Quantum Factor Graphs: Closing-the-Box Operation and Variational Approaches

End-of-Second-Year Oral Exam

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August 29, 2016
Overview

Marginal problems

\[ \sum \prod_{x \in F} f_a(x \partial a) \]

where \( f_a \) is a non-negative function on \( \bigotimes_{i \in \partial a} x_i \).
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- Closing-the-box Approach;
- Variational Approach (Bethe Approximation).
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Marginal problems in Quantum Setup

\[ \text{Tr} \left[ \exp \left( \sum_{a \in \mathcal{F}} \log \rho_a \right) \right] \]

where \( \rho_a \) is a PSD operator on \( \bigotimes_{i \in \partial a} \mathcal{H}_i \).
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Quantum Sum-Product Algorithm

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Outline

1. Factor Graphs/Preliminaries
2. Quantum Factor Graphs (QFGs)
3. Closing-the-box Operations on QFGs
4. Variational Approach on QFGs
5. Numerical Result of QSPA
6. Conclusion & Outlook
Factor Graphs and Normal Factor Graphs

*Factor graphs*, or classical factor graph (CFG), describe factorizations.

\[ g(x_1, x_2, x_3, x_4) = f_A(x_1, x_3) \cdot f_B(x_1, x_2, x_3) \cdot f_C(x_3, x_4). \]
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In general, we associate the factorization

\[ g(x) \triangleq \prod_{a \in \mathcal{F}} f_a(x_a) \]

to a factor graph with variable node set \( \mathcal{V} \), function node set \( \mathcal{F} \), and edge set \( \mathcal{E} \subseteq \mathcal{V} \times \mathcal{F} \) given by

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\[ f_C \]

\[ \mathcal{V} \]
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\[ x_1 \]
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Example 2 (LDPC Code described by CFG)

\[
\begin{array}{c}
\text{y}_1 \\
\text{p}_{Y_1|X_1} \\
\text{y}_2 \\
\text{p}_{Y_2|X_2} \\
\text{y}_3 \\
\text{p}_{Y_3|X_3} \\
\vdots \\
\text{y}_n \\
\text{p}_{Y_n|X_n} \\
\end{array}
\]
Factor graphs are popular in describing (large-scale) probability systems.

\[ x_i, y_i \in \mathbb{F}_2 \quad \forall i \in \{1, \cdots, n\}; \]

\[ f_+ (x) \triangleq \mathbb{1} \left\{ \sum_{i \text{ incoming}} x_i = 0 \right\}. \]

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A problem of interest:

Calculate the marginal distribution of $$X_i$$ given fixed $$\{y_i\}_{i=1}^n.$$
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\[ g_y(x) = \prod_i p_{Y_i=y_i|X_i}(x_i) \cdot \prod_k f_k(x) \]

\[ \propto p_{Y=y|X}(x) \]

\[ \sum_{x_j, j \neq i} g_y(x) \propto p_{Y=y|X_i}(x_i) \]

Symbol-wise ML decoding
Definition 3 (Partition Function/Sum)

In many applications, we are interested in calculating summations like (or similar to)

\[ Z \triangleq \sum_x g(x) = \sum_x \prod_{a \in \mathcal{F}} f_a(x_{\partial a}), \]

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**Example 1 (continue)**

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In general, calculation of \( Z \) is NP hard.
Example 1 Sum over local variables first...

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Partition Sum and the Closing-the-box Operations

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= \sum_{x_3} \left( \hat{f}_{AB}(x_3) \right) \cdot \hat{f}_C(x_3) = Z
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Closing-the-box in general

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Sum-Product Algorithm on a tree

Example 1

Closing the boxes from the inner ones to outer ones will yield the partition sum $Z$.

Distributive Law on $\mathbb{R}$
Sum-Product Algorithm on a tree

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Closing the boxes from the inner ones to outer ones will yield the partition sum $Z$.

Distributive Law on $\mathbb{R}$

Sum-Product Algorithm for Trees

Require: Acyclic factor graph $G = (F, V, E)$; root $r \in V$; height of the tree $h \geq 0$.

Ensure: Partition sum $Z$

1. for $d = h - 1, \cdots, 0$ do
2. for all $i \in V$ d-step reachable\(^a\) from $r$ do
3. Let $f^{(i)}$ be the parent factor\(^b\) of $i$;
4. $f^{(i)} \leftarrow \sum_{x_i} \prod_{a \in \partial i} f_a(x_i)$;
5. end for
6. end for
7. $Z \leftarrow f(r)$.

\(^a\)i.e., there exists a path connecting $r$ and $i$ passing through $d$ factors.

\(^b\)i.e. the unique factor node that is both on the path from $r$ to $i$ and also adjacent to $i$. 
Sum-Product Algorithm on a tree

Example 1

Closing the boxes from the inner ones to outer ones will yield the partition sum \( Z \).

Distributive Law on \( \mathbb{R} \)

Message-Passing Algorithm

Sum-Product Algorithm for Trees

Require: Acyclic factor graph \( G = (\mathcal{F}, \mathcal{V}, \mathcal{E}) \);
\text{root } r \in \mathcal{V}; \text{ height of the tree } h \geq 0.

Ensure: Partition sum \( Z \)

1: \textbf{for } \( d = h - 1, \cdots, 0 \) \textbf{do}
2: \hspace{1em} \textbf{for all } \( i \in \mathcal{V} \) \( d \)-step reachable\(^a\) from \( r \) \textbf{do}
3: \hspace{2em} Let \( f(i) \) be the parent factor\(^b\) of \( i \);
4: \hspace{2em} \( f(i) \leftarrow \sum_{x_i} \prod_{a \in \partial i} f_a(x_i) \);
5: \hspace{1em} \textbf{end for}
6: \textbf{end for}
7: \( Z \leftarrow f(r) \).

\(^a\)i.e., there exists a path connecting \( r \) and \( i \) passing through \( d \) factors.

\(^b\)i.e. the unique factor node that is both on the path from \( r \) to \( i \) and also adjacent to \( i \).
Sum-Product Algorithm for Trees

**Require:** Acyclic factor graph $G = (\mathcal{F}, \mathcal{V}, \mathcal{E})$;
root $r \in \mathcal{V}$; height of the tree $h \geq 0$.

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1. for $d = h - 1, \cdots, 0$ do
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\(^a\)i.e., there exists a path connecting $r$ and $i$ passing through $d$ factors.
\(^b\)i.e., the unique factor node that is both on the path from $r$ to $i$ and also adjacent to $i$. 

---

Example 1

Closing the boxes from the inner ones to outer ones will yield the partition sum $Z$. 

**Message-Passing Algorithm**
Sum-Product Algorithm as a Message Passing Algorithm

**Sum-Product Algorithm**

**Require:** Factor graph $\mathcal{G} = (\mathcal{F}, \mathcal{V}, \mathcal{E})$;

**Ensure:** ???

1: for all $(i, a) \in \mathcal{E}$ do
2:    $m_{i \rightarrow a} \leftarrow 1$;
3:    $m_{a \rightarrow i} \leftarrow 1$;
4: end for
5: repeat
6:   for all $(i, a) \in \mathcal{E}$ do
7:       $m_{i \rightarrow a}(x_i) \leftarrow \prod_{c \in \partial i \setminus a} m_{a \rightarrow i}(x_i)$;
8:   end for
9:   for all $(i, a) \in \mathcal{E}$ do
10:      $m_{a \rightarrow i}(x_i) \leftarrow \sum_{x_{\partial a \setminus i}} f_a(x_{\partial a}) \cdot \prod_{j \in \partial a \setminus i} m_{j \rightarrow a}(x_j)$;
11: end for
12: until ________
**Sum-Product Algorithm**

**Require:** Factor graph $\mathcal{G} = (\mathcal{F}, \mathcal{V}, \mathcal{E})$;

**Ensure:** ???

1. for all $(i, a) \in \mathcal{E}$ do
2. \hspace{1em} $m_{i \rightarrow a} \leftarrow 1$;
3. \hspace{1em} $m_{a \rightarrow i} \leftarrow 1$;
4. end for
5. repeat
6. for all $(i, a) \in \mathcal{E}$ do
7. \hspace{1em} $m_{i \rightarrow a}(x_i) \leftarrow \prod_{c \in \partial_i \setminus a} m_{a \rightarrow i}(x_i)$;
8. end for
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11. end for
12. until _________
Sum-Product Algorithm

**Require:** Factor graph $\mathcal{G} = (\mathcal{F}, \mathcal{V}, \mathcal{E})$;

**Ensure:** ???

1. **for all** $(i, a) \in \mathcal{E}$ **do**
2. $m_{i \rightarrow a} \leftarrow 1$
3. $m_{a \rightarrow i} \leftarrow 1$
4. **end for**

5. **repeat**
6. **for all** $(i, a) \in \mathcal{E}$ **do**
7. $m_{i \rightarrow a}(x_i) \propto \prod_{c \in \partial_i \setminus a} m_{a \rightarrow i}(x_i)$
8. **end for**
9. **for all** $(i, a) \in \mathcal{E}$ **do**
10. $m_{a \rightarrow i}(x_i) \propto \sum_{x_{\partial a \setminus i}} f_a(x_{\partial a}) \cdot \prod_{j \in \partial a \setminus i} m_{j \rightarrow a}(x_j)$
11. **end for**
12. **until** ________
Sum-Product Algorithm

**Require:** Factor graph $\mathcal{G} = (\mathcal{F}, \mathcal{V}, \mathcal{E})$;

**Ensure:** 

1. for all $(i, a) \in \mathcal{E}$ do
2. $m_{i \rightarrow a} \leftarrow 1$;
3. $m_{a \rightarrow i} \leftarrow 1$;
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5. repeat
6. for all $(i, a) \in \mathcal{E}$ do
7. $m_{i \rightarrow a}(x_i) \propto \prod_{c \in \partial_i \setminus a} m_{a \rightarrow i}(x_i)$;
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11. end for
12. until ________
Sum-Product Algorithm

**Require:** Factor graph $\mathcal{G} = (\mathcal{F}, \mathcal{V}, \mathcal{E})$;

**Ensure:**

1. for all $(i, a) \in \mathcal{E}$ do
2. $m_{i \rightarrow a} \leftarrow 1$;
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11. end for
12. until convergence
**Sum-Product Algorithm as a Message Passing Algorithm**

**Sum-Product Algorithm**

**Require:** Factor graph $\mathcal{G} = (\mathcal{F}, \mathcal{V}, \mathcal{E})$;

**Ensure:** ???

1. for all $(i, a) \in \mathcal{E}$ do
2. $m_{i \rightarrow a} \leftarrow 1$;
3. $m_{a \rightarrow i} \leftarrow 1$;
4. end for
5. repeat
6. for all $(i, a) \in \mathcal{E}$ do
7. $m_{i \rightarrow a}(x_i) \propto \prod_{c \in \partial_i \setminus a} m_{a \rightarrow i}(x_i)$;
8. end for
9. for all $(i, a) \in \mathcal{E}$ do
10. $m_{a \rightarrow i}(x_i) \propto \sum_{x_{\partial a \setminus i}} f_a(x_{\partial a}) \cdot \prod_{j \in \partial a \setminus i} m_{j \rightarrow a}(x_j)$;
11. end for
12. until convergence
In acyclic case, it will always converge.

