一般化された確率伝搬法の数学的構造

東北大学大学院情報科学研究科
田中和之
kazu@smapip.is.tohoku.ac.jp
http://www.smapip.is.tohoku.ac.jp/~kazu/
Introduction

Factor Graph and Loopy Belief Propagation

Generalized Belief Propagation

Simplified Cluster Variation Method

Factor Graph による確率伝搬法の表現を一般化された確率伝搬法 (Generalized Belief Propagation) と Simplified Cluster Variation Method の定式化の立場から導出する。
Generalized Belief Propagation

Cluster: Set of nodes

Subcluster $\alpha = \gamma \cap \gamma'$ $\iff$ $\gamma \supseteq \alpha$ and $\gamma' \supseteq \alpha$

Basic Cluster Set $C$: $\forall \gamma \in C$ and $\forall \gamma' \in C$ $\Rightarrow$ $\gamma \cap \gamma' \notin C$

Subcluster Set: $\{\alpha | \alpha = \gamma \cap \gamma' \text{ for } \forall \gamma \in C \text{ and } \forall \gamma' \in C\}$

Every subcluster of the element of $C$ does not belong to $C$.

Example: System consisting of 4 nodes

$$\mu(\gamma) = -1 - \sum_{\gamma' \subset \gamma} \mu(\gamma')$$

$\{1,2\} \supseteq 1, \{1,2\} \supseteq 2, \{2,3\} \supseteq 2, \{2,3\} \supseteq 3$

$\{3,4\} \supseteq 3, \{3,4\} \supseteq 4, \{1,4\} \supseteq 1, \{1,4\} \supseteq 4$

$$\mu(\{1,2\}) = \mu(\{2,3\}) = \mu(\{3,4\}) = \mu(\{1,4\}) = -1$$

$$\mu(1) = \mu(2) = \mu(3) = \mu(4) = 1$$
**Generalized Belief Propagation**

**KL Divergence**

\[
D[P_V, Q_V] = \sum_{\tilde{X}_V} Q_V(\tilde{X}_V) \ln \left( \frac{Q_V(\tilde{X}_V)}{P_V(\tilde{X}_V)} \right)
\]

\[
P_V(\tilde{X}_V) \propto \prod_{\gamma \in C} W_\gamma(\tilde{X}_\gamma)
\]

Marginals are determined so as to minimize \(D_{GBP}[\{Q_\alpha\}]\)

\[
D_{GBP}[\{Q_\alpha\}] = \sum_{\alpha} \sum_{\tilde{X}_\alpha} Q_\alpha(\tilde{X}_\alpha) \ln \left( \frac{Q_\alpha(\tilde{X}_\alpha)}{W_\alpha(\tilde{X}_\alpha)} \right)
\]

**Example**

\[
D_{GBP}[\{Q_\alpha\}] = D[W_{12}, Q_{12}] + D[W_{23}, Q_{23}]
+ D[W_{34}, Q_{34}] + D[W_{41}, Q_{42}]
- D[W_1, Q_1] - D[W_2, Q_2]
- D[W_2, Q_2]
\]
Selection of Basic Cluster in LBP and GBP

LBP
(Bethe Approx.)

GBP
(Square Approx. in CVM; Kikuchi Approx.)

Ω
Generalized Belief Propagation

$V$: すべての頂点の集合

$C = \{\gamma | |\gamma| = 3\}$: 3個の頂点からなるハイパエッジの集合

$B = \{\beta | \beta = \gamma \cap \gamma', \forall \gamma \in C, \forall \gamma' \in C\}$

$A = \{i | i = \beta \cap \beta', \forall \beta \in B, \forall \beta' \in B\}$

$C$に属するハイパエッジの副クラスターの集合

$B$の要素はノードとエッジのみ

$A$に属するのエッジの副クラスターの集合

$A$の要素はノードのみ
Generalized Belief Propagation

\[ V = \{1,2,3,4,5\} \]

\[ C = \{ \gamma \mid \gamma = \{i,j,k\}, i \in V, j \in V, k \in V \} \]

\[ B = \{ \beta \mid \beta = \gamma \cap \gamma', \forall \gamma \in C, \forall \gamma' \in C \} \]

\[ A = \{ i \mid i = \beta \cap \beta', \forall \beta \in B, \forall \beta' \in B \} \]

