The Bethe Fartition Function and the SPA for Factor Graphs based on Homogeneous Real Stable Polynomials

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Main results

Consider a **standard factor graph (S-FG)** N where **each local function** is defined based on a (possibly different) **multi-affine homogeneous real stable** (MAHRS) polynomial.

Then we prove that

1. The **projection** of the **local marginal polytope** (LMP) on the **edges** in N equals the **convex hull** of the set of **valid configurations** $\mathrm{conv}(\mathcal{C})$.

2. For the **typical** case where the S-FG has a **sum-product algorithm (SPA) fixed point** consisting of **positive-valued messages only**, the SPA finds the value of the **Bethe partition function** $Z_{\mathrm{B}}(\mathsf{N})$ **exponentially fast**.

3. The **Bethe free energy function** F_{B} has some **convexity properties**.

Outline

An introductory example

A setup based on binary matrices with prescribed row sums and column sums

Graphical-model-based approximation method

Main results

A more general setup

Main results for a more general setup

Numerical results

Future works and connection to other works

Outline

- **An introductory example**

  A setup based on binary matrices with prescribed row sums and column sums

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  Main results for a more general setup

  Numerical results

  Future works and connections to other works

An introductory example

Consider the set of all **binary 3×3 matrices**.

We want to know the number of **binary** 3×3 matrices with **row sums** and **column sums** equaling **two**.

The following are **example binary** 3×3 matrices:

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \end{pmatrix} \qquad \begin{pmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \\ 1 & 0 & 1 \end{pmatrix} \qquad \begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \\ 1 & 1 & 0 \end{pmatrix}.$$

An introductory example

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$$\underbrace{\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \end{pmatrix}}_{\times}, \quad \underbrace{\begin{pmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \\ 1 & 0 & 1 \end{pmatrix}}_{\checkmark}, \quad \underbrace{\begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \\ 1 & 1 & 0 \end{pmatrix}}_{\checkmark}.$$

The number of such matrices is **3!**.

An introductory example

$$\begin{pmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \\ 1 & 0 & 1 \end{pmatrix}, \qquad \begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \\ 1 & 1 & 0 \end{pmatrix}.$$

- These binary matrices can be viewed as **binary contingency tables** of size 3×3 with **row sums** and **column sums** equaling **two**.
- The number of such **binary contingency tables** is $3!$.

Outline

Setup

Definition

1. $[n] \triangleq \{1, 2, \ldots, n\}$ for $n \in \mathbb{Z}_{\geq 1}$ and $[m] \triangleq \{1, 2, \ldots, m\}$ for $m \in \mathbb{Z}_{\geq 1}$.

2. $\boldsymbol{x} = \big(x(i,j)\big)_{i\in[n], j\in[m]}$: a **$\{0,1\}$-valued matrix** of size $n \times m$.

3. For the ***i*-th row** $\boldsymbol{x}(i,:)$, we introduce an integer r_i and impose a **constraint** on the **row sum**:

$$\mathcal{X}_{r_i} = \left\{ \boldsymbol{x}(i,:) \,\middle|\, \sum_{j\in[m]} x(i,j) = r_i \right\}.$$

4. For the ***j*-th column** $\boldsymbol{x}(:,j)$, we introduce an integer c_j and impose a **constraint** on the **column sum**:

$$\mathcal{X}_{c_j} = \left\{ \boldsymbol{x}(:,j) \,\middle|\, \sum_{i\in[n]} x(i,j) = c_j \right\}.$$

Setup

Definition

5. The set of **valid configurations** is defined to be

$$\mathcal{C} \triangleq \left\{ \boldsymbol{x} \in \{0,1\}^{n\times n} \;\middle|\; \begin{array}{l} \boldsymbol{x}(i,:) \in \mathcal{X}_{r_i},\ \forall i \in [n], \\ \boldsymbol{x}(:,j) \in \mathcal{X}_{c_j},\ \forall j \in [m] \end{array} \right\},$$

the set of **binary matrices** such that the **i-th row sum** is r_i and the **j-th column sum** is c_j.