- \( b_i(x_i) \triangleq \prod_{a \in \partial i} m_{a \to i}(x_i) \propto \sum_{x \in V} g(x) \);
- \( b_a(x_{\partial a}) \triangleq f_a(x_{\partial a}) \cdot \prod_{i \in \partial a} m_{i \to a}(x_i) \propto \sum_{x \in V \setminus \partial a} g(x) \).
Sum-Product Algorithm and the Variational Approach

In acyclic case, it will always converge.

- \( b_i(x_i) \triangleq \prod_{a \in \partial_i} m_{a \rightarrow i}(x_i) \propto \sum_{x_{\mathcal{V} \setminus i}} g(x); \)
- \( b_a(x_{\partial a}) \triangleq f_a(x_{\partial a}) \cdot \prod_{i \in \partial a} m_{i \rightarrow a}(x_j) \propto \sum_{x_{\mathcal{V} \setminus \partial a}} g(x). \)

In general case, if it converges, then: [Yedidia et al., 2005]

The above \( \{b_i\}_{i \in \mathcal{V}} \) and \( \{b_a\}_{a \in \mathcal{F}} \) correspond to the \textit{interior stationary points} of the \textit{constrained Bethe approximation problem}:

\[
\begin{align*}
    \min_{\mathcal{F}} & \quad \text{Bethe} \left( \{b_a\}_{a \in \mathcal{F}}, \{b_i\}_{i \in \mathcal{V}} \right) \\
    \text{subject to} & \quad b_{i}(x_{i}) = \sum_{x_{\partial i}} b_{a}(x_{\partial a}) b_{a}(x_{\partial a}) \quad \forall x_{i}, \forall (i, a) \in \mathcal{E}.
\end{align*}
\]
Sum-Product Algorithm and the Variational Approach

In acyclic case, it will always converge.

- \( b_i(x_i) \triangleq \prod_{a \in \partial_i} m_{a \rightarrow i}(x_i) \propto \sum_{x_{\mathcal{V}\setminus i}} g(x) \);
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In general case, if it converges, then: [Yedidia et al., 2005]

The above \( \{b_i\}_{i \in \mathcal{V}} \) and \( \{b_a\}_{a \in \mathcal{F}} \) correspond to the interior stationary points of the constrained Bethe approximation problem:

\[
\min \quad F_{\text{Bethe}} \left( (b_a)_{a \in \mathcal{F}}, (b_i)_{i \in \mathcal{V}} \right) \\
\triangleq - \sum_{a \in \mathcal{F}} \sum_{x_{\partial a}} b_a(x_{\partial a}) \log f_a(x_{\partial a}) - \sum_{a \in \mathcal{F}} \mathcal{H}(b_a) + \sum_{i \in \mathcal{V}} (d_i - 1) \cdot \mathcal{H}(b_i)
\]

s.t. \( b_a \) probability on \( x_{\partial a} \), \( b_i \) probability on \( x_i \), \( \forall a \in \mathcal{F}, \forall i \in \mathcal{V} \)

\( b_i(x_i) = \sum_{x_{\partial a \setminus i}} b_a(x_{\partial a}) \) \( \forall x_i, \forall (i,a) \in \mathcal{E} \)
Outline

1. Factor Graphs/Preliminaries
2. Quantum Factor Graphs (QFGs)
3. Closing-the-box Operations on QFGs
4. Variational Approach on QFGs
5. Numerical Result of QSPA
6. Conclusion & Outlook
Definition 4 ([Leifer and Poulin, 2008])

A quantum Factor graph (QFG) \((\mathcal{V}, \mathcal{F}, \mathcal{E})\) with local factors \(\{\rho_a\}\) describes the “factorization”

\[
\rho \triangleq \bigotimes_{a \in \mathcal{F}} \rho_a = \exp \left[ \sum_{a \in \mathcal{F}} \log(\rho_a) \right],
\]

(1)

where, for each \(a \in \mathcal{F}\), positive definite operator \(\rho_a\) is an operator on \(\bigotimes_{i \in \partial a} \mathcal{H}_i\).
Quantum Factor Graphs (QFGs)

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Example 5

\[
\begin{array}{c}
\rho_A \\
\mathcal{H}_1 \\
\rho_B \\
\mathcal{H}_2 \\
\rho_C
\end{array}
\]

A QFG describing \(\rho = \rho_A \otimes \rho_B \otimes \rho_C\).

\(\rho_A \in \mathcal{L}^+ (\mathcal{H}_1)\)
\(\rho_B \in \mathcal{L}^+ (\mathcal{H}_1 \otimes \mathcal{H}_2)\)
\(\rho_C \in \mathcal{L}^+ (\mathcal{H}_2)\)

Here, \(\mathcal{L}^+ (\mathcal{H})\) stands for the set of all positive semi-definite operators on the Hilbert space \(\mathcal{H}\).
For $\rho_A, \rho_B \in \mathcal{L}^{++}(\mathcal{H})$, define [Warmuth, 2005]

$$\rho_A \circ \rho_B \triangleq \exp(\log(\rho_A) + \log(\rho_B)),$$

where $\exp$ and $\log$ denote the operator exponential and the operator natural logarithm, respectively.
Quantum Factor Graphs (QFGs)

For $\rho_A, \rho_B \in \mathcal{L}^{++}(\mathcal{H})$, define [Warmuth, 2005]

$$\rho_A \odot \rho_B \triangleq \exp(\log(\rho_A) + \log(\rho_B)),$$

where $\exp$ and $\log$ denote the operator exponential and the operator natural logarithm, respectively. By the Lie Product formula, we have

$$\rho_A \odot \rho_B = \lim_{n \to \infty} \left( \rho_A^{\frac{1}{n}} \rho_B^{\frac{1}{n}} \right)^n.$$
Quantum Factor Graphs (QFGs)

For $\rho_A, \rho_B \in \mathcal{L}^{++}(\mathcal{H})$, define [Warmuth, 2005]

$$\rho_A \circ \rho_B \triangleq \exp(\log(\rho_A) + \log(\rho_B)),$$

(2)

where $\exp$ and $\log$ denote the operator exponential and the operator natural logarithm, respectively. By the Lie Product formula, we have

$$\rho_A \circ \rho_B = \lim_{n \to \infty} \left( \rho_A^{\frac{1}{n}} \rho_B^{\frac{1}{n}} \right)^n.$$

(3)

Equation (3) can be used to generalize the $\circ$ product to PSD operators.
For $\rho_A, \rho_B \in \mathcal{L}^{++}(\mathcal{H})$, define [Warmuth, 2005]

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$$\rho_A \circ \rho_B = \lim_{n \to \infty} \left(\rho_A^{\frac{1}{n}} \rho_B^{\frac{1}{n}}\right)^n.\quad (3)$$

Equation (3) can be used to generalize the $\circ$ product to PSD operators.

**Properties of $\circ$**

- **Associativity:** $(\rho_A \circ \rho_B) \circ \rho_C = \rho_A \circ (\rho_B \circ \rho_C)$;
- **Commutativity:** $\rho_A \circ \rho_B = \rho_B \circ \rho_A$;
- **Closeness:** $\rho_A \circ \rho_B$ is positive (semi) definite if $\rho_A, \rho_B$ are positive (semi) definite.
Quantum Factor Graphs (QFGs)

For $\rho_A, \rho_B \in \mathcal{L}^{++} (\mathcal{H})$, define [Warmuth, 2005]

$$\rho_A \circ \rho_B \triangleq \exp(\log(\rho_A) + \log(\rho_B)),$$  \hspace{1cm} (2)

where $\exp$ and $\log$ denote the operator exponential and the operator natural logarithm, respectively. By the Lie Product formula, we have

$$\rho_A \circ \rho_B = \lim_{n \to \infty} \left( \rho_A^{\frac{1}{n}} \rho_B^{\frac{1}{n}} \right)^n.$$  \hspace{1cm} (3)

Equation (3) can be used to generalize the $\circ$ product to PSD operators.

Properties of $\circ$

- **Associativity:** $(\rho_A \circ \rho_B) \circ \rho_C = \rho_A \circ (\rho_B \circ \rho_C)$;
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$\langle \mathcal{L}^+ (\mathcal{H}), \circ \rangle$ (or $\langle \mathcal{L}^{++} (\mathcal{H}), \circ \rangle$) is an Abelian group.
Quantum Factor Graphs (QFGs)

For $\rho_A, \rho_B \in \mathcal{L}^{++}(\mathcal{H})$, define [Warmuth, 2005]

$$\rho_A \otimes \rho_B \triangleq \exp(\log(\rho_A) + \log(\rho_B)),$$

where exp and log denote the operator exponential and the operator natural logarithm, respectively. By the Lie Product formula, we have

$$\rho_A \otimes \rho_B = \lim_{n \to \infty} \left(\rho_A^{\frac{1}{n}} \rho_B^{\frac{1}{n}}\right)^n.$$

Equation (3) can be used to generalize the $\otimes$ product to PSD operators.

Properties of $\otimes$

- **Associativity**: $(\rho_A \otimes \rho_B) \otimes \rho_C = \rho_A \otimes (\rho_B \otimes \rho_C)$;
- **Commutativity**: $\rho_A \otimes \rho_B = \rho_B \otimes \rho_A$;
- **Closeness**: $\rho_A \otimes \rho_B$ is positive (semi) definite if $\rho_A, \rho_B$ are positive (semi) definite.

$\langle \mathcal{L}^+(\mathcal{H}), \otimes \rangle$ (or $\langle \mathcal{L}^{++}(\mathcal{H}), \otimes \rangle$) is an Abelian group.
Quantum Factor Graphs

Example 5: continue

A QFG describing \( \rho = \rho_A \otimes \rho_B \otimes \rho_C \).
Quantum Factor Graphs

Example 5: continue

A QFG describing $\rho = \rho_A \otimes \rho_B \otimes \rho_C$.

Suppose $\mathcal{H}_1 = \mathcal{H}_2 = \mathbb{C}^2$, and

$$\rho_A = \begin{bmatrix} +3 & -1 \\ -1 & +3 \end{bmatrix}, \quad \rho_B = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \rho_C = \begin{bmatrix} +3 & -1 \\ -1 & +3 \end{bmatrix}.$$
Quantum Factor Graphs

Example 5: continue

A QFG describing $\rho = \rho_A \otimes \rho_B \otimes \rho_C$.

