Graphical models and message-passing
Part I: Basics and MAP computation

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Tutorial materials (slides, monograph, lecture notes) available at:
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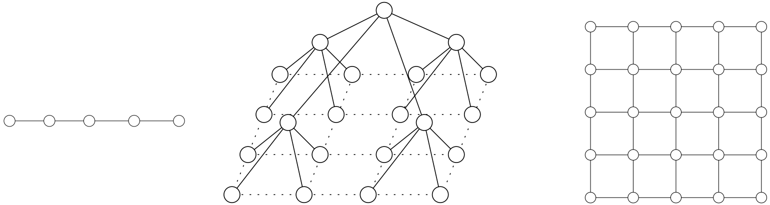
Introduction

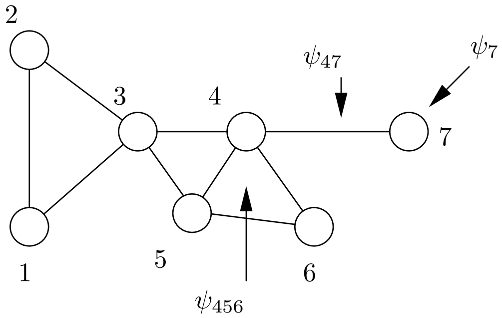
- graphical model:
  - $*$ graph $G = (V, E)$ with N vertices
  - $*$ random vector: $(X_1, X_2, \ldots, X_N)$



(a) Markov chain (b) Multiscale quadtree (c) Two-dimensional grid

- useful in many statistical and computational fields:
  - machine learning, artificial intelligence
  - computational biology, bioinformatics
  - statistical signal/image processing, spatial statistics
  - statistical physics
  - communication and information theory

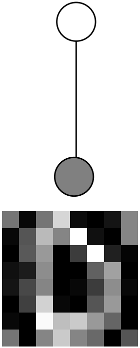
Graphs and factorization



- clique C is a fully connected subset of vertices
- compatibility function ψ_C defined on variables $x_C = \{x_s, s \in C\}$
- factorization over all cliques

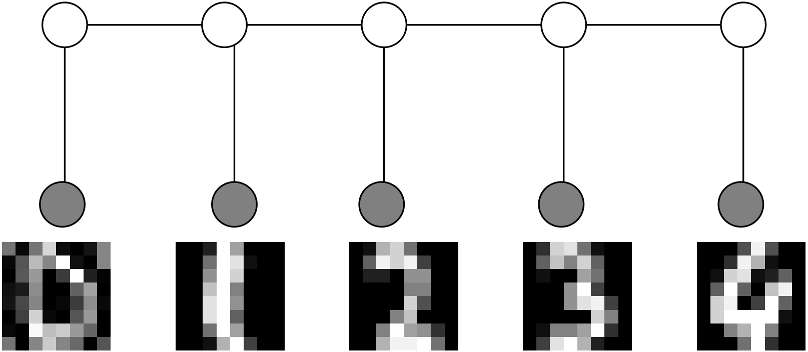
$$p(x_1, \ldots, x_N) = \frac{1}{Z} \prod_{C \in \mathfrak{C}} \psi_C(x_C).$$

Example: Optical digit/character recognition



- **Goal:** correctly label digits/characters based on "noisy" versions
- E.g., mail sorting; document scanning; handwriting recognition systems

Example: Optical digit/character recognition



- **Goal:** correctly label digits/characters based on "noisy" versions
- strong sequential dependencies captured by (hidden) Markov chain
- "message-passing" spreads information along chain

(Baum & Petrie, 1966; Viterbi, 1967, and many others)

Example: Image processing and denoising

- 8-bit digital image: matrix of intensity values $\{0, 1, \ldots 255\}$
- enormous redundancy in "typical" images (useful for denoising, compression, etc.)

