Estimating the Capacity of the 2-D Hard Square Constraint Using Generalized Belief Propagation

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1-D RLL Constraints

Let $0 \leq d < k \leq \infty$ be fixed integers (k is allowed to be ∞).

Definition

A binary sequence $x_1 x_2 \ldots x_n \in \{0, 1\}^n$ satisfies the (one-dimensional) (d, k)-runlength-limited (RLL) constraint if any pair of successive 1s in the sequence is separated by at least d and at most k 0s.

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Codes consisting of sequences satisfying a (d, k)-RLL constraint are used for writing information on magnetic and optical recording devices such as hard drives and CDs/DVDs.

The maximum rate of such a code is given by the capacity of the (d, k)-RLL constraint, defined as

$$C_{d,k} = \lim_{n \to \infty} \frac{1}{n} \log_2 Z_n^{(d,k)}$$

where $Z_n^{(d,k)}$ denotes the number of binary length-n sequences satisfying the constraint.

The 1-D $(1, \infty)$-RLL Constraint

A binary sequence satisfies the $(1, \infty)$-RLL constraint if it does not contain 1s in adjacent (i.e., consecutive) positions.

Some easy facts about $Z_n := Z_n^{(1,\infty)}$:

- Z_n, $n = 1, 2, 3, \ldots$, forms a Fibonacci sequence

$$Z_1 = 2, \quad Z_2 = 3, \quad \text{and} \quad Z_n = Z_{n-1} + Z_{n-2} \text{ for all } n \geq 3$$

- $C_{1,\infty} := \lim_{n \to \infty} \frac{1}{n} \log_2 Z_n = \log_2 \frac{1+\sqrt{5}}{2} = 0.6942\ldots$

The 2-D Hard Square Constraint

Definition

A binary $m \times n$ array satisfies the 2-D hard square constraint (also called the 2-D $(1, \infty)$-RLL constraint) if no row or column of the array contains 1s in adjacent positions.

Each such array can also be viewed as an independent set in the $m \times n$ grid graph.

The Hard-Square Entropy Constant

Let $Z_{m,n}$ denote the number of such $m \times n$ arrays.

It can be shown (for example, using subadditivity arguments) that the limit

$$\eta = \lim_{m,n\to\infty} \frac{1}{mn} \log_2(Z_{m,n})$$

exists. This limit is called the hard-square entropy constant.

Open Problem: Determine the hard-square entropy constant η.

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Open Problem: Determine the hard-square entropy constant η.

What is known:

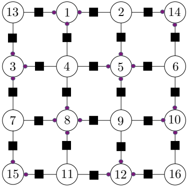
- Various upper and lower bounds, resulting in the numerical estimate

  $$\eta = 0.58789116\ldots$$

  [Justesen & Forchhammer, 1999]

- η is computable to within an accuracy of $\frac{1}{N}$ in time polynomial in N [Pavlov, 2010]

Binary Ising Model on the 2-D Lattice



- $m \times n$ grid with mn vertices and $2mn - (m + n)$ edges
- Variable $x_i \in \{0, 1\}$ at each vertex i
- Pairwise function $f : \{0, 1\} \times \{0, 1\} \to \mathbb{R}_+$
- Defines a joint distribution on $\{0, 1\}^{m \times n}$:

$$p(\mathbf{x}) = \frac{1}{Z} \prod_{i \sim j} f(x_i, x_j)$$

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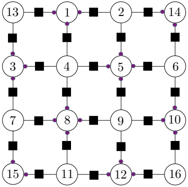

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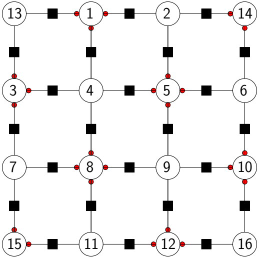
- Quantity of interest:

$$Z = \sum_{\mathbf{x}} \prod_{i \sim j} f(x_i, x_j)$$

Called the partition function.

Special Case: Hard-Square Model



$$f(a,b) = \mathbf{1}_{(a,b)\neq(1,1)}$$

The partition function here is precisely $Z_{m,n}$.

Gibbs Free Energy

Define the energy of a configuration $\mathbf{x} \in \{0,1\}^{m \times n}$ to be

$$E(\mathbf{x}) = -\sum_{i \sim j} \log f(x_i, x_j)$$

so that $p(\mathbf{x}) = \frac{1}{Z} \exp(-E(\mathbf{x}))$.

