Variational Methods, Belief Propagation, & Graphical Models

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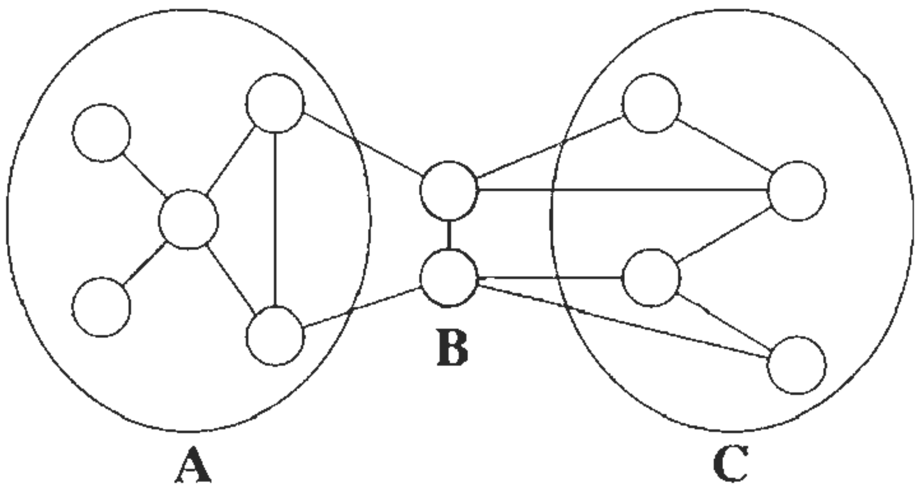
Undirected Graphical Models

An undirected graph $\mathcal{G}$ is defined by

$\mathcal{V} \longrightarrow$ set of N nodes $\{1, 2, \ldots, N\}$

$\mathcal{E} \longrightarrow$ set of edges (s, t) connecting nodes $s, t \in \mathcal{V}$

Nodes $s \in \mathcal{V}$ are associated with random variables x_s



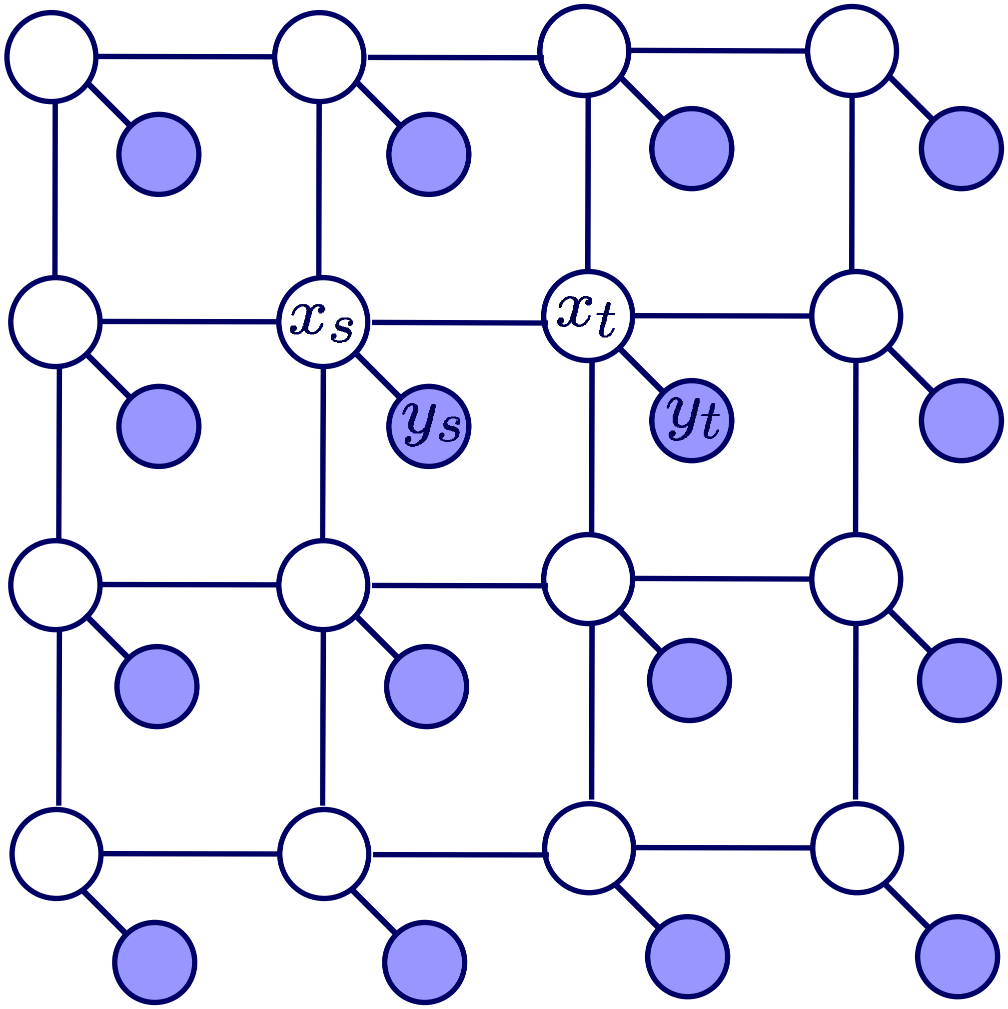
Graph Separation

$\updownarrow$

Conditional Independence

$$p(x_A, x_C | x_B) = p(x_A | x_B) p(x_C | x_B)$$

Nearest-Neighbor Grids



Low Level Vision

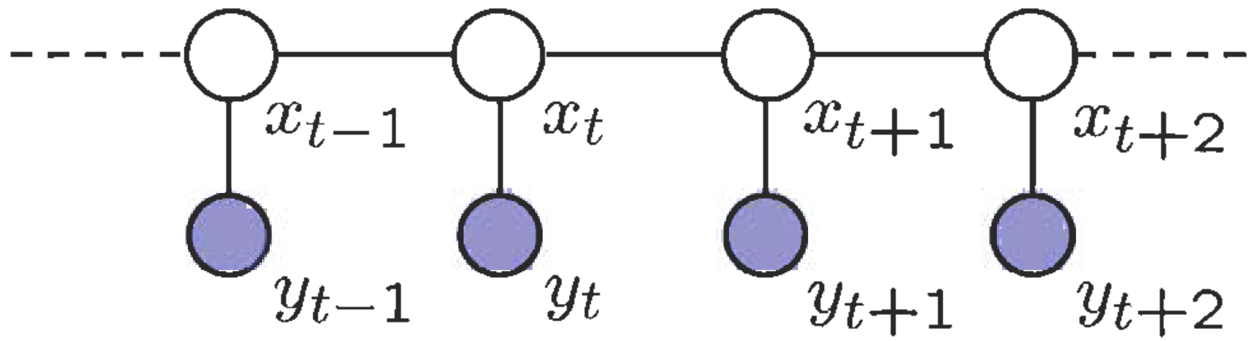
- Image denoising
- Stereo
- Optical flow
- Shape from shading
- Superresolution
- Segmentation

