

Belief Propagation and Free Energy

David Kappel

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Outline

Bayesian Networks, Markov Random Fields and Factor Graphs

Standard Belief Propagation

Free Energies

Summary

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Bayesian Networks

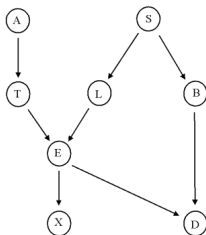
- ▶ Popular graphical model in AI literature.
- ▶ Directed graph structure.
- ▶ Applications: Medical diagnosis, language understanding, heuristic search ...

"Asia" Medical Diagnosis

Medical system modelling statistical dependencies between symptoms, test results and diseases:

- ▶ A recent trip to Asia (A) increases the chances to tuberculosis (T).
- ▶ Smoking (S) is a risk factor for both lung cancer (L) and bronchitis (B).
- ▶ The presence of either (E) tuberculosis or lung cancer can be detected by an X-ray results (X), but the X-ray alone cannot distinguish between them.
- ▶ Dyspnoea (D) (shortness of breath) may be caused by bronchitis (B), or either (E) tuberculosis or lung cancer.

"Asia" Medical Diagnosis



$$p(\mathbf{x}) = p(x_A)p(x_S)p(x_T | x_A)p(x_B | x_S) \times \quad (1) \\ p(x_E | x_L, x_T)p(x_D | x_B, x_E)p(x_X | x_E)$$

Bayesian Networks

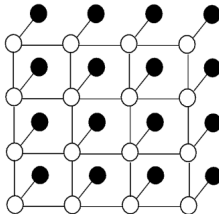
joint probability:

$$p(x_1, x_2, \dots, x_N) = \prod_{i=1}^N p(x_i \mid \text{Par}(x_i)) \quad (2)$$

marginal probability:

$$p(x_i) = \sum_{\{x\} \setminus x_i} p(x_1, x_2, \dots, x_N) \quad (3)$$

Pairwise Markov Random Fields



- ▶ Undirected graph model.
- ▶ Low level computer vision, image y_i , scene x_i .

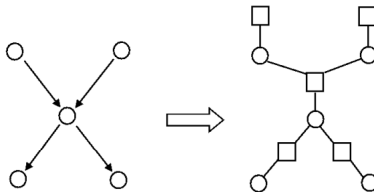
Pairwise Markov Random Fields

- ▶ evidence function $\phi_i(x_i, y_i)$
- ▶ compatibility function $\psi_{ij}(x_i, x_j)$

joint probability:

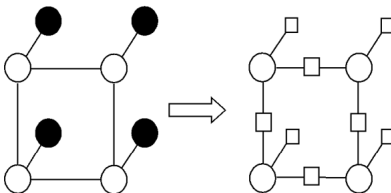
$$p(\mathbf{x}, \mathbf{y}) = \frac{1}{Z} \prod_{(i,j)} \psi_{ij}(x_i, x_j) \prod_i \phi_i(x_i, y_i) \quad (4)$$

Converting Bayesian Networks to Factor Graphs



Factor graph functions $\psi_a(\{x\}_a)$ directly correspond to Bayesian network probabilities $p(x_i \mid \text{Par}(x_i))$.

Converting Markov Random Fields to Factor Graphs



- ▶ Observed nodes replaced by single node functions $\phi_i(x_i, y_i)$
- ▶ Two node functions $\psi_{ij}(x_i, x_j)$ linking hidden nodes

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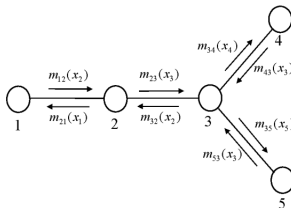
Standard Belief Propagation

joint probability:

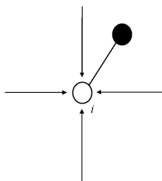
$$p(\mathbf{x}) = \frac{1}{Z} \prod_{(i,j)} \psi_{ij}(x_i, x_j) \prod_i \phi_i(x_i) \quad (5)$$

marginal probability:

$$p(x_i) = \sum_{\mathbf{x} \setminus x_i} p(x_1, x_2, \dots, x_N) \quad (6)$$



Message Passing



$$b_i(x_i) = k\phi_i(x_i) \prod_{j \in N(x_i)} m_{ij}(x_i) \quad (7)$$

$$m_{ij}(x_i) \leftarrow \sum_{x_i} \phi_i(x_i) \psi_{ij}(x_i, x_j) \prod_{k \in N(x_i) \setminus j} m_{ki}(x_i) \quad (8)$$