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For an arbitrary probability distribution $b(\mathbf{x})$ on $\{0,1\}^{m \times n}$, define

- the average energy

$$U(b) = \sum_{\mathbf{x}} b(\mathbf{x}) E(\mathbf{x})$$

- the entropy

$$H(b) = -\sum_{\mathbf{x}} b(\mathbf{x}) \log b(\mathbf{x})$$

- the Gibbs free energy

$$F(b) = U(b) - H(b)$$

A Variational Principle

$$-\log Z = \min_b F(b)$$

Proof: Write

$$\begin{aligned} F(b) &= -\log Z + \sum_{\mathbf{x}} b(\mathbf{x}) \log \frac{b(\mathbf{x})}{p(\mathbf{x})} \\ &= -\log Z + D(b \parallel p) \end{aligned}$$

The Bethe Free Energy

Let $(b_{i,j}(x_i, x_j))$ and $(b_i(x_i))$ be "beliefs" defined for all edges $i \sim j$ and vertices i, respectively. These must satisfy the following:

- the $b_{i,j}$s and b_is are probability mass functions on $\{0,1\}^2$ and $\{0,1\}$, respectively
- $\sum_{x_j} b_{i,j}(x_i, x_j) = b_i(x_i)$ (consistency)

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We then define

- the Bethe average energy

$$U_{\mathrm{B}}(\{b_{i,j}\}, \{b_i\}) = \sum_{i \sim j} \sum_{(a,b) \in \{0,1\}^2} b_{i,j}(a,b) \log f(a,b)$$

- the Bethe entropy

$$H_{\mathrm{B}}(\{b_{i,j}\}, \{b_i\}) = \sum_{i \sim j} H(b_{i,j}) - \sum_i (d_i - 1) H(b_i)$$

  where d_i denotes the degree of the vertex i.

- the Bethe free energy

$$F_{\mathrm{B}}(\{b_{i,j}\}, \{b_i\}) = U_{\mathrm{B}}(\{b_{i,j}\}, \{b_i\}) - H_{\mathrm{B}}(\{b_{i,j}\}, \{b_i\})$$

The Bethe Approximation

$$-\log Z_{\mathrm{B}} := \min_{\{b_{i,j}\},\{b_i\}} F_{\mathrm{B}}(\{b_{i,j}\},\{b_i\})$$

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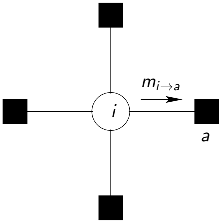
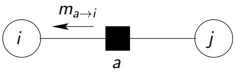
Theorem (Yedidia, Freeman and Weiss, 2001)

Stationary points of the Bethe free energy functional correspond to the beliefs at fixed points of the belief propagation algorithm.

Belief Propagation (The Sum-Product Algorithm)





Message update rules:

- $m_{i \to a}(x_i) = \prod_{c \in N(i) \setminus a} m_{c \to i}(x_i)$
- $m_{a \to i}(x_i) = \sum_{x_j} f(x_i, x_j) m_{j \to a}(x_j)$

Beliefs:

- $b_i(x_i) \propto \prod_{a \in N(i)} m_{a \to i}(x_i)$
- $b_a(x_i, x_j) \propto f(x_i, x_j) m_{i \to a}(x_i) m_{j \to a}(x_j)$

(the use of $\propto$ indicates that the beliefs must be normalized to sum to 1)

How Good is the Bethe Approximation?

For beliefs $\{b_{i,j}\}$ and $\{b_i\}$ at a fixed point of the BP algorithm, define

$$Z_{\mathrm{BP}}(\{b_{i,j}\},\{b_i\}) := \exp\big(-F_{\mathrm{B}}(\{b_{i,j}\},\{b_i\})\big)$$

Theorem (Wainwright, Jaakkola and Willsky, 2003)

At any fixed point of the BP algorithm,

$$\frac{Z}{Z_{\mathrm{BP}}(\{b_{i,j}\},\{b_i\})} = \sum_{\mathbf{x}} \frac{\prod_{i\sim j} b_{i,j}(x_i,x_j)}{\prod_i b_i(x_i)^{d_i-1}}$$

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Theorem (Chertkov and Chernyak, 2006)

At any fixed point of the BP algorithm,

$$\frac{Z}{Z_{\mathrm{BP}}(\{b_{i,j}\},\{b_i\})} = 1 + \textit{ a finite series of correction terms}$$

How Good is the Bethe Approximation?

