Today's lecture

Approximate inference in graphical models.

- Forward and Backward KL divergence
- Variational Inference
- Mean Field: Naive and Structured
- Marginal Polytope
- Local Polytope
- Relaxation methods
- Loopy BP
- LP relaxations for MAP inference

Figures from D. Sontag, Murphy's book

Approximate marginal inference

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- Almost all approximate inference algorithms in practice are
  - Variational algorithms (e.g., mean-field, loopy belief propagation)
  - Sampling methods (e.g., Gibbs sampling, MCMC)

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- The KL-divergence is asymmetric

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- What can we do?

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- The KL is always non-negative, so we see that $J(q)$ is an upper bound on the negative log likelihood (NLL)

$$J(q) = KL(q||p) - \log Z \geq -\log Z = -\log p(\mathcal{D})$$

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- This is the expected NLL plus a penalty term that measures how far apart the two distributions are

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- They differ only when q is minimized over a restricted set of probability distribution $Q = \{q_1, \cdots\}$, and $p \neq q$. Why?

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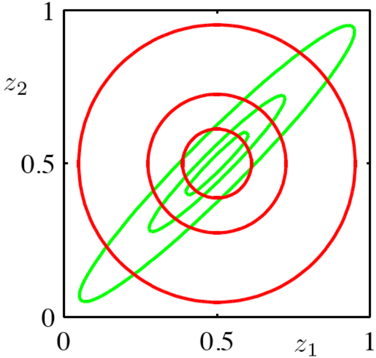
KL divergence - M projection

$$q^* = arg \min_{q \in Q} KL(p||q) = \sum_{\mathbf{x}} p(\mathbf{x}) \log \frac{p(\mathbf{x})}{q(\mathbf{x})}$$

$p(\mathbf{x})$ is a 2D Gaussian and Q is the set of all Gaussian distributions with diagonal covariance matrices



p=Green, q^*=Red

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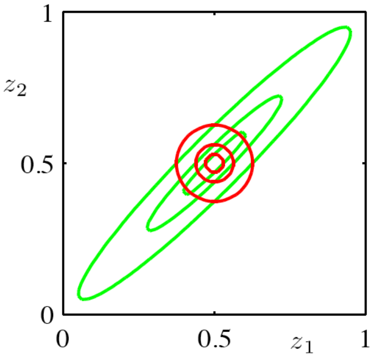

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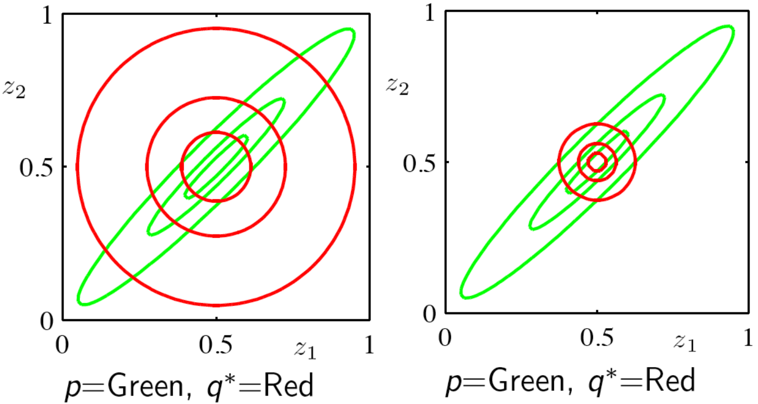
KL Divergence (single Gaussian)

- In this example, both the M-projection and I-projection find an approximate $q(\mathbf{x})$ that has the correct mean (i.e., $\mathbb{E}_p(\mathbf{z}) = \mathbb{E}_q(\mathbf{x})$)



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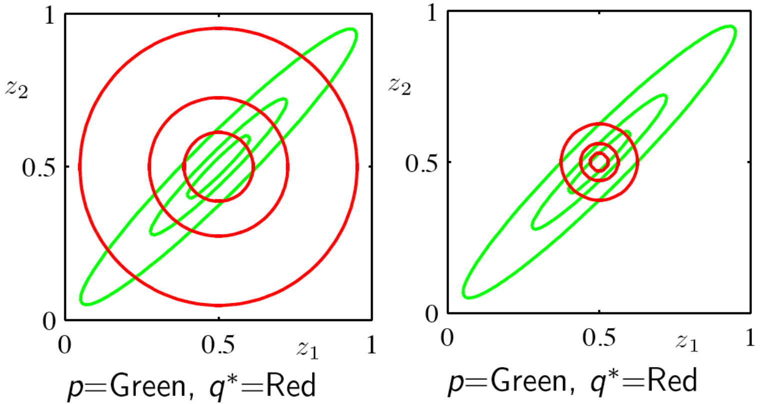

What if $p(\mathbf{x})$ is multimodal?