Suppose $\mathcal{H}_1 = \mathcal{H}_2 = \mathbb{C}^2$, and

$$
\begin{align*}
\rho_A &= \begin{bmatrix}
  +3 & -1 \\
  -1 & +3 
\end{bmatrix}, \\
\rho_B &= \begin{bmatrix}
  0 & 1 \\
  1 & 0 
\end{bmatrix}, \\
\rho_C &= \begin{bmatrix}
  +3 & -1 \\
  -1 & +3 
\end{bmatrix}. 
\end{align*}
$$

We have,

$$
\rho = \rho_A \otimes \rho_B \otimes \rho_C = \begin{bmatrix}
  9 & -3 & -3 & 1 \\
  -3 & 9 & 1 & -3 \\
  -3 & 1 & 9 & -3 \\
  1 & -3 & -3 & 9 
\end{bmatrix}.
$$
Quantum Partition-Sum Problem

Definition 6 (Partition Function/Sum)

In a number of applications, we are interested in calculating

$$Z \triangleq \text{Tr} (\rho) = \text{Tr} \left( \bigotimes_{a \in \mathcal{F}} \rho_a \right) = \text{Tr} \left( \exp \left[ \sum_{a \in \mathcal{F}} \log (\rho_a) \right] \right),$$

which is defined to be the *partition function/sum* of a QFG.
Quantum Partition-Sum Problem

Definition 6 (Partition Function/Sum)

In a number of applications, we are interested in calculating

$$Z \triangleq \text{Tr} (\rho) = \text{Tr} \left( \bigotimes_{a \in \mathcal{F}} \rho_a \right) = \text{Tr} \left( \exp \left[ \sum_{a \in \mathcal{F}} \log(\rho_a) \right] \right),$$

which is defined to be the *partition function/sum* of a QFG.

In general calculation of the partition function/sum of a QFG is NP hard.
Outline

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Closing-the-box operations and partial trace functions

Closing the box in CFG

\[
Z = \sum_{x_1, x_2} f_A(x_1) f_B(x_1, x_2) f_C(x_2)
\]
Closing-the-box operations and partial trace functions

Closing the box in CFG

\[ Z = \sum_{x_1, x_2} f_A(x_1) f_B(x_1, x_2) f_C(x_2) = \sum_{x_1} f_A(x_1) \sum_{x_2} f_B(x_1, x_2) f_C(x_2) \]
Closing-the-box operations and partial trace functions

Closing the box in CFG $\implies$ Applying distributive law

\[
Z = \sum_{x_1, x_2} f_A(x_1) f_B(x_1, x_2) f_C(x_2) = \sum_{x_1} f_A(x_1) \sum_{x_2} f_B(x_1, x_2) f_C(x_2)
\]
Closing-the-box operations and partial trace functions

Closing the box in QFG

\[ Z = \text{Tr}(\rho_A \otimes \rho_B \otimes \rho_C) \]
Closing-the-box operations and partial trace functions

Closing the box in QFG

\[ Z = \text{Tr}(\rho_A \odot \rho_B \odot \rho_C) \overset{?}{=} \text{Tr}_1(\rho_A \odot \text{Tr}_2(\rho_B \odot \rho_C)) \]
Closing-the-box operations and partial trace functions

Closing the box in QFG $\implies$ Distributive law over (partial) trace

\[
Z = \text{Tr}(\rho_A \otimes \rho_B \otimes \rho_C) \overset{?}{=} \text{Tr}_1(\rho_A \otimes \text{Tr}_2(\rho_B \otimes \rho_C))
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Closing-the-box operations and partial trace functions

Closing the box in QFG $\implies$ Distributive law over (partial) trace

\[
Z = \text{Tr}(\rho_A \otimes \rho_B \otimes \rho_C) = \text{Tr}_1(\rho_A \otimes \text{Tr}_2(\rho_B \otimes \rho_C))
\]

However, in general,

\[
\text{Tr}(\rho_A \otimes \rho_B \otimes \rho_C) = \text{Tr}_1(\text{Tr}_2(\rho_A \otimes \rho_B \otimes \rho_C)) \neq \text{Tr}_1(\rho_A \otimes \text{Tr}_2(\rho_B \otimes \rho_C)).
\]
Closing-the-box operations and partial trace functions

Closing the box in QFG $\implies$ Distributive law over (partial) trace

\[ Z = \text{Tr}(\rho_A \otimes \rho_B \otimes \rho_C) \stackrel{?}{=} \text{Tr}_1 (\rho_A \otimes \text{Tr}_2 (\rho_B \otimes \rho_C)) \]

However, in general,

\[ \text{Tr}(\rho_A \otimes \rho_B \otimes \rho_C) = \text{Tr}_1 (\text{Tr}_2 (\rho_A \otimes \rho_B \otimes \rho_C)) \neq \text{Tr}_1 (\rho_A \otimes \text{Tr}_2 (\rho_B \otimes \rho_C)). \]

Example 7

Let $\mathcal{H}_1 = \mathcal{H}_2 \triangleq \mathbb{C}^2$. Suppose $\rho_A \triangleq \frac{1}{2} \cdot \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}$, $\rho_B \otimes \rho_C \triangleq \text{diag}(0, 1, 1, 0)$. In this case, $\text{Tr}(\rho_A \otimes \rho_B \otimes \rho_C) = 0$ and $\text{Tr}_1 (\rho_A \otimes \text{Tr}_2 (\rho_B \otimes \rho_C)) = 1$. 
Cases when factors are close to identity matrix

Oftentimes, we can still have an approximate closing-the-box rule.

**Lemma 8**

We have bounds

\[ S(\kappa(\rho_A))^{-1} \leq \frac{\text{Tr}(\rho_A \otimes \rho_B \otimes \rho_C)}{\text{Tr}_1(\rho_A \otimes \text{Tr}_2(\rho_B \otimes \rho_C))} \leq S(\kappa(\rho_A)). \]

**Given**

- \( \rho_A \in \mathcal{L}^{++}(\mathcal{H}_1); \)
- \( \rho_B \in \mathcal{L}^{++}(\mathcal{H}_1 \otimes \mathcal{H}_2); \)
- \( \rho_C \in \mathcal{L}^{++}(\mathcal{H}_2); \)
- \( \kappa(\cdot) \geq 1 \) is the condition number function;
- \( S(\cdot) \) is the Specht ratio function defined as

\[ S(r) \triangleq \frac{(r - 1) \cdot r^{\frac{1}{r-1}}}{e \cdot \log r}. \]
Cases when factors are close to identity matrix

Oftentimes, we can still have an approximate closing-the-box rule.

Lemma 8

We have bounds

\[ S(\kappa(\rho_A)) - 1 \leq \frac{\text{Tr}(\rho_A \otimes \rho_B \otimes \rho_C)}{\text{Tr}_1(\rho_A \otimes \text{Tr}_2(\rho_B \otimes \rho_C))} \leq S(\kappa(\rho_A)). \]

Given

- \( \rho_A \in \mathcal{L}^{++}(\mathcal{H}_1); \)
- \( \rho_B \in \mathcal{L}^{++}(\mathcal{H}_1 \otimes \mathcal{H}_2); \)
- \( \rho_C \in \mathcal{L}^{++}(\mathcal{H}_2); \)
- \( \kappa(\cdot) \geq 1 \) is the condition number function;
- \( S(\cdot) \) is the Specht ratio function defined as

\[ S(r) \triangleq \frac{(r - 1) \cdot r^{\frac{1}{r-1}}}{e \cdot \log r}. \]

The proof utilizes the Golden–Thompson inequality [Bourin and Seo, 2007].
Cases when factors are close to identity matrix

Oftentimes, we can still have an approximate closing-the-box rule.

**Lemma 8**

We have bounds

\[
S(\kappa(\rho_A))^{-1} \leq \frac{\text{Tr}(\rho_A \odot \rho_B \odot \rho_C)}{\text{Tr}_1(\rho_A \odot \text{Tr}_2(\rho_B \odot \rho_C))} \leq S(\kappa(\rho_A)).
\]

The proof utilizes the Golden–Thompson inequality [Bourin and Seo, 2007]. Considering \( \rho_A \approx I \),
Cases when factors are close to identity matrix

Oftentimes, we can still have an approximate closing-the-box rule.

**Lemma 8**

We have bounds

\[
S\left(\kappa(\rho_A)\right)^{-1} \leq \frac{\text{Tr}(\rho_A \odot \rho_B \odot \rho_C)}{\text{Tr}_1(\rho_A \odot \text{Tr}_2(\rho_B \odot \rho_C))} \leq S\left(\kappa(\rho_A)\right).
\]

The proof utilizes the Golden–Thompson inequality [Bourin and Seo, 2007]. Considering \(\rho_A \approx I\), we expect to have

\[
\text{Tr}(\rho_A \odot \rho_B \odot \rho_C) \approx \text{Tr}_1(\rho_A \odot \text{Tr}_2(\rho_B \odot \rho_C)).
\]
Type-1 Approximation

when \( \rho_A \) is “close” to identity matrix \( I \)

\[
Z = \text{Tr}(\rho_A \otimes \rho_B \otimes \rho_C)
\]

\[
\text{Tr}_1(\rho_A \otimes \text{Tr}_2(\rho_B \otimes \rho_C))
\]
Type-1 Approximation

when $\rho_A$ is “close” to identity matrix $I$

$Z = \text{Tr}(\rho_A \odot \rho_B \odot \rho_C)$

$\approx \text{Tr}_1(\rho_A \odot \text{Tr}_2(\rho_B \odot \rho_C))$
Type-1 Approximation

when $\rho_1$ is “close” to identity matrix $I$

$Z = \text{Tr}(\rho_1 \odot \rho_{1,2})$

$\approx \text{Tr}_1(\rho_1 \odot \text{Tr}_2(\rho_{1,2}))$
Type-1 Approximation

when $\rho_1$ or $\rho_{1,2}$ is “close” to identity matrix $I$

\[ Z = \text{Tr}(\rho_1 \otimes \rho_{1,2}) \]

\[ \approx \text{Tr}_1(\rho_1 \otimes \text{Tr}_2(\rho_{1,2})) \]
Type-1 Approximation

when $\rho_1$ or $\rho_{1,2}$ is "close" to identity matrix $I$

$$Z = \text{Tr}(\rho_1 \odot \rho_{1,2})$$

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Type-1 Approximation

when $\rho_1$ or $\rho_{1,2}$ is “close” to identity matrix $I$

$Z = \text{Tr}(\rho_1 \otimes \rho_{1,2})$ ~

$\text{Tr}_1(\rho_1 \otimes \text{Tr}_2(\rho_{1,2}))$

Lemma (Type-1 Approximation)

Given $X \in \mathcal{L}^H(\mathcal{H}_1)$, and $Y \in \mathcal{L}^H(\mathcal{H}_1 \otimes \mathcal{H}_2)$, for $t$ close to 0, we have

$$\text{Tr}_2[(I + tX) \otimes (I + tY)] = (I + tX) \otimes \text{Tr}_2(I + tY) + O(t^3).$$  \hspace{1cm} (4)

Theorem (Type-1 Approximation)

Following the same setup, we have

$$\text{Tr}[(I + tX) \otimes (I + tY)] = \text{Tr}_1[(I + tX) \otimes \text{Tr}_2(I + tY)] + O(t^4).$$  \hspace{1cm} (5)
Type-1 Approximation

when $\rho_1$ or $\rho_{1,2}$ is “close” to identity matrix $I$

$Z = \text{Tr}(\rho_1 \odot \rho_{1,2})$

“Linear” close to $I$: i.e., $\rho_1 = I + tX$ and $\rho_{1,2} = I + tY$. 

\[ \text{Tr}_1(\rho_1 \odot \text{Tr}_2(\rho_{1,2})) \]
Type-1 Approximation

when \(\rho_1\) or \(\rho_{1,2}\) is “close” to identity matrix \(I\)

\[
Z = \text{Tr}(\rho_1 \otimes \rho_{1,2})
\]

“Linear” close to \(I\): i.e., \(\rho_1 = I + tX\) and \(\rho_{1,2} = I + tY\).