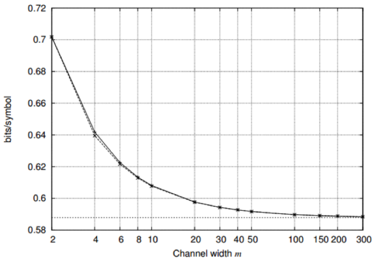
Theorem (Ruozzi, 2012)

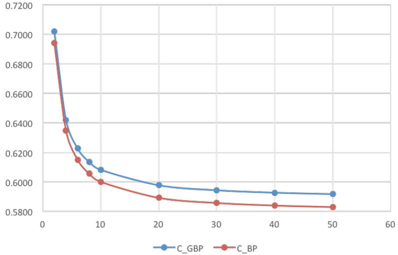
For the binary Ising model considered here,

$$Z \geq Z_{\mathrm{B}}.$$

Numerical Results for the Hard-Square Model

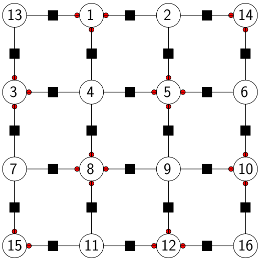
Recall: $\eta = 0.58789116\ldots$.

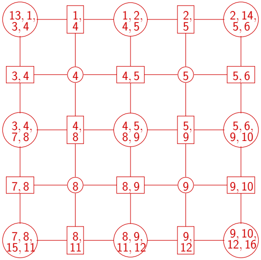




[Plot above is from Sabato and Molkaraie, 2012]

Regions and Region Graphs





$\mathcal{R} = \mathcal{R}_0 \cup \mathcal{R}_1 \cup \mathcal{R}_2$, where

- $\mathcal{R}_0$: all the 2x2 subgrids
- $\mathcal{R}_1$: all the non-boundary edges (intersections of regions in $\mathcal{R}_0$)
- $\mathcal{R}_2$: all the non-boundary vertices (intersections of regions in $\mathcal{R}_1$)

Region-Based Beliefs

Beliefs $b_R(\mathbf{x}_R)$ are defined for all regions $R \in \mathcal{R}$. These must satisfy the following:

- each b_R is a probability mass function on $\{0,1\}^{|R|}$, where $|R|$ denotes the size (number of vertices) of the region R;
- for regions $P \subset R$, we have $\sum_{\mathbf{x}_{R \setminus P}} b_R(\mathbf{x}_R) = b_P(\mathbf{x}_P)$ (consistency)

Region-Based Free Energy

Given a set of beliefs $\{b_R : R \in \mathcal{R}\}$, we define for each region $R \in \mathcal{R}$:

- the average energy of R

$$U_R = \sum_{\mathbf{x}_R \in \{0,1\}^{|R|}} \sum_{i,j \in R : i \sim j} b_R(\mathbf{x}_R) \log f(x_i, x_j)$$

- the entropy of b_R

$$H_R = -\sum_{\mathbf{x}_R} b_R(\mathbf{x}_R) \log b_R(\mathbf{x}_R)$$

- the free energy of R

$$F_R = U_R - H_R$$

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- the free energy of R

$$F_R = U_R - H_R$$

The region-based free energy of the model $(\mathcal{R}, \{b_R\})$ is defined as

$$F_{\mathcal{R}}(\{b_R\}) = \sum_{R \in \mathcal{R}_0} F_R - \sum_{R \in \mathcal{R}_1} F_R + \sum_{R \in \mathcal{R}_2} F_R$$

The Kikuchi Approximation

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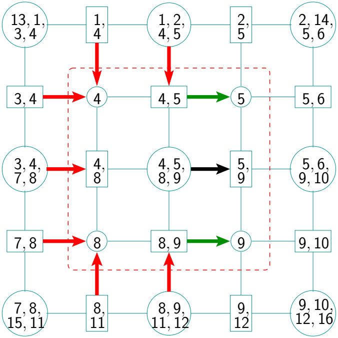
GBP Message Updates (The Parent-to-Child Algorithm)



$$m_{(4,5,8,9)\to(5,9)}(x_5, x_9) = \frac{\sum_{x_4, x_8} f(x_4, x_5) f(x_4, x_8) f(x_8, x_9) \prod \text{(red messages)}}{\prod \text{(green messages)}}$$