M projection (Mixture of Gaussians)

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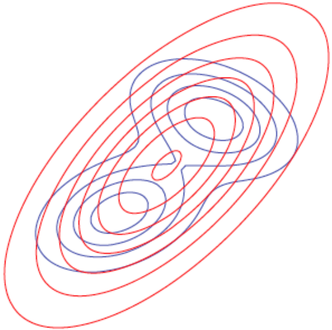
$p(\mathbf{x})$ is a mixture of two 2D Gaussians and Q is the set of all 2D Gaussian distributions (with arbitrary covariance matrices)



M-projection yields a distribution $q(\mathbf{x})$ with the correct mean and covariance.

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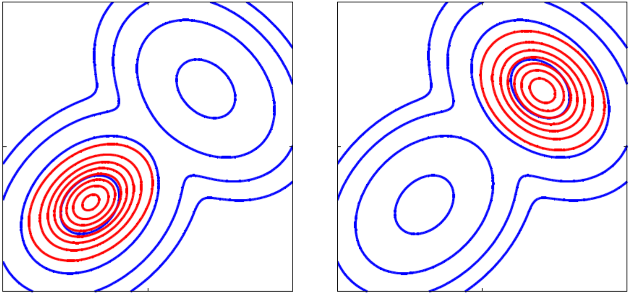

p=Blue, q^*=Red (two local minima!)

The I-projection does not necessarily yield the correct moments

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- We can do the maximization one node at a time, in an iterative fashion

Mean Field Updates

- Focus on q_j (holding all other terms constant)

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&= \sum_{\mathbf{x}_j} q_j(\mathbf{x}_j) \sum_{\mathbf{x}_{-j}} \prod_{i \neq j} q_i(\mathbf{x}_i) \log \tilde{p}(\mathbf{x}) - \\
&\quad \sum_{\mathbf{x}_j} q_j(\mathbf{x}_j) \sum_{\mathbf{x}_{-j}} \prod_{i \neq j} q_i(\mathbf{x}_i) \left[\sum_{k \neq j} \log q_k(x_k) + \log q_j(\mathbf{x}_j) \right] \\
&= \sum_{\mathbf{x}_j} q_j(\mathbf{x}_j) \log f_j(\mathbf{x}_j) - \sum_{\mathbf{x}_j} q_j(\mathbf{x}_j) \log q_j(\mathbf{x}_j) + \text{const}
\end{aligned}
$$

Mean Field Updates

- Focus on q_j (holding all other terms constant)

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where
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- So we average out all the variables except x_j, and can rewrite $L(q_j)$ as

$$
L(q_j) = -KL(q_j || f_j)
$$

Variational Inference for Graphical Models

- Suppose that we have an arbitrary graphical model

$$p(\mathbf{x}; \theta) = \frac{1}{Z(\theta)} \prod_{c \in C} \phi_c(\mathbf{x}_c) = \exp\left(\sum_{c \in C} \theta_c(\mathbf{x}_c) - \ln Z(\theta) \right)$$

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Mean Field for Variational Inference

$$\max_{q\in Q} \sum_{c\in C} \sum_{\mathbf{x}_c} q(\mathbf{x}_c)\theta_c(\mathbf{x}_c) + H(q(\mathbf{x}))$$

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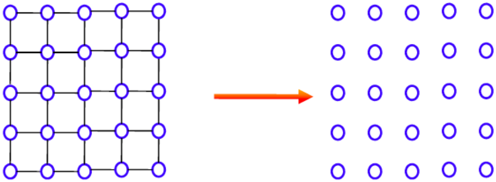
- Although this function is concave and thus in theory should be easy to optimize, we need some compact way of representing $q(\mathbf{x})$
- **Mean field**: assume a factored representation of the joint distribution



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

This is called "naive" mean field

Naive Mean Field

- Suppose that Q consists of all fully factorized distributions, then we can simplify

