DIFFUSION METHODS FOR CLASSIFICATION WITH PAIRWISE RELATIONSHIPS

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Abstract. We define two algorithms for propagating information in classification problems with pairwise relationships. The algorithms are based on contraction maps and are related to non-linear diffusion and random walks on graphs. The approach is also related to message passing algorithms, including belief propagation and mean field methods. The algorithms we describe are guaranteed to converge on graphs with arbitrary topology. Moreover they always converge to a unique fixed point, independent of initialization. We prove that the fixed points of the algorithms under consideration define lower bounds on the energy function and the max-marginals of a Markov random field. The theoretical results also illustrate a relationship between message passing algorithms and value iteration for an infinite horizon Markov decision process. We illustrate the practical application of the algorithms under study with numerical experiments in image restoration and stereo depth estimation.

1. Introduction. In many classification problems there are relationships among a set of items to be classified. For example, in image reconstruction problems adjacent pixels are likely to belong to the same object or image segment. This leads to relationships between the labels of different pixels in an image. Energy minimization methods based on Markov random fields (MRF) address these problems in a common framework [3,14,21]. Within this framework we introduce two new algorithms for classification with pairwise information. These algorithms are based on contraction maps and are related to non-linear diffusion and random walks on graphs.

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The setting under consideration is as follows. Let G = (V, E) be an undirected simple graph and let L be a set of labels. A labeling of V is a function $x : V \to L$ assigning a label from L to each vertex in V. Local information is modeled by a cost $g_i(a)$ for assigning label a to vertex i. Information on label compatibility for neighboring vertices is modeled by a cost $h_{ij}(a, b)$ for assigning label a to vertex i and label b to vertex j. The cost for a labeling x is defined by an energy function,

$$F(x) = \sum_{i \in V} g_i(x_i) + \sum_{\{i,j\} \in E} h_{ij}(x_i, x_j).$$
(1)

In the context of MRFs the energy function defines a Gibbs distribution on random variables X associated with the vertices V,

$$p(X = x) = \frac{1}{Z} \exp(-F(x)).$$
 (2)

Minimizing the energy F(x) corresponds to maximizing p(X = x). This approach has been applied to a variety of problems in image processing and computer vision [10]. A classical example involves restoring corrupted images [4,11]. In image restoration there is a grid of pixels and the problem is to estimate an intensity value for each pixel. To restore an image I one looks for an image J that is similar to I and is smooth almost everywhere. Similarity between I and J is defined by local costs at each pixel. The smoothness constraint is defined by pairwise costs between neighboring pixels in J.

1.1. Basic definitions and overview of results. Let G = (V, E) be an undirected, simple, connected graph, with more than one vertex. For simplicity let $V = \{1, \ldots, n\}$. Let N(i) and d(i) denote, respectively, the set of neighbors and the degree of vertex i,

$$N(i) = \{ j \in V \mid \{i, j\} \in E \}, \quad d(i) = |N(i)|$$

Let L be a set of labels. For each vertex $i \in V$ we have a non-negative cost for assigning label a to vertex i, denoted by $g_i(a)$. These costs capture local information about the label of each vertex. For each edge $\{i, j\} \in E$ we have a non-negative cost for assigning label a to vertex i and label b to vertex j, denoted equally by $h_{ij}(a, b)$ or $h_{ji}(b, a)$. These costs capture relationships between labels of neighboring vertices.

 $g_i: L \to [0, \infty)$ for $i \in V$;

 $h_{ij}, h_{ji}: L^2 \to [0, \infty)$ for $\{i, j\} \in E$ with $h_{ij}(a, b) = h_{ji}(b, a)$.

Let $x \in L^V$ denote a labeling of V with labels from L. A cost for x that takes into account both local information at each vertex and the pairwise relationships can be defined by an energy function $F: L^V \to \mathbb{R}$,

$$F(x) = \sum_{i \in V} g_i(x_i) + \sum_{\{i,j\} \in E} h_{ij}(x_i, x_j).$$
(3)

This leads to a natural optimization problem where we look for a labeling x with minimum energy.

Throughout the paper we assume L is finite. The optimization problem defined by F is NP-hard even when |L| = 2 as it can be used to solve the independent set problem on G. It can also be used to solve coloring with k colors when |L| = k. The optimization problem can be solved in polynomial time using dynamic programming when G is a tree

[1]. More generally dynamic programming leads to polynomial optimization algorithms when the graph G is chordal (triangulated) and has bounded tree-width.

Min-sum (max-product) belief propagation [14,21] is a local message passing algorithm that is equivalent to dynamic programming when G is a tree. Both dynamic programming and belief propagation aggregate local costs by sequential propagation of information along the edges in E.

For $i \in V$ we define the value function $f_i : L \to \mathbb{R}$,

$$f_i(\tau) = \min_{\substack{x \in L^V \\ x_i = \tau}} F(x).$$
(4)

In the context of MRFs the value functions are also known as *max-marginals*. The value functions are also what is computed by the dynamic programming and belief propagation algorithms for minimizing F when G is a tree. Each value function defines a cost for assigning a label to a vertex that takes into account the whole graph. If x^* minimizes F(x), then x_i^* minimizes $f_i(\tau)$, and when $f_i(\tau)$ has a unique minimum we can minimize F(x) by selecting

$$x_i^* = \operatorname{argmin} f_i(\tau). \tag{5}$$

A local belief is a function $\gamma: L \to \mathbb{R}$. A field of beliefs specifies a local belief for each vertex in V, and is an element of

$$(\mathbb{R}^L)^V = \{ \varphi = (\varphi_1, \dots, \varphi_N) \mid \varphi_i : L \to \mathbb{R} \}.$$
(6)

We define two algorithms in terms of maps,

$$T: (\mathbb{R}^L)^V \to (\mathbb{R}^L)^V,$$
$$S: (\mathbb{R}^L)^V \to (\mathbb{R}^L)^V.$$

The maps T and S are closely related. Both maps are contractions, but each of them has its own unique fixed point. Each of these maps can be used to define an algorithm to optimize F(x) based on fixed point iterations and local decisions.