6. We want to compute the number of the **valid configurations** $|\mathcal{C}|$.

Outline

Graphical-model-based approximation method

Main idea

1. Define a **standard factor graph (S-FG)** N whose partition function equals

$$Z(\mathsf{N}) = |\mathcal{C}|.$$

2. Run the **sum product algorithm (SPA)**, a.k.a. **belief propagation** (BP), on the S-FG N to compute the **Bethe approximation of** $|\mathcal{C}|$, denoted by $Z_{\mathrm{B}}(\mathsf{N})$.

Graphical-model-based approximation method

Example

Consider $n = m = 3$ **and** $r_i = c_j = 2$, *i.e.*, $\boldsymbol{x} \in \{0,1\}^{3\times 3}$.

The i**-th row** $\boldsymbol{x}(i,:) \in \mathcal{X}_{r_i}$ and the j**-th column** $\boldsymbol{x}(:,j) \in \mathcal{X}_{c_j}$, where

$$\mathcal{X}_{r_i} = \{(1,1,0),(0,1,1),(1,0,1)\}, \quad \mathcal{X}_{c_j} = \{(1,1,0)^\mathsf{T},(0,1,1)^\mathsf{T},(1,0,1)^\mathsf{T}\}.$$

1. The **local functions**:

$$f_{\mathrm{l},i}\big(\boldsymbol{x}(i,:)\big) \triangleq \begin{cases} 1 & \text{if } \boldsymbol{x}(i,:) \in \mathcal{X}_{r_i} \\ 0 & \text{otherwise} \end{cases}, \quad f_{\mathrm{r},j}\big(\boldsymbol{x}(:,j)\big) \triangleq \begin{cases} 1 & \text{if } \boldsymbol{x}(:,j) \in \mathcal{X}_{c_j} \\ 0 & \text{otherwise} \end{cases}.$$

2. The **support** of the local functions:

$$\mathcal{X}_{f_{\mathrm{l},i}} \triangleq \left\{\boldsymbol{x}(i,:) \in \{0,1\}^3 \;\middle|\; f_{\mathrm{l},i}\big(\boldsymbol{x}(i,:)\big) > 0\right\} = \mathcal{X}_{r_i},$$
$$\mathcal{X}_{f_{\mathrm{r},j}} \triangleq \left\{\boldsymbol{x}(:,j) \in \{0,1\}^3 \;\middle|\; f_{\mathrm{r},j}\big(\boldsymbol{x}(:,j)\big) > 0\right\} = \mathcal{X}_{c_j}.$$

Graphical-model-based approximation method

3. The $\{0,1\}$-valued **global function**:

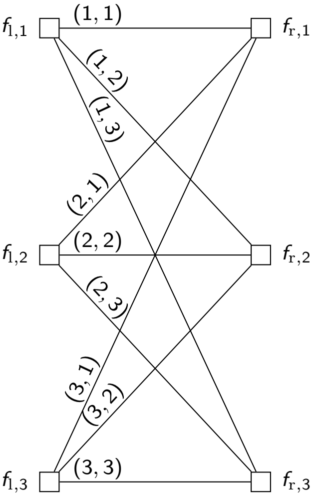
$$g(\boldsymbol{x}) \triangleq f_{\mathrm{l},1}\big(x(1,1), x(1,2), x(1,3)\big) \cdot f_{\mathrm{l},2}\big(x(2,1), x(2,2), x(2,3)\big) \cdots f_{\mathrm{r},2}\big(x(1,2), x(2,2), x(3,2)\big) \cdot f_{\mathrm{r},3}\big(x(1,3), x(2,3), x(3,3)\big).$$

The **previously defined** set of **valid configurations** is equal to the **support** of the global function:

$$\mathcal{C} = \left\{ \boldsymbol{x} \in \{0,1\}^{3\times 3} \;\middle|\; g(\boldsymbol{x}) > 0 \right\}.$$

4. The **partition function**:

$$Z(\mathsf{N}) \triangleq \sum_{\boldsymbol{x} \in \{0,1\}^{3\times 3}} g(\boldsymbol{x}) = |\mathcal{C}|.$$



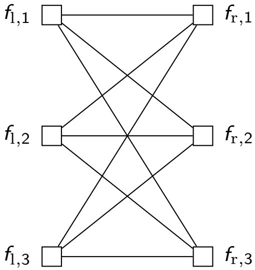
Graphical-model-based approximation method

5. The **Bethe approximation** of the partition function, *i.e.*, the **Bethe partition function**, is defined to be

$$Z_{\mathrm{B}}(\mathsf{N}) \triangleq \exp\left(-\min_{\boldsymbol{\beta}\in\mathcal{L}(\mathsf{N})} F_{\mathrm{B}}(\boldsymbol{\beta})\right),$$

where F_{B} is the **Bethe free energy (BFE)** function,

where $\mathcal{L}(\mathsf{N})$ is the **local marginal polytope** (LMP) (see, *e.g.*, [Wainwright and Jordan, 2008]).