$x_s \longrightarrow$ unobserved or hidden variable

$y_s \longrightarrow$ local observation of x_s

Hidden Markov Models (HMMs)

Visual Tracking



$$\boxed{p(x,y) = p(x_0) \prod_{t=1}^{T} p(x_t \mid x_{t-1}) p(y_t \mid x_t)}$$

"Conditioned on the present, the past and future are statistically independent"

Other Graphical Models

Images removed due to copyright considerations.

Articulated Models

Pictorial Structures (Constellation Models)

Outline

Inference in Graphical Models

- Pairwise Markov random fields
- Belief propagation for trees

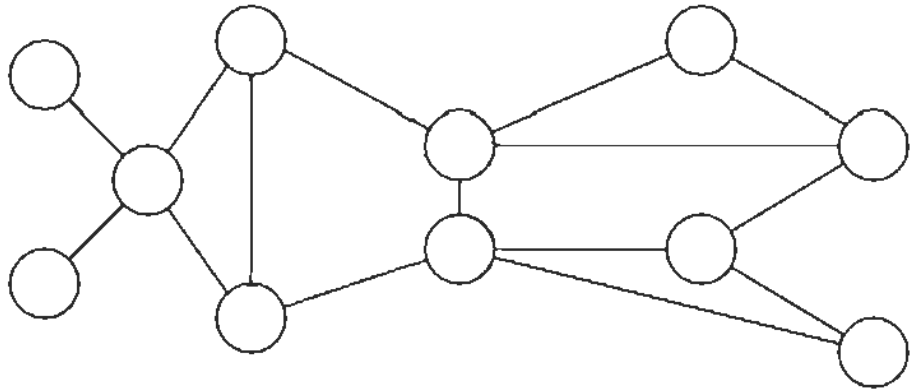
Variational Methods

- Mean field
- Bethe approximation & BP

Extensions of Belief Propagation

- Efficient message passing implementation
- Generalized BP
- Particle filters and nonparametric BP

Pairwise Markov Random Fields



$$p(x \mid y) = \frac{1}{Z} \prod_{(s,t)\in\mathcal{E}} \psi_{st}(x_s, x_t) \prod_{s\in\mathcal{V}} \psi_s(x_s, y)$$

$\mathcal{V} \longrightarrow$ set of N nodes $\{1, 2, \ldots, N\}$

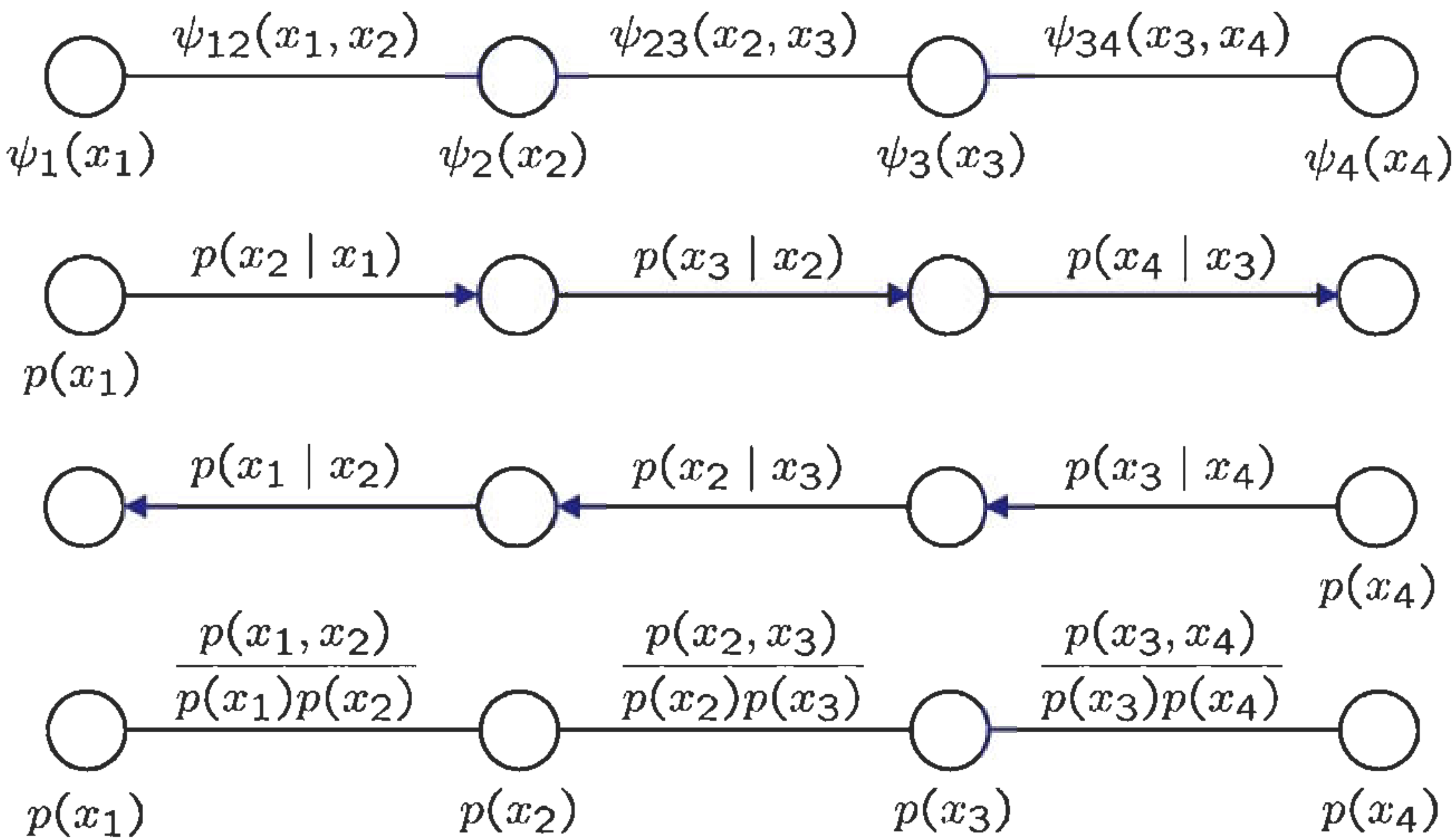
$\mathcal{E} \longrightarrow$ set of edges (s, t) connecting nodes $s, t \in \mathcal{V}$