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subject to the constraints

$$q_i(x_i) \geq 0 \qquad \forall i \in V, x_i$$

$$\sum_{x_i} q_i(x_i) = 1 \qquad \forall i \in V$$

Naive Mean Field for Pairwise MRFs

- For pairwise MRFs we have

$$\max_q \sum_{ij \in E} \sum_{x_i, x_j} \theta_{ij}(x_i, x_j) q_i(x_i) q_j(x_j) - \sum_{i \in V} \sum_{x_i} q_i(x_i) \ln q_i(x_i) \quad (1)$$

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  1. For each $i \in V$
     - Fully maximize Eq. (1) wrt $\{q_i(x_i), \forall x_i\}$
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- Constructing the Lagrangian, taking the derivatives and setting to zero yields the update

$$q_i(x_i) \leftarrow \frac{1}{Z_i} \exp\left\{ \theta_i(x_i) + \sum_{j \in N(i)} \sum_{x_j} q_j(x_j) \theta_{ij}(x_i, x_j) \right\}$$

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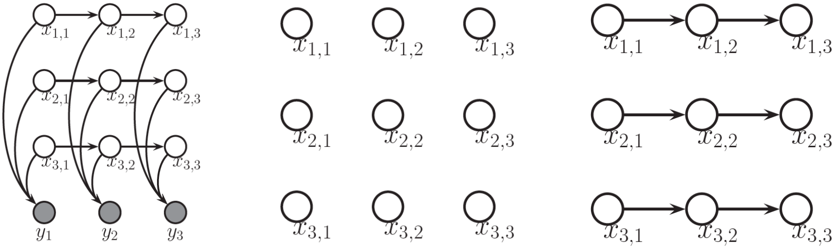
- See *Mean field example for the Ising Model*, Murphy 21.3.2

Structured mean-field approximations

- Rather than assuming a fully-factored distribution for q, we can use a structured approximation, such as a spanning tree

Structured mean-field approximations

- Rather than assuming a fully-factored distribution for q, we can use a structured approximation, such as a spanning tree
- For example, for a factorial HMM, a good approximation may be a product of chain-structured models (see Murphy 21.4.1)



Approximate Inference via Loopy BP

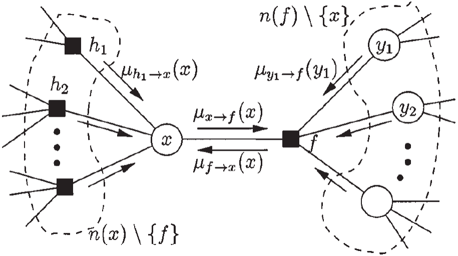
- Mean field inference approximates posterior as product of marginal distributions
- Allows use of different forms for each variable: useful when inferring statistical parameters of models, or regression weights
- An alternative approximate inference algorithm is **loopy belief propagation**
- Same algorithm shown to do exact inference in trees last class
- In loopy graphs, BP not guaranteed to give correct results, may not converge, but often works well in practice

Loopy BP on Pairwise Models

Algorithm 22.1: Loopy belief propagation for a pairwise MRF

Input: node potentials $\psi_s(x_s)$, edge potentials $\psi_{st}(x_s, x_t)$;
Initialize messages $m_{s \to t}(x_t) = 1$ for all edges $s - t$;
Initialize beliefs $\text{bel}_s(x_s) = 1$ for all nodes s;
repeat
    Send message on each edge
    $m_{s \to t}(x_t) = \sum_{x_s} \left(\psi_s(x_s) \psi_{st}(x_s, x_t) \prod_{u \in \text{nbr}_s \setminus t} m_{u \to s}(x_s) \right)$;
    Update belief of each node $\text{bel}_s(x_s) \propto \psi_s(x_s) \prod_{t \in \text{nbr}_s} m_{t \to s}(x_s)$;
until *beliefs don't change significantly*;
Return marginal beliefs $\text{bel}_s(x_s)$;

Loopy BP for Factor Graph



$$m_{i \to f}(x_i) = \prod_{h \in M(i) \setminus f} m_{h \to i}(x_i)$$

$$m_{f \to i}(x_i) = \sum_{\mathbf{x}_c \setminus x_i} f(\mathbf{x}_c) \prod_{j \in N(f) \setminus i} m_{j \to f}(x_j)$$

$$\mu_i(x_i) \propto \prod_{f \in M(i)} m_{f \to i}(x_i)$$

Convergence of LBP

- Can we predict when will converge?