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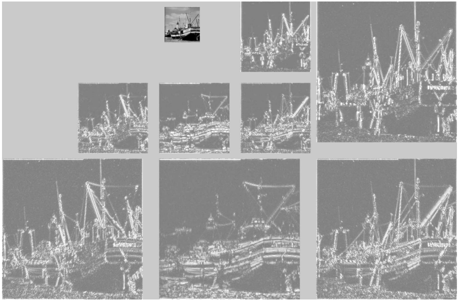
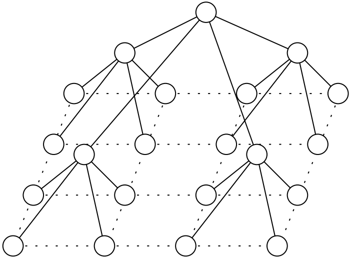




- 8-bit digital image: matrix of intensity values $\{0, 1, \dots 255\}$
- enormous redundancy in "typical" images (useful for denoising, compression, etc.)
- multiscale tree used to represent coefficients of a multiscale transform (e.g., wavelets, Gabor filters etc.)

(e.g., Willsky, 2002)

Example: Depth estimation in computer vision

Stereo pairs: two images taken from horizontally-offset cameras

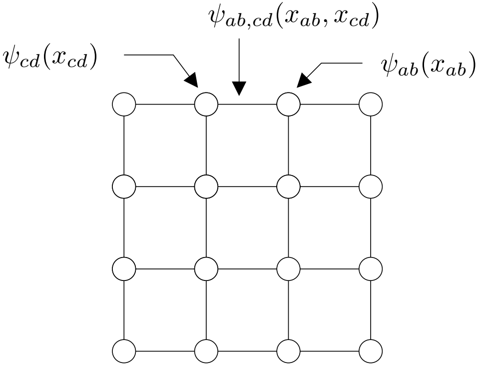
Modeling depth with a graphical model

Introduce variable at pixel location (a, b):

$$x_{ab} \equiv \text{Offset between images in position } (a, b)$$

Left image

Right image



Use message-passing algorithms to estimate most likely offset/depth map.

(Szeliski et al., 2005)

Many other examples

- natural language processing (e.g., parsing, translation)
- computational biology (gene sequences, protein folding, phylogenetic reconstruction)
- social network analysis (e.g., politics, Facebook, terrorism.)
- communication theory and error-control decoding (e.g., turbo codes, LDPC codes)
- satisfiability problems (3-SAT, MAX-XORSAT, graph colouring)
- robotics (path planning, tracking, navigation)
- sensor network deployments (e.g., distributed detection, estimation, fault monitoring)
- ...

Core computational challenges

Given an undirected graphical model (Markov random field):

$$p(x_1, x_2, \ldots, x_N) \;=\; \frac{1}{Z} \prod_{C \in \mathcal{C}} \psi_C(x_C)$$

How to efficiently compute?

- most probable configuration (MAP estimate):

$$\textbf{Maximize}: \qquad \widehat{x} = \arg \max_{\mathbf{x} \in \mathcal{X}^N} p(x_1, \ldots, x_N) \;=\; \arg \max_{\mathbf{x} \in \mathcal{X}^N} \prod_{C \in \mathcal{C}} \psi_C(x_C).$$

- the data likelihood or normalization constant

$$\textbf{Sum/integrate}: \qquad Z \;=\; \sum_{x \in \mathcal{X}^N} \prod_{C \in \mathcal{C}} \psi_C(x_C)$$

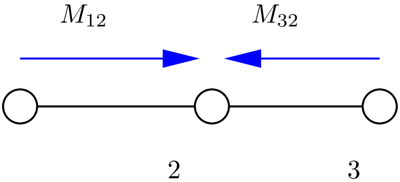
- marginal distributions at single sites, or subsets:

$$\textbf{Sum/integrate}: \qquad p(X_s = x_s) = \frac{1}{Z} \sum_{x_t,\; t \neq s} \prod_{C \in \mathcal{C}} \psi_C(x_C)$$

§1. Max-product message-passing on trees

Goal: Compute most probable configuration (MAP estimate) on a tree:

$$\widehat{x} \;=\; \arg\max_{\mathbf{x}\in\mathcal{X}^N} \left\{ \prod_{s\in V} \exp(\theta_s(x_s)) \prod_{(s,t)\in E} \exp(\theta_{st}(x_s, x_t)) \right\}.$$

