### From Belief Propagation to Generalised Belief Propagation

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#### Outline

- Backgrounds on Graphical Models
- Backgrounds on Statistical Physics
- Region-Based Approximation
- A Special Case: Bethe Approximation and Recovering BP
- Region Graph Method and Generalized Belief Propagation (GBP)
- GBP for Estimating the Partition Function of the 2D Ising Model

# Backgrounds on Graphical Models

#### Graphical Models Is All About Factorization

• Consider n random variables $X_1, \ldots, X_n$  where  $X_i \in \mathcal{X}_i$ 

$$p(x_1,\ldots,x_n) = \prod_{a \in A} \psi_a(x_a)$$

Probabilistic notions such as conditional independence <==> Graph-theoretic notions such as cliques and separation

- Generally two types of graphical models are common in practice
  - Bayesian Network (directed graphical models)
  - Markov Random Field (undirected graphical models)

#### Bayesian Network

 $\pi(i)$ 

 The probability distribution is factorized according to a directed acyclic graph

$$p(x_1, \dots, x_n) = \prod_{i \in V} p_i(x_i | x_{\pi(i)})$$
$$p_i(x_i | x_{\pi(i)}) \ge 0$$
$$\int p_i(x_i | x_{\pi(i)}) = 1$$

•  $p_i(x_i|x_{\pi(i)})$  is indeed a conditional probability distribution

- Let G(V, E) be an undirected graph and  $p(x_V) > 0$ 
  - Global Markov Property:

 $\forall W \subseteq V : \quad p(x_W | x_{V \setminus W}) = p(x_W | x_{\Delta W})$ 



• Let G(V, E) be an undirected graph and  $p(x_V) > 0$ 



• Example:



$$p(x_1, \dots, x_7) = \frac{1}{Z} \psi_{1234}(x_1, \dots, x_4) \psi_{456}(x_4, x_5, x_6) \psi_{67}(x_6, x_7)$$

• Example:



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#### Factor Graph

Let V = {1,...,n} and A indexes the factors
=> A factor graph is a bipartite graph G = (V, A, E)

$$p(\boldsymbol{x}) \triangleq p(x_1, \dots, x_n) = \frac{1}{Z} \prod_{a \in A} \psi_a(\boldsymbol{x}_a)$$
$$Z = \sum_{\boldsymbol{x}} \prod_{a \in A} \psi_a(\boldsymbol{x}_a)$$



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• Example:  $V = \{1, ..., 7\}$  and  $A = \{a, b, c\}$ 



#### Two Important Problems!

• Computing the marginal distribution  $p(\mathbf{x}_W)$  over a particular subset  $W \subset V$  of nodes

$$p(\boldsymbol{x}_W) = \sum_{\boldsymbol{x} \setminus \boldsymbol{x}_W} p(\boldsymbol{x})$$

• Computing a mode of the density

 $\underset{\boldsymbol{x}\in\mathcal{X}^n}{\arg\max} p(\boldsymbol{x})$ 

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#### In general, these problems are hard!

• Example: Consider binary random variables  $X_0, \ldots, X_{100}$ . To compute  $p(x_0)$  we need to sum over an exponential number of terms:

$$p(x_0) = \sum_{x_1, \dots, x_{100} \in \{0, 1\}} p(x_0, x_1, \dots, x_{100})$$

- The partition function Z of a graphical model encodes important information about the underlying distribution
  - Z is an important quantity for physicist => from Z we can compute experimentally measurable quantities
  - If all  $\psi_a$  are hard constraints => Z counts the number of valid configuration in the system

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Z = number of valid Sudoku configurations

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• Message update rules:

 $n_{i \to a}(x_i) = \prod_{c \in N(i) \setminus a} m_{c \to i}(x_i)$ 



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• Message update rules:







• How to compute the marginals?

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• How to compute the marginals?



BP is exact on trees, but only gives an approximation on graphs with cycles!