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  - Unroll messages across time in a *computation tree*: T iterations of LBP is exact computation in tree of height $T+1$
  - if leaves' effect on root diminishes over time will converge

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- Can we make it more likely to converge?
  - Damp the messages to avoid oscillations
  - Can we speed up convergence?
- Change from synchronous to asynchronous updates
  - Update sets of nodes at a time, e.g., spanning trees (*tree reparameterization)*

LBP as Variational Inference

- More theoretical analysis of LBP from variational point of view: (Wainwright & Jordan, 2008)

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LBP as Variational Inference

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- Simplify by considering pairwise UGMs, discrete variables

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$$p(\mathbf{x};\theta) = \frac{1}{Z(\theta)} \prod_{c \in C} \phi_c(\mathbf{x}_c) = \exp\left(\sum_{c \in C} \theta_c(\mathbf{x}_c) - \ln Z(\theta)\right)$$

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The log-partition Function

- Since $KL(q||p) \geq 0$ we have

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which implies

$$\ln Z(\theta) \geq \sum_{c \in C} \mathbb{E}_q[\theta_c(\mathbf{x}_c)] + H(q(\mathbf{x}))$$

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$$-\sum_{c \in C} \mathbb{E}_q[\theta_c(\mathbf{x}_c)] + \ln Z(\theta) - H(q(\mathbf{x})) \geq 0$$

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- This casts exact inference as a variational optimization problem

Rewriting Objective in terms of Moments

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where M is the **marginal polytope**, having all valid marginal vectors

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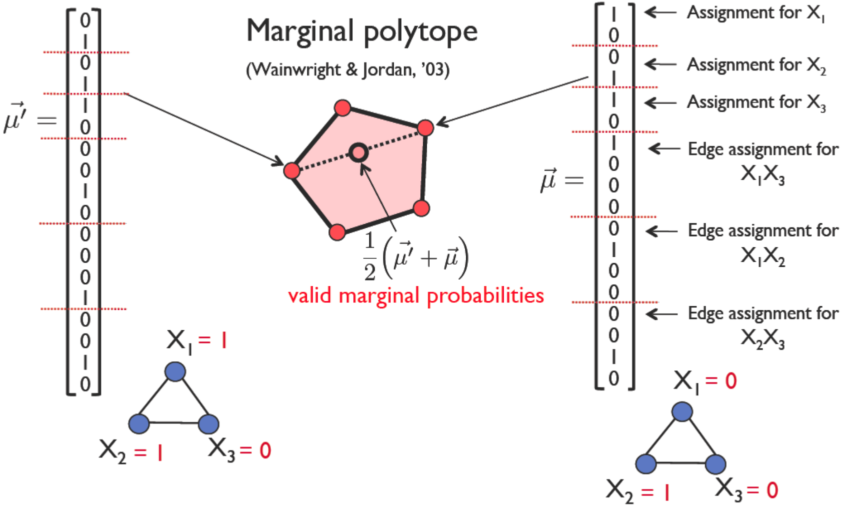
- For a discrete-variable MRF, the sufficient statistic vector $\mathbf{f}(\mathbf{x})$ is simply the concatenation of indicator functions for each clique of variables that appear together in a potential function
- For example, if we have a pairwise MRF on binary variables with $m = |V|$ variables and $|E|$ edges, $d = 2m + 4|E|$

Marginal Polytope for Discrete MRFs



Relaxation

$$\ln Z(\theta) = \max_{\mu \in M} \sum_{c \in C} \sum_{\mathbf{x}_c} \theta_c(\mathbf{x}_c)\mu_c(\mathbf{x}_c) + H(\mu)$$

We still haven't achieved anything, because:

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- We replace $H(\mu)$ with a function $\tilde{H}(\mu)$ which approximates $H(\mu)$

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- For every "cluster" of variables to choose a local assignment

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- The local consistency polytope, M_L is defined by these constraints
- The μ_i and μ_{ij} are called pseudo-marginals

polytope for a tree-structured MRF, and the pseudomarginals are the marginals. marginal polytope, i.e., $M \subseteq M_L$

Mean-field vs relaxation

$$\max_{q \in Q} \sum_{c \in C} \sum_{\mathbf{x}_c} q(\mathbf{x}_c)\theta_c(\mathbf{x}_c) + H(q(\mathbf{x}))$$