6. Then we run the **sum-product algorithm (SPA)**, a.k.a. **belief propagation (BP)**, on the S-FG N to get $Z_{\mathrm{B}}(\mathsf{N})$.

Outline

An introductory example

A setup based on binary matrices with prescribed row sums and column sums

Graphical-model-based approximation method

- **Main results**

A more general setup

Main results for a more general setup

Numerical results

Future works and connection to other works

Main results

1. The **projection** of the **LMP** on the **edges** in N **equals** conv($\mathcal{C}$).
   (For general S-FGs, this projection is a **relaxation** of conv($\mathcal{C}$), *i.e.*, conv($\mathcal{C}$) is a **strict subset** of this **projection**.)

2. For the **typical case** where N has an **SPA fixed point** consisting of **positive-valued messages only**, the SPA finds the value of Z_{B}(N) **exponentially fast**.

3. The **BFE function** has some **convexity properties**.

Comments

- A **generalization** of parts of the results in [Vontobel, 2013].
- Even though the S-FG has a **non-trivial cyclic structure**, the SPA has **a good performance**.

Main results

Comments

For the setup where $n = m$, $r_i = 1$, and $c_j = 1$, it holds that

- $\mathcal{C} = \{\boldsymbol{x} \mid \boldsymbol{x}$ is a **permutation matrix** of size n-by-$n\}$
- The **projection** of the **LMP** on the **edges** equals the set of **doubly stochastic matrices** of size n-by-n.

Birkhoff–von Neumann theorem

The set of **doubly stochastic matrices** of size n-by-n is the **convex hull** of the set of the **permutation matrices** of size n-by-n.

The main result that $\text{conv}(\mathcal{C})$ equals the **projection** of the **LMP** on the **edges** for our considered S-FG, can be viewed as a **generalization**.

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Graphical-model-based approximation method

Main results

- **A more general setup**

Main results for a more general setup

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A more general setup

An example S-FG

Consider $n = m = 3$ **and** $r_i = c_j = 2$. Then

$$f_{1,i}\big(\boldsymbol{x}(i,:)\big) = \begin{cases} 1 & \text{if } \boldsymbol{x}(i,:) \in \{(1,1,0),(0,1,1),(1,0,1)\} \\ 0 & \text{otherwise} \end{cases},$$

which corresponds to a **multi-affine homogeneous real stable (MAHRS) polynomial** w.r.t. the **indeterminates** in $\boldsymbol{L} \triangleq \big(L_1, L_2, L_3\big) \in \mathbb{C}^3$:

$$\begin{aligned} p_i(\boldsymbol{L}) &= \sum_{\boldsymbol{x}(i,:)\in\{0,1\}^3} f_{1,i}\big(\boldsymbol{x}(i,:)\big) \cdot \prod_{j\in[3]} \big(L_j\big)^{\boldsymbol{x}(i,j)} \\ &= L_1 \cdot L_2 + L_2 \cdot L_3 + L_1 \cdot L_3, \end{aligned}$$

Remark

- For details of **real stable polynomials**, see, *e.g.*, [Gharan, 2020]

Consider a **more general** setup where **each local function** is defined based on a **(possibly different) MAHRS polynomial**.

Do the previous results **hold** in this **more general setup**?

Yes!