$Z \longrightarrow$ normalization constant (partition function)

- Product of arbitrary positive *clique potential* functions
- Guaranteed Markov with respect to corresponding graph

Markov Chain Factorizations

$$p(x \mid y) = \frac{1}{Z} \prod_{(s,t) \in \mathcal{E}} \psi_{st}(x_s, x_t) \prod_{s \in \mathcal{V}} \psi_s(x_s, y)$$



Energy Functions

$$
\begin{aligned}
p(x \mid y) &= \frac{1}{Z} \prod_{(s,t)\in\mathcal{E}} \psi_{st}(x_s, x_t) \prod_{s\in\mathcal{V}} \psi_s(x_s, y) \\
&= \frac{1}{Z} \exp\left\{ - \sum_{(s,t)\in\mathcal{E}} \phi_{st}(x_s, x_t) - \sum_{s\in\mathcal{V}} \phi_s(x_s, y) \right\} \\
&= \frac{1}{Z} \exp\{-E(x)\}
\end{aligned}
$$

$$\phi_{st}(x_s, x_t) = -\log \psi_{st}(x_s, x_t) \qquad \phi_s(x_s) = -\log \psi_s(x_s)$$

- Interpretation inspired by statistical physics
- Justifications from probability (notational convenience)

Probabilistic Inference

$$p(x \mid y) = \frac{1}{Z} \prod_{(s,t)\in\mathcal{E}} \psi_{st}(x_s, x_t) \prod_{s\in\mathcal{V}} \psi_s(x_s, y)$$

Maximum a Posteriori (MAP) Estimate

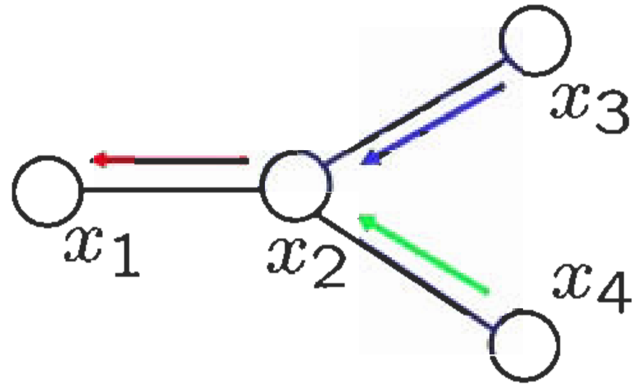
$$\hat{x} = \arg\max_{x} \; p(x \mid y)$$

Posterior Marginal Densities

$$p_t(x_t \mid y) = \sum_{x_{\mathcal{V}\setminus t}} p(x \mid y)$$

- Bayes least squares estimate
- Maximizer of the Posterior Marginals (MPM)
- Measures of confidence in these estimates

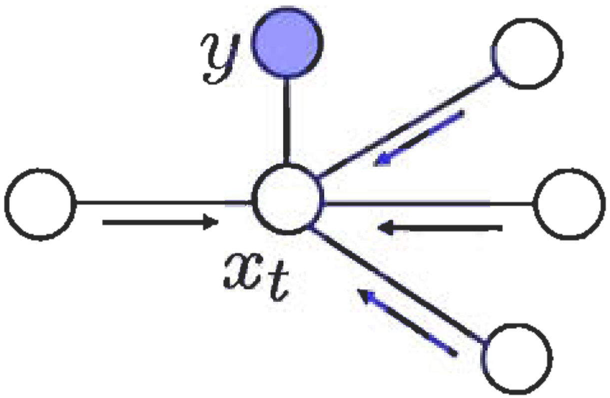
Inference via the Distributed Law



$$
\begin{aligned}
p_1(x_1) &= \sum_{x_2,x_3,x_4} \psi_1(x_1)\psi_{12}(x_1,x_2)\psi_2(x_2)\psi_{23}(x_2,x_3)\psi_3(x_3)\psi_{24}(x_2,x_4)\psi_4(x_4) \\
&= \psi_1(x_1) \sum_{x_2,x_3,x_4} \psi_{12}(x_1,x_2)\psi_2(x_2)\psi_{23}(x_2,x_3)\psi_3(x_3)\psi_{24}(x_2,x_4)\psi_4(x_4) \\
&= \psi_1(x_1) \sum_{x_2} \psi_{12}(x_1,x_2)\psi_2(x_2) \sum_{x_3,x_4} \psi_{23}(x_2,x_3)\psi_3(x_3)\psi_{24}(x_2,x_4)\psi_4(x_4) \\
&= \psi_1(x_1) \underbrace{\sum_{x_2} \psi_{12}(x_1,x_2)\psi_2(x_2) \underbrace{\left[\sum_{x_3} \psi_{23}(x_2,x_3)\psi_3(x_3)\right]}_{m_{32}(x_2)} \cdot \underbrace{\left[\sum_{x_4} \psi_{24}(x_2,x_4)\psi_4(x_4)\right]}_{m_{42}(x_2)}}_{m_{21}(x_1) = \sum_{x_2} \psi_{12}(x_1,x_2)\psi_2(x_2)m_{32}(x_2)m_{42}(x_2)}
\end{aligned}
$$

Belief Propagation (Sum-Product)

BELIEFS: Posterior marginals (possibly approximate)

