, and a constraint that the two replicas are either at point A, which is at $(r_x = 0, r_y = 0)$ or at point B, which is at $(r_x = 3, r_y = 1)$. We can consider the Divide projection to move the replica vector to the nearest of points A and B, and the Concur projection to set r_x and r_y to their mean value.

The only solution that satisfies all the constraints is the point A, where $r_x = r_y = 0$. But let's see what happens when we start at some point near B like point D in figure 18. The Divide projection takes us to the nearest point

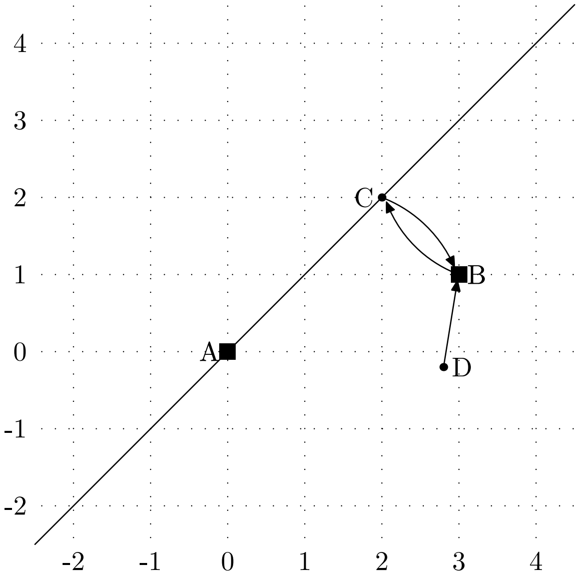


Fig. 18 An example of a trap resulting from alternating projections. If one alternately projects to the nearest point that satisfies the constraint to be at A or B, and then the nearest point where the replica values are equal (the diagonal line), one may be trapped in a short cycle (B to C to B and so on) and never find the true solution at A.

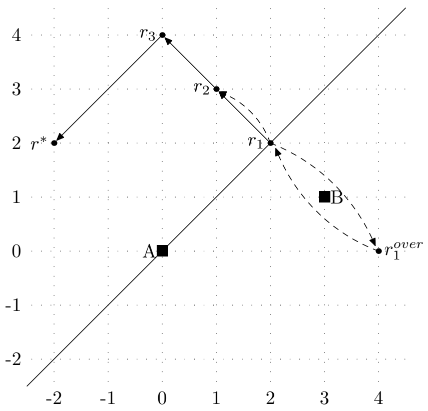
of A or B, which is B, then the Concur projection takes us to the nearest point on the diagonal line, which is C, then we go back to B, and so on. We never find the true solution at A.

13 Difference-Map Dynamics

To make progress, we need a way to turn pairs of points in replica space where the Divide constraints and Concur constraints come close, but do not intersect (like points B and C in figure 18) into repellers in the dynamics rather than traps. The "Difference-Map" (DM) dynamics does that [59]. We first consider a particular version of DM, where the replica update rule is

$$\mathbf{r}_{t+1} = P_C(\mathbf{r}_t + 2[P_D(\mathbf{r}_t) - \mathbf{r}_t])) - [P_D(\mathbf{r}_t) - \mathbf{r}_t]. \tag{16}$$

To parse this complicated looking equation, it is useful to think of the difference-map dynamics as breaking up into a three-step process [60]. The expression $[P_D(\mathbf{r}_t) - \mathbf{r}_t]$ represents the change to the current values of the replicas resulting from the Divide projection. In the first step, the values of the replicas move *twice* the desired amount indicated by the Divide projection. We can refer to these new values of the replicas as the "overshot" values $\mathbf{r}_t^{over} = \mathbf{r}_t + 2[P_D(\mathbf{r}_t) - \mathbf{r}_t]$. Next the Concur projection is applied to the overshot values to obtain the "concurred" values of the replicas $\mathbf{r}_t^{conc} = P_C(\mathbf{r}_t^{over})$.



t	$\boldsymbol{r}_t$	$P_D(\boldsymbol{r}_t)$	$\boldsymbol{r}_t^{over}$	$\boldsymbol{r}_t^{conc}$
1	$(2,2)$	$(3,1)$	$(4,0)$	$(2,2)$
2	$(1,3)$	$(3,1)$	$(5,-1)$	$(2,2)$
3	$(0,4)$	$(0,0)$	$(0,-4)$	$(-2,-2)$
4	$(-2,2)$	$(0,0)$	$(2,-2)$	$(0,0)$
5	$(-2,2)$			

Fig. 19 An example showing how DM dynamics avoids traps. If we start at the point r_1, an alternating projections dynamics would be trapped between point B and r_1, and never find the solution at A. DM dynamics will instead be repelled from the trap and move to r_2 (via the three sub-steps denoted with dashed lines r_1^{over}, $r_1^{conc} = r_1$, and r_2), then move to r_3, and then end at the fixed point $r_4 = r^*$, which corresponds to the solution at A.