Taylor Series Expansion:

\[
\overline{\text{Tr}}(\rho_1 \otimes \rho_{1,2}) =
\]

\[
\overline{\text{Tr}}_1(\rho_1 \otimes \overline{\text{Tr}}_2(\rho_{1,2})) =
\]
Type-1 Approximation

when $\rho_1$ or $\rho_{1,2}$ is "close" to identity matrix $I$

$Z = \text{Tr}(\rho_1 \otimes \rho_{1,2})$

"Linear" close to $I$: i.e., $\rho_1 = I + tX$ and $\rho_{1,2} = I + tY$.

Taylor Series Expansion:

$\text{Tr}(\rho_1 \otimes \rho_{1,2}) = 1 + t \cdot \text{Tr}(X + Y) + t^2 \cdot \frac{\text{Tr}(XY + YX)}{2} + t^3 \cdot 0$

$+ t^4 \cdot \frac{\text{Tr}(XYX - XX^2)}{12} + \cdots$

$\text{Tr}_1(\rho_1 \otimes \text{Tr}_2(\rho_{1,2})) = 1 + t \cdot \text{Tr}_1(X + \text{Tr}_2(Y)) + t^2 \cdot \frac{\text{Tr}_1[X\text{Tr}_2(Y) + \text{Tr}_2(Y)X]}{2}$

$+ t^4 \cdot \frac{\text{Tr}_1[X\text{Tr}_2(Y)X\text{Tr}_2(Y) - XX\text{Tr}_2(Y)^2]}{12} + \cdots$
Type-1 Approximation

when $\rho_1$ or $\rho_{1,2}$ is "close" to identity matrix $I$

$Z = \text{Tr}(\rho_1 \odot \rho_{1,2})$

$\approx \text{Tr}_1(\rho_1 \odot \text{Tr}_2(\rho_{1,2}))$

"Linear" close to $I$: i.e., $\rho_1 = I + tX$ and $\rho_{1,2} = I + tY$.

Taylor Series Expansion:

$\overline{\text{Tr}}(\rho_1 \odot \rho_{1,2}) = 1 + t \cdot \overline{\text{Tr}}(X + Y) + t^2 \cdot \frac{\overline{\text{Tr}}(XY + YX)}{2} + t^3 \cdot 0$

$+ t^4 \cdot \frac{\overline{\text{Tr}}(XYX - X^2Y^2)}{12} + \cdots$

$\overline{\text{Tr}}_1(\rho_1 \odot \overline{\text{Tr}}_2(\rho_{1,2})) = 1 + t \cdot \overline{\text{Tr}}_1(X + \overline{\text{Tr}}_2(Y)) + t^2 \cdot \frac{\overline{\text{Tr}}_1[X \overline{\text{Tr}}_2(Y) + \overline{\text{Tr}}_2(Y)X]}{2}$

$+ t^3 \cdot \frac{\overline{\text{Tr}}_1[X \overline{\text{Tr}}_2(Y)X \overline{\text{Tr}}_2(Y) - X^2 \overline{\text{Tr}}_2(Y)^2]}{12} + \cdots$
Type-2 Approximation

when $\rho_1$ or $\rho_{1,2}$ is “close” to identity matrix $I$

$Z = \text{Tr}(\rho_1 \otimes \rho_{1,2})$

$\approx \text{Tr}_1(\rho_1 \otimes \text{Tr}_2(\rho_{1,2}))$
Type-2 Approximation

when $\rho_1$ or $\rho_{1,2}$ is “close” to identity matrix $I$

$$Z = \text{Tr}(\rho_1 \otimes \rho_{1,2})$$

$$\rho_1 \xrightarrow{H_1} \rho_{1,2} \xrightarrow{H_2}$$

$\approx$

$$\text{Tr}_1(\rho_1 \otimes \text{Tr}_2(\rho_{1,2}))$$

Lemma (Type-2 Approximation)

Given $X \in \mathcal{L}^H(H_1)$, and $Y \in \mathcal{L}^H(H_1 \otimes H_2)$, for $t$ close to 0, we have

$$\text{Tr}_2\left[e^{tX} \otimes e^{tY}\right] = e^{tX} \otimes \text{Tr}_2(e^{tY}) + O(t^3).$$

(4)

Theorem (Type-2 Approximation)

Following the same setup, we have

$$\text{Tr}\left[e^{tX} \otimes e^{tY}\right] = \text{Tr}_1\left[e^{tX} \otimes \text{Tr}_2(e^{tY})\right] + O(t^4).$$

(5)
Type-2 Approximation

when $\rho_1$ or $\rho_{1,2}$ is "close" to identity matrix $I$

\[ Z = \text{Tr}(\rho_1 \odot \rho_{1,2}) \approx \text{Tr}_1(\rho_1 \odot \text{Tr}_2(\rho_{1,2})) \]

"Exponential" close to $I$: i.e., $\rho_1 = e^{tX}$ and $\rho_{1,2} = e^{tY}$. 
Type-2 Approximation

when \( \rho_1 \) or \( \rho_{1,2} \) is "close" to identity matrix \( I \)

\[
Z = \text{Tr}(\rho_1 \otimes \rho_{1,2})
\]

"Exponential" close to \( I \): i.e., \( \rho_1 = e^{tX} \) and \( \rho_{1,2} = e^{tY} \).

Taylor Series Expansion:

\[
\overline{\text{Tr}}(\rho_1 \otimes \rho_{1,2}) = \\
\overline{\text{Tr}}_1(\rho_1 \otimes \overline{\text{Tr}}_2(\rho_{1,2})) = 
\]
Type-2 Approximation

when $\rho_1$ or $\rho_{1,2}$ is “close” to identity matrix $I$

$Z = \text{Tr}(\rho_1 \circ \rho_{1,2})$

$\approx \text{Tr}_1(\rho_1 \circ \text{Tr}_2(\rho_{1,2}))$

“Exponential” close to $I$: i.e., $\rho_1 = e^{tX}$ and $\rho_{1,2} = e^{tY}$.

Taylor Series Expansion:

$$\overline{\text{Tr}}(\rho_1 \circ \rho_{1,2}) = 1 + t \cdot \overline{\text{Tr}}(\tilde{X} + Y) + \frac{t^2}{2!} \cdot \overline{\text{Tr}}(\tilde{X} + Y)^2 + \frac{t^3}{3!} \cdot \overline{\text{Tr}}(\tilde{X} + Y)^3 + \frac{t^4}{4!} \cdot \overline{\text{Tr}}(\tilde{X} + Y)^4 + \cdots$$

$$\overline{\text{Tr}}_1(\rho_1 \circ \text{Tr}_2(\rho_{1,2})) = 1 + t \cdot \overline{\text{Tr}}_1\left(X + \text{Tr}_2(Y)\right) + \frac{t^2}{2} \cdot \overline{\text{Tr}}_1\left(X^2 + X\text{Tr}_2(Y) + \text{Tr}_2(Y)X + \text{Tr}_2(Y^2)\right)$$

$$+ \frac{t^3}{6} \cdot \overline{\text{Tr}}_1\left(X^3 + 3 \cdot X^2 \cdot \text{Tr}_2(Y) + 3 \cdot X \cdot \text{Tr}_2(Y^2) + \text{Tr}_2(Y^3)\right) + \cdots$$
**Type-2 Approximation**

When $\rho_1$ or $\rho_{1,2}$ is "close" to identity matrix $I$,

$$Z = \text{Tr}(\rho_1 \odot \rho_{1,2}) \approx \text{Tr}_1(\rho_1 \odot \text{Tr}_2(\rho_{1,2}))$$

"Exponential" close to $I$: i.e., $\rho_1 = e^{tX}$ and $\rho_{1,2} = e^{tY}$.

Taylor Series Expansion:

$$\overline{\text{Tr}}(\rho_1 \odot \rho_{1,2}) = 1 + t \cdot \overline{\text{Tr}}(\tilde{X} + Y) + \frac{t^2}{2!} \cdot \overline{\text{Tr}}((\tilde{X} + Y)^2) + \frac{t^3}{3!} \cdot \overline{\text{Tr}}((\tilde{X} + Y)^3) + \frac{t^4}{4!} \cdot \overline{\text{Tr}}((\tilde{X} + Y)^4) + \cdots$$

$$\overline{\text{Tr}}_1(\rho_1 \odot \text{Tr}_2(\rho_{1,2})) = 1 + t \cdot \overline{\text{Tr}}_1(X + \text{Tr}_2(Y)) + \frac{t^2}{2} \cdot \overline{\text{Tr}}_1(X^2 + X\text{Tr}_2(Y) + \text{Tr}_2(Y)X + \text{Tr}_2(Y^2))$$

$$+ \frac{t^3}{6} \cdot \overline{\text{Tr}}_1(X^3 + 3 \cdot X^2 \cdot \text{Tr}_2(Y) + 3 \cdot X \cdot \text{Tr}_2(Y^2) + \text{Tr}_2(Y^3)) + \cdots$$
**t-close Approximation**

**Definition (t-close to I)**

A set of operators \( \{\rho_k\}_k \) are said to be *t-close to I*, if

\[
\rho_k = I + t\chi_k \quad \text{or} \quad \rho_k = e^{t\chi_k} \quad \forall k,
\]

for some Hermitian operators \( \{\chi_k\}_k \), and \( t \) close to 0.
**t-close Approximation**

**Definition (t-close to I)**

A set of operators \( \{ \rho_k \} \) are said to be **t-close to I**, if

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\rho_k = I + t \chi_k \quad \text{or} \quad \rho_k = e^{t \chi_k} \quad \forall k,
\]

for some Hermitian operators \( \{ \chi_k \} \), and \( t \) close to 0.