For $z \in \{T, S\}$ we start from an initial field of beliefs φ^0 and sequentially compute

$$\varphi^{k+1} = z(\varphi^k).$$

Both $S^k(\varphi^0)$ and $T^k(\varphi^0)$ converge to the unique fixed points of S and T, respectively. After convergence to a fixed point φ (or a bounded number of iterations in practice) we select a labeling x by selecting the label minimizing the belief at each vertex (breaking ties arbitrarily),

$$x_i = \operatorname*{argmin}_{\tau} \varphi_i(\tau). \tag{7}$$

The algorithms we consider depend on parameters $p \in (0, 1)$, q = 1 - p and weights $w_{ij} \in [0, 1]$ for each $i \in V$ and $j \in N(i)$. The weights from each vertex are constrained to sum to one,

$$\sum_{\in N(i)} w_{ij} = 1 \qquad \forall i \in V.$$
(8)

These weights can be interpreted in terms of transition probabilities for a random walk on G. In a uniform random walk we have $w_{ij} = 1/d(i)$. Non-uniform weights can be

used to capture additional information about an underlying application. For example, in the case of stereo depth estimation (Section 5.2) we have used non-uniform weights that reflect color similarity between neighboring pixels. We note, however, that while we may interpret the results of the fixed point algorithms in terms of transition probabilities in a random walk, the algorithms we study are deterministic.

The maps S and T we consider are defined as follows.

Definition 1.1.

$$(T\varphi)_i(\tau) = pg_i(\tau) + \sum_{j \in N(i)} \min_{u_j \in L} \frac{p}{2} h_{ij}(\tau, u_j) + qw_{ji}\varphi_j(u_j),$$
(9)

$$(S\varphi)_i(\tau) = pg_i(\tau) + \sum_{j \in N(i)} w_{ij} \min_{u_j \in L} ph_{ij}(\tau, u_j) + q\varphi_j(u_j).$$
(10)

The map defined by T corresponds to a form of non-linear diffusion of beliefs along the edges of G. The map defined by S corresponds to value iteration for a Markov decision process (MDP) [2] defined by random walks on G. We show that both S and T are contractions. Let $\bar{\varphi}$ be the fixed point of T and let $\hat{\varphi}$ be the fixed point of S. We show $\bar{\varphi}$ defines a lower bound on the energy function F, and that $\hat{\varphi}$ defines lower bounds on the value functions f_i ,

$$\sum_{i \in V} \bar{\varphi}_i(x_i) \le F(x) \qquad \forall x \in L^V, \tag{11}$$

$$\hat{\varphi}_i(\tau) \le f_i(\tau) \qquad \forall i \in V, \ \tau \in L.$$
 (12)

In Section 3 we study the fixed point iteration algorithm defined by T and the relationship between $\bar{\varphi}$ and F. To the extent that $\sum_{i \in V} \bar{\varphi}_i(x_i)$ approximates F(x) this justifies selecting a labeling x by minimizing $\bar{\varphi}_i$ at each vertex. This approach is related to mean field methods and variational inference with the Gibbs distribution p(X = x)[14,21].

In Section 4 we study the algorithm defined by S and the relationship between $\hat{\varphi}_i$ and f_i . To the extent that $\hat{\varphi}_i(\tau)$ approximates $f_i(\tau)$ this justifies selecting a labeling x by minimizing $\hat{\varphi}_i$ at each vertex. We also show a connection between the fixed point $\hat{\varphi}$ and optimal policies of a Markov decision process. The process is defined in terms of random walks on G, with transition probabilities given by the weights w_{ij} .

1.2. Examples. Figure 1 shows two examples of fixed points of T when the graph G = (V, E) is a cycle with 5 vertices. In this case we have a binary labeling problem $L = \{1, 2\}$. The local costs are all zero except that vertex 1 has a preference for label 2. This is encoded by a cost for label 1,

$$g_1(1) = 1, (13)$$

$$g_1(2) = 0,$$
 (14)

$$g_i(a) = 0 \qquad \forall i \neq 1, \ a \in L.$$
(15)

In Figure 1(a) we have pairwise costs that encourage equal labels for neighboring vertices,

$$h_{ij}(a,b) = \begin{cases} 0, & a = b, \\ 1, & a \neq b. \end{cases}$$
(16)



FIG. 1. The fixed points of T on two problems defined on the graph above. In this case $L = \{1, 2\}$. In both cases the local costs g_i are all zero except for vertex 1 who has a preference towards label 2. In (a) the pairwise costs encourage neighboring vertices to take the same label. In (b) the pairwise costs encourage neighboring vertices to take different labels.

In Figure 1(b) we have pairwise costs that encourage different labels for neighboring vertices,

$$h_{ij}(a,b) = \begin{cases} 1, & a = b, \\ 0, & a \neq b. \end{cases}$$
(17)

Figure 1 shows a graphical representation of the local costs for each vertex, and the value of $\bar{\varphi}$, the fixed point of T, on each example. In Figure 1(a) local selection of x_i minimizing $\bar{\varphi}_i$ leads to x = (2, 2, 2, 2, 2, 2). In Figure 1(b) local selection of x_i minimizing $\bar{\varphi}_i$ leads to x = (2, 1, 2, 2, 1). In both examples the resulting labeling x is the global minimum of F(x). For these examples we used p = 0.1 and $w_{ij} = 1/d(i)$.