Finally the overshoot (that is, the extra motion in the first step) is subtracted from the result of the Concur projection to obtain the replica value for the next iteration $\mathbf{r}_{t+1} = \mathbf{r}_t^{conc} - [P_D(\mathbf{r}_t) - \mathbf{r}_t]$.

In figure 19 we return to our previous example to illustrate that the DM dynamics do not get stuck in a trap. Suppose that we now start initially at point $\mathbf{r}_1 = (2,2)$. The Divide projection would take us to point B, but the overshoot takes us twice as far to $\mathbf{r}_1^{over} = (4,0)$. The Concur projection takes us back to $\mathbf{r}_1^{conc} = (2,2)$. Finally, the amount by which we overshot is subtracted so that $\mathbf{r}_2 = (1,3)$. The next full iteration takes us to $\mathbf{r}_3 = (0,4)$ (sub-steps are tabulated in figure 19). Now however, we are closer to A then to B. Therefore, the next overshoot takes us to $\mathbf{r}_3^{over} = (0,-4)$, from which we would move to $\mathbf{r}_3^{conc} = (-2,-2)$, and $\mathbf{r}_4 = (-2,2)$. Finally, at $\mathbf{r}_4$ we have reached a fixed point in the dynamics, because $\mathbf{r}_5 = \mathbf{r}_4$.

It can be proven that if a fixed point $\mathbf{r}^*$ in the DM dynamics is reached such that $\mathbf{r}_{t+1} = \mathbf{r}_t = \mathbf{r}^*$, then that fixed point must *correspond* to a solution $\mathbf{r}_{sol}$ that can be obtained using $\mathbf{r}_{sol} = P_D(\mathbf{r}^*)$. Thus, applying one more Divide projection to our fixed point, we arrive at our solution at $(0,0)$.

Of course, the DM dynamics is not a panacea. It is possible for example for the replica vector to fall into a more complicated cycle and fail to find a fixed point. More generically, it is believed that when DM fails to converge, it typically follows chaotic dynamics. Empirically, though, it is now clear that the DM dynamics can effectively solve a great variety of problems (e.g. graph coloring, solving diophantine equations, Sudoku, spin glass ground states, phase retrieval, random satisfiability, sphere packing, heteropolymer folding) that would be insoluble with the more naive alternating projections approach [59,61].

It is natural to wonder to what extent the DM equation (16) can be modified, to perhaps improve convergence; for example can that funny-looking 2 that defines how much one overshoots be changed into a parameter? It turns out the value 2 is a good choice: smaller values and you don't always escape from a trap, larger ones and you start shooting away at an exponentially growing rate, which can cause problems.

However, you might also notice that equation (16) does not treat the Divide and Concur projections symmetrically. What if we swap the roles of P_C and P_D? It turns out that works fine, typically about as well as the original version. So is there a parameterized version of DM that lets us move smoothly from the original version given by equation (16) to the version with P_C and P_D swapped? Such a parameterization has indeed been devised [4, 59]. For many problems a parameter value that gives a version of DM partway between the original and the swapped version, but still rather close to either the original or swapped version, works best [61].

14 DC as a Message-passing Algorithm

Nevertheless, the standard DM dynamics given by equation (16) has an important conceptual advantage—it makes it easier to see that DC is a message-passing algorithm closely analogous to BP [60]. Recall that each iteration of the standard DM dynamics can be interpreted as a three-step process: first overshoot, then concur, then correct.

The overshoot computation is done using the Divide projection at the constraint nodes. One can interpret the replica values before the overshoot as "messages" from the variable nodes to the factor nodes, and the resulting overshot values as messages from the factor nodes to the variable nodes.