**Lemma 9 (t-close Approximation)**

Given \( \rho_1 \in \mathcal{L}^+ (\mathcal{H}_1) \), and \( \rho_{1,2} \in \mathcal{L}^H (\mathcal{H}_1 \otimes \mathcal{H}_2) \), \( t \) close to I, we have

\[
\text{Tr}_2 [\rho_1 \odot \rho_{1,2}] = \rho_1 \odot \text{Tr}_2 (\rho_{1,2}) + O(t^3).
\]  
(4)

**Theorem 10 (t-close Approximation)**

Following the same setup, we have

\[
\text{Tr} [\rho_1 \odot \rho_{1,2}] = \text{Tr}_1 [\rho_1 \odot \text{Tr}_2 (\rho_{1,2})] + O(t^4). 
\]  
(5)
Numerical Result of Closing-the-Box Approximation

We are interested in a numerical comparison between

$$\text{Tr}_1(\text{Tr}_2(\rho_1 \circ \rho_{1,2})) \text{ and } \text{Tr}_1(\rho_1 \circ \text{Tr}_2(\rho_{1,2})).$$

for random $\rho_1 \in \mathcal{L}^+ (\mathbb{C}^2)$ and $\rho_{1,2} \in \mathcal{L}^+ (\mathbb{C}^4)$. 
We are interested in a numerical comparison between

\[ \text{Tr}_1(\text{Tr}_2(\rho_1 \odot \rho_{1,2})) \text{ and } \text{Tr}_1(\rho_1 \odot \text{Tr}_2(\rho_{1,2})). \]

for random \( \rho_1 \in \mathcal{L}^+ (\mathbb{C}^2) \) and \( \rho_{1,2} \in \mathcal{L}^+ (\mathbb{C}^4) \).
We are interested in a numerical comparison between

\[ \text{Tr}_1(\text{Tr}_2(\rho_1 \odot \rho_{1,2})) \text{ and } \text{Tr}_1(\rho_1 \odot \text{Tr}_2(\rho_{1,2})). \]

for random \( \rho_1 \in \mathcal{L}^+ (\mathbb{C}^2) \) and \( \rho_{1,2} \in \mathcal{L}^+ (\mathbb{C}^4). \)

\[ \rho = U^H \Lambda U \]
Numerical Result of Closing-the-Box Approximation

We are interested in a numerical comparison between

$$\text{Tr}_1(\text{Tr}_2(\rho_1 \odot \rho_{1,2})) \text{ and } \text{Tr}_1(\rho_1 \odot \text{Tr}_2(\rho_{1,2})).$$

for random $\rho_1 \in \mathcal{L}^+ (\mathbb{C}^2)$ and $\rho_{1,2} \in \mathcal{L}^+ (\mathbb{C}^4)$.

- Unitary matrix $U = [u_1, \cdots, u_n]$ with $u_1 \perp \cdots \perp u_n$
  uniformly distributed on $\mathbb{C}^n$ unit sphere.

$$\rho = U^H \Lambda U$$
Numerical Result of Closing-the-Box Approximation

We are interested in a numerical comparison between

$$\text{Tr}_1(\text{Tr}_2(\rho_1 \circ \rho_{1,2}))$$

and

$$\text{Tr}_1(\rho_1 \circ \text{Tr}_2(\rho_{1,2}))$$.

for random $\rho_1 \in \mathcal{L}^+ (\mathbb{C}^2)$ and $\rho_{1,2} \in \mathcal{L}^+ (\mathbb{C}^4)$.

- Unitary matrix $U = [u_1, \cdots, u_n]$ with $u_1 \perp \cdots \perp u_n$

uniformly distributed on $\mathbb{C}^n$ unit sphere.

$$\rho = U^H \Lambda U$$
Numerical Result of Closing-the-Box Approximation

We are interested in a numerical comparison between

\[ \text{Tr}_1(\text{Tr}_2(\rho_1 \circ \rho_{1,2})) \text{ and } \text{Tr}_1(\rho_1 \circ \text{Tr}_2(\rho_{1,2})). \]

for random \( \rho_1 \in \mathcal{L}^+ (\mathbb{C}^2) \) and \( \rho_{1,2} \in \mathcal{L}^+ (\mathbb{C}^4) \).

- Unitary matrix \( U = [u_1, \cdots, u_n] \) with \( u_1 \perp \cdots \perp u_n \)
  uniformly distributed on \( \mathbb{C}^n \) unit sphere.

\[ \rho = U^H \Lambda U \]
We are interested in a numerical comparison between

$$\text{Tr}_1(\text{Tr}_2(\rho_1 \odot \rho_{1,2})) \text{ and } \text{Tr}_1(\rho_1 \odot \text{Tr}_2(\rho_{1,2})).$$

for random $\rho_1 \in \mathcal{L}^+ (\mathbb{C}^2)$ and $\rho_{1,2} \in \mathcal{L}^+ (\mathbb{C}^4)$.

- Unitary matrix $U = [u_1, \cdots, u_n]$ with $u_1 \perp \cdots \perp u_n$
- Uniformly distributed on $\mathbb{C}^n$ unit sphere.
Numerical Result of Closing-the-Box Approximation

We are interested in a numerical comparison between

\[ \text{Tr}_1(\text{Tr}_2(\rho_1 \circ \rho_{1,2})) \quad \text{and} \quad \text{Tr}_1(\rho_1 \circ \text{Tr}_2(\rho_{1,2})). \]

for random \( \rho_1 \in \mathcal{L}^+ (\mathbb{C}^2) \) and \( \rho_{1,2} \in \mathcal{L}^+ (\mathbb{C}^4) \).

- Unitary matrix \( U = [u_1, \cdots, u_n] \) with \( u_1 \perp \cdots \perp u_n \) uniformly distributed on \( \mathbb{C}^n \) unit sphere.

\[ \rho = U^H \Lambda U \]
Numerical Result of Closing-the-Box Approximation

We are interested in a numerical comparison between

\[ \text{Tr}_1(\text{Tr}_2(\rho_1 \odot \rho_{1,2})) \text{ and } \text{Tr}_1(\rho_1 \odot \text{Tr}_2(\rho_{1,2})). \]

for random \( \rho_1 \in \mathcal{L}^+ (\mathbb{C}^2) \) and \( \rho_{1,2} \in \mathcal{L}^+ (\mathbb{C}^4) \).

\[ \rho = U^H \Lambda U \]

- Unitary matrix \( U = [u_1, \cdots, u_n] \) with \( u_1 \perp \cdots \perp u_n \) uniformly distributed on \( \mathbb{C}^n \) unit sphere.

- Diagonal matrix \( \Lambda = \text{diag}(\lambda_1, \cdots, \lambda_n) \) with \( \{\lambda_k\}_k \) to be i.i.d.
We are interested in a numerical comparison between

$$\text{Tr}_1(\text{Tr}_2(\rho_1 \odot \rho_{1,2})) \quad \text{and} \quad \text{Tr}_1(\rho_1 \odot \text{Tr}_2(\rho_{1,2})).$$

for random $\rho_1 \in \mathcal{L}^+ (\mathbb{C}^2)$ and $\rho_{1,2} \in \mathcal{L}^+ (\mathbb{C}^4)$.

- Unitary matrix $U = [u_1, \cdots, u_n]$ with $u_1 \perp \cdots \perp u_n$ uniformly distributed on $\mathbb{C}^n$ unit sphere.

- Diagonal matrix $\Lambda = \text{diag}(\lambda_1, \cdots, \lambda_n)$ with $\{\lambda_k\}_k$ to be i.i.d.

Consider the statistics of the relative error:

$$\eta \triangleq \frac{|\text{Tr}_1[\rho_A \odot \text{Tr}_2(\rho_B)] - \text{Tr}_1[\text{Tr}_2(\rho_A \odot \rho_B)]|}{\text{Tr}_1[\text{Tr}_2(\rho_A \odot \rho_B)].}$$
Numerical Result of Closing-the-Box Approximation

Frequency Density = Frequency Interval Length

- - - $|\mathcal{N}(\mu,\sigma^2)|$ distributed Eigenvalues ($\mu = 1$, $\sigma = 0.25$)
- - - - $|\mathcal{N}(\mu,\sigma^2)|$ distributed Eigenvalues ($\mu = 1$, $\sigma = 0.5$)
- - - - - $|\mathcal{N}(\mu,\sigma^2)|$ distributed Eigenvalues ($\mu = 1$, $\sigma = 1$)
- - - - - - - Uniformly distributed Eigenvalues ($a = 0$, $b = 1$)

Relative Error $\eta$
Numerical Result of Closing-the-Box Approximation

Relative Error $\eta$

Frequency Density = \frac{\text{Frequency}}{\text{Interval Length}}

$|\mathcal{N}(\mu, \sigma^2)|$ distributed Eigenvalues ($\mu = 1, \sigma = 0.25$)

$|\mathcal{N}(\mu, \sigma^2)|$ distributed Eigenvalues ($\mu = 1, \sigma = 0.5$)

$|\mathcal{N}(\mu, \sigma^2)|$ distributed Eigenvalues ($\mu = 1, \sigma = 1$)

Uniformly distributed Eigenvalues ($a = 0, b = 1$)
Corollary 11 (Closing-the-box on a Chain QFG)

Consider the chain QFG above where \( \{\rho_k\}_k \) are \( t \)-close to \( I \). Then,

\[
\text{Tr} \{ \rho_1 \circ \rho_2 \circ \cdots \circ \rho_{N-1} \circ \rho_N \} = \text{Tr} \{ \rho_1 \circ \rho_2 \circ \cdots \circ \rho_{N-1} \circ \rho_N \} + O(t^4)
\]
Corollary 11 (Closing-the-box on a Chain QFG)

Consider the chain QFG above where \( \{\rho_k\}_k \) are \( t \)-close to \( I \). Then,

\[
\text{Tr} \left\{ \rho_1 \odot \rho_2 \odot \cdots \odot \rho_{N-1} \odot \rho_N \right\} \\
= \text{Tr}_{\geq 2} \left\{ \text{Tr}_1(\rho_1 \odot \rho_2) \odot \cdots \odot \rho_{N-1} \odot \rho_N \right\} + O(t^4)
\]

(6)
Corollary 11 (Closing-the-box on a Chain QFG)

Consider the chain QFG above where \( \{\rho_k\}_k \) are \( t \)-close to \( I \). Then,

\[
\text{Tr} \{\rho_1 \circ \rho_2 \circ \cdots \circ \rho_{N-1} \circ \rho_N\} \\
= \text{Tr}_{\geq 2} \{\text{Tr}_1(\rho_1 \circ \rho_2) \circ \cdots \circ \rho_{N-1} \circ \rho_N\} + O(t^4) \\
= \text{Tr}_{\geq 3} \{\text{Tr}_2[\text{Tr}_1(\rho_1 \circ \rho_2) \circ \rho_3] \circ \cdots \circ \rho_{N-1} \circ \rho_N\} + O(t^4)
\]
Corollary 11 (Closing-the-box on a Chain QFG)

Consider the chain QFG above where \( \{\rho_k\}_k \) are \( t \)-close to \( I \). Then,

\[
\text{Tr} \{\rho_1 \otimes \rho_2 \otimes \cdots \otimes \rho_{N-1} \otimes \rho_N\} \\
= \text{Tr}_{\geq 2} \{\text{Tr}_1(\rho_1 \otimes \rho_2) \otimes \cdots \otimes \rho_{N-1} \otimes \rho_N\} + O(t^4) \\
= \text{Tr}_{\geq 3} \{\text{Tr}_2[\text{Tr}_1(\rho_1 \otimes \rho_2) \otimes \rho_3] \otimes \cdots \otimes \rho_{N-1} \otimes \rho_N\} + O(t^4) \\
= \text{Tr}_{N-1} \{\text{Tr}_{N-2} [\text{Tr}_{N-3} (\cdots \text{Tr}_1(\rho_1 \otimes \rho_2) \cdots) \otimes \rho_{N-1}] \otimes \rho_N\} + O(t^4).
\]
Closing-the-box Operations on QFGs

Closing-the-box on a Tree QFG
Applying the same trick on a tree QFG

Quantum Sum-Product Algorithm for Trees

Require:
Acyclic QFG $G = (F, V, E)$; root $r \in V$; height of the tree $h \geq 0$; local operators $\{\rho_a\}_{a \in \text{local}}$.