Of course in general local minimization of $\bar{\varphi}$ does not lead to a labeling minimizing F(x) and it would be interesting to characterize when this happens.

1.3. Related work. For general graphs G, when the pairwise costs $h_{ij}(a, b)$ define a metric over L there are polynomial time approximation algorithms for the optimization problem defined by F [13]. In some important cases the optimization problem can be solved using graph cuts and maximum flow algorithms [6, 7, 12, 15]. This includes in particular the case of MAP estimation for an Ising model with an external field [12].

The algorithms we study are closely related to message passing methods, in particular to min-sum (or equivalently max-product) belief propagation (BP) [14,21]. When

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the graph G is a tree, BP converges and solves the optimization problem defined by F. Unfortunately BP is not guaranteed to converge and it can have multiple fixed points for general graphs. Some form of dampening can help BP converge in practice. The algorithms we study provide a simple alternative to min-sum belief propagation that is guaranteed to converge to a unique fixed point, regardless of initialization. The algorithms are also guaranteed to converge "quickly".

One approach for solving the optimization problem defined by F involves using a linear program (LP) relaxation. The optimization problem can be posed using an LP with a large number of constraints and relaxed to obtain a tractable LP over the *local polytope* [20]. Several message passing methods have been motivated in terms of this LP [17]. There are also recent methods which use message passing in the inner loop of an algorithm that converges to the optimal solution of the local polytope LP relaxation [18,19]. In Section 3.1 we characterize the fixed point of S using a different LP.

The mean-field algorithm [14, 21] is an iterative method for approximating the Gibbs distribution p(x) by a factored distribution q(x),

$$q(x) = \prod_{i \in V} q_i(x_i).$$
(18)

The mean-field approach involves minimization of the KL divergence between p and q using fixed point iterations that repeatedly update the factors q_i defining q. A drawback of the approach is that the fixed point is not unique and the method is sensitive to initialization.

The algorithm defined by T is related to the mean-field method in the sense that the fixed points of T appear to approximate F(x) by a function H(x) that is a sum of local terms,

$$H(x) = \sum_{i \in V} \bar{\varphi}_i(x_i).$$
(19)

We do not know, however, if there is a measure under which the resulting H(x) is an optimal approximation to F(x) within the class of functions defined by a sum of local terms.

2. Preliminaries. The algorithms we study are efficient in the following sense. Let m = |E| and k = |L|. Each iteration in the fixed point algorithm involves evaluating T or S. This can be done in $O(mk^2)$ by "brute-force" evaluation of the expressions in Definition 1.1. In many applications, including in image restoration and stereo matching, the pairwise cost h_{ij} has special structure that allows for faster computation using the techniques described in [9]. This leads to an O(mk) algorithm for each iteration of the fixed point methods. Additionally, the algorithms are easily parallelizable.

The fixed point algorithms defined by T and S converge quickly because the maps are contractions in $(\mathbb{R}^L)^V$.

Let $z: \mathbb{R}^K \to \mathbb{R}^K$ and ||x|| be a norm in \mathbb{R}^K . For $\gamma \in (0,1)$, z is a γ -contraction if

$$||z(x) - z(y)|| \le \gamma ||x - y||.$$
(20)

When z is a contraction it has a unique fixed point \bar{x} . It also follows directly from the contraction property that fixed point iteration $x_k = z(x_{k-1})$ converges to \bar{x} quickly,

$$\|x_k - \bar{x}\| \le \gamma^k \|x_0 - \bar{x}\|.$$
(21)

The weights w_{ij} in the definition of T and S define a random process that generates random walks on G. We have a Markov chain with state space V. Starting from a vertex Q_0 we generate an infinite sequence of random vertices (Q_0, Q_1, \ldots) with transition probabilities

$$p(Q_{t+1} = j | Q_t = i) = w_{ij}.$$
(22)

A natural choice for the weights is $w_{ij} = 1/d(i)$, corresponding to moving from *i* to *j* with uniform probability over N(i). This choice leads to uniform random walks on *G* [16].

We consider in $(\mathbb{R}^L)^V$ the partial order

$$\varphi \le \psi \iff \varphi_i(\tau) \le \psi_i(\tau) \quad \forall i \in V \; \forall \tau \in L.$$
(23)

It follows trivially from the definitions of T and S that both maps preserve order in $(\mathbb{R}^L)^V$,

$$\varphi \le \psi \Rightarrow T\varphi \le T\psi, \ S\varphi \le S\psi.$$
(24)

We claim that for any $\alpha \in \mathbb{R}^V$,

$$\sum_{i \in V} \sum_{j \in N(i)} w_{ji} \alpha_j = \sum_{j \in V} \alpha_j.$$
(25)

This follows from re-ordering the double summation and the constraints that the weights out of each vertex sum to one,

$$\sum_{i \in V} \sum_{j \in N(i)} w_{ji} \alpha_j = \sum_{j \in V} \sum_{i \in N(j)} w_{ji} \alpha_j = \sum_{j \in V} \alpha_j.$$

We note that the algorithms defined by T and S are related in the following sense. For a regular graph with degree d, if we let $w_{ij} = 1/d$ the maps T and S are equivalent up to rescaling if the costs in T and S are rescaled appropriately.