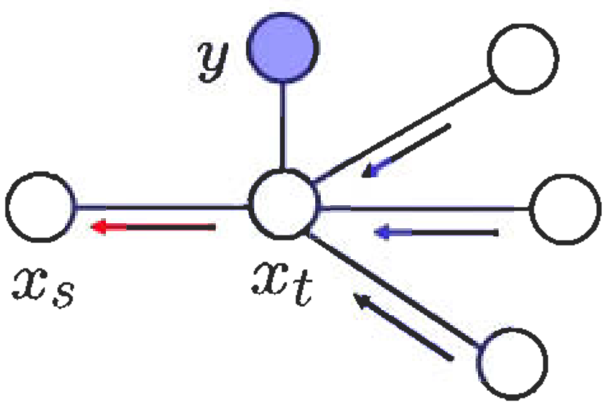


$$q_t(x_t \mid y) = \alpha \psi_t(x_t, y) \prod_{u \in \Gamma(t)} m_{ut}(x_t)$$

$\Gamma(t) \longrightarrow$ *neighborhood* of node *t* (adjacent nodes)

MESSAGES: Sufficient statistics (possibly approximate)

$$m_{ts}(x_s) = \alpha \sum_{x_t} \psi_{st}(x_s, x_t) \psi_t(x_t, y) \prod_{u \in \Gamma(t) \setminus s} m_{ut}(x_t)$$



I) Message Product
II) Message Propagation

Belief Propagation for Trees

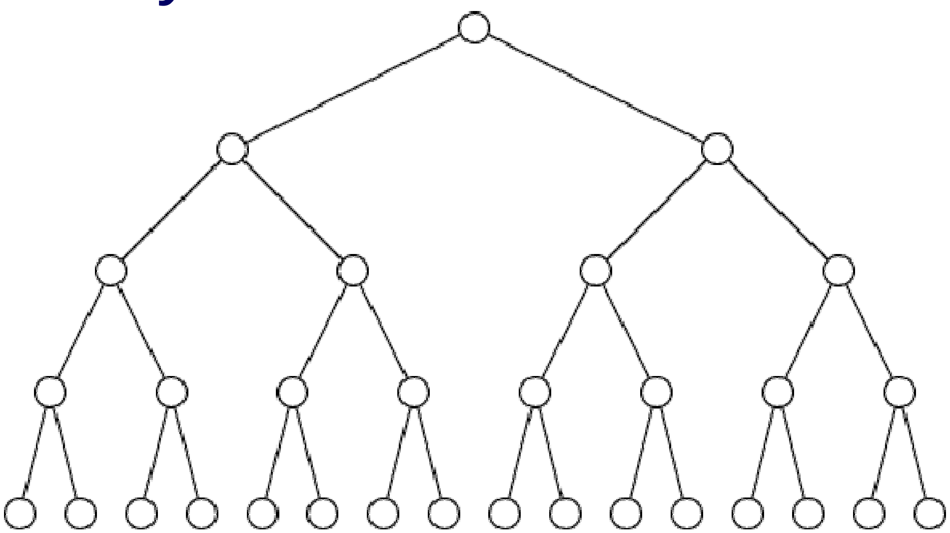
- Dynamic programming algorithm which exactly computes all marginals
- On Markov chains, BP equivalent to alpha-beta or forward-backward algorithms for HMMs
- Sequential *message schedules* require each message to be updated only once
- Computational cost:

$N \longrightarrow$ *number of nodes*

$M \longrightarrow$ *discrete states for each node*

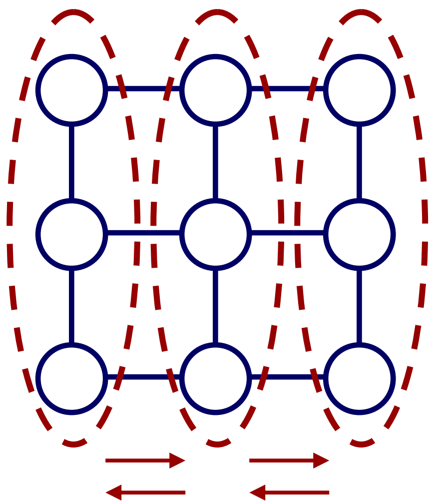
Belief Prop: $\mathcal{O}(NM^2)$

Brute Force: $\mathcal{O}(M^N)$



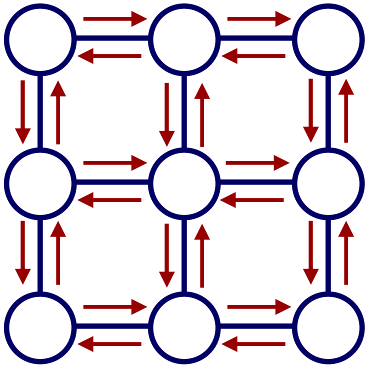
Inference for Graphs with Cycles

- For graphs with cycles, the dynamic programming BP derivation breaks



Junction Tree Algorithm

- Cluster nodes to break cycles
- Run BP on the tree of clusters
- Exact, but often intractable



Loopy Belief Propagation

- Iterate local BP message updates on the graph with cycles
- Hope beliefs converge
- Empirically, often very effective…

A Brief History of Loopy BP

- *1993:* Turbo codes (and later LDPC codes, rediscovered from Gallager's *1963* thesis) revolutionize error correcting codes *(Berrou et. al.)*
- *1995-1997:* Realization that turbo decoding algorithm is equivalent to loopy BP *(MacKay & Neal)*
- *1997-1999:* Promising results in other domains, & theoretical analysis via computation trees *(Weiss)*
- *2000:* Connection between loopy BP & variational approximations, using ideas from statistical physics *(Yedidia, Freeman, & Weiss)*
- *2001-2005:* Many results interpreting, justifying, and extending loopy BP

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Approximate Inference Framework

$$p(x \mid y) = \frac{1}{Z} \prod_{(s,t)\in\mathcal{E}} \psi_{st}(x_s, x_t) \prod_{s\in\mathcal{V}} \psi_s(x_s, y)$$