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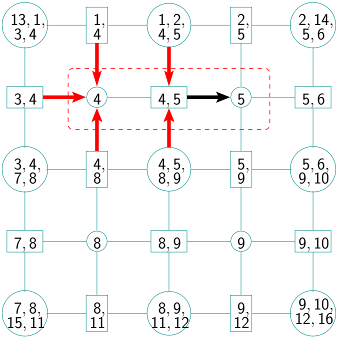
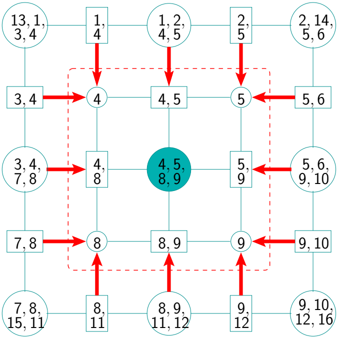


$$m_{(4,5)\to(5)}(x_5) = \sum_{x_4} f(x_4, x_5) \prod \text{(red messages)}$$

GBP Beliefs (The Parent-to-Child Algorithm)



$$b_{(4,5,8,9)}(x_4, x_5, x_8, x_9) \;\; \propto \;\; f(x_4, x_5) f(x_4, x_8) f(x_5, x_9) f(x_8, x_9) \prod \text{(red messages)}$$

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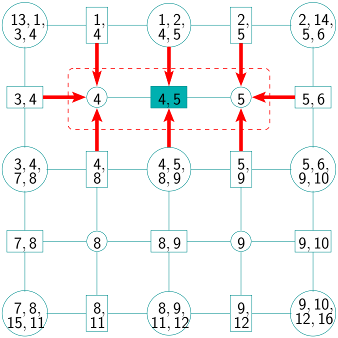
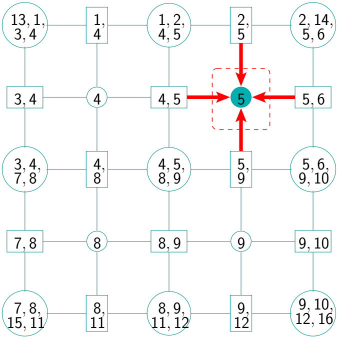


$$b_{(4,5)}(x_4, x_5) \quad \propto \quad f(x_4, x_5) \prod \text{(red messages)}$$

GBP Beliefs (The Parent-to-Child Algorithm)

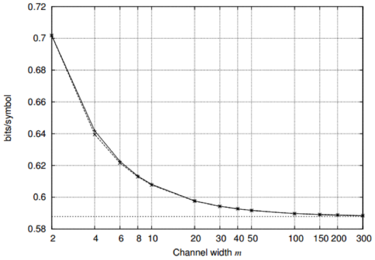


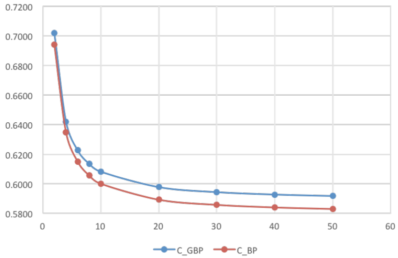
$$b_{(5)}(x_5) \propto \prod \text{(red messages)}$$

How Good is the Kikuchi Approximation?

Looking at the hard-square model again . . .

Recall: $\eta = 0.58789116\ldots$.





[Plot above is from Sabato and Molkaraie, 2012]

What We Conjecture

Conjecture (Chan et al., ISIT'14)

For the binary Ising model considered here,

$$\frac{1}{mn}\log Z - \frac{1}{mn}\log Z_{\mathcal{R}} = o(1)$$

where $o(1)$ *is a positive term that goes to* 0 *as* $m, n \to \infty$*.*

In other words, we conjecture that

$$\frac{Z}{Z_{\mathcal{R}}} = \exp\big(mn\, o(1)\big).$$

Attacking the Conjecture: The Opening Gambit

For beliefs $\{b_R\}$ at a fixed point of the GBP algorithm, define

$$Z_{\mathrm{GBP}}(\{b_R\}) := \exp\big(-F_{\mathcal{R}}(\{b_R\})\big)$$

Theorem (Chan et al., ISIT'14)