3. Algorithm defined by T (Diffusion). In this section we study the fixed point algorithm defined by T. We show that T is a contraction in $(\mathbb{R}^L)^V$ and that the fixed point of T defines a "factored" lower bound on F.

We start by showing that T is a contraction with respect to the norm on $(\mathbb{R}^L)^V$ defined by

$$\|\varphi\|_{\infty,1} = \sum_{i \in V} \|\varphi_i\|_{\infty}.$$
(26)

LEMMA 3.1 (Contraction). For any $\varphi, \psi \in (\mathbb{R}^L)^V$

$$\|(T\varphi)_i - (T\psi)_i\|_{\infty} \le q \sum_{j \in N(i)} w_{ji} \|\varphi_j - \psi_j\|_{\infty} \qquad \forall i \in V,$$
(27)

$$\|(T\varphi) - (T\psi)\|_{\infty,1} \le q \|\varphi - \psi\|_{\infty,1}.$$
(28)

Proof. Take $i \in V$ and $\tau \in L$. For any $x \in L^V$

$$\begin{aligned} (T\varphi)_{i}(\tau) &= pg_{i}(\tau) + \sum_{j \in N(i)} \min_{u_{j} \in L} \frac{p}{2} h_{ij}(\tau, u_{j}) + qw_{ji}\varphi_{j}(u_{j}) \\ &\leq pg_{i}(\tau) + \sum_{j \in N(i)} \frac{p}{2} h_{ij}(\tau, x_{j}) + qw_{ji}\varphi_{j}(x_{j}) \\ &\leq pg_{i}(\tau) + \sum_{j \in N(i)} \frac{p}{2} h_{ij}(\tau, x_{j}) + qw_{ji}(\psi_{j}(x_{j}) + |\varphi_{j}(x_{j}) - \psi_{j}(x_{j})|) \\ &\leq pg_{i}(\tau) + \sum_{j \in N(i)} \frac{p}{2} h_{ij}(\tau, x_{j}) + qw_{ji}(\psi_{j}(x_{j}) + \|\varphi_{j} - \psi_{j}\|_{\infty}). \end{aligned}$$

Since the inequality defined by the first and last terms above holds for any x, it holds when x minimizes the last term. Therefore

$$(T\varphi)_i(\tau) \le (T\psi)_i(\tau) + q \sum_{j \in N(i)} w_{ji} \|\varphi_j - \psi_j\|_{\infty}.$$

Since this inequality holds interchanging φ with ψ we have

$$|(T\varphi)_i(\tau) - (T\psi)_i(\tau)| \le q \sum_{j \in N(i)} w_{ji} \|\varphi_j - \psi_j\|_{\infty}.$$

Taking the τ maximizing the left hand side proves (27). To prove (28), we sum the inequalities (27) for all $i \in V$ and use (25).

The contraction property above implies the fixed point algorithm defined by T converges to a unique fixed point independent on initialization. It also implies the distance to the fixed point decreases quickly, and we can bound the distance to the fixed point using either the initial distance to the fixed point or the distance between consecutive iterates (a readily available measure).

THEOREM 3.2. The map T has a unique fixed point $\bar{\varphi}$ and for any $\varphi \in (\mathbb{R}^L)^V$ and integer $k \geq 0$,

$$\|\bar{\varphi} - T^k \varphi\|_{\infty,1} \le q^k \|\bar{\varphi} - \varphi\|_{\infty,1},\tag{29}$$

$$\|\bar{\varphi} - \varphi\|_{\infty,1} \le \frac{1}{p} \|T\varphi - \varphi\|_{\infty,1}.$$
(30)

Proof. Existence and uniqueness of the fixed point, as well as the first inequality follows trivially from Lemma 3.1. To prove the second inequality observe that since $T^k \varphi$ converges to $\bar{\varphi}$,

$$\|\bar{\varphi}-\varphi\|_{\infty,1} \le \sum_{k=0}^{\infty} \|T^{k+1}\varphi - T^k\varphi\|_{\infty,1} \le \sum_{k=0}^{\infty} q^k \|T\varphi - \varphi\|_{\infty,1}.$$
 (31)

Now note that since $p \in (0, 1)$ and p + q = 1,

$$\sum_{k=0}^{\infty} q^k p = 1 \implies \sum_{k=0}^{\infty} q^k = \frac{1}{p}.$$
(32)

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The map T and the energy function F are related as follows.

Proposition 3.3. For any $\varphi \in (\mathbb{R}^L)^V$ and $x \in L^V$

$$\sum_{i \in V} (T\varphi)_i(x_i) \le pF(x) + q \sum_{i \in V} \varphi_i(x_i).$$
(33)

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Proof. Direct use of the definition of T yields

$$\begin{split} \sum_{i \in V} (T\varphi)_i(x_i) &= \sum_{i \in V} pg_i(x_i) + \sum_{j \in N(i)} \min_{\substack{u_j \in L}} \frac{p}{2} h_{ij}(x_i, u_j) + qw_{ji}\varphi_j(u_j) \\ &\leq \sum_{i \in V} pg_i(x_i) + \sum_{j \in N(i)} \frac{p}{2} h_{ij}(x_i, x_j) + qw_{ji}\varphi_j(x_j) \\ &= p\left(\sum_{i \in V} g_i(x_i) + \sum_{i \in V} \sum_{j \in N(i)} \frac{1}{2} h_{ij}(x_i, x_j)\right) + q \sum_{i \in V} \sum_{j \in N(i)} w_{ji}\varphi_j(x_j) \\ &= pF(x) + q \sum_{j \in V} \varphi_j(x_j), \end{split}$$

where the last equality follows from the fact that $h_{ij}(x_i, x_j) = h_{ji}(x_j, x_i)$ and equation (25).