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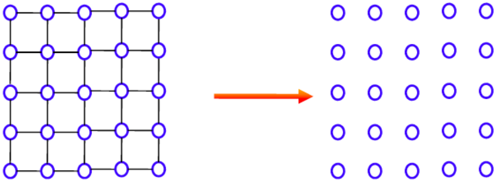
- **Mean-field** algorithms assume a factored representation of the joint distribution



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

Naive Mean-Field

- Using the same notation naive mean-field is:

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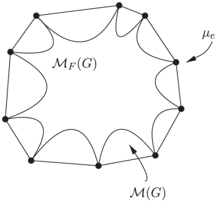

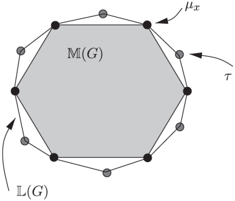

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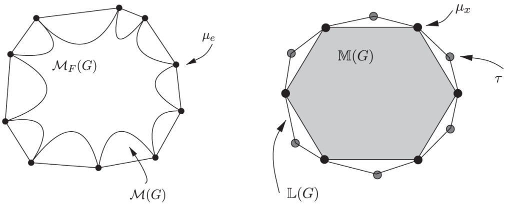

- We obtain a lower bound on the partition function, i.e., (*) $\leq \ln Z(\theta)$

MAP Inference

- Recall the MAP inference task

$$\arg\max_{\mathbf{x}} p(\mathbf{x}), \qquad p(\mathbf{x}) = \frac{1}{Z} \prod_{c \in C} \phi_c(\mathbf{x}_c)$$

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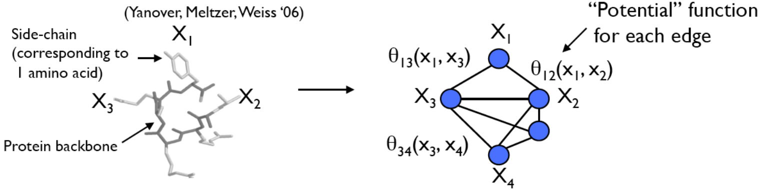
- Since the log is monotonic, let $\theta_c(\mathbf{x}_c) = \log \phi_c(\mathbf{x}_c)$

$$\arg\max_{\mathbf{x}} \sum_{c \in C} \theta_c(\mathbf{x}_c)$$

  This is called the **max-sum**

Application: protein side-chain placement

- Find "minimum energy" configuration of amino acid side-chains along fixed carbon backbone:



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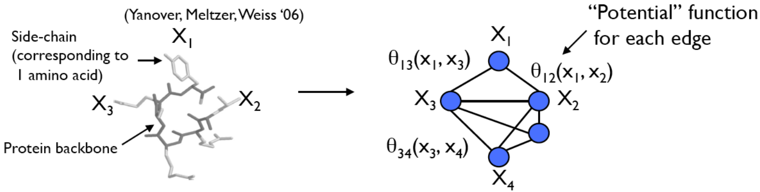

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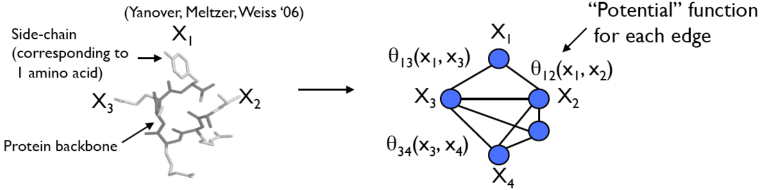
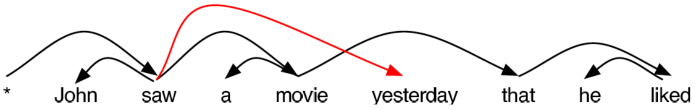


- Orientations of the side-chains are represented by discretized angles called rotamers
- Rotamer choices for nearby amino acids are energetically coupled (attractive and repulsive forces)

Application: Dependency parser

- Given a sentence, predict the dependency tree that relates the words



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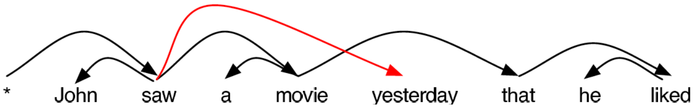