At a fixed point of the GBP algorithm,

$$\frac{Z}{Z_{\mathrm{GBP}}(\{b_R\})} = \sum_{\mathbf{x}} \frac{\prod_{R \in \mathcal{R}_0 \cup \mathcal{R}_2} b_R(\mathbf{x}_R)}{\prod_{R \in \mathcal{R}_1} b_R(\mathbf{x}_R)}$$

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Compare this with

Theorem (Wainwright, Jaakkola and Willsky, 2003)

At any fixed point of the BP algorithm,

$$\frac{Z}{Z_{\mathrm{BP}}(\{b_{i,j}\}, \{b_i\})} = \sum_{\mathbf{x}} \frac{\prod_{i \sim j} b_{i,j}(x_i, x_j)}{\prod_i b_i(x_i)^{d_i - 1}}$$

Question to be Addressed

Question

For the binary Ising model considered here, is it true that the beliefs $\{b_R\}$ *at a fixed point of GBP satisfy*

$$\frac{1}{mn}\log\sum_{\mathbf{x}}\frac{\prod_{R\in\mathcal{R}_0\cup\mathcal{R}_2} b_R(\mathbf{x}_R)}{\prod_{R\in\mathcal{R}_1} b_R(\mathbf{x}_R)} = o(1)$$

where $o(1)$ *is a positive term that goes to* 0 *as* $m, n \to \infty$*?*

What We Can Prove . . .

Theorem (Chan et al., ISIT'14)

For a binary Ising model of size at most 5×5*, or size equal to* $3 \times n$ *(or* $n \times 3$*) we have*

$$\sum_{\mathbf{x}} \frac{\prod_{R \in \mathcal{R}_0 \cup \mathcal{R}_2} b_R(\mathbf{x}_R)}{\prod_{R \in \mathcal{R}_1} b_R(\mathbf{x}_R)} \geq 1$$

at any fixed point of GBP. Consequently,

$$Z \geq Z_{\mathrm{GBP}}(\{b_R\})$$

at any fixed point of GBP.

A Key Tool: Log-Supermodularity

A function $g : \{0,1\}^k \to \mathbb{R}_+$ is called log-supermodular if

$$g(\mathbf{x})g(\mathbf{y}) \leq g(\mathbf{x} \vee \mathbf{y})g(\mathbf{x} \wedge \mathbf{y})$$

for all $\mathbf{x}, \mathbf{y} \in \{0,1\}^k$.

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Log-supermodularity is preserved under

- multiplication: g_1, g_2 log-supermodular $\implies$ $g_1 g_2$ log-supermodular
- marginalization: g log-supermodular $\implies$ $\sum_{x_1} g(\mathbf{x})$ log-supermod

  (this follows from the Ahlswede-Daykin four functions theorem)

Log-Supermodularity of Functions with Binary Inputs

- A function $f : \{0,1\}^2 \to \mathbb{R}_+$ is log-supermodular iff

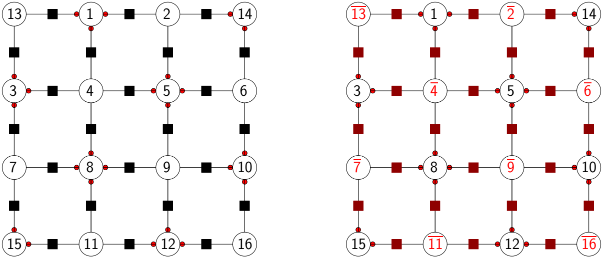
$$f(01)f(10) \leq f(00)f(11)$$

- If $f : \{0,1\}^2 \to \mathbb{R}_+$ is **not** log-supermodular, then the function

$$\bar{f}(a,b) = f(a, 1-b)$$

  is log-supermodular.