Now we show the fixed point of T defines a lower bound on F in terms of a sum of local terms.

THEOREM 3.4. Let $\bar{\varphi}$ be the fixed point of T and

$$H(x) = \sum_{i \in V} \bar{\varphi}_i(x_i).$$

Then $0 \leq \bar{\varphi}$ and $H(x) \leq F(x)$.

Proof. The fact that $H(x) \leq F(x)$ follows directly from Proposition 3.3.

To prove $0 \leq \bar{\varphi}$ consider the sequence $(0, T0, T^20, \ldots)$. The non-negativity of g_i and h_{ij} implies $0 \leq T0$. Since T is order preserving (24) it follows by induction that $T^k 0 \leq T^{k+1}0$ for all $k \geq 0$. Since the sequence is pointwise non-decreasing and converges to $\bar{\varphi}$ we have $0 \leq \bar{\varphi}$.

Theorem 3.4 allows us to compute both a lower and an upper bound on the optimal value of F, together with a solution where F attains the upper bound.

COROLLARY 3.5. Let $\bar{\varphi}$ be the fixed point of T and

$$\bar{x}_i = \operatorname{argmin} \bar{\varphi}_i(\tau) \ \forall i \in V;$$

then for any x^* minimizing F,

$$\sum_{i \in V} \bar{\varphi}_i(\bar{x}_i) \le F(x^*) \le F(\bar{x}).$$

Proof. If x^* is a minimizer of F, then the inequality $F(x^*) \leq F(\bar{x})$ holds trivially. We can use the definition of \bar{x} to conclude that

$$\sum_{i \in V} \bar{\varphi}_i(\bar{x}_i) \le \sum_{i \in V} \bar{\varphi}_i(x_i^*) \le F(x^*),$$

where the second inequality follows from Theorem 3.4.

3.1. Linear programming formulation. Here we provide an LP characterizing for the fixed point of T. We note that the LP formulation described here is different from the standard LP relaxation for minimizing F(x) which involves the local polytope described in [20].

Consider the following LP which depends on a vector of coefficients a in $(\mathbb{R}^L)^V$,

$$\max_{\varphi} a^{T} \varphi$$
$$\varphi_{i}(u_{i}) \leq pg_{i}(u_{i}) + \sum_{j \in N(i)} \frac{p}{2} h_{ij}(u_{i}, u_{j}) + qw_{ji}\varphi_{j}(u_{j}) \qquad \forall i \in V, \forall u \in L^{V}.$$

Note that the constraints in the LP are equivalent to $\varphi \leq T\varphi$. Next we show that this LP has a unique solution which equals the fixed point of T whenever every coefficient is positive, independent of their specific values. For example, $\bar{\varphi}$ is the optimal solution when a is the vector of ones.

THEOREM 3.6. If a is a non-negative vector the fixed point of T is an optimal solution for the LP. If a is a positive vector the fixed point of T is the unique optimal solution for the LP.

Proof. Let $\bar{\varphi}$ be the fixed point of T. First note that $\bar{\varphi}$ is a feasible solution since $\bar{\varphi} \leq T\bar{\varphi}$.

Let $\varphi \in (\mathbb{R}^L)^V$ be any feasible solution for the LP. The linear constraints are equivalent to $\varphi \leq T\varphi$. Since T preserves order it follows by induction that $T^k\varphi \leq T^{k+1}\varphi$ for all $k \geq 0$. Since the sequence $(\varphi, T\varphi, T^2\varphi, \ldots)$ converges to $\bar{\varphi}$ and it is pointwise nondecreasing we conclude $\varphi \leq \bar{\varphi}$.

If a is non-negative we have $a^T \varphi \leq a^T \bar{\varphi}$ and therefore $\bar{\varphi}$ must be an optimal solution for the LP. If a is positive and $\varphi \neq \bar{\varphi}$ we have $a^T \varphi < a^T \bar{\varphi}$. This proves the fixed point is the unique optimal solution for the LP.

4. Algorithm defined by S (Optimal control). In this section we study the algorithm defined by S. We start by showing that S corresponds to value iteration for an infinite horizon discounted Markov decision process (MDP) [2].

An infinite horizon discounted MDP is defined by a tuple (Q, A, c, t, γ) where Q is a set of states, A is a set of actions, and γ is a discount factor in \mathbb{R} . The cost function $c: Q \times A \to \mathbb{R}$ specifies a cost c(s, a) for taking action a on state s. The transition probabilities $t: Q \times A \times Q \to \mathbb{R}$ specify the probability t(s, a, s') of moving to state s' if we take action a in state s.

Let o be an infinite sequence of state and action pairs, $o = ((s_1, a_1), (s_2, a_2), \ldots) \in (Q \times A)^{\infty}$. The (discounted) cost of o is

$$c(o) = \sum_{k=0}^{\infty} \gamma^k c(s_k, a_k).$$
(34)

A policy for the MDP is defined by a map $\pi : Q \to A$, specifying an action to be taken at each state. The value of a state s under the policy π is the expected cost of an infinite sequence of state and action pairs generated using π starting at s,

$$v_{\pi}(s) = E[c(o)|\pi, s_1 = s].$$
(35)

An optimal policy π^* minimizes $v_{\pi}(s)$ for every starting state. Value iteration computes v_{π^*} as the fixed point of $\mathcal{L} : \mathbb{R}^Q \to \mathbb{R}^Q$,

$$(\mathcal{L}v)(s) = \min_{a \in A} c(s, a) + \gamma \sum_{s' \in Q} t(s, a, s')v(s').$$

$$(36)$$

The map \mathcal{L} is known to be a γ -contraction [2] with respect to the $\|\cdot\|_{\infty}$ norm.