Ensure:
Approximate Partition sum $Z_1$: for $d = h - 1, \cdots, 0$ do
for all $i \in V$ d-step reachable from $r$ do
Let $\rho(i)$ be the parent factor of $i$;
$\rho(i) \leftarrow \text{Tr}_i(\bigotimes_{a \in \partial i} f_a(x_i))$;
end for
end for
$\tilde{Z} \leftarrow \rho(r)$.
Closing-the-box on a Tree QFG

Applying the same trick on a tree QFG

Quantum Sum-Product Algorithm for Trees

Require:

Acyclic QFG $G = (F, V, E)$; root $r \in V$; height of the tree $h \geq 0$; local operators $\{\rho_a\}$ at close to $I$.

Ensure:

Approximate Partition sum $Z_1$:

1. For $d = h - 1, \ldots, 0$

2. For all $i \in V$ $d$-step reachable from $r$

3. Let $\rho(i)$ be the parent factor of $i$;

4. $\rho(i) \leftarrow \text{Tr}_{i}(\bigotimes_{a \in \partial i} f_a(x_i))$;

5. End for

6. End for

7. $\tilde{Z} \leftarrow \rho(r)$.

Michael X. CAO (IE@CUHK)
Closing-the-box on a Tree QFG

Applying the same trick on a tree QFG
Closing-the-box Operations on QFGs

Closing-the-box on a Tree QFG
Applying the same trick on a tree QFG

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Acyclic QFG $G = (F, V, E)$; root $r \in V$; height of the tree $h \geq 0$; local operators $\{\rho_a\}$ $a$-close to $I$.

Ensure:
Approximate Partition sum $\tilde{Z}$:
for $d = h - 1, \ldots, 0$
  for all $i \in V$ $d$-step reachable from $r$
    Let $\rho_i$ be the parent factor of $i$
    $\rho_i \leftarrow \text{Tr}_i(\bigotimes_{a \in \partial_i} f_a(x_i))$
  end for
end for
$\tilde{Z} \leftarrow \rho_r$. 
Closing-the-box on a Tree QFG

Applying the same trick on a tree QFG
Quantum Sum-Product Algorithm for Trees

Require:
- Acyclic QFG \( G = (F, V, E); \) root \( r \in V \); height of the tree \( h \geq 0 \);
- Local operators \( \{\rho_a\}_{a \in \text{local}} \) close to \( I \).

Ensure:
- Approximate Partition sum \( Z \)

1: for \( d = h-1, \cdots, 0 \) do
2: for all \( i \in V \) \text{d-step reachable from } r \) do
3: Let \( \rho_i \) be the parent factor of \( i \);
4: \( \rho_i \leftarrow \text{Tr}_i (\bigotimes_{a \in \partial_i} f_a(x_i)) \);
5: end for
6: end for
7: \( \tilde{Z} \leftarrow \rho_r \).
Closing-the-box Operations on QFGs

Closing-the-box on a Tree QFG

Applying the same trick on a tree QFG

Quantum Sum-Product Algorithm for Trees

**Require:** Acyclic QFG $\mathcal{G} = (\mathcal{F}, \mathcal{V}, \mathcal{E})$; root $r \in \mathcal{V}$; height of the tree $h \geq 0$; local operators $\{\rho_a\}_a$ $t$-close to $I$.

**Ensure:** Approximate Partition sum $Z$

1: for $d = h - 1, \ldots, 0$ do
2: for all $i \in \mathcal{V}$ d-step reachable from $r$ do
3: Let $\rho^{(i)}$ be the parent factor of $i$;
4: $\rho^{(i)} \leftarrow \text{Tr}_i \left( \bigotimes_{a \in \partial i} f_a(x_i) \right)$;
5: end for
6: end for
7: $\tilde{Z} \leftarrow \rho^{(r)}$. 

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Closing-the-box on a Tree QFG
Applying the same trick on a tree QFG

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Ensure: Approximate Partition sum $\tilde{Z}$

1: for $d = h - 1, \cdots, 0$ do
2: for all $i \in \mathcal{V}$ d-step reachable from $r$ do
3: Let $\rho^{(i)}$ be the parent factor of $i$;
4: $\rho^{(i)} \leftarrow \text{Tr}_i \left( \bigotimes_{a \in \partial_i} f_a(x_i) \right)$;
5: end for
6: end for
7: $\tilde{Z} \leftarrow \rho^{(r)}$. 

Michael X. CAO (IE@CUHK)
Quantum Factor Graphs
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Quantum Sum-Product Algorithm (QSPA)

Quantum Sum-Product Algorithm [Leifer and Poulin, 2008]

Require: QFG $\mathcal{G} = (\mathcal{F}, \mathcal{V}, \mathcal{E})$;
Ensure: ???

1: for all $(i, a) \in \mathcal{E}$ do
2: \quad $m_{i \rightarrow a} \leftarrow l \in \mathcal{L}(\mathcal{H}_i)$;
3: \quad $m_{a \rightarrow i} \leftarrow l \in \mathcal{L}(\mathcal{H}_i)$;
4: end for
5: repeat
6: \quad for all $(i, a) \in \mathcal{E}$ do
7: \quad \quad $m_{i \rightarrow a} \propto \bigodot_{c \in \partial_i \setminus a} m_{a \rightarrow i}$;
8: \quad end for
9: \quad for all $(i, a) \in \mathcal{E}$ do
10: \quad \quad $m_{a \rightarrow i} \propto \text{Tr}_{\partial a \setminus i} \left( \rho_a \bigodot \bigodot_{j \in \partial a \setminus i} m_{j \rightarrow a} \right)$;
11: \quad end for
12: until converge
Lemma 12

Consider a QFG with no cycles.
Lemma 12

Consider a QFG with no cycles. Given \( t \)-close density operators

\[
\{ \sigma_a \in \mathcal{L}_1^+ (\mathcal{H}_a) \}_{a \in \mathcal{F}}, \{ \sigma_i \in \mathcal{L}_1^+ (\mathcal{H}_i) \}_{i \in \mathcal{V}}
\]
satisfying the local marginal constrains

\[
\sigma_i = \text{Tr}_{\partial a \setminus i} (\sigma_a) \quad \forall (i, a) \in \mathcal{E}.
\]
Lemma 12

Consider a QFG with no cycles. Given $t$-close density operators

$$\{\sigma_a \in \mathcal{L}_1^+ (\mathcal{H}_a)\}_{a \in \mathcal{F}}, \{\sigma_i \in \mathcal{L}_1^+ (\mathcal{H}_i)\}_{i \in \mathcal{V}}$$

satisfying the local marginal constraints

$$\sigma_i = \text{Tr}_{\partial a \setminus i} (\sigma_a) \quad \forall (i, a) \in \mathcal{E}.$$ 

There exists a global density operator $\tilde{\sigma}$

$$\sigma_a \approx \text{Tr}_{\mathcal{V} \setminus \partial a} (\tilde{\sigma}) \quad \forall a \in \mathcal{F}, \quad \sigma_i \approx \text{Tr}_{\mathcal{V} \setminus i} (\tilde{\sigma}) \quad \forall i \in \mathcal{V}.$$
Lemma 12

Consider a QFG with no cycles. Given \( t \)-close density operators

\[
\{ \sigma_a \in \mathcal{L}^+_1(\mathcal{H}_a) \}_{a \in \mathcal{F}}, \{ \sigma_i \in \mathcal{L}^+_1(\mathcal{H}_i) \}_{i \in \mathcal{V}}
\]

satisfying the local marginal constrains

\[
\sigma_i = \text{Tr}_{\partial a \setminus i} (\sigma_a) \quad \forall (i, a) \in \mathcal{E}.
\]

There exists a global density operator \( \tilde{\sigma} \)

\[
\sigma_a \approx \text{Tr}_{\mathcal{V} \setminus \partial a} (\tilde{\sigma}) \quad \forall a \in \mathcal{F}, \quad \sigma_i \approx \text{Tr}_{\mathcal{V} \setminus i} (\tilde{\sigma}) \quad \forall i \in \mathcal{V}.
\]

**Proof [Idea]** Just consider the closing-the-box operations on

\[
\tilde{\sigma} = \exp \left[ \sum_{a \in \mathcal{F}} \log(\sigma_a) - \sum_{i \in \mathcal{V}} (d_i - 1) \log(\sigma_i) \right].
\]
Lemma 12

Consider a QFG with no cycles. Given $t$-close density operators

$$\{\sigma_a \in \mathcal{L}_1^+ (\mathcal{H}_a)\}_{a \in \mathcal{F}}, \{\sigma_i \in \mathcal{L}_1^+ (\mathcal{H}_i)\}_{i \in \mathcal{V}}$$

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$$\sigma_a \approx \text{Tr}_{\mathcal{V} \setminus \partial a} (\tilde{\sigma}) \quad \forall a \in \mathcal{F}, \quad \sigma_i \approx \text{Tr}_{\mathcal{V} \setminus i} (\tilde{\sigma}) \quad \forall i \in \mathcal{V}.$$ 

Proof [Idea] Just consider the closing-the-box operations on

$$\tilde{\sigma} = \exp \left[ \sum_{a \in \mathcal{F}} \log(\sigma_a) - \sum_{i \in \mathcal{V}} (d_i - 1) \log(\sigma_i) \right].$$

[Remark] If $\sigma$ is the “true” global density operator, then $\tilde{\sigma} \approx \sigma$. 
Outline

1. Factor Graphs/Preliminaries
2. Quantum Factor Graphs (QFGs)
3. Closing-the-box Operations on QFGs
4. Variational Approach on QFGs
5. Numerical Result of QSPA
6. Conclusion & Outlook
Definition 13

In analogy to CFGs, we define the quantum Helmholtz energy and quantum Gibbs free energy as

\[
F_H \triangleq - \log(Z),
\]

\[
F_{\text{Gibbs}}(\sigma) \triangleq - \sum_{a \in \mathcal{F}} \langle \sigma, \log \rho_a \rangle - S(\sigma)
\]

\[
= - \sum_{a \in \mathcal{F}} \langle \text{Tr}_\mathcal{V}\partial_a(\sigma), \log \rho_a \rangle - S(\sigma).
\]

where \( S(\cdot) \) stands for the von Neumann entropy function.
Quantum Helmholtz Energy and Gibbs Free Energy

**Definition 13**

In analogy to CFGs, we define the quantum Helmholtz energy and quantum Gibbs free energy as

$$F_H \triangleq - \log(Z),$$

$$F_{\text{Gibbs}}(\sigma) \triangleq - \sum_{a \in \mathcal{F}} \langle \sigma, \log \rho_a \rangle - S(\sigma)$$

$$= - \sum_{a \in \mathcal{F}} \langle \text{Tr}_{\mathcal{V}\backslash \partial a}(\sigma), \log \rho_a \rangle - S(\sigma).$$

where $S(\cdot)$ stands for the von Neumann entropy function.