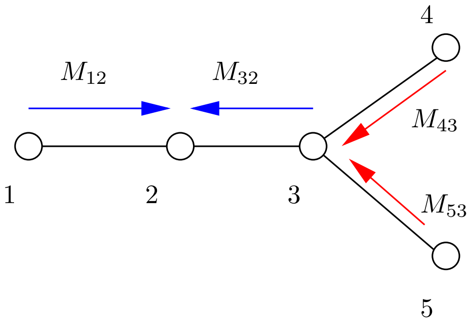


$$\max_{x_1, x_2, x_3} p(\mathbf{x}) \;=\; \max_{x_2} \left[\exp(\theta_2(x_2)) \prod_{t\in 1,3} \left\{ \max_{x_t} \exp[\theta_t(x_t) + \theta_{2t}(x_2, x_t)] \right\} \right]$$

Max-product strategy: "Divide and conquer": break global maximization into simpler sub-problems. (Lauritzen & Spiegelhalter, 1988)

Max-product on trees

Decompose: $\max_{x_1,x_2,x_3,x_4,x_5} p(\mathbf{x}) \;=\; \max_{x_2} \Big[\exp(\theta_1(x_1)) \; \prod_{t \in N(2)} M_{t2}(x_2)\Big].$

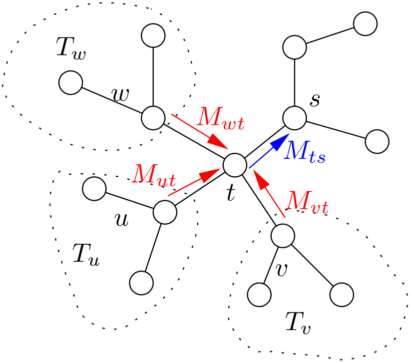


Update messages:

$$M_{32}(x_2) \;=\; \max_{x_3} \left[\exp(\theta_3(x_3) + \theta_{23}(x_2, x_3)) \prod_{v \in N(3) \backslash 2} M_{v3}(x_3)\right]$$

Putting together the pieces

Max-product is an exact algorithm for any tree.



$M_{ts} \equiv$ message from node t to s
$\mathcal{N}(t) \equiv$ neighbors of node t

Update: $\quad \mathbf{M_{ts}(x_s)} \leftarrow \max_{x'_t \in \mathcal{X}_t} \Big\{ \exp\Big[\theta_{st}(x_s, x'_t) + \theta_t(x'_t)\Big] \prod_{v \in \mathcal{N}(t)\backslash s} \mathbf{M_{vt}(x_t)} \Big\}$

Max-marginals: $\quad \widetilde{p}_s(x_s;\theta) \propto \exp\{\theta_s(x_s)\} \prod_{t \in \mathcal{N}(s)} M_{ts}(x_s)$.

Summary: max-product on trees

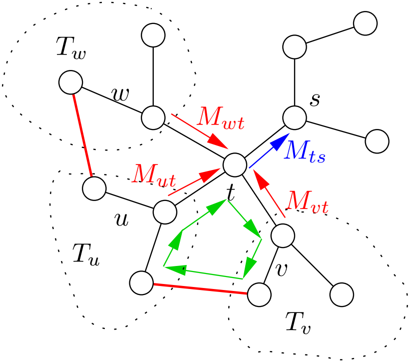
- converges in at most graph diameter # of iterations
- updating a single message is an $\mathcal{O}(m^2)$ operation
- overall algorithm requires $\mathcal{O}(Nm^2)$ operations

- upon convergence, yields the exact *max-marginals*:

$$\widetilde{p}_s(x_s) \propto \exp\{\theta_s(x_s)\} \prod_{t \in \mathcal{N}(s)} M_{ts}(x_s).$$

- when $\arg max_{x_s} \widetilde{p}_s(x_s) = \{x^s\}$ for all $s \in V$, then $x^* = (x_1^*, \ldots, x_N^*)$ is the *unique MAP solution*
- otherwise, there are multiple MAP solutions and one can be obtained by back-tracking

§2. Max-product on graph with cycles?