A Local Transformation



A binary Ising model defined by local functions f is equivalent to a binary Ising model defined by $\bar{f}$:

- The partition functions are equal: $Z(f) = Z(\bar{f})$
- For each set of beliefs $\{b_R\}$, there exists a corresponding $\{\bar{b}_R\}$ such that

$$\sum_{\mathbf{x}} \frac{\prod_{R \in \mathcal{R}_0 \cup \mathcal{R}_2} b_R(\mathbf{x}_R)}{\prod_{R \in \mathcal{R}_1} b_R(\mathbf{x}_R)} = \sum_{\mathbf{x}} \frac{\prod_{R \in \mathcal{R}_0 \cup \mathcal{R}_2} \bar{b}_R(\mathbf{x}_R)}{\prod_{R \in \mathcal{R}_1} \bar{b}_R(\mathbf{x}_R)}$$

Ising Models with Log-Supermodular Local Functions

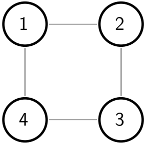
Lemma

In a binary Ising model with log-supermodular local functions, the BP and GBP message update rules preserve log-supermodularity of messages.

Thus, if BP and GBP are initialized with log-supermodular messages, then

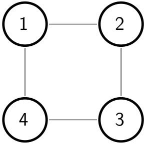
- the messages in subsequent iterations of BP and GBP remain log-supermodular, and
- the BP-based beliefs $b_{i,j}, b_i$ and the GBP-based beliefs b_R are all log-supermodular.

The 2×2 Grid



The Kikuchi approximation is exact: $Z_{\mathcal{R}} = Z$.

The 2×2 Grid



The Kikuchi approximation is exact: $Z_{\mathcal{R}} = Z$.

Theorem

For the 2×2 grid, at any fixed point of BP, we have

$$\frac{Z}{Z_{\mathrm{BP}}(\{b_{i,j}\},\{b_i\})} = 1 + \frac{\Delta_{1,2}\Delta_{2,3}\Delta_{3,4}\Delta_{4,1}}{\prod_i b_i(0)b_i(1)},$$

where $\Delta_{i,j} = b_{i,j}(00)b_{i,j}(11) - b_{i,j}(01)b_{i,j}(10)$.

Proof of 2×2 Theorem

- Start with Wainwright-Jaakkola-Willsky:

$$\frac{Z}{Z_{\mathrm{BP}}(\{b_{i,j}\}, \{b_i\})} = \sum_{x_1,\ldots,x_4} \frac{\prod_{i\sim j} b_{i,j}(x_i, x_j)}{\prod_i b_i(x_i)}$$
$$= \sum_{x_1,\ldots,x_4} \prod_i b_i(x_i) \prod_{i\sim j} \frac{b_{i,j}(x_i, x_j)}{b_i(x_i) b_j(x_j)}$$

- Verify that

$$\frac{b_{i,j}(x_i, x_j)}{b_i(x_i) b_j(x_j)} = 1 + \frac{s(x_i) s(x_j) \Delta_{ij}}{b_i(x_i) b_j(x_j)},$$

where $s(0) = -1$ and $s(1) = +1$.

- Hence,

$$\frac{Z}{Z_{\mathrm{BP}}(\{b_{i,j}\}, \{b_i\})} = \sum_{x_1,\ldots,x_4} \prod_i b_i(x_i) \prod_{i\sim j} \left(1 + \frac{s(x_i) s(x_j) \Delta_{ij}}{b_i(x_i) b_j(x_j)}\right)$$

Proof (cont'd)

- Expand out the product $\prod_{i\sim j}\left(1+\frac{s(x_i)s(x_j)\Delta_{ij}}{b_i(x_i)b_j(x_j)}\right)$:

$$\frac{Z}{Z_{\mathrm{BP}}} = \sum_{x_1,\dots,x_4} \prod_i b_i(x_i)\left(1+\cdots+\frac{\prod_{i\sim j}\Delta_{i,j}}{\prod_i b_i(x_i)^2}\right)$$

- Note that

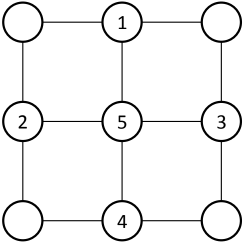
$$\sum_{x_1,\dots,x_4} \prod_i b_i(x_i) \;=\; \prod_i \sum_{x_i} b_i(x_i) \;=\; 1.$$

and

$$\begin{aligned}\sum_{x_1,\dots,x_4} \prod_i b_i(x_i)\frac{\prod_{i\sim j}\Delta_{i,j}}{\prod_i b_i(x_i)^2} &= \prod_{i\sim j}\Delta_{i,j}\sum_{x_1,\dots,x_4}\frac{1}{\prod_i b_i(x_i)}\\ &= \prod_{i\sim j}\Delta_{i,j}\prod_i\sum_{x_i}\frac{1}{b_i(x_i)}\\ &= \prod_{i\sim j}\Delta_{i,j}\prod_i\frac{1}{b_i(0)b_i(1)}\end{aligned}$$

All other terms $\sum_{x_1,\dots,x_4} \prod_i b_i(x_i)(\cdots)$ vanish.