Direct calculation yields

$$F_{\text{Gibbs}}(\sigma) = F_H + S(\sigma \parallel \tilde{\rho}) \geq F_H.$$
Quantum Helmholtz Energy and Gibbs Free Energy

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In analogy to CFGs, we define the quantum Helmholtz energy and quantum Gibbs free energy as

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F_H \triangleq - \log(Z),
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\]

\[
= - \sum_{a \in F} \langle \text{Tr}_{Y \setminus \partial a}(\sigma), \log \rho_a \rangle - S(\sigma).
\]

where \( S(\cdot) \) stands for the von Neumann entropy function.

Direct calculation yields

\[
F_{\text{Gibbs}}(\sigma) = F_H + S(\sigma \parallel \tilde{\rho}) \geq F_H.
\]

In other words,

\[
F_H = \min_{\sigma \in L_1^+(\mathcal{H})} F_{\text{Gibbs}}(\sigma).
\]
Definition 13

In analogy to CFGs, we define the quantum Helmholtz energy and quantum Gibbs free energy as

\[ F_H \triangleq -\log(Z), \]
\[ F_{\text{Gibbs}}(\sigma) \triangleq -\sum_{a \in \mathcal{F}} \langle \sigma, \log \rho_a \rangle - S(\sigma) \]
\[ = -\sum_{a \in \mathcal{F}} \langle \text{Tr}_{\mathcal{V}\setminus \partial a}(\sigma), \log \rho_a \rangle - S(\sigma). \]

Direct calculation yields

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Thus, we transfer the calculation of \( Z \) into the optimization problem above.

where \( S(\cdot) \) stands for the von Neumann entropy function.
Definition 13

In analogy to CFGs, we define the quantum Helmholtz energy and quantum Gibbs free energy as

\[
F_H \triangleq - \log(Z),
\]

\[
F_{\text{Gibbs}}(\sigma) \triangleq - \sum_{a \in \mathcal{F}} \langle \sigma, \log \rho_a \rangle - S(\sigma)
= - \sum_{a \in \mathcal{F}} \langle \text{Tr}_{\mathcal{\mathcal{Y}}} \partial_a(\sigma), \log \rho_a \rangle - S(\sigma).
\]

where \(S(\cdot)\) stands for the von Neumann entropy function.

Direct calculation yields

\[
F_{\text{Gibbs}}(\sigma) = F_H + S(\sigma \| \tilde{\rho}) \geq F_H.
\]

In other words,

\[
F_H = \min_{\sigma \in \mathcal{L}_1^+(\mathcal{H})} F_{\text{Gibbs}}(\sigma).
\]

Thus, we transfer the calculation of \(Z\) into the optimization problem above. However, this optimization problem is in general not tractable.
Quantum Bethe Free Energy

In acyclic cases, by Lemma 12, we can approximate $\sigma$ by $\tilde{\sigma}$. Thus, intuitively,
Quantum Bethe Free Energy

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$$F_{\text{Gibbs}} = - \sum_{a \in \mathcal{F}} \langle \text{Tr}_{\mathcal{V}\setminus\partial a}(\sigma), \log \rho_a \rangle - S(\sigma)$$
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$$\approx -\sum_{a \in \mathcal{F}} \langle \text{Tr}_{\mathcal{V}\setminus \partial a}(\sigma), \log \rho_a \rangle - S(\tilde{\sigma})$$
Quantum Bethe Free Energy

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$$\approx - \sum_{a \in \mathcal{F}} \langle \text{Tr}_{\mathcal{V} \setminus \partial a} \sigma, \log \rho_a \rangle - S(\tilde{\sigma})$$

$$\approx - \sum_{a \in \mathcal{F}} \langle \text{Tr}_{\mathcal{V} \setminus \partial a} \sigma, \log \rho_a \rangle - \sum_{a \in \mathcal{F}} S(\sigma_a) + \sum_{i \in \mathcal{V}} (d_i - 1) \cdot S(\sigma_i)$$
Quantum Bethe Free Energy

In acyclic cases, by Lemma 12, we can approximate $\sigma$ by $\tilde{\sigma}$. Thus, intuitively,

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$$\approx -\sum_{a \in \mathcal{F}} \langle \text{Tr}_{\mathcal{V} \backslash \partial_a} \sigma, \log \rho_a \rangle - \sum_{a \in \mathcal{F}} S(\sigma_a) + \sum_{i \in \mathcal{V}} (d_i - 1) \cdot S(\sigma_i)$$

**Definition 14 (Quantum Bethe free energy)**

We define the quantum Bethe free energy function of a QFG to be

$$F_{\text{Bethe}}((\sigma_a)_{a \in \mathcal{F}}, (\sigma_i)_{i \in \mathcal{V}}) \triangleq -\sum_{a \in \mathcal{F}} \langle \sigma_a, \log \rho_a \rangle - \sum_{a \in \mathcal{F}} S(\sigma_a) + \sum_{i \in \mathcal{V}} (d_i - 1) \cdot S(\sigma_i),$$

where $(\sigma_a)_{a \in \mathcal{F}}$ and $(\sigma_i)_{i \in \mathcal{V}}$ are density operators.
**Theorem (\(F_{\text{Bethe}}\) approximate \(F_{\text{Gibbs}}\))**

Consider a QFG with no cycles. Suppose the global density operator \(\sigma\) and its marginals density operator \(\sigma_a \triangleq \operatorname{Tr}_{\{V\setminus a\}}(\sigma)\) for all \(a \in \mathcal{F}\), and \(\sigma_i = \operatorname{Tr}_{\{V\setminus i\}}(\sigma)\) for all \(i \in \mathcal{V}\) are all \(t\)-close to identity. Then,

\[
F_{\text{Gibbs}}(\sigma) = F_{\text{Bethe}}((\sigma_a)_{a \in \mathcal{F}}, (\sigma_i)_{i \in \mathcal{V}}) + O(t^3).
\]

**Definition 14 (Quantum Bethe free energy)**

We define the *quantum Bethe free energy function* of a QFG to be

\[
F_{\text{Bethe}}((\sigma_a)_{a \in \mathcal{F}}, (\sigma_i)_{i \in \mathcal{V}}) \triangleq -\sum_{a \in \mathcal{F}} \langle \sigma_a, \log \rho_a \rangle - \sum_{a \in \mathcal{F}} S(\sigma_a) + \sum_{i \in \mathcal{V}} (d_i - 1) \cdot S(\sigma_i),
\]

(7)

where \((\sigma_a)_{a \in \mathcal{F}}\) and \((\sigma_i)_{i \in \mathcal{V}}\) are density operators.
Definition 15 (Constrained Quantum Bethe Approximation Problem)

\[
\begin{align*}
\min & \quad F_{\text{Gibbs}}(\sigma) \\
\text{s.t.} & \quad \sigma \in \mathcal{L}_1^+(\mathcal{H})
\end{align*}
\]
Constrained Quantum Bethe Approximation Problem

Definition 15 (Constrained Quantum Bethe Approximation Problem)

\[
\begin{align*}
& \text{min} \quad F_{\text{Bethe}} \left( (\sigma_a)_{a \in \mathcal{F}}, (\sigma_i)_{i \in \mathcal{V}} \right) \\
& \text{s.t.} \quad \sigma_a \in \mathcal{L}_1^+ (\mathcal{H}_a) \quad \forall a \in \mathcal{F} \\
& \quad \sigma_i \in \mathcal{L}_1^+ (\mathcal{H}_i) \quad \forall i \in \mathcal{V} \\
& \quad \sigma_i = \text{Tr}_{\partial a \setminus i} (\sigma_a) \quad \forall (i, a) \in \mathcal{E}
\end{align*}
\]
**Constrained Quantum Bethe Approximation Problem**

**Definition 15 (Constrained Quantum Bethe Approximation Problem)**

\[
\begin{align*}
\min & \quad F_{\text{Bethe}} ((\sigma_a)_{a \in \mathcal{F}}, (\sigma_i)_{i \in \mathcal{V}}) \\
\text{s.t.} & \quad \sigma_a \in \mathcal{L}_1^+ (\mathcal{H}_a) \quad \forall a \in \mathcal{F} \\
& \quad \sigma_i \in \mathcal{L}_1^+ (\mathcal{H}_i) \quad \forall i \in \mathcal{V} \\
& \quad \sigma_i = \text{Tr}_{\partial a \setminus i} (\sigma_a) \quad \forall (i, a) \in \mathcal{E}
\end{align*}
\]
Variational Approach on QFGs

Constrained Quantum Bethe Approximation Problem

Definition 15 (Constrained Quantum Bethe Approximation Problem)

\[
\min \quad F_{\text{Bethe}} \left( (\sigma_a)_{a \in \mathcal{F}}, (\sigma_i)_{i \in \mathcal{V}} \right)
\]

s.t.

\[
\sigma_a \in \mathcal{L}_1^+(\mathcal{H}_a) \quad \forall a \in \mathcal{F}
\]

\[
\sigma_i \in \mathcal{L}_1^+(\mathcal{H}_i) \quad \forall i \in \mathcal{V}
\]

\[
\sigma_i = \text{Tr}_{\partial a \setminus i}(\sigma_a) \quad \forall (i, a) \in \mathcal{E}
\]