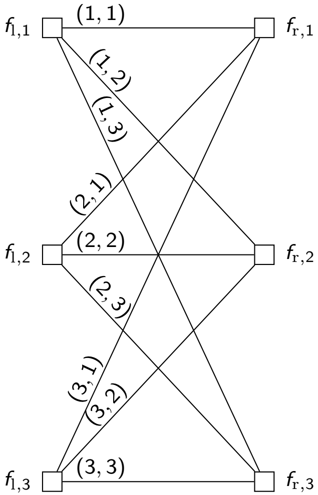
An MAHRS Polynomials-based S-FG

The standard factor graph (S-FG) N consists of

1. **edges**: $(1,1),(1,2),\ldots,(3,3)$;
2. **Binary** matrix

$$\boldsymbol{x} \triangleq \begin{pmatrix} x(1,1) & x(1,2) & x(1,3) \\ x(2,1) & x(2,2) & x(2,3) \\ x(3,1) & x(3,2) & x(3,3) \end{pmatrix}.$$

3. **Nonnegative-valued** local functions $f_{\mathrm{l},1},\ldots,f_{\mathrm{r},3}$;



An MAHRS Polynomials-based S-FG

6. The **local function** $f_{\mathrm{l},i}$ on the **LHS** is defined to be the mapping:

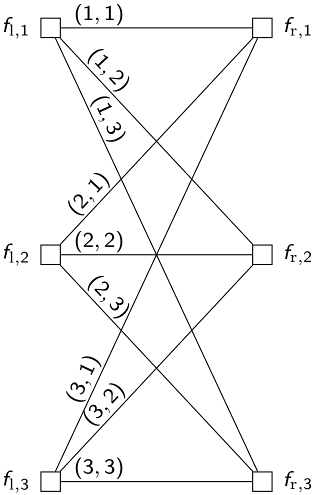
$$\{0,1\}^3 \to \mathbb{R}_{\geq 0}, \quad \boldsymbol{x}(i,:) \mapsto f_{\mathrm{l},i}\big(\boldsymbol{x}(i,:)\big)$$

such that it corresponds to an **MAHRS polynomial**.

7. The **support** of $f_{\mathrm{l},i}$:

$$\mathcal{X}_{f_{\mathrm{l},i}} \triangleq \left\{ \boldsymbol{x}(i,:) \in \{0,1\}^3 \;\middle|\; f_{\mathrm{l},i}\big(\boldsymbol{x}(i,:)\big) > 0 \right\}.$$

8. A **similar idea** in the definitions of $f_{\mathrm{r},j}$ and $\mathcal{X}_{f_{\mathrm{r},j}}$ on the **RHS**.



An MAHRS Polynomials-based S-FG

9. The **nonnegative-valued global function**:

$$g(\boldsymbol{x}) \triangleq f_{\mathrm{l},1}\big(\boldsymbol{x}(1,:)\big) \cdot f_{\mathrm{l},2}\big(\boldsymbol{x}(2,:)\big) \cdot f_{\mathrm{l},3}\big(\boldsymbol{x}(3,:)\big) \cdot f_{\mathrm{r},1}\big(\boldsymbol{x}(:,1)\big) \cdot f_{\mathrm{r},2}\big(\boldsymbol{x}(:,2)\big) \cdot f_{\mathrm{r},3}\big(\boldsymbol{x}(:,3)\big).$$

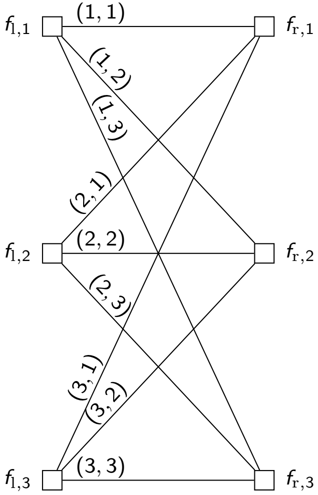
10. The set of **valid configurations**:

$$\mathcal{C} \triangleq \left\{\boldsymbol{x} \in \{0,1\}^{3\times 3} \;\middle|\; g(\boldsymbol{x}) > 0\right\},$$

which is also the **support** of the **global function**.

11. The **partition function**:

$$Z(\mathsf{N}) \triangleq \sum_{\boldsymbol{x}\in\mathcal{C}} g(\boldsymbol{x}).$$



Outline

Known results

Consider an **S-FG** N where **each local function** is defined based on a (possibly different) **MAHRS** polynomial.

Remarks

- Exactly computing $Z(\mathsf{N})$ is a **#P-complete problem** in general.
- **Run the SPA** to find the value of the **Bethe partition function** $Z_{\mathrm{B}}(\mathsf{N})$ that **approximates** $Z(\mathsf{N})$.
- [Straszak and Vishnoi, 2019, Theorem 3.2]: $Z_{\mathrm{B}}(\mathsf{N}) \leq Z(\mathsf{N})$.
- **Other real-stable-polynomial-based approximation of** $Z(\mathsf{N})$ [Gurvits, 2015, Brändén et al., 2023].