# Backgrounds on Statistical Physics

#### Boltzmann Law

 A fundamental result of statistical mechanics is that, in thermal equilibrium, the probability of a state will be given by Boltzmann's distribution:

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

Alternative point of view



#### Energy Assigned to a Factor Graph

- Consider factor graph G = (V, A, E)
  - For probability distribution

$$p(\boldsymbol{x}) = \frac{1}{Z} \prod_{a \in A} f_a(\boldsymbol{x}_a)$$

we can define energy of state x as

$$E(\boldsymbol{x}) = -\sum_{a \in A} \ln f_a(\boldsymbol{x}_a)$$

#### (Helmholtz) Free Energy

• Free energy of a system is defined as

$$F_H \triangleq U - H$$

• *U* is average energy:

$$U \triangleq \sum_{\boldsymbol{x}} p(\boldsymbol{x}) E(\boldsymbol{x})$$

• *H* is entropy:

$$H = -\sum_{\boldsymbol{x}} p(\boldsymbol{x}) \ln p(\boldsymbol{x})$$

- $p(\boldsymbol{x})$  is the actual probability distribution of the system
- Note that we have  $F_H = -\ln Z$

Variational Approach (Gibbs Free Energy)

• Instead of true probability distribution p(x) consider some other distribution b(x). Then define

 $F(b) \triangleq U(b) - H(b)$ 

• where 
$$U(b) \triangleq \sum_{x} b(x) E(x)$$
$$H(b) \triangleq \sum_{x} b(x) \ln b(x)$$
• We can show 
$$x$$

$$F(b) = F_H + D(b||p)$$

= F(b) takes its minimum at b(x) = p(x)

#### Variational Approach

• Consider the following optimization problem

 $F_{H} = \begin{cases} \min F(b) \\ \text{s.t. } b \text{ is a joint probability distribution over } \boldsymbol{x} \end{cases}$ 

- This optimization problem provides an exact procedure for computing the partition function (in fact  $F_H$ ) and recovering p(x)
- Bad news: this problem is at least as hard as the original problem of partition function computation

As n becomes large, this method is intractable!

• Good news: we can use it to develop approximation methods!

# A General Approach to Upper Bound $F_H$

• A more practical approach to upper bound  $F_H$  is to minimize F(b) over a restricted class of probability distribution



• Example: mean-field approximation

$$b_{\rm MF} = \prod_{i \in V} b_i(x_i)$$

 We can extend this method by considering more complicated form for b(x) that leads to a tractable distribution.
=> Example: structured mean-field approach

#### A General Approximation Approach

$$\min_{b} F(b)$$
  
s.t.  $0 \le b(\boldsymbol{x}) \le 1, \quad \forall \boldsymbol{x}$   
$$\sum_{\boldsymbol{x}} b(\boldsymbol{x}) = 1$$

#### A General Approximation Approach


### A General Approximation Approach





All distributions

**Region-Based Approximation** 











• Break the factor graph into regions



• Approximate the overall free energy as: the sum of the free energy of all the regions

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• Approximate the overall free energy as: the sum of the free energy of all the regions

$$F_{\mathcal{R}} \approx \sum_{R \in \mathcal{R}} F_R(b_R)$$

Heuristic: to have a good approximation => Find good set of regions

• A region *R* of a factor graph consists of  $V_R$  and  $A_R$  such that: if  $a \in A_R \Rightarrow N(a) \in V_R$ 



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• Associated quantities of a region:

Region Energy
$$E_R(\boldsymbol{x}_R) \triangleq -\sum_{a \in A_R} \log f_a(\boldsymbol{x}_a)$$

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Region Energy	Region Entropy	Region Average Energy
$E_R(\boldsymbol{x}_R) \triangleq -\sum_{a \in A_R} \log f_a(\boldsymbol{x}_a)$	$H_R(b_R) \triangleq -\sum_{\boldsymbol{x}_R} b_R(\boldsymbol{x}_R) \log b_R(\boldsymbol{x}_R)$	$U_R(b_R) \triangleq \sum_{\boldsymbol{x}_R} b_R(\boldsymbol{x}_R) E_R(\boldsymbol{x}_R)$