M_{ts}	$\equiv$	message from node t to s
$\mathcal{N}(t)$	$\equiv$	neighbors of node t

- max-product can be applied to graphs with cycles (no longer exact)
- empirical performance is often very good

Partial guarantees for max-product

- single-cycle graphs and Gaussian models
  (Aji & McEliece, 1998; Horn, 1999; Weiss, 1998, Weiss & Freeman, 2001)

- local optimality guarantees:
  - "tree-plus-loop" neighborhoods (Weiss & Freeman, 2001)
  - optimality on more general sub-graphs (Wainwright et al., 2003)

- existence of fixed points for general graphs (Wainwright et al., 2003)

- exactness for certain matching problems (Bayati et al., 2005, 2008, Jebara & Huang, 2007, Sanghavi, 2008)

- no general optimality results

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- no general optimality results

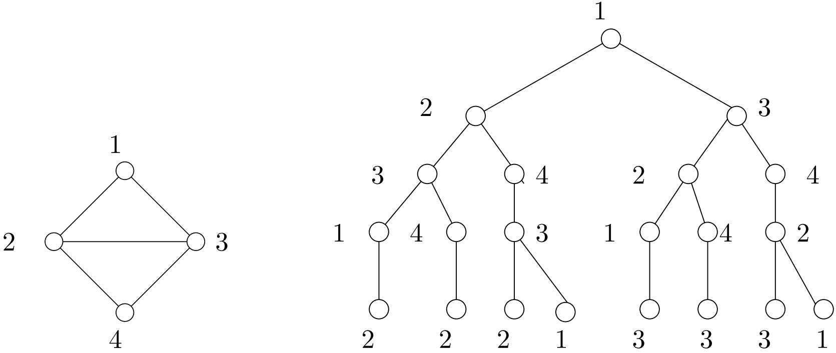
Questions:

- Can max-product return an incorrect answer with high confidence?
- Any connection to classical approaches to integer programs?

Standard analysis via computation tree

- standard tool: computation tree of message-passing updates

(Gallager, 1963; Weiss, 2001; Richardson & Urbanke, 2001)



(a) Original graph (b) Computation tree (4 iterations)

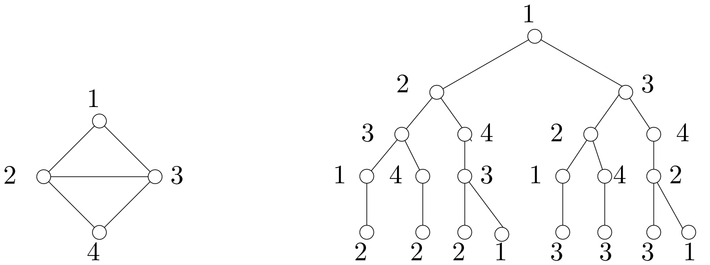
- level t of tree: all nodes whose messages reach the root (node 1) after t iterations of message-passing

Example: Inexactness of standard max-product

(Wainwright et al., 2005)

Intuition:

- max-product solves (exactly) a modified problem on computation tree
- nodes *not equally weighted* in computation tree ⇒ max-product can output an incorrect configuration

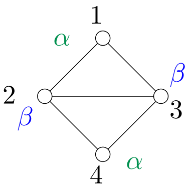


(a) Diamond graph G_{dia} (b) Computation tree (4 iterations)

- for example: asymptotic node fractions ω in this computation tree:

$$\begin{bmatrix}\omega(1) & \omega(2) & \omega(3) & \omega(4)\end{bmatrix} = \begin{bmatrix}0.2393 & 0.2607 & 0.2607 & 0.2393\end{bmatrix}$$

A whole family of non-exact examples



$$\theta_s(x_s) \quad \begin{cases} \alpha x_s & \text{if } s = 1 \text{ or } s = 4 \\ \beta x_s & \text{if } s = 2 \text{ or } s = 3 \end{cases}$$

$$\theta_{st}(x_s, x_t) = \begin{cases} -\gamma & \text{if } x_s \neq x_t \\ 0 & \text{otherwise} \end{cases}$$

- for γ sufficiently large, optimal solution is always either $1^4 = \begin{bmatrix} 1 & 1 & 1 & 1 \end{bmatrix}$ or $(-1)^4 = \begin{bmatrix} (-1) & (-1) & (-1) & (-1) \end{bmatrix}$
- first-order LP relaxation always exact for this problem
- max-product and LP relaxation give *different* decision boundaries:

Optimal/LP boundary: $\quad \widehat{\mathbf{x}} = \begin{cases} 1^4 & \text{if } 0.25\alpha + 0.25\beta \geq 0 \\ (-1)^4 & \text{otherwise} \end{cases}$