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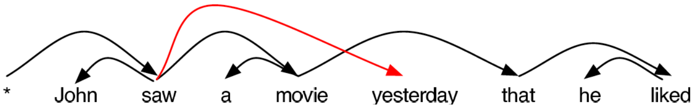

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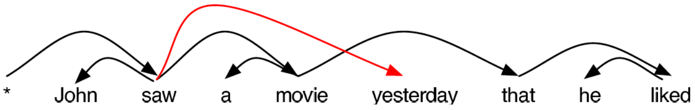

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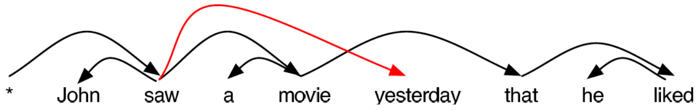

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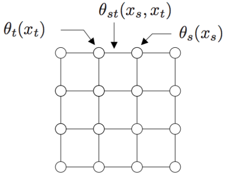
- m words $\Rightarrow m(m-1)$ binary arc selection variables $x_{ij} \in \{0,1\}$
- We represent the problem as

$$\max_{\mathbf{x}} \theta_T(\mathbf{x}) + \sum_{ij} \theta_{ij}(x_{ij}) + \sum_{i} \theta_{i|}(\mathbf{x}_{i|})$$

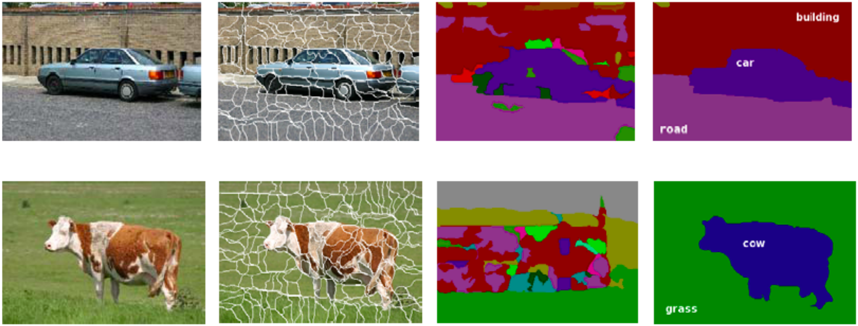
with $\mathbf{x}_{|i} = \{x_{ij}\}_{j \neq i}$ (all outgoing edges)

Application: Semantic Segmentation

- Use Potts to encode that neighboring pixels are likely to have the same discrete label and hence belong to the same segment



$$p(\mathbf{x}, \theta) = \max_{\mathbf{x}} \sum_i \theta_i(x_i) + \sum_{i,j} \theta_{i,j}(x_i, x_j)$$



MAP as an integer linear program (ILP)

- MAP as a discrete optimization problem is

$$\mathbf{x}^* = arg \max_{\mathbf{x}} \sum_{i \in V} \theta_i(x_i) + \sum_{ij \in E} \theta_{ij}(x_i, x_j)$$

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- What is the dimension of μ, if binary variables?
- Are these two problems equivalent?

Constraints

$$\max_{\mu} \sum_{i \in V} \sum_{x_i} \theta_i(x_i)\mu_i(x_i) + \sum_{ij} \theta_{ij}(x_i, x_j)\mu_{ij}(x_i, x_j)$$

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- For every "cluster" of variables to choose a local assignment

$$\begin{array}{rcll} \mu_i(x_i) & \in & \{0,1\} & \forall i \in V, x_i \\ \sum_{x_i} \mu_i(x_i) & = & 1 & \forall i \in V \\ \mu_{ij}(x_i, x_j) & \in & \{0,1\} & \forall i,j \in E, x_i, x_j \\ \sum_{x_i, x_j} \mu_{ij}(x_i, x_j) & = & 1 & \forall i,j \in E \end{array}$$

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\end{aligned}$$

- Enforce that these local assignments are globally consistent

$$\begin{aligned}
\mu_i(x_i) &= \sum_{x_j} \mu_{ij}(x_i, x_j) \quad \forall ij \in E, x_i \\
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- Many extremely good off-the-shelf solvers, such as CPLEX and Gurobi
- But it might be too slow...