- Choose a family of approximating distributions which is tractable. The simplest example:

$$q(x) = \prod_{s\in\mathcal{V}} q_s(x_s)$$

- Define a distance to measure the quality of different approximations. Two possibilities:

$$D(p \,||\, q) = \sum_x p(x \mid y) \log \frac{p(x \mid y)}{q(x)}$$

$$D(q \,||\, p) = \sum_x q(x) \log \frac{q(x)}{p(x \mid y)}$$

- Find the approximation minimizing this distance

Fully Factored Approximations

$$p(x \mid y) = \frac{1}{Z} \prod_{(s,t)\in\mathcal{E}} \psi_{st}(x_s, x_t) \prod_{s\in\mathcal{V}} \psi_s(x_s, y)$$

$$q(x) = \prod_{s\in\mathcal{V}} q_s(x_s)$$

$$D(p \,||\, q) = \sum_x p(x \mid y) \log \frac{p(x \mid y)}{q(x)}$$

$$= \left[\sum_{s\in\mathcal{V}} H_s(p_s) - H(p) \right] + \sum_{s\in\mathcal{V}} D(p_s \,||\, q_s)$$

Marginal Entropies

Joint Entropy

- Trivially minimized by setting $q_s(x_s) = p_s(x_s \mid y)$
- Doesn't provide a computational method…

Variational Approximations

$$D(q(x) \,||\, p(x \mid y)) = \sum_x q(x) \log \frac{q(x)}{p(x \mid y)}$$

$$\begin{aligned}
\log p(y) &= \log \sum_x p(x, y) \\
&= \log \sum_x q(x) \frac{p(x, y)}{q(x)} && \textit{(Multiply by one)} \\
&\geq \underbrace{\sum_x q(x) \log \frac{p(x, y)}{q(x)}}_{= -D(q(x) \,||\, p(x \mid y)) + \log p(y)} && \textit{(Jensen's inequality)}
\end{aligned}$$

- Minimizing KL divergence maximizes a lower bound on the data likelihood

Free Energies

$$p(x \mid y) = \frac{1}{Z} \exp\{-E(x)\}$$

$$\begin{aligned} D(q \,||\, p) &= \sum_x q(x) \log q(x) - \sum_x q(x) \log p(x \mid y) \\ &= \underbrace{\underbrace{-H(q)}_{\text{Negative Entropy}} + \underbrace{\sum_x q(x) E(x)}_{\text{Average Energy}}}_{\text{Gibbs Free Energy}} + \underbrace{\log Z}_{\text{Normalization}} \end{aligned}$$

- Free energies equivalent to KL divergence, up to a normalization constant

Mean Field Free Energy

$$\boxed{\begin{aligned} p(x \mid y) &= \frac{1}{Z} \exp\left\{ - \sum_{(s,t)\in\mathcal{E}} \phi_{st}(x_s, x_t) - \sum_{s\in\mathcal{V}} \phi_s(x_s, y) \right\} \\ q(x) &= \prod_{s\in\mathcal{V}} q_s(x_s) \end{aligned}}$$

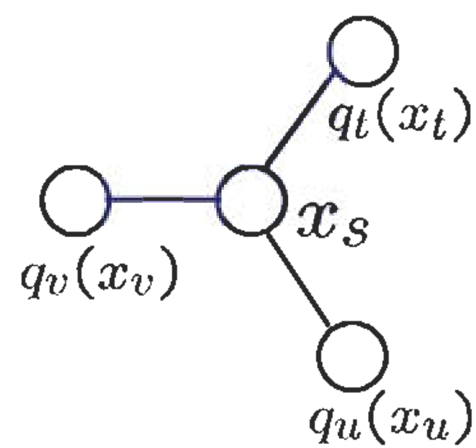
$$\begin{aligned} D(q \,||\, p) &= -H(q) + \sum_x q(x) E(x) + \log Z \\ &= - \sum_{s\in\mathcal{V}} H_s(q_s) + \sum_{(s,t)\in\mathcal{E}} q_s(x_s) q_t(x_t) \phi_{st}(x_s, x_t) \\ &\quad \cdots + \sum_{s\in\mathcal{V}} q_s(x_s) \phi_s(x_s) + \log Z \end{aligned}$$

Mean Field Equations

$$D(q \,||\, p) = -\sum_{s \in \mathcal{V}} H_s(q_s) + \sum_{(s,t) \in \mathcal{E}} q_s(x_s) q_t(x_t) \phi_{st}(x_s, x_t)$$
$$\cdots + \sum_{s \in \mathcal{V}} q_s(x_s) \phi_s(x_s) + \log Z$$

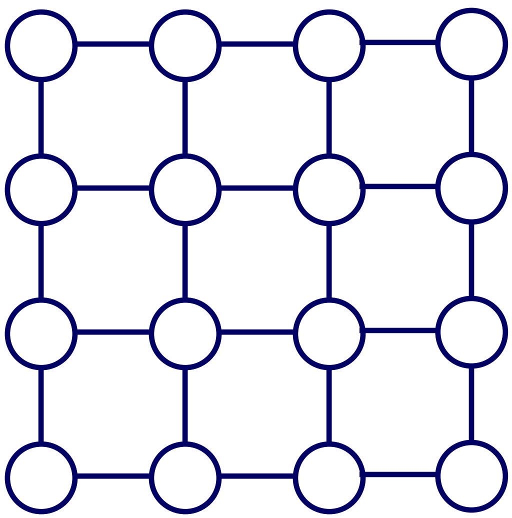
- Add Lagrange multipliers to enforce $\sum_{x_s} q_s(x_s) = 1$
- Taking derivatives and simplifying, we find a set of fixed point equations:

$$q_s(x_s) = \alpha \psi_s(x_s) \prod_{t \in \Gamma(s)} \prod_{x_t} \psi_{st}(x_s, x_t)^{q_t(x_t)}$$