Max-product boundary: $\quad \widehat{\mathbf{x}} = \begin{cases} 1^4 & \text{if } 0.2393\alpha + 0.2607\beta \geq 0 \\ (-1)^4 & \text{otherwise} \end{cases}$

§3. A more general class of algorithms

- by introducing weights on edges, obtain a more general family of *reweighted max-product algorithms*
- with suitable edge weights, connected to linear programming relaxations
- many variants of these algorithms:
  - tree-reweighted max-product (W., Jaakkola & Willsky, 2002, 2005)
  - sequential TRMP (Kolmogorov, 2005)
  - convex message-passing (Weiss et al., 2007)
  - dual updating schemes (e.g., Globerson & Jaakkola, 2007)

Tree-reweighted max-product algorithms

(Wainwright, Jaakkola & Willsky, 2002)

Message update from node t to node s:

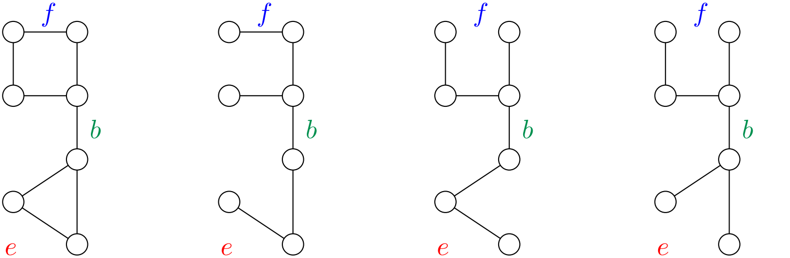
$$M_{ts}(x_s) \quad \leftarrow \quad \kappa \max_{x'_t \in \mathcal{X}_t} \Bigg\{ \exp \Big[\underbrace{\frac{\theta_{st}(x_s, x'_t)}{\rho_{st}}}_{\text{reweighted edge}} + \theta_t(x'_t) \Big] \frac{\prod_{v \in \mathcal{N}(t) \backslash s} \overbrace{\big[M_{vt}(x_t)\big]^{\rho_{vt}}}^{\text{reweighted messages}}}{\underbrace{\big[M_{st}(x_t)\big]^{(1-\rho_{ts})}}_{\text{opposite message}}} \Bigg\}.$$

Properties:

1. Modified updates remain *distributed* and *purely local* over the graph.
2. Key differences:
   - Messages are reweighted with $\rho_{st} \in [0, 1]$.
   - Potential on edge (s, t) is rescaled by $\rho_{st} \in [0, 1]$.
   - Update involves the reverse direction edge.
3. The choice $\rho_{st} = 1$ for all edges (s, t) recovers standard update.

Edge appearance probabilities

Experiment: What is the probability ρ_e that a given edge $e \in E$ belongs to a tree T drawn randomly under $\boldsymbol{\rho}$?



(a) Original (b) $\rho(T^1) = \frac{1}{3}$ (c) $\rho(T^2) = \frac{1}{3}$ (d) $\rho(T^3) = \frac{1}{3}$

In this example: $\rho_b = 1$; $\rho_e = \frac{2}{3}$; $\rho_f = \frac{1}{3}$.

The vector $\boldsymbol{\rho_e} = \{ \rho_e \mid e \in E \}$ must belong to the *spanning tree polytope*. (Edmonds, 1971)

§4. Reweighted max-product and linear programming

- MAP as integer program: $f^* = \max_{\mathbf{x} \in \mathcal{X}^N} \Big\{ \sum_{s \in V} \theta_s(x_s) + \sum_{(s,t) \in E} \theta_{st}(x_s, x_t) \Big\}$

- define local marginal distributions (e.g., for $m = 3$ states):

$$\mu_s(x_s) = \begin{bmatrix} \mu_s(0) \\ \mu_s(1) \\ \mu_s(2) \end{bmatrix} \qquad \mu_{st}(x_s, x_t) = \begin{bmatrix} \mu_{st}(0,0) & \mu_{st}(0,1) & \mu_{st}(0,2) \\ \mu_{st}(1,0) & \mu_{st}(1,1) & \mu_{st}(1,2) \\ \mu_{st}(2,0) & \mu_{st}(2,1) & \mu_{st}(2,2) \end{bmatrix}$$

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- alternative formulation of MAP as linear program?