The second step is to concur the overshot replica values, and make them equal at each variable node. This exactly parallels the BP step where one computes a belief at each variable from the incoming messages.

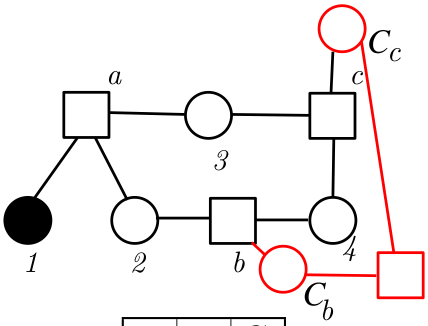
Finally, the third step is to correct the concurred replica values neighboring variable nodes by subtracting the original overshoot. This parallels the BP step (see equation (6)) where one computes the messages from variable nodes to factor nodes by subtracting the incoming message from the belief.

To summarize, although the details of the update rules are different, the DC overshot replica values correspond to BP messages from factor nodes to variable nodes, the DC concurred replica values correspond to BP beliefs, and the DC corrected replica values correspond to BP messages from variable nodes to factor nodes [60].

15 DC for Optimization

We have seen how to use DC to solve *constraint satisfaction* problems; now I will show that *optimization* problems can be converted into constraint satisfaction problems. In some cases, this is relatively easy; if we know some conditions on the optimum configuration (e.g. the stationarity conditions) we can impose those as constraints.

x_1	x_2	x_3	C_a
0	0	0	∞
0	0	1	0
0	1	0	0
0	1	1	∞
1	0	0	0
1	0	1	∞
1	1	0	∞
1	1	1	0



x_3	x_4	C_c
0	0	0.4
0	1	1.9
0	2	0.2
1	0	4.9
1	1	0.3
1	2	2.4

x_2	x_4	C_b
0	0	1.2
0	1	1.7
0	2	3.2
1	0	1.9
1	1	0.6
1	2	1.4

Fig. 20 A constraint graph derived from the factor graph shown in figure 2. The red circles represent new cost variable nodes corresponding to the soft cost functions in the original factor graph. The red square represents a global constraint on the maximum summed cost.

Another possibility, which may be less elegant but which is always available, is to introduce "cost variables" corresponding to the cost functions of a factor graph. Consider for example the *factor* graph that we first introduce in figure 2, and the *constraint* graph derived from it shown in figure 20. For each soft local cost, we introduce a new variable corresponding to that cost, and modify the soft factor into a corresponding hard constraint. For example, for the constraint b in the constraint graph illustrated, we require that if x_2 and x_4 equal 0, then the cost variable C_b must equal 1.2.

All the cost variables can then be tied together in a new global hard constraint, which says that the sum of the cost variables must be less than some desired maximum cost. If we like, we can continually tighten the desired maximum cost in an outer loop on the algorithm.

This technique, which can generally convert an optimization problem into a constraint satisfaction problem to which DC can be applied, has been used to develop DC decoders for LDPC codes [60,61], and DC algorithms that optimize heteropolymer energy functions [62].

16 Advantages and Disadvantages of DC Compared with BP

As an optimization or constraint satisfaction algorithm, DC presents several notable advantages compared with BP algorithms. First of all, as we have emphasized, DC has no difficulties dealing with continuous variables.

A second, less obvious, advantage is that DC, unlike BP, performs very well even when the hidden variables have no good "local evidence." BP algorithms often converge to a fixed point with non-informative beliefs in the absence of local evidence.

Consider, for example, the problem of packing hard spheres (or other geometrical objects) as densely as possible into a finite volume such as the interior of a cube, for which DC is the state-of-the-art algorithm [63]. Because there is no local evidence saying that any particular sphere should be in a particular part of the volume, if one applied BP the messages sent from variables representing sphere centers to the constraints would start off generally non-informative, simply "saying" that the cost of being anywhere in the cube was equal. Those messages would be a fixed point of the dynamics: the BP algorithm would get no traction. Even starting with random messages, a BP algorithm for this problem would nearly inevitably converge to non-informative messages. DC on the other hand, is forced to make a single guess for each message at all times. Even starting with some initial random guesses for the positions of the sphere centers, it gradually works its way to a solution that satisfies all the hard constraints.

A third advantage of DC is that it is much easier to introduce complicated hard constraints, as might naturally arise in computer vision or control problems.