Now we show that S is equivalent to value iteration for an MDP defined by random walks on G. Intuitively we have states defined by a vertex $i \in V$ and a label $a \in L$. An action involves selecting a different label for each possible next vertex, and the next vertex is selected according to a random walk defined by the weights w_{ij} .

LEMMA 4.1. Define an MDP (Q, A, c, t, γ) as follows. The states are pairs of vertices and labels $Q = V \times L$. The actions specify a label for every possible next vertex $A = L^V$. The discount factor is $\gamma = q$. The transition probabilities and cost function are defined by

$$t((i,\tau), u, (j,\tau')) = \begin{cases} w_{ij}, & j \in N(i), \ \tau' = u_j, \\ 0 & \text{otherwise}, \end{cases}$$
(37)

$$c((i,\tau),u) = pg_i(\tau) + \sum_{j \in N(i)} pw_{ij}h_{ij}(\tau, u_j).$$
(38)

The map S is equivalent to value iteration for this MDP. That is, if $\varphi_i(\tau) = v((i, \tau))$, then

$$(S\varphi)_i(\tau) = (\mathcal{L}v)((i,\tau)).$$

Proof. The result follows directly from the definition of the MDP, \mathcal{L} and S.

$$(\mathcal{L}v)((i,\tau)) = \min_{u \in L^V} c((i,\tau), u) + \gamma \sum_{(j,\tau') \in Q} t((i,\tau), u, (j,\tau'))v(j,\tau')$$
(39)

$$= \min_{u \in L^{V}} pg_{i}(\tau) + \sum_{j \in N(i)} pw_{ij}h_{ij}(\tau, u_{j}) + q \sum_{j \in N(i)} w_{ij}v(j, u_{j})$$
(40)

$$= pg_i(\tau) + \sum_{j \in N(i)} w_{ij} \min_{u_j \in L} ph_{ij}(\tau, u_j) + qv(j, u_j)$$
(41)

$$= (S\varphi)_i(\tau). \tag{42}$$

The relationship to value iteration shows S is a contraction and we have the following results regarding fixed point iterations with S.

THEOREM 4.2. The map S has a unique fixed point $\hat{\varphi}$ and for any $\varphi \in (\mathbb{R}^L)^V$ and integer $k \ge 0$,

$$\|\hat{\varphi} - S^k \varphi\|_{\infty} \le q^k \|\hat{\varphi} - \varphi\|_{\infty},\tag{43}$$

$$\|\hat{\varphi} - \varphi\|_{\infty} \le \frac{1}{p} \|S\varphi - \varphi\|_{\infty}.$$
(44)

Proof. The first inequality follows directly from Lemma 4.1 and the fact that \mathcal{L} is a γ -contraction with $\gamma = q$. The proof of the second inequality is similar to the proof of the analogous result for the map T in Theorem 3.2.

4.1. Random walks. The formalism of MDPs is quite general, and encompasses the fixed point algorithm defined by S. In this section we further analyze this fixed point algorithm and provide an interpretation using one-dimensional problems defined by random walks on G.

The weights w_{ij} define a random process that generates infinite walks on G. Starting from some vertex in V we repeatedly move to a neighboring vertex, and the probability of moving from $i \in V$ to $j \in N(i)$ in one step is given by w_{ij} .

An infinite walk $\omega = (\omega_1, \omega_2, \ldots) \in V^{\infty}$ can be used to define an energy on an infinite sequence of labels $z = (z_1, z_2, \ldots) \in L^{\infty}$,

$$F_{\omega}(z) = \sum_{t=0}^{\infty} pq^{t} g_{\omega_{t}}(z_{t}) + pq^{t} h_{\omega_{t}\omega_{t+1}}(z_{t}, z_{t+1}).$$
(45)

The energy $F_{\omega}(z)$ can be seen as the energy of a pairwise classification problem on a graph G' = (V', E') that is an infinite path,

$$V' = \{1, 2, \ldots\},\tag{46}$$

$$E' = \{\{1, 2\}, \{2, 3\}, \ldots\}.$$
(47)

The graph G' can be interpreted as a one-dimensional "unwrapping" of G along the walk ω . This unwrapping defines a map from vertices in the path G' to vertices in G.

Consider a policy $\pi: V \times L \times V \to L$ that specifies z_{k+1} in terms of ω_k, z_k and ω_{k+1} ,

$$z_{k+1} = \pi(\omega_k, z_k, \omega_{k+1}).$$
(48)

Now consider the expected value of $F_{\omega}(z)$ when ω is a random walk starting at $i \in V$ and z is a sequence of labels defined by the policy π starting with $z_1 = \tau$,

$$v_{\pi}(i,\tau) = E[F_{\omega}(z)|\omega_1 = i, z_1 = \tau, z_{k+1} = \pi(\omega_k, z_k, \omega_{k+1})].$$
(49)

There is an optimal policy π^* that minimizes $v_{\pi}(i,\tau)$ for every $i \in V$ and $\tau \in L$. Let $\hat{\varphi}$ be the fixed point of S. Then $\hat{\varphi}_i(\tau) = v_{\pi^*}(i,\tau)$. This follows directly from the connection between S and the MDP described in the last section.

4.2. Bounding the value functions of F. Now we show that $\hat{\varphi}$ defines lower bounds on the value functions (max-marginals) f_i defined in (4). We start by showing that f_i can be lower bounded by f_j for $j \in N(i)$.