$$g^* = \max_{(\mu_s, \mu_{st}) \in \mathbb{M}(G)} \left\{ \sum_{s \in V} \mathbb{E}_{\mu_s}[\theta_s(x_s)] + \sum_{(s,t) \in E} \mathbb{E}_{\mu_{st}}[\theta_{st}(x_s, x_t)] \right\}$$

$$\text{Local expectations:} \qquad \mathbb{E}_{\mu_s}[\theta_s(x_s)] := \sum_{x_s} \mu_s(x_s) \theta_s(x_s).$$

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$$\text{Local expectations:} \qquad \mathbb{E}_{\mu_s}[\theta_s(x_s)] \quad := \quad \sum_{x_s} \mu_s(x_s) \theta_s(x_s).$$

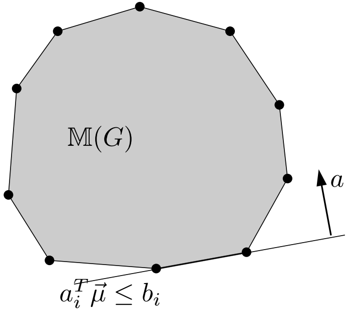
Key question: What constraints must local marginals $\{\mu_s, \mu_{st}\}$ satisfy?

Marginal polytopes for general undirected models

- $\mathbb{M}(G) \equiv$ set of all *globally realizable* marginals $\{\mu_s, \mu_{st}\}$:

$$\left\{ \vec{\mu} \in \mathbb{R}^d \;\middle|\; \mu_s(x_s) \;=\; \sum_{x_t, t \neq s} p_\mu(\mathbf{x}), \text{ and } \mu_{st}(x_s, x_t) \;=\; \sum_{x_u, u \neq s,t} p_\mu(\mathbf{x}) \right\}$$

for some $p_\mu(\cdot)$ over $(X_1, \ldots, X_N) \in \{0, 1, \ldots, m-1\}^N$.



- polytope in $d = m|V| + m^2|E|$ dimensions (m per vertex, m^2 per edge)
- with m^N vertices
- number of facets?

Marginal polytope for trees

- $\mathbb{M}(T) \equiv$ special case of marginal polytope for tree T
- local marginal distributions on nodes/edges (e.g., $m = 3$)

$$\mu_s(x_s) = \begin{bmatrix} \mu_s(0) \\ \mu_s(1) \\ \mu_s(2) \end{bmatrix} \qquad \mu_{st}(x_s, x_t) = \begin{bmatrix} \mu_{st}(0,0) & \mu_{st}(0,1) & \mu_{st}(0,2) \\ \mu_{st}(1,0) & \mu_{st}(1,1) & \mu_{st}(1,2) \\ \mu_{st}(2,0) & \mu_{st}(2,1) & \mu_{st}(2,2) \end{bmatrix}$$

Deep fact about tree-structured models: If $\{\mu_s, \mu_{st}\}$ are non-negative and *locally consistent*:

$$\textbf{Normalization}: \quad \sum_{x_s} \mu_s(x_s) = 1$$

$$\textbf{Marginalization}: \quad \sum_{x_t'} \mu_{st}(x_s, x_t') = \mu_s(x_s),$$

then on any tree-structured graph T, they are *globally consistent.*

Follows from junction tree theorem (Lauritzen & Spiegelhalter, 1988).

Max-product on trees: Linear program solver

- MAP problem as a simple linear program:

$$f(\widehat{x}) = \arg\max_{\vec{\mu} \in \mathbb{M}(T)} \left\{ \sum_{s \in V} \mathbb{E}_{\mu_s}[\theta_s(x_s)] + \sum_{(s,t) \in E} \mathbb{E}_{\mu_{st}}[\theta_{st}(x_s, x_t)] \right\}$$

subject to $\vec{\mu}$ in tree marginal polytope:

$$\mathbb{M}(T) = \left\{ \vec{\mu} \geq 0, \quad \sum_{x_s} \mu_s(x_s) = 1, \qquad \sum_{x_t'} \mu_{st}(x_s, x_t') = \mu_s(x_s) \right\}.$$