A fourth advantage of DC is that it cannot be trapped at a fixed point that is not a solution of the problem. BP, on the other hand, can converge to non-solutions, such as the "trapping sets" that cause "error floors" in BP decoders of some LDPC codes [64]. DC LDPC decoders do not get stuck in traps, as we would expect, but unfortunately they often decode to codewords that are less likely than the transmitted codeword, a failure mode not seen in BP [60]. Working from the idea of combining the advantages of BP and DC, my colleagues Yige Wang, Stark Draper and I recently proposed a hybrid "difference-map BP" decoder that heuristically imports a difference-map dynamics into a min-sum BP decoder. Difference-map BP has proven to significantly improve error floor performance compared to standard BP decoders, and also turns out to be closely related to the "splitting" BP algorithm [60].

DC also has some disadvantages in comparison with BP. Most significantly, it fundamentally only tracks a single value for each variable, so it cannot compute marginal probabilities like the sum-product algorithm does, or properly account for a probabilistic weighted sum over states.

DC also is often somewhat slow in converging to a solution. A related issue is that the convergence rate of DC depends crucially on the metric chosen. Even if we restrict ourselves to the natural Euclidean metric, it is very important how one scales the different variables in a problem (e.g. for a particular problem, it matters significantly whether one measures distances for a particular variable in units of millimeters or kilometers, and costs in units of dollars or cents). Currently, the best way to scale variables in DC is somewhat of a mystery.

Finally, unlike many versions of BP, DC is *not* guaranteed to give correct answers for constraint graphs or factor graphs without cycles. It does, however, have its own set of guarantees, which we turn to next.

17 Justifications for and History of DC

Let's begin by considering when the alternating projections algorithm can be guaranteed to find a satisfying solution to a constraint satisfaction problem. Suppose that we have two constraints that we want to satisfy. In our case we consider the collection of Divide constraints to be one constraint, and the collection of Concur constraints to be the the other constraint. Each of the two constraints can be considered to be sets of points in some space (in our case consider that to be the space of replica vectors).

A set of points is defined to be *convex* if the segment of points connecting any two points in the set is also contained in the set. It turns out (see the monograph by Bauschke and Combettes [65] for a full mathematical treatment of the topics discussed in this section) that if two sets of points are convex, alternately projecting from a point in one set to the nearest point in the other is guaranteed to converge a point in the intersection of the two sets. In that case, the alternating projections algorithm is also known as the "Projections onto Convex Sets" algorithm. It follows that if the sets of replica vectors that satisfy the Divide and Concur constraints are each convex, than the alternating projections algorithm will converge to a solution.

Notice however that the alternating projections algorithm is only guaranteed to be weakly convergent—the algorithm sometimes bounces from one convex set to the other, getting ever closer to the intersection of the two sets, but never actually reaching it in a finite number of iterations. Think for example, of the case when the two convex sets are each a line that intersects at a point.

Just as for alternating projections, one can prove that the DM projection dynamics also always converges to the intersection of two convex sets, and in some cases (but not always) it accelerates convergence compared to alternating projections. In fact, for some cases where alternating projections converges only weakly, DM converges in a finite number of iterations. So for the problem of finding the intersection of two convex sets, the DM is a handy alternative algorithm to alternating projections: it also always converges to a solution, and sometimes is much faster.

It is easy to show that the set of replica values satisfying the Concur constraints is automatically convex. It is also true that an intersection of convex sets is convex, which means that if all the sets of replica values satisfying the local Divide constraints are convex, the overall Divide constraint is also convex.

Historically, the "difference-map" dynamics given by equation (16) were first investigated in 1956 by Douglas and Rachford [66] as an improved iterative method for solving partial differential equations, and extended into a projection operator splitting method by Lions and Mercier in 1979 [67]. The surprisingly successful application of the DM algorithm to the *non-convex* phase retrieval problem [69] sparked the more recent investigations into why DM dynamics should also be useful for non-convex problems [68], their application to many other problems [59], and finally the formulation of the DC algorithm [4], which makes clear that the approach can be applied to general constraint satisfaction and optimization problems, albeit without the guarantees that obtain when it is applied to convex problems.

To summarize, just as BP algorithms converge to exact solutions on tree factor graphs but still can give very useful results for problems defined on general graphs, the DC algorithm converges to exact solutions when the constraint solution sets are convex, but can still give very useful results for problems defined using general constraints.

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