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Free Energies

- ▶ A system of N particles.
- ▶ Each which can in one of a discrete number of states.
- ▶ The state of the system: $\mathbf{x} = \{x_1, x_2, \dots, x_N\}$
- ▶ Each state has a corresponding energy $E(\mathbf{x})$

Boltzmann's law:

$$p(\mathbf{x}) = \frac{1}{Z} e^{-E(\mathbf{x})/T} \quad (9)$$

The Potts and Ising Models

- ▶ field $h_i(x_i, y_i) = \ln \phi_i(x_i, y_i)$
- ▶ interaction $J_{ij}(x_i, x_j) = \ln \psi_{ij}(x_i, x_j)$

Potts model energy:

$$E(\mathbf{x}) = - \sum_{(i,j)} J_{ij}(x_i, x_j) - \sum_i h_i(x_i, y_i) \quad (10)$$

Boltzmann law:

$$p(\mathbf{x}) = \frac{1}{Z} e^{-E(\mathbf{x})/T}$$

$$\rightarrow p(\mathbf{x}) = \frac{1}{Z} \prod_{(i,j)} \psi_{ij}(x_i, x_j) \prod_i \phi_i(x_i, y_i)$$

The Helmholtz free energy

- ▶ Important quantity in statistical mechanics.
- ▶ Many techniques exist which give good approximations.

partition function (normalisation constant):

$$Z = \sum_{\mathbf{x} \in S} e^{-E(\mathbf{x})/T} \quad (11)$$

Helmholtz Free Energy:

$$F_H = -\ln Z \quad (12)$$

Variational approach:

- ▶ True probability distribution $p(\mathbf{x})$.
- ▶ Trail probability distribution $b(\mathbf{x})$.

Gibbs Free Energy:

$$F(b) = U(b) - H(b) \quad (13)$$

Average energy:

$$U(b) = \sum_{\mathbf{x} \in S} b(\mathbf{x}) E(\mathbf{x}) \quad (14)$$

Variational entropy:

$$H(b) = - \sum_{\mathbf{x} \in S} b(\mathbf{x}) \ln b(\mathbf{x}) \quad (15)$$

Gibbs Free Energy

$$\begin{aligned} F(b) &= U(b) - H(b) \\ &= \sum_{\mathbf{x} \in S} b(\mathbf{x}) E(\mathbf{x}) + \sum_{\mathbf{x} \in S} b(\mathbf{x}) \ln b(\mathbf{x}) \\ &= \sum_{\mathbf{x} \in S} b(\mathbf{x}) (E(\mathbf{x}) + \ln b(\mathbf{x})) \end{aligned}$$

using Boltzmann's law:

$$\begin{aligned} p(\mathbf{x}) &= \frac{1}{Z} e^{-E(\mathbf{x})} \\ E(\mathbf{x}) &= -\ln Z - \ln p(\mathbf{x}) \\ E(\mathbf{x}) &= F_H - \ln p(\mathbf{x}) \end{aligned}$$

Gibbs Free Energy

$$\begin{aligned} F(b) &= \sum_{\mathbf{x} \in S} b(\mathbf{x}) (F_H - \ln p(\mathbf{x}) + \ln b(\mathbf{x})) \\ &= F_H + \sum_{\mathbf{x} \in S} b(\mathbf{x}) \ln \frac{b(\mathbf{x})}{p(\mathbf{x})} \\ &= F_H + D_{KL}(b|p) \end{aligned}$$

With $D_{KL}(b|p)$, the Kullback-Leibler divergence.

Gibbs Free Energy

- ▶ BP is equal to minimizing the variational free energy.
- ▶ If graph is loop-free the solution is exact.
- ▶ If graph has loops the results are equal to the Bethe approximation from statistical mechanics.

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- ▶ Different disciplines have yielded different approaches and models.
- ▶ Yet, the methods are similar and can be converted into each other.
- ▶ Belief Propagation can be understood as a solution to an energy minimisation problem.

Questions?

References

- ▶ Belief propagation and its relation to free energy [1, 3].
- ▶ Further readings on graphical models [2].



Jonathan S. Yedidia, William T. Freeman, and Yair Weiss.

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Technical report, Mitsubishi Electric Research Laboratories, 2002.



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