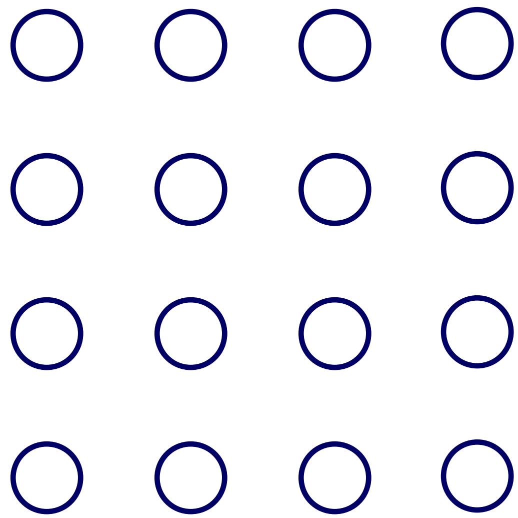


- Updating one marginal at a time gives convergent coordinate descent

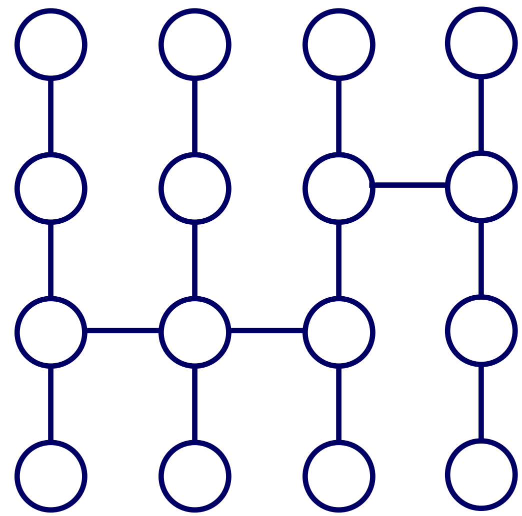
Structured Mean Field



Original Graph



Naïve Mean Field

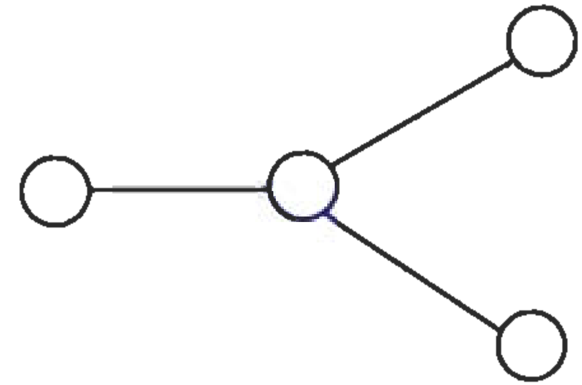


Structured Mean Field

- Any subgraph for which inference is tractable leads to a mean field style approximation for which the update equations are tractable

Tree Structured Free Energies

- Trees *exactly* factorize as



$$q(x) = \prod_{(s,t)\in\mathcal{E}} \frac{q_{st}(x_s, x_t)}{q_s(x_s)q_t(x_t)} \prod_{s\in\mathcal{V}} q_s(x_s)$$

- We may then optimize over *all* distributions which are Markov with respect to a tree-structured graph:

$$D(q \,||\, p) = -H(q) + \sum_x q(x)E(x) + \log Z$$

$$\sum_x q(x)E(x) = \sum_{(s,t)\in\mathcal{E}} q_{st}(x_s, x_t)\phi_{st}(x_s, x_t) + \sum_{s\in\mathcal{V}} q_s(x_s)\phi_s(x_s)$$

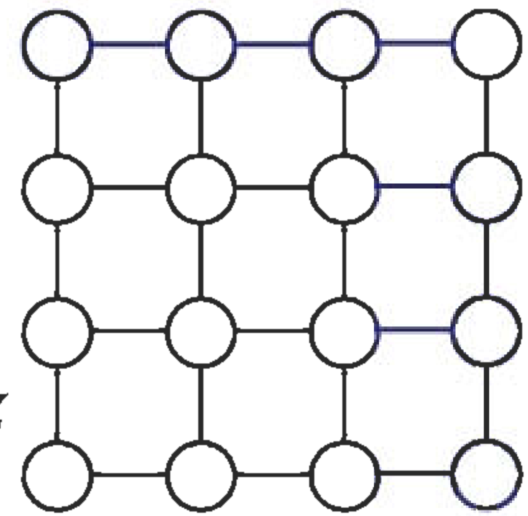
$$H(q) = \sum_{s\in\mathcal{V}} H_s(q_s) - \sum_{(s,t)\in\mathcal{E}} I_{st}(q_{st})$$

Marginal Entropies

Mutual Information

Bethe Free Energy

- Bethe approximation uses the tree-structured free energy form even though the graph has cycles



$$D(q \,||\, p) = -H(q) + \sum_x q(x)E(x) + \log Z$$

Average Energy (exact for pairwise MRFs)

$$\sum_x q(x)E(x) = \sum_{(s,t)\in\mathcal{E}} q_{st}(x_s, x_t)\phi_{st}(x_s, x_t) + \sum_{s\in\mathcal{V}} q_s(x_s)\phi_s(x_s)$$

Approximate Entropy

$$H(q) \approx \sum_{s\in\mathcal{V}} H_s(q_s) - \sum_{(s,t)\in\mathcal{E}} I_{st}(q_{st})$$

Minimizing Bethe Free Energy

$$D(q \,||\, p) = -H(q) + \sum_x q(x)E(x) + \log Z$$

$$\sum_x q(x)E(x) = \sum_{(s,t)\in\mathcal{E}} q_{st}(x_s, x_t)\phi_{st}(x_s, x_t) + \sum_{s\in\mathcal{V}} q_s(x_s)\phi_s(x_s)$$

$$H(q) \approx \sum_{s\in\mathcal{V}} H_s(q_s) - \sum_{(s,t)\in\mathcal{E}} I_{st}(q_{st})$$

- Add Lagrange multipliers to enforce normalizations:

$$\lambda_{st}(x_t) \longleftrightarrow \sum_{x_s} q_{st}(x_s, x_t) = q_t(x_t) \qquad\qquad \sum_{x_s} q_s(x_s) = 1$$

- Taking derivatives and simplifying,

$$q_t(x_t) = \alpha \exp\left\{\phi_t(x_t) + \frac{1}{|\Gamma(t)| - 1} \sum_{s\in\Gamma(t)} \lambda_{st}(x_t)\right\}$$

$$q_{st}(x_s, x_t) = \alpha \exp\left\{\phi_{st}(x_s, x_t) + \phi_s(x_s) + \phi_t(x_t) + \lambda_{ts}(x_s) + \lambda_{st}(x_t)\right\}$$