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Region (Gibbs) Free Energy

 $F_R(b_R) \triangleq U_R(b_R) - H_R(b_R)$ 

### **Region-Based Approximation**

• Region-based (approximate) entropy:

$$H_{\mathcal{R}}(\{b_R\}) \triangleq \sum_{R \in \mathcal{R}} c_R H_R(b_R)$$

• Region-based average energy:

$$U_{\mathcal{R}}(\{b_R\}) \triangleq \sum_{R \in \mathcal{R}} c_R U_R(b_R)$$

• Region-based (Gibbs) free energy:

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### Valid Region-Based Approximation

• Definition: A set of regions  $\mathcal{R}$  and associated counting numbers  $C_R$  give a valid approximation if:

$$\sum_{R \in \mathcal{R}} c_R I_{A_R}(a) = \sum_{R \in \mathcal{R}} c_R I_{V_R}(i) = 1, \qquad \forall i \in V \text{ and } \forall a \in A$$

- Why valid region-based approximation?
  - If  $b_R(\boldsymbol{x}) = p_R(\boldsymbol{x}) \Rightarrow U = U_R(\{b_R\})$
  - In general  $H \neq H_{\mathcal{R}}(\{b_R\})$  but H is equal to  $H_{\mathcal{R}}(\{b_R\})$ up to total number of degrees of freedom in the system

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#### Region-Based Approximation (Constraints on Beliefs)

1. Normalization:  $\forall R \in \mathcal{R}, b_R(\boldsymbol{x}_R)$  forms a probability function:

$$\sum_{\boldsymbol{x}_R} b_R(\boldsymbol{x}_R) = 1$$

2. Local consistency: if the set of variable nodes  $W \subseteq R \cap S$ :

$$\sum_{oldsymbol{x}_R ackslash oldsymbol{x}_W} b_R(oldsymbol{x}_R) = \sum_{oldsymbol{x}_S ackslash oldsymbol{x}_W} b_S(oldsymbol{x}_S)$$



3. Inequality:  $0 \le b_R(\boldsymbol{x}_R) \le 1$ 

The above expressions give a set of local constraints!

A Special Case: Bethe Approximation and Recovering BP

- Two types of regions, large and small:  $\mathcal{R} = \mathcal{R}_L \cup \mathcal{R}_S$
- n regions in  $\mathcal{R}_S$  each contains one variable node
- m regions in  $\mathcal{R}_L$  each contains one factor node and the neighboring variable nodes



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$$\mathcal{R}_L: (a, 1, 2, 4, 5)(b, 2, 5)(c, 2, 3, 5, 6)$$
  
 $\mathcal{R}_S: (1)(2)(3)(4)(5)(6)$ 

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$$c_{R} = 1$$

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$$R = \{i\} \Rightarrow c_{R} = 1 - d_{i}$$

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Good news: this choice of counting numbers give a valid approximation for variational free energy!







#### Bethe Approximation (Constraints on Beliefs)

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  - Normalization:  $\sum_{\boldsymbol{x}_a} b_a(\boldsymbol{x}_a) = \sum_{x_i} b_i(x_i) = 1, \quad \forall i \in V \text{ and } \forall a \in A$
  - Consistency:  $\sum_{\boldsymbol{x}_a \setminus x_i} b_a(\boldsymbol{x}_a) = b_i(x_i), \quad \forall a \in A \text{ and } \forall i \in N(a)$
  - Inequality:  $0 \le b(\boldsymbol{x}_a) \le 1$ ,  $0 \le b_i(x_i) \le 1$ ,  $\forall a \in A \text{ and } \forall i \in V$

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### Connection Between Bethe Approximation and BP

• Theorem:


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#### • Theorem:

 $\begin{array}{c} \begin{array}{c} \text{Interior stationary points of} \\ \text{Bethe Free Energy} \end{array} & \begin{array}{c} & \\ \end{array} & \\ \end{array} & \begin{array}{c} \text{BP fixed points with} \\ \text{positive beliefs} \end{array} \end{array}$   $\begin{array}{c} \text{min } F_{\text{Bethe}} = \min_{b} \left[ U_{\text{Bethe}} - H_{\text{Bethe}} \right] \\ \text{s.t. } \sum_{x_a} b_a(x_a) = 1 \\ \sum_{x_a} b_a(x_a) = b_i(x_i) \end{array}$   $\begin{array}{c} \text{min } F_{\text{Bethe}} = \min_{b} \left[ U_{\text{Bethe}} - H_{\text{Bethe}} \right] \\ \text{ni}_{i \to a}(x_i) = \sum_{x_a \setminus x_i} f_a(x_a) \prod_{j \in N(a) \setminus i} n_{j \to a}(x_j) \\ n_{i \to a}(x_i) = \prod_{c \in N(i) \setminus a} m_{c \to i}(x_i) \\ \text{min } F_{a \to i}(x_i) = \sum_{x_a \setminus x_i} b_a(x_a) = b_i(x_i) \end{array}$ 