PROPOSITION 4.3. Let $i \in V$ and $j \in N(i)$. Then

$$f_i(u_i) \ge pg_i(u_i) + \min_{u_j} ph_{ij}(u_i, u_j) + qf_j(u_j),$$
(50)

$$f_i(u_i) \ge pg_i(u_i) + \sum_{j \in N(i)} w_{ij} \min_{u_j} ph_{ij}(u_i, u_j) + qf_j(u_j).$$
(51)

Proof. The second inequality follows from the first one by taking a convex combination over $j \in N(i)$. To prove the first inequality note that,

$$f_i(u_i) = \min_{\substack{x \in L^V \\ x = -u_i}} F(x) \tag{52}$$

$$= \min_{u_j \in L} \min_{\substack{x \in L^V\\x_i=u_i, x_j=u_j}} F(x)$$
(53)

$$= \min_{u_j \in L} \min_{\substack{x \in L^V\\x_i=u_i, x_j=u_j}} pF(x) + qF(x)$$
(54)

$$\geq pg_i(u_i) + \min_{u_j \in L} ph_{ij}(u_i, u_j) + \min_{\substack{x \in L^V \\ x_i = u_i, x_j = u_j}} qF(x)$$
(55)

$$\geq pg_i(x_i) + \min_{u_j \in L} ph_{ij}(u_i, u_j) + \min_{\substack{x \in L^V\\ x_i = u_i}} qF(x)$$
(56)

$$= pg_i(x_i) + \min_{u_j \in L} ph_{ij}(u_i, u_j) + qf_j(u_j).$$
(57)

The first inequality above follows from $F(x) \ge g_i(x_i) + h_{ij}(x_i, x_j)$ since all the terms in F(x) are non-negative. The second inequality follows from the fact that we are minimizing F(x) over x with fewer restrictions.

The map S and the value functions are related as follows.

PROPOSITION 4.4. Let $f = (f_1, \ldots, f_N) \in (\mathbb{R}^L)^V$ be a field of beliefs defined by the value functions

$$Sf \le f.$$
 (58)

Proof. The result follows directly from Proposition 4.3. \Box Now we show that the fixed point of S defines lower bounds on the value functions.

THEOREM 4.5. Let $\hat{\varphi}$ be the fixed point of S. Then

$$0 \le \hat{\varphi}_i(\tau) \le f_i(\tau).$$

Proof. Since the costs g_i and h_{ij} are non-negative we have $0 \leq S0$. Using the fact that S preserves order we can conclude $0 \leq \hat{\varphi}$.

Since $Sf \leq f$ and S preserves order, $S^k f \leq f$ for all k. To end the proof, take the limit $k \to \infty$ at the left hand side of this inequality.

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5. Numerical experiments. In this section we illustrate the practical feasibility of the proposed algorithms with preliminary experiments in computer vision problems.

5.1. Image restoration. The goal of image restoration is to estimate a clean image z from a noisy, or corrupted, version y. A classical approach to solve this problem involves looking for a piecewise smooth image x that is similar to y [5,11]. In the weak membrane model [5] the local costs $g_i(a)$ penalize differences between x and y while the pairwise costs $h_{ij}(a,b)$ penalize differences between neighboring pixels in x. In this setting, the graph G = (V, E) is a grid in which the vertices V correspond to pixels and the edges E connect neighboring pixels. The labels L are possible pixel values and a labeling x defines an image. For our experiments we use $L = \{0, \ldots, 255\}$ corresponding to the possible values in an 8-bit image.

To restore y we define the energy F(x) using

$$g_i(x_i) = (y_i - x_i)^2;$$
 (59)

$$h_{ij}(x_i, x_j) = \lambda \min((x_i - x_j)^2, \tau).$$
 (60)

The local cost $g_i(x_i)$ encourages x_i to be similar to y_i . The pairwise costs depend on two parameters $\lambda, \tau \in \mathbb{R}$. The cost $h_{ij}(x_i, x_j)$ encourages x_i to be similar to x_j but also allows for large differences since the cost is bounded by τ . The value of λ controls the relative weight of the local and pairwise costs. Small values of λ lead to images x that are very similar to the noisy image y, while large values of λ lead to images x that are smoother.

Figure 2 shows an example result of image restoration using the algorithm defined by T. The example illustrates the algorithm is able to recover a clean image that is smooth almost everywhere while at the same time preserving sharp discontinuities at the boundaries of objects. For comparison we also show the results of belief propagation. In this example the noisy image y was obtained from a clean image z by adding independent noise to each pixel using a Gaussian distribution with standard deviation $\sigma = 20$. The



Original Image

Noisy Image

Output of TRMS error = 8.9 Energy = 1519837

Output of BP RMS error = 10.7Energy = 650296

FIG. 2. Image restoration using the fixed point algorithm defined by T and BP. The algorithms were run for 100 iterations.

TABLE 1. Results of restoration using T, S and belief propagation (BP). The goal of restoration is to recover the original image z. We show the energy of the restored image x and the root mean squared error (RMSE) between x and z. We show the results of the different algorithms for different values of the parameter λ . Both T and S obtain lower RMSE compared to BP even though BP generally obtains results with significantly lower energy.