The 3×3 Grid



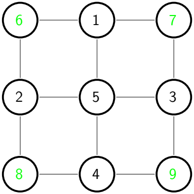
Theorem

For the 3×3 *grid, at any fixed point of GBP, the ratio* $Z/Z_{\mathrm{GBP}}(\{b_R\})$ *is given by*

$$1 + b_5(0)\left(\frac{\Delta(0)}{b_{51}(00)b_{51}(01)}\right)^4 + b_5(1)\left(\frac{\Delta(1)}{b_{51}(10)b_{51}(11)}\right)^4,$$

where $\Delta(x) = b_{512}(x00)b_{512}(x11) - b_{512}(x01)b_{512}(x10)$.

Proof of 3×3 Theorem



- Start with

$$\frac{Z}{Z_{\mathrm{GBP}}(\{b_R\})} = \sum_{x_1,\ldots,x_9} \frac{b(x_{1526})b(x_{1537})b(x_{2548})b(x_{3549})b(x_5)}{b(x_{15})b(x_{25})b(x_{35})b(x_{45})}$$

- Marginalize out x_6, x_7, x_8, x_9:

$$\frac{Z}{Z_{\mathrm{GBP}}(\{b_R\})} = \sum_{x_1,\ldots,x_5} \frac{b(x_{152})b(x_{153})b(x_{254})b(x_{354})b(x_5)}{b(x_{15})b(x_{25})b(x_{35})b(x_{45})}$$

Proof (cont'd)

- Now, define

$$B(\mathbf{x}) = \frac{b(x_{15})b(x_{25})b(x_{35})b(x_{45})}{b(x_5)^3}$$

and write $\frac{Z}{Z_{\mathrm{GBP}}(\{b_R\})}$ as

$$\sum_{x_1,\ldots,x_5} B(\mathbf{x}) \cdot \frac{b(x_{152})b(x_5)}{b(x_{15})b(x_{25})} \cdot \frac{b(x_{153})b(x_5)}{b(x_{15})b(x_{35})} \cdot \frac{b(x_{254})b(x_5)}{b(x_{25})b(x_{45})} \cdot \frac{b(x_{354})b(x_5)}{b(x_{35})b(x_{45})}$$

- Next, verify that

$$\frac{b(x_{i5j})b(x_5)}{b(x_{i5})b(x_{j5})} = 1 + \frac{s(x_i)s(x_j)\Delta_{5ij}(x_5)}{b(x_{i5})b(x_{j5})}$$

where $s(0) = -1$ and $s(1) = +1$.

Plug this back into the expression for $\frac{Z}{Z_{\mathrm{GBP}}(\{b_R\})}$ and simplify.

Proof (cont'd)

- Upon simplification, we obtain

$$\frac{Z}{Z_{\mathrm{GBP}}(\{b_R\})} = 1 + \sum_{x_5} \frac{\Delta(x_5)^4}{b(x_5)^3} \sum_{x_1,\dots,x_4} \prod_{i=1}^{4} \frac{1}{b(x_{i5})}$$

- This further simplifies to

$$\begin{aligned}\frac{Z}{Z_{\mathrm{GBP}}(\{b_R\})} &= 1 + \sum_{x_5} \frac{\Delta(x_5)^4}{b(x_5)^3} \left(\frac{1}{b(x_5 0)} + \frac{1}{b(x_5 1)} \right)^4 \\ &= 1 + \sum_{x_5} b(x_5) \left(\frac{\Delta(x_5)}{b(x_5 0) b(x_5 1)} \right)^4\end{aligned}$$

□

References

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[2] C.L. Chan, M. Jafari Siavoshani, S. Jaggi, N. Kashyap, and P.O. Vontobel, "Generalized Belief Propagation for Estimating the Partition Function of the 2D Ising Model," in *Proc. 2015 IEEE Int. Symp. Inf. Theory (ISIT 2015)*, Hong Kong, China, June 2015.