$$\sum_{x_i} b_i(x_i) = 1$$
$$0 \le b_a(\boldsymbol{x}_a) \le 1$$
$$0 \le b_i(x_i) \le 1$$

#### • Theorem:

Interior stationary points of BP fixed points with **Bethe Free Energy** positive beliefs  $m_{a \to i}(x_i) = \sum f_a(\boldsymbol{x}_a) \prod n_{j \to a}(x_j)$  $\min_{L} F_{\text{Bethe}} = \min_{L} \left[ U_{\text{Bethe}} - H_{\text{Bethe}} \right]$  $\boldsymbol{x}_a \setminus x_i \qquad j \in N(a) \setminus i$ s.t.  $\sum_{\boldsymbol{x}_a} b_a(\boldsymbol{x}_a) = 1$  $\sum_{\boldsymbol{x}_a \setminus x_i} b_a(\boldsymbol{x}_a) = b_i(x_i)$  $\sum_{x_i} b_i(x_i) = 1$  $n_{i \to a}(x_i) = \prod m_{c \to i}(x_i)$  $c \in N(i) \setminus a$ Leads to the interior stationary points  $0 \leq b_a(\boldsymbol{x}_a) \leq 1$  $0 \leq b_i(x_i) \leq 1$ 

#### • Theorem:

Interior stationary points of Bethe Free Energy

$$\min_{b} F_{\text{Bethe}} = \min_{b} \left[ U_{\text{Bethe}} - H_{\text{Bethe}} \right]$$

s.t. 
$$\sum_{\boldsymbol{x}_a} b_a(\boldsymbol{x}_a) = 1$$
$$\sum_{\boldsymbol{x}_a \setminus x_i} b_a(\boldsymbol{x}_a) = b_i(x_i)$$
$$\sum_{\boldsymbol{x}_i} b_i(x_i) = 1$$

$$0 \le b_a(\boldsymbol{x}_a) \le 1$$

 $0 \le b_i(x_i) \le 1$ 

$$m_{a \to i}(x_i) = \sum_{\boldsymbol{x}_a \setminus x_i} f_a(\boldsymbol{x}_a) \prod_{j \in N(a) \setminus i} n_{j \to a}(x_j)$$

$$n_{i \to a}(x_i) = \prod_{c \in N(i) \setminus a} m_{c \to i}(x_i)$$

BP fixed points with

positive beliefs

Leads to the interior stationary points

#### Proof Idea (using Lagrange method)

- Write the Lagrangian of the Bethe optimization problem
- Take derivative of  ${\cal L}$  and find the stationary points of  $F_{
  m Bethe}$
- By appropriate change of variables, connect them to BP update rule

# Region Graph Method and Generalized Belief Propagation





























• Definition: region graph  $\mathcal{G}_{RG} = (\mathcal{V}_{RG}, \mathcal{E}_{RG})$ each vertex —> a region of the original factor graph G = (V, A, E)



• Counting numbers:  $c_v = 1 - \sum_{u \in \mathcal{A}(v)} c_u$ ,  $\forall v \in \mathcal{G}_{RG}$  —> a valid approximation!



- Counting numbers:  $c_v = 1 \sum_{u \in \mathcal{A}(v)} c_u$ ,  $\forall v \in \mathcal{G}_{RG} \longrightarrow a \text{ valid approximation}!$
- $\forall \alpha \in V \cup A \longrightarrow \mathcal{G}_{RG}(\alpha)$  is a connected graph!