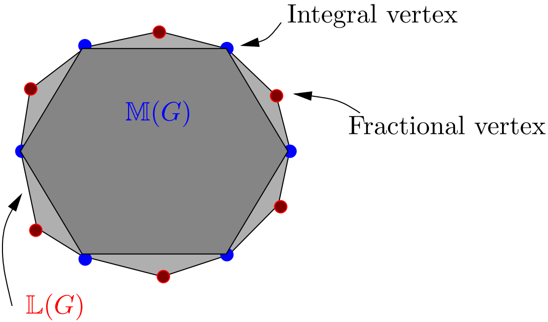
Max-product and LP solving:

- on tree-structured graphs, max-product is a dual algorithm for solving the tree LP. (Wai. & Jordan, 2003)
- max-product message $M_{ts}(x_s) \equiv$ Lagrange multiplier for enforcing the constraint $\sum_{x_t'} \mu_{st}(x_s, x_t') = \mu_s(x_s)$.

Tree-based relaxation for graphs with cycles

Set of *locally consistent pseudomarginals* for general graph G:

$$\mathbb{L}(G) \; = \; \left\{ \vec{\tau} \in \mathbb{R}^d \;\mid\; \vec{\tau} \geq 0, \; \sum_{x_s} \tau_s(x_s) = 1, \quad \sum_{x_t} \tau_{st}(x_s, x'_t) = \tau_s(x_s) \right\}.$$

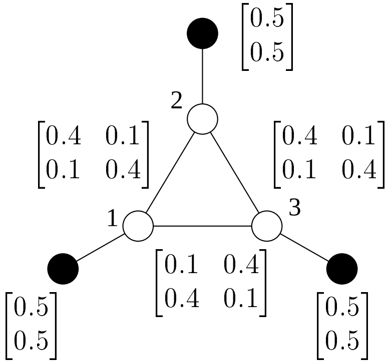


Key: For a general graph, $\mathbb{L}(G)$ is an outer bound on $\mathbb{M}(G)$, and yields a *linear-programming relaxation* of the MAP problem:

$$f(\widehat{x}) \; = \; \max_{\vec{\mu} \in \mathbb{M}(G)} \theta^T \vec{\mu} \; \leq \; \max_{\vec{\tau} \in \mathbb{L}(G)} \theta^T \vec{\tau}.$$

Looseness of $\mathbb{L}(G)$ with graphs with cycles

Locally consistent (pseudo)marginals



Pseudomarginals satisfy the "obvious" local constraints:

Normalization: $\sum_{x'_s} \tau_s(x'_s) = 1$ for all $s \in V$.

Marginalization: $\sum_{x'_s} \tau_s(x'_s, x_t) = \tau_t(x_t)$ for all edges (s, t).

TRW max-product and LP relaxation

First-order (tree-based) LP relaxation:

$$f(\widehat{x}) \;\leq\; \max_{\vec{\tau} \in \mathbb{L}(G)} \left\{ \sum_{s \in V} \mathbb{E}_{\tau_s}[\theta_s(x_s)] + \sum_{(s,t) \in E} \mathbb{E}_{\tau_{st}}[\theta_{st}(x_s, x_t)] \right\}$$

Results: (Wainwright et al., 2005; Kolmogorov & Wainwright, 2005):

(a) **Strong tree agreement** Any TRW fixed-point that satisfies the strong tree agreement condition specifies an optimal LP solution.

(b) **LP solving:** For any binary pairwise problem, TRW max-product solves the first-order LP relaxation.

(c) **Persistence for binary problems:** Let $S \subseteq V$ be the subset of vertices for which there exists a single point $x_s^* \in \arg\max_{x_s} \nu_s^*(x_s)$. Then for *any optimal solution*, it holds that $y_s = x_s^*$.

On-going work on LPs and conic relaxations

- tree-reweighted max-product solves first-order LP for any binary pairwise problem (Kolmogorov & Wainwright, 2005)
- convergent dual ascent scheme; LP-optimal for binary pairwise problems (Globerson & Jaakkola, 2007)
- convex free energies and zero-temperature limits (Wainwright et al., 2005, Weiss et al., 2006; Johnson et al., 2007)
- coding problems: adaptive cutting-plane methods (Taghavi & Siegel, 2006; Dimakis et al., 2006)
- dual decomposition and sub-gradient methods: (Feldman et al., 2003; Komodakis et al., 2007, Duchi et al., 2007)
- solving higher-order relaxations; rounding schemes (e.g., Sontag et al., 2008; Ravikumar et al., 2008)