Linear Programing Relaxation for MAP

$$MAP(\theta) = \max_{\mu} \sum_{i \in V} \sum_{x_i} \theta_i(x_i)\mu_i(x_i) + \sum_{ij} \theta_{ij}(x_i, x_j)\mu_{ij}(x_i, x_j)$$

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- Relax integrality constraints, allowing the variables to be between 0 and 1

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Loopy Belief Propagation (Max Product)

- Introducing Lagrange multipliers and solving we get (see Murphy 22.3.5.4)

$$M_{i \to j}(x_i) \propto \max_{x_j} \left[\exp\{\theta_{ij}(x_i, x_j) + \theta_j(x_j)\} \prod_{u \in N(j) \setminus i} M_{u \to j}(x_j) \right]$$

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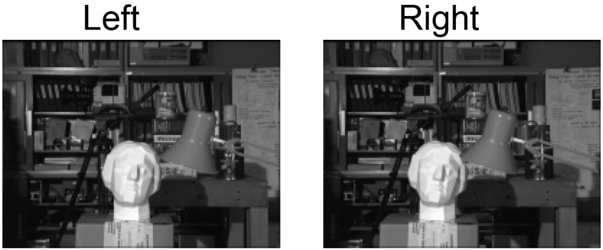
Stereo Estimation

- Tsukuba images from Middlebury stereo database



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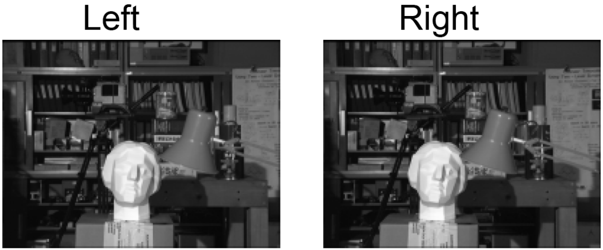

- MRF for each pixel, with states the disparity

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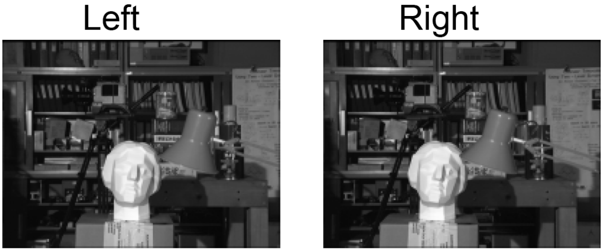

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where pixel $p_i = (x, y)$

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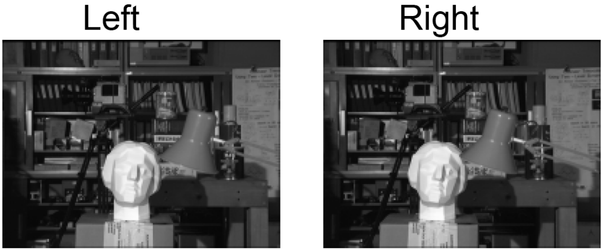

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- The pairwise factor θ_{ij} between neighboring pixels favor smoothness

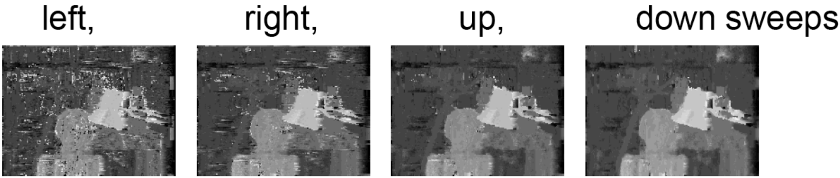
Stereo Estimation

- If we only use the unary terms. How would you do inference in this case?

Stereo Estimation

- If we only use the unary terms. How would you do inference in this case?

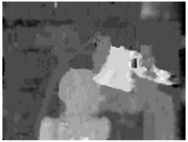
- If full graphical model



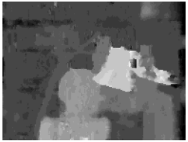
[Credit: Coughlan BP Tutorial]

Subsequent iterations:

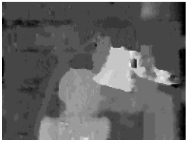
2



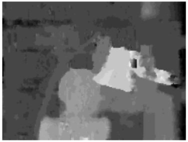
3



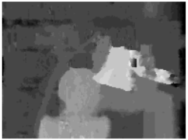
4



5



… 20



Note:

Little change after first few iterations.

Model can be improved to give better results

-- this is just a simple example to illustrate BP.

[Credit: Coughlan BP Tutorial]