Bethe and Belief Propagation

Bethe Fixed Points

$$q_t(x_t) = \alpha \psi_t(x_t) \exp \left\{ \frac{1}{|\Gamma(t)| - 1} \sum_{s \in \Gamma(t)} \lambda_{st}(x_t) \right\}$$

$$q_{st}(x_s, x_t) = \alpha \psi_{st}(x_s, x_t) \psi_s(x_s) \psi_t(x_t) \exp \{\lambda_{ts}(x_s) + \lambda_{st}(x_t)\}$$

Belief Propagation

$$q_t(x_t) = \alpha \psi_t(x_t, y) \prod_{u \in \Gamma(t)} m_{ut}(x_t)$$

$$q_{st}(x_s, x_t) = \alpha \psi_{st}(x_s, x_t) \psi_s(x_s) \psi_t(x_t) \prod_{u \in \Gamma(s) \backslash t} m_{us}(x_s) \prod_{v \in \Gamma(t) \backslash s} m_{vt}(x_t)$$

$$m_{ts}(x_s) = \alpha \sum_{x_t} \psi_{st}(x_s, x_t) \psi_t(x_t, y) \prod_{u \in \Gamma(t) \backslash s} m_{ut}(x_t)$$

Correspondence

$$\boxed{\lambda_{st}(x_t) = \log \prod_{u \in \Gamma(t) \backslash s} m_{ut}(x_t)}$$

Implications for Loopy BP

Bethe Free Energy is an Approximation

- BP may have multiple fixed points (non-convex)
- BP is not guaranteed to converge
- Few general guarantees on BP's accuracy

Characterizations of BP Fixed Points

- All graphical models have at least one BP fixed point
- Stable fixed points are local minima of Bethe
- For graphs with cycles, BP is almost never exact
- As cycles grow long, BP becomes exact (coding)

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Double-Loop Algorithms

(Yuille & Rangarajan, Neural Comp. 2003)

$$D(q \,||\, p) = -H(q) + \sum_x q(x)E(x) + \log Z$$

$$\sum_x q(x)E(x) = \sum_{(s,t)\in\mathcal{E}} q_{st}(x_s, x_t)\phi_{st}(x_s, x_t) + \sum_{s\in\mathcal{V}} q_s(x_s)\phi_s(x_s)$$

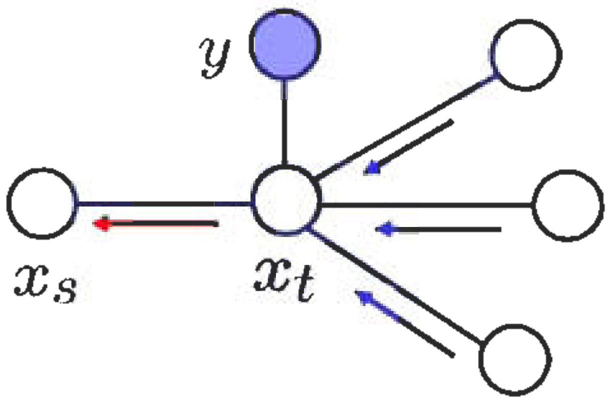
$$H(q) \approx \sum_{s\in\mathcal{V}} H_s(q_s) - \sum_{(s,t)\in\mathcal{E}} I_{st}(q_{st})$$

- Directly minimize Bethe free energy
- Guaranteed to converge to a local optimum
- Much slower than loopy BP
- Some theory and experimental results suggesting that when BP doesn't converge, it's a sign that Bethe approximation is bad

Efficient Message Updates

(Felzenszwalb & Huttenlocher)

$$m_{ts}(x_s) = \alpha \sum_{x_t} \psi_{st}(x_s, x_t)\psi_t(x_t, y) \prod_{u \in \Gamma(t) \backslash s} m_{ut}(x_t)$$



$N \longrightarrow$ *number of nodes*

$M \longrightarrow$ *discrete states for each node*

- Message update is matrix-vector product $(\mathcal{O}(M^2))$
- For pairwise potentials which depend only on the difference $(x_s - x_t)$, this becomes a convolution
  - FFT message updates in $\mathcal{O}(M \log M)$
  - Other approximations sometimes allow $\mathcal{O}(M)$

Dynamic Quantization

(Coughlan et. al., ECCV 2002 & 2004 CVPR GMBV workshop)

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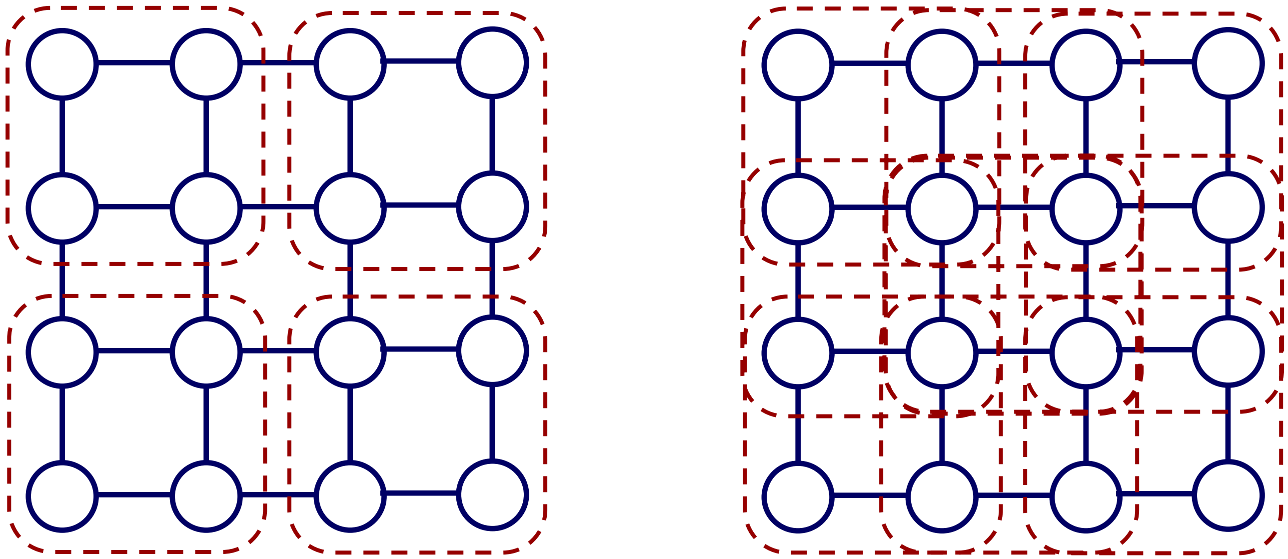
- Deformable template: State at each node is discretization of position and orientation of some point along the letter contour
- Rules for pruning unlikely states based on local evidence, and current message estimates, allow efficient, nearly *globally optimal* matching