Hierarchies of conic programming relaxations

- tree-based LP relaxation using $\mathbb{L}(G)$: first in a hierarchy of hypertree-based relaxations (Wainwright & Jordan, 2004)
- hierarchies of SDP relaxations for polynomial programming (Lasserre, 2001; Parrilo, 2002)
- intermediate between LP and SDP: second-order cone programming (SOCP) relaxations (Ravikumar & Lafferty, 2006; Kumar et al., 2008)
- all relaxations: particular outer bounds on the marginal polyope

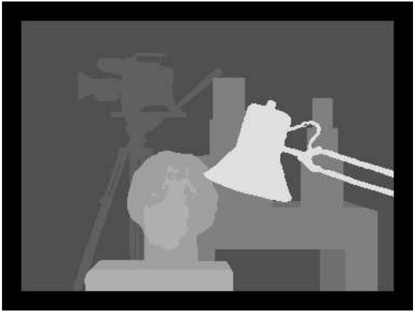
Key questions:

- when are particular relaxations tight?
- when does more computation (e.g., LP $\rightarrow$ SOCP $\rightarrow$ SDP) yield performance gains?

Stereo computation: Middlebury stereo benchmark set

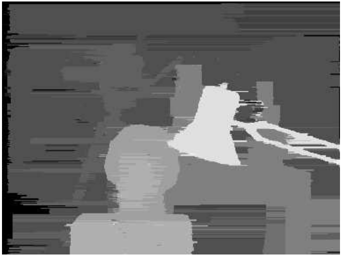
- standard set of benchmarked examples for stereo algorithms (Scharstein & Szeliski, 2002)
- Tsukuba data set: Image sizes $384 \times 288 \times 16$ ($W \times H \times D$)

(a) Original image

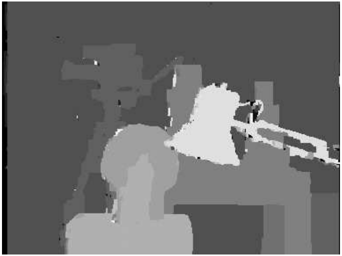


(b) Ground truth disparity

Comparison of different methods

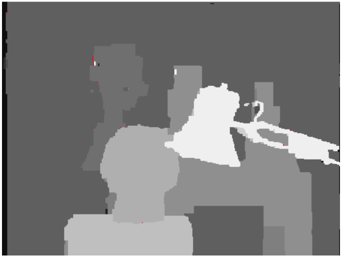


(a) Scanline dynamic programming



(b) Graph cuts

(c) Ordinary belief propagation

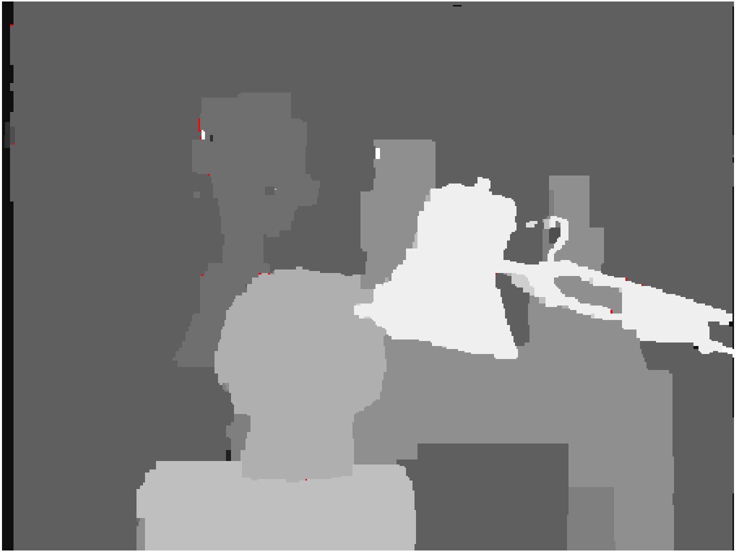


(d) Tree-reweighted max-product

(a), (b): Scharstein & Szeliski, 2002; (c): Sun et al., 2002 (d): Weiss, et al., 2005;

Ordinary belief propagation

Tree-reweighted max-product



Ground truth