# The Region-Based Approximation)

• The region-based (Gibbs) free energy approximation

$$F_{\mathcal{R}}(\{b_R\}) = \sum_{R \in \mathcal{R}} c_R F_R(b_R)$$

• Approximate free energy optimization problem:  $\min_{\{b_R\}} F_{\mathcal{R}}(\{b_R\})$ 

s.t. 
$$\sum_{\boldsymbol{x}_P \setminus \boldsymbol{x}_C} b_P(\boldsymbol{x}_P) = b_C(\boldsymbol{x}_C)$$
  
 $\sum_{\boldsymbol{x}_R} b_R(\boldsymbol{x}_R) = 1$   
 $0 \le b_R(\boldsymbol{x}_R) \le 1$ 

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$$b_P \propto (m_{A \to P} \ m_{B \to P}) (m_{C \to R} \ m_{C \to G} \ m_{E \to G}) \prod_{a \in A_P} f_a(\boldsymbol{x}_a)$$



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$$b_R \propto (m_{P \to R} \ m_{C \to R}) (m_{D \to F} \ m_{C \to G} \ m_{E \to G}) \prod_{a \in A_R} f_a(\boldsymbol{x}_a)$$



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$$b_R(oldsymbol{x}_R) = \sum_{oldsymbol{x}_P ackslash oldsymbol{x}_R} b_P(oldsymbol{x}_P)$$



# Connection Between Region Graph Method and GBP

• Theorem:



 In contrast to Bethe approximation: people started from the region-based approximation and using Lagrange method derived the GBP algorithm

# Generalized Belief Propagation

- Generalized belief propagation has other variations:
  - Parent to child algorithm
  - Child to parent algorithm
  - two-way algorithm
- The BP algorithm is a special case of all the above algorithms if the regions are chosen according to Bethe approximation
- The GBP is more complex than BP but it provides more flexibility in terms of choosing the regions (i.e. how to approximate Gibbs free energy)

#### Generalized Belief Propagation for Estimating the Partition Function of the 2D Ising Model

joint work with

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# 2D Ising Model

- Motivated by a 2D run-length limited (RLL) constraints problem
  - A symmetric (d, k) RLL constraint imposes (horizontally and vertically):
    - At least d zero symbols between two ones
    - At most k zero symbols between two ones
- Sabato, G. and Molkaraie observed that GBP can potentially outperform BP approximating capacity of an RLL problem

### Capacity of 2D (1, $\infty$ )-RLL Constraint


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• C\_GBP • C\_BP

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• C\_GBP • C\_BP

$$C(m,m) = \frac{\log_2 Z(m,m)}{m \times m}$$

### 2D Binary Ising Model

























































$$F_{\mathcal{R}}(\{b_R\}) = \sum_{R \in \mathcal{R}} c_R F_R(b_R)$$



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## Previous Work and Our Result

• Previous work:

For any binary log-supermodular graphical model, for any fixed pound of BP, we have

$$Z \ge Z_{\rm BP}(\{b_i, b_a\}).$$
  $F_{\rm B}(\{b_i, b_a\}) = -\log Z_{\rm BP}(\{b_i, b_a\})$ 

• Our result:

For  $R_{m \times n}$  based on 2D Ising model of size no large than 5 x 5 or 3 x n, for any fixed pound of GBP, we have

$$Z \geq Z_{\mathcal{R},\text{GBP}}(\{b_R\}). \qquad F_{\mathcal{R}}(\{b_R\}) = -\log Z_{\mathcal{R},\text{GBP}}(\{b_R\})$$

• Conjecture:

The above statement is true for any  $R_{m \times n}$  based on 2D Ising model of any size

## Proof Idea

• First, we show that

$$\frac{Z}{Z_{\mathcal{R},\mathrm{GBP}}(\{b_R\})} = \sum_{\boldsymbol{x}} \prod_{R \in \mathcal{R}} (b_R(\boldsymbol{x}_R))^{c_R}$$

- Using result of Ruozzi, we can show that the 2D Ising model can be transformed to a log-supermodular graphical model
  - This transformation preserves the partition function and also does not change the fixed-point-based approximation of partition function using GBP
- Next, we analyze the above ratio for binary pairwise graphical models with log-supermodular factor function

# Thank You!


## Some of the References

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