Generalized Belief Propagation

(Yedidia, Freeman, & Weiss, NIPS 2000)



- Big idea: cluster nodes to break shortest cycles
- Non-overlapping clusters: exactly equivalent to loopy BP on the graph of cluster nodes
- Overlapping clusters: higher-order Kikuchi free energies ensure that information not over-counted

BP for Continuous Variables

$$q_t(x_t) = \alpha \psi_t(x_t, y) \prod_{u \in \Gamma(t)} m_{ut}(x_t)$$

$$m_{ts}(x_s) = \alpha \int_{x_t} \psi_{st}(x_s, x_t) \psi_t(x_t, y) \prod_{u \in \Gamma(t) \setminus s} m_{ut}(x_t) \, dx_t$$

Jointly Gaussian Variables

- Messages represented by mean and covariance
- BP updates are generalizations of the Kalman filter
- If BP converges, means exact, but variances approximate

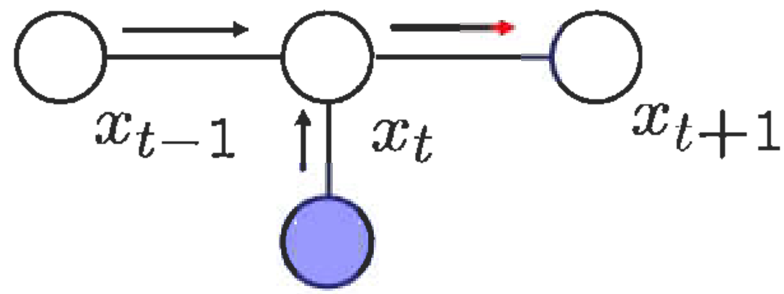
Continuous Non-Gaussian Variables

- Closed parametric forms usually do not exist
- Discretization can be intractable in as few as 2-3 dim.

Particle Filters

Condensation, Sequential Monte Carlo, Survival of the Fittest,…

- Nonparametric approximation to optimal BP estimates
- Represent messages and posteriors using a set of samples, found by simulation



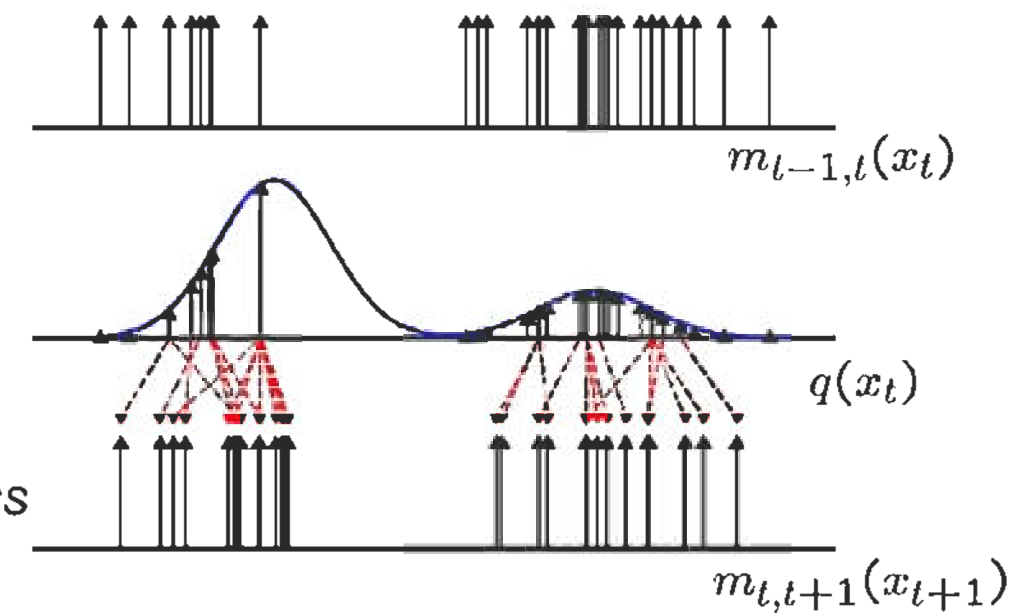
Sample-based density estimate

↓

Weight by observation likelihood

↓

Resample & propagate by dynamics



Nonparametric Belief Propagation

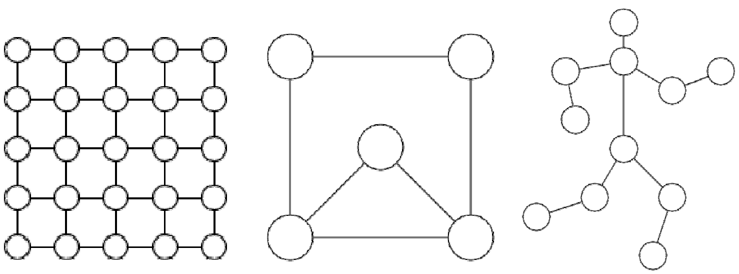
(Sudderth, Ihler, Freeman, & Willsky)

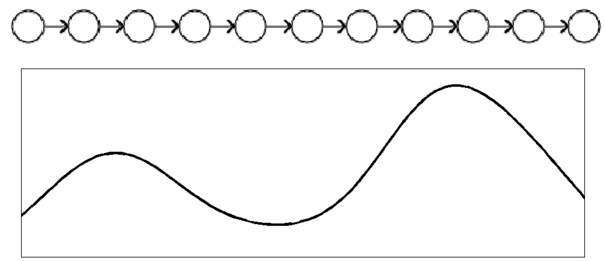
Belief Propagation

- General graphs
- Discrete or Gaussian

Particle Filters

- Markov chains
- General potentials





Nonparametric BP

- General graphs
- General potentials