	Т		S		BP	
λ	Energy	RMSE	Energy	RMSE	Energy	RMSE
0.01	659210	10.1	842459	9.1	211646	15.8
0.02	943508	9.0	1220572	8.7	337785	13.4
0.05	1519837	8.9	1873560	10.9	650296	10.7
0.10	2089415	11.0	2506230	14.8	1080976	10.1
0.20	2700193	14.8	2942392	17.7	1730132	12.9

input image has 122 by 179 pixels. We used $\lambda = 0.05$ and $\tau = 100$ to define the pairwise costs. For the algorithm defined by T we used uniform weights, $w_{ij} = 1/d(i)$ and p = 0.001. Both the algorithms defined by T and belief propagation were run for 100 iterations. We based our implementations on the belief propagation code from [8], which provides efficient methods for handling truncated quadratic discontinuity costs. The algorithm defined by T took 16 seconds on a 1.6Ghz Intel Core i5 laptop computer while belief propagation took 18 seconds.

The goal of restoration is to recover a clean image z. We evaluate the restored image x by computing the root mean squared error (RMSE) between x and z. We see in Figure 2 that when $\lambda = 0.05$ and $\tau = 100$ the result of T has lower RMSE value compared to the result of BP, even though the result of T has significantly higher energy. We also evaluate the results of T, S and BP using different values of λ in Table 1. For all of these experiments we used $\tau = 100$ and ran each algorithm for 100 iterations. The minimum RMSE obtained by T and S is lower than the minimum RMSE obtained by BP considering different values for λ , even though T and S always find solutions that have higher energy compared to BP. This suggests the algorithms we propose do a good job aggregating local information using pairwise constraints, but the energy minimization problem defined by F(x) may not be the ideal formulation of the restoration problem.

5.2. Stereo depth estimation. In stereo matching we have two images I_l and I_r taken at the same time from different viewpoints. Most pixels in one image have a corresponding pixel in the other image, being the projection of the same three-dimensional point. The difference in the coordinates of corresponding pixels is called the disparity. We assume the images are rectified such that a pixel (x, y) in I_l matches a pixel (x - d, y) in I_r with $d \ge 0$. For rectified images the distance of a three-dimensional point to the image plane is inversely proportional to the disparity.

In practice we consider the problem of labeling every pixel in I_l with an integer disparity in $L = \{0, \ldots, D\}$. In this case a labeling x is a disparity map for I_l . The local costs $g_i(a)$ encourage pixels in I_l to be matched to pixels of similar color in I_r . The pairwise costs $h_{ij}(a, b)$ encourage piecewise smooth disparity maps.

The model we used in our stereo experiment is defined by

$$g_i(a) = \min(\gamma, ||I_l(i) - I_r(i - (a, 0))||_1);$$
(61)

$$h_{ij}(a,b) = \begin{cases} 0, & a = b, \\ \alpha, & |a - b| = 1, \\ \beta, & |a - b| > 1. \end{cases}$$
(62)

Here $I_l(i)$ is the value of pixel i in I_l while $I_r(i-(a,0))$ is the value of the corresponding pixel in I_r assuming a disparity a for i. The ℓ_1 norm $||I_l(i) - I_r(i - (a, 0))||_1$ defines a distance between RGB values (matching pixels should have similar color). The color distance is truncated by γ to allow for some large color differences which occur due to









Ground truth

Result of S

FIG. 3. Stereo disparity estimation using the fixed point algorithm defined by S on the Tsukuba image pair. The algorithm was run for 1,000 iterations.

specular reflections and occlusions. The pairwise costs depend on two parameter $\alpha, \beta \in \mathbb{R}$ with $\alpha < \beta$. The pairwise costs encourage the disparity neighboring pixels to be similar or differ by 1 (to allow for slanted surfaces), but also allows for large discontinuities which occur at object boundaries.

Figure 3 shows an example result of disparity estimation using the fixed point algorithm defined by S. In this example we used non-uniform weights w_{ij} to emphasize the relationships between neighboring pixels of similar color, since those pixels are most likely to belong to the same object/surface. The parameters we used for the results in Figure 3 were defined by,

$$w_{ii} \propto 0.01 + e^{-0.2||I_l(i) - I_l(j)||_1},\tag{63}$$

p = 0.0001, $\alpha = 500$, $\beta = 1000$, and $\gamma = 20$. The input image has 384 by 288 pixels and the maximum disparity is D = 15. The fixed point algorithm was run for 1,000 iterations which took 13 seconds on a laptop computer.

We note that the results in Figure 3 are similar to results obtained by min-sum belief propagation shown in [8].

6. Conclusion and future work. The experimental results in the last section illustrate the practical feasibility of the algorithms under study. Our theoretical results prove these algorithms are guaranteed to converge to unique fixed points on graphs with arbitrary topology and with arbitrary pairwise relationships. This includes the case of repulsive interactions which often leads to convergence problems for message passing methods.

Our results can be extended to other contraction maps similar to T and S and alternative methods for computing the fixed points of these maps. Some specific directions for future work are as follows.

- (1) Asynchronous updates. It is possible to define algorithms that update the beliefs of a single vertex at a time in any order. As long as all vertices are updated infinitely many times, the resulting algorithms converge to the same fixed point as the parallel update methods examined in this work. We conjecture that in a sequential computation, the sequential update of vertices in a "sweep" would converge faster than a "parallel" update. Moreover, after a sequential update of all vertices, the neighbors of those vertices with greater change should be the first ones to be updated in the next "sweep".
- (2) Non-backtracking random walks. The algorithms defined by S and T can be understood in terms of random walks on G. It is possible to define alternative algorithms based on non-backtracking random walks. In particular, starting with the MDP in Section 4 we can increase the state-space Q to keep track of the last vertex visited in the walk and define transition probabilities that avoid the previous vertex when selecting the next one. The resulting value iteration algorithm becomes very similar to belief propagation and other message passing methods that involve messages defined on the edges of G.

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