Main results

Consider an **S-FG** N where **each local function** is defined based on a (possibly different) **MAHRS** polynomial.

- The **support** $\mathcal{X}_{f_{\mathrm{l},i}}$ on the LHS corresponds to **a set of bases of a matroid** [Brändén, 2007].
- The support of the **product** of the **local functions** on the **LHS** is $\{\mathcal{X}_{f_{\mathrm{l},1}} \times \mathcal{X}_{f_{\mathrm{l},2}} \times \cdots \times \mathcal{X}_{f_{\mathrm{l},n}}\}$.
- Similarly for the local functions and the **support** on the **LHS**.
- The support of the **global function** equals the **intersection** of the bases of **matroids**:

$$\mathcal{C} = \{\mathcal{X}_{f_{\mathrm{l},1}} \times \mathcal{X}_{f_{\mathrm{l},2}} \times \cdots \times \mathcal{X}_{f_{\mathrm{l},n}}\} \bigcap \{\mathcal{X}_{f_{\mathrm{r},1}} \times \mathcal{X}_{f_{\mathrm{r},2}} \times \cdots \times \mathcal{X}_{f_{\mathrm{r},m}}\}$$

Main results

1. The **convex hull** $\mathrm{conv}(\mathcal{C})$ is the **projection of the LMP** on the **edges**.
   (Based on results on intersection of matroids [Oxley, 2011].)

2. For the typical case where the S-FG has an SPA **fixed point** consisting of **positive-valued messages only**, the SPA finds the value of $Z_{\mathrm{B}}(\mathsf{N})$ **exponentially fast**.
   (Based on the properties of **real stable polynomials** in [Brändén, 2007].)

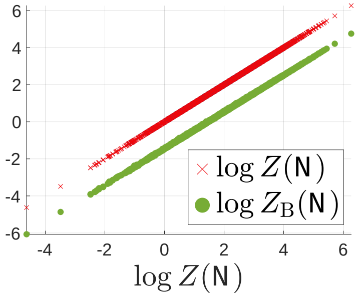
3. The **Bethe free energy function** F_{B} has some **convexity properties**.
   The proof of the convexity is **new**.
   (Based on the **dual** form of $Z_{\mathrm{B}}(\mathsf{N})$ in [Straszak and Vishnoi, 2019, Anari and Gharan, 2021].)

Outline

Numerical results

Setup

- We first consider the case $n = m = 6$ **and** $r_i = c_j = 2$.
- We independently randomly generate 3000 **instances** of N.



Observation

- $Z_{\mathrm{B}}(\mathrm{N}) \leq Z(\mathrm{N})$ ([Straszak and Vishnoi, 2019, Theroem 3.2]).
- $Z_{\mathrm{B}}(\mathrm{N})$ provides a **good estimate** of $Z(\mathrm{N})$ in this case.

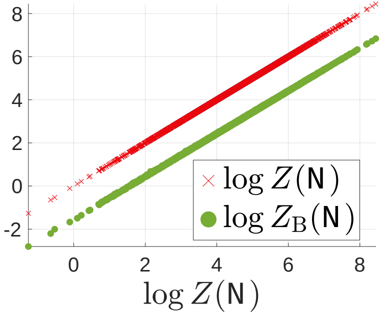
Numerical results

Setup

Consider **the same setup** as the previous case, but with $n = m = 6$ **replaced** by $n = m = 7$.

Observation

We can make **similar observations**.



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A more general setup

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Numerical results

- **Future works and connection to other works**

Future work

- Consider a **more general** S-FG, where each local function corresponds to a **more general** polynomial.
- Prove the **convergence** of the SPA for a **more general** S-FG.

Connection to other works

- **Polynomial approaches** to approximate **partition functions**.
  [Gurvits, 2011, Straszak and Vishnoi, 2017, Anari and Gharan, 2021]

- The properties of **real stable** polynomials and the **partition functions**.
  [Brändén, 2014, Borcea and Brändén, 2009, Borcea et al., 2009]

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Thank you!

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