The Lagrangian is given by

\[
L \triangleq F_{\text{Bethe}} + \sum_{a \in \mathcal{F}} \gamma_a \cdot (\text{Tr}(\sigma_a) - 1) + \sum_{i \in \mathcal{V}} \gamma_i \cdot (\text{Tr}(\sigma_i) - 1)
\]

\[
+ \sum_{(i, a) \in \mathcal{E}} \text{Tr} \left( \lambda_{a, i} \cdot (\sigma_i - \text{Tr}_{\partial a \setminus i}(\sigma_a)) \right).
\]
Constrained Quantum Bethe Approximation Problem

Stationary condition

\[ \frac{\partial L}{\partial \gamma_a} = \frac{\partial L}{\partial \gamma_i} = 0 \]

\[ \frac{d}{dt} L(\lambda_{a,i}^* + tC) \bigg|_{t=0} = 0 \]

\[ \frac{d}{dt} L(\sigma_a^* + tC) \bigg|_{t=0} = 0 \]

\[ \frac{d}{dt} L(\sigma_i^* + tC) \bigg|_{t=0} = 0 \]
Constrained Quantum Bethe Approximation Problem

Stationary condition

\[ \frac{\partial L}{\partial \gamma_a} = \frac{\partial L}{\partial \gamma_i} = 0 \]

We have \( \forall a \in F, \forall i \in V \)

\[ \frac{d}{dt} L (\lambda_{a,i}^* + tC) \bigg|_{t=0} = 0 \]

\[ \frac{d}{dt} L (\sigma_a^* + tC) \bigg|_{t=0} = 0 \]

\[ \frac{d}{dt} L (\sigma_i^* + tC) \bigg|_{t=0} = 0 \]

\[ \sigma_a^* = \exp \left[ \log \rho_a + \sum_{i \in \partial a} \lambda_{a,i}^* - (1 + \gamma_a^*) I \right] \]

\[ \sigma_i^* = \exp \left[ \frac{1}{d_i - 1} \cdot \left( (1 + \gamma_i^*) I + \sum_{a \in \partial i} \lambda_{a,i}^* \right) \right]. \]
Constrained Quantum Bethe Approximation Problem

Stationary condition

\[ \frac{\partial L}{\partial \gamma_a} = \frac{\partial L}{\partial \gamma_i} = 0 \quad \text{We have } \forall a \in \mathcal{F}, \forall i \in \mathcal{V} \]

\[ \frac{d}{dt} L(\lambda_{a,i}^* + tC) \bigg|_{t=0} = 0 \quad \sigma_a^* = \exp \left[ \log \rho_a + \sum_{i \in \partial a} \lambda_{a,i}^* - (1 + \gamma_a^*) I \right] \]

\[ \sigma_i^* = \exp \left[ \frac{1}{d_i - 1} \cdot \left( (1 + \gamma_i^*) I + \sum_{a \in \partial i} \lambda_{a,i}^* \right) \right]. \]

Now, suppose \( \{ m_{i \rightarrow a} \}_{(i,a) \in \mathcal{E}} \) and \( \{ m_{a \rightarrow i} \}_{(i,a) \in \mathcal{E}} \) are given s.t.

\[ \lambda_{a,i}^* = \log m_{i \rightarrow a} \]

\[ \lambda_{a,i}^* = \sum_{c \in \partial i \setminus a} \log m_{c \rightarrow i} \quad \forall (i, a) \in \mathcal{E}. \]
Variational Approach on QFGs

Constrained Quantum Bethe Approximation Problem

Stationary condition

\[
\frac{\partial L}{\partial \gamma_a} = \frac{\partial L}{\partial \gamma_i} = 0
\]

We have \( \forall a \in \mathcal{F}, \forall i \in \mathcal{V} \)

\[
\frac{d}{dt} L (\lambda_{a,i}^* + tC) \bigg|_{t=0} = 0
\]

\[
\sigma_a^* \propto \exp \left[ \log(\rho_a) + \sum_{i \in \partial a} \log(m_{i \rightarrow a}) \right]
\]

\[
\frac{d}{dt} L (\sigma_a^* + tC) \bigg|_{t=0} = 0
\]

\[
\sigma_i^* \propto \exp \left[ \sum_{a \in \partial i} \log(m_{a \rightarrow i}) \right]
\]

\[
\frac{d}{dt} L (\sigma_i^* + tC) \bigg|_{t=0} = 0
\]

Now, suppose \( \{m_{i \rightarrow a}\}_{(i,a) \in \mathcal{E}} \) and \( \{m_{a \rightarrow i}\}_{(i,a) \in \mathcal{E}} \) are given s.t.

\[
\lambda_{a,i}^* = \log m_{i \rightarrow a}
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\[
\lambda_{a,i}^* = \sum_{c \in \partial i \setminus a} \log m_{c \rightarrow i} \quad \forall (i,a) \in \mathcal{E}.
\]
Constrained Quantum Bethe Approximation Problem

Stationary condition

\[
\frac{\partial L}{\partial \gamma_a} = \frac{\partial L}{\partial \gamma_i} = 0
\]

We have \( \forall a \in \mathcal{F}, \forall i \in \mathcal{V} \)

\[
\frac{d}{dt} L(\lambda^*_{a,i} + tC) \bigg|_{t=0} = 0
\]

\[
\sigma^*_{a} \propto \exp \left[ \log(\rho_a) + \sum_{i \in \partial a} \log(m_{i \rightarrow a}) \right]
\]

\[
\frac{d}{dt} L(\sigma^*_{a} + tC) \bigg|_{t=0} = 0
\]

\[
\sigma^*_i \propto \exp \left[ \sum_{a \in \partial i} \log(m_{a \rightarrow i}) \right]
\]

\[
\frac{d}{dt} L(\sigma^*_{i} + tC) \bigg|_{t=0} = 0
\]

\[
m_{i \rightarrow a} \propto \exp \left[ \sum_{c \in \partial i \setminus a} \log(m_{c \rightarrow i}) \right],
\]

\[
m_{a \rightarrow i} \propto \text{Tr}_{\partial a \setminus i} \left\{ \exp \left[ \log(\rho_a) + \sum_{j \in \partial a \setminus i} \log(m_{j \rightarrow a}) \right] \right\}.
\]
Constrained Quantum Bethe Approximation Problem

Theorem 16 (Interior Stationary Points)

\( \{(\sigma_a^*)_{a \in \mathcal{F}}, (\sigma_i^*)_{i \in \mathcal{V}}\} \) is an internal stationary point of the constrained quantum Bethe approximation problem if and only if, for all \( a \in \mathcal{F}, i \in \mathcal{V}, \)

\[
\sigma_a^* \propto \exp \left[ \log(\rho_a) + \sum_{i \in \partial a} \log(m_{i \to a}) \right]
\]

\[
\sigma_i^* \propto \exp \left[ \sum_{a \in \partial i} \log(m_{a \to i}) \right]
\]

with \( \{m_{i \to a}, m_{a \to i}\}_{(i,a) \in \mathcal{E}} \) defined before.
Constrained Quantum Bethe Approximation Problem

**Theorem 16 (Interior Stationary Points)**

\[ \{(\sigma_a^*)_{a \in \mathcal{F}}, (\sigma_i^*)_{i \in \mathcal{V}}\} \text{ is an internal stationary point of the constrained quantum Bethe approximation problem if and only if, for all } a \in \mathcal{F}, i \in \mathcal{V}, \]

\[ \sigma_a^* \propto \exp \left[ \log(\rho_a) + \sum_{i \in \partial a} \log(m_{i \rightarrow a}) \right] \]

\[ \sigma_i^* \propto \exp \left[ \sum_{a \in \partial i} \log(m_{a \rightarrow i}) \right] \]

with \( \{m_{i \rightarrow a}, m_{a \rightarrow i}\}_{(i,a) \in \mathcal{E}} \) defined before.

If QSPA converges, then it converges to an internal stationary point of the constrained quantum Bethe approximation problem.
Outline

1. Factor Graphs/Preliminaries
2. Quantum Factor Graphs (QFGs)
3. Closing-the-box Operations on QFGs
4. Variational Approach on QFGs
5. Numerical Result of QSPA
6. Conclusion & Outlook
For the QFG below, we generate the factors $\{\rho_k\}_{k=1}^6$ (independently) in the same fashion as in the last numerical example.

We apply the QSPA to the QFG on the LHS, and estimate $Z$ by $Z_{\text{QSPA}} = -\log(F^* \text{Bethe}).$

Relative error: $\eta \equiv \frac{|Z_{\text{QSPA}} - Z|}{Z}.$
For the QFG below, we generate the factors $\{\rho_k\}_{k=1}^6$ (independently) in the same fashion as in the last numerical example.

We apply the QSPA to the QFG on the LHS, and estimate $Z$ by

$$Z^{QSPA} = -\log(F^\ast_{\text{Bethe}}).$$
For the QFG below, we generate the factors $\{\rho_k\}_{k=1}^6$ (independently) in the same fashion as in the last numerical example.

We apply the QSPA to the QFG on the LHS, and estimate $Z$ by

$$Z^{QSPA} = -\log(F_{\text{Bethe}}^*).$$

Relative error:

$$\eta \triangleq \frac{|Z^{QSPA} - Z|}{Z}.$$
Numerical Result

- $|\mathcal{N}(\mu, \sigma)|$ distributed Eigenvalues ($\mu = 1, \sigma = 1$)
- Uniformly distributed Eigenvalues ($a = 0, b = 1$)
The closing-the-box operations on QFGs holds approximately, namely,

\[ \text{Tr}(\rho_A \odot \rho_B \odot \rho_C) \approx \text{Tr}_1(\rho_A \odot \text{Tr}_2(\rho_B \odot \rho_C)) \]

for \( \rho_A, \rho_B, \rho_C \) close to identity matrix.
Conclusion

1. The closing-the-box operations on QFGs holds approximately, namely,

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for $\rho_A$, $\rho_B$, $\rho_C$ close to identity matrix.

2. The fixed-points of QSPA correspond to the interior stationary points of quantum Bethe free energy minimization problem.
Conclusion & Outlook

Outlook

On-going Migration of other methods to QFGs, e.g., of loop calculus [Chernyak and Chertkov, 2007], graph cover [Vontobel, 2013];

Near Future Implications of the theory on QSPA for practical problems;

Convergence condition of QSPA (nontrivial special cases QSPA will always converge);

Future Minimum mathematical requirements s.t. the Sum-Product algorithm works (approximately).

Sufficient condition: commutative ring \(\langle F, +, \cdot \rangle\).
Outlook

**On-going** Migration of other methods to QFGs, e.g., of loop calculus [Chernyak and Chertkov, 2007], graph cover [Vontobel, 2013];
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**Sufficient condition**: commutative ring $\langle \mathbb{F}_R \rightarrow \mathbb{R}, +, \cdot \rangle$. 
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References II


Q&A

1. Factor Graphs/Preliminaries
2. Quantum Factor Graphs (QFGs)
3. Closing-the-box Operations on QFGs
4. Variational Approach on QFGs
5. Numerical Result of QSPA
6. Conclusion & Outlook