\[ C = \{ \{1,2,3\}, \{1,3,4\}, \{1,4,5\}, \{1,2,5\} \} \]

\[ B = \{ \{1,2\}, \{1,3\}, \{1,4\}, \{1,5\} \} \]

\[ A = \{1\} \]
Generalized Belief Propagation

\[
\sum \sum \sum \sum \sum_{X_3 X_4} = \sum \sum \sum \sum \sum_{X_3 X_4 X_5}
\]

\[
\sum \sum \sum \sum \sum_{X_2 X_3 X_4} = \sum \sum \sum \sum \sum_{X_2 X_3 X_4 X_5}
\]

\[
\sum \sum \sum \sum \sum_{X_2} = \sum \sum \sum \sum \sum_{X_2 X_5}
\]

\[
\sum \sum \sum \sum \sum_{X_1} = \sum \sum \sum \sum \sum_{X_1 X_2 X_5}
\]
Generalized Belief Propagation

Marginal Probabilities are determined so as to minimize the Kikuchi Free Energy under some Reducibility Conditions.

Kikuchi Free Energy

Reducibility Conditions
Generalized Belief Propagation

\[ P_{125}(x_1, x_2, x_5) \propto W_{125}(x_1, x_2, x_5) \]
\[ \times M_{23 \rightarrow 1}(x_1) M_{3 \rightarrow 12}(x_1, x_2) \]
\[ \times M_{45 \rightarrow 1}(x_1) M_{4 \rightarrow 15}(x_1, x_5) \]
\[ \times M_{3 \rightarrow 1}(x_1) M_{4 \rightarrow 1}(x_1) M_{43 \rightarrow 1}(x_1) \]

\[ C = \{\{1,2,3\}, \{1,3,4\}, \{1,4,5\}, \{1,2,5\}\} \]
\[ B = \{\{1,2\}, \{1,3\}, \{1,4\}, \{1,5\}\} \]
\[ A = \{1\} \]
Generalized Belief Propagation

\[ P_{12}(x_1, x_2) \propto M_{23\rightarrow 1}(x_1)M_{3\rightarrow 12}(x_1, x_2) \]
\[ \times M_{25\rightarrow 1}(x_1)M_{5\rightarrow 12}(x_1, x_2) \]
\[ \times M_{3\rightarrow 1}(x_1)M_{4\rightarrow 1}(x_1)M_{5\rightarrow 1}(x_1) \]
\[ \times M_{43\rightarrow 1}(x_1)M_{45\rightarrow 1}(x_1) \]

\[ C = \{\{1,2,3\}, \{1,3,4\}, \{1,4,5\}, \{1,2,5\}\} \]
\[ B = \{\{1,2\}, \{1,3\}, \{1,4\}, \{1,5\}\} \]
\[ A = \{1\} \]
Generalized Belief Propagation

\[ \sum X_5 \]

\[ \sum X_5 \]

\[ \sum X_5 \]
Generalized Belief Propagation

\[
\sum_{X_2} = \sum_{X_2} = \sum_{X_2}
\]
Generalized Belief Propagation

\[ \sum X_2 \sum X_5 = \sum X_2 \sum X_5 \]
Generalized Belief Propagation

\[
P_1(X_1) = \sum_{X_2} P_{12}(X_1, X_2)
\]

\[
P_1(X_1) = \sum_{X_2} \sum_{X_5} P_{125}(X_1, X_2, X_5)
\]

\[
P_{12}(X_1, X_2) = \sum_{X_5} P_{125}(X_1, X_2, X_5)
\]
Generalized Belief Propagation

Marginal Probabilities are determined so as to minimize the Kikuchi Free Energy under some Reducibility Conditions.

\[ \sum X_5 = \sum \sum X_2 X_5 \]

Reducibility Conditions
Marginal Probabilities are determined so as to minimize the Kikuchi Free Energy under some Reducibility Conditions.

\[
\sum_{X_1} \frac{\langle X_1 \rangle_{12}}{\langle X_1 \rangle_{125}} = \sum_{X_1} \sum_{X_5} \frac{\langle X_1 \rangle_{\{1,2,5\}}}{\langle X_1 \rangle_{\{1,2,3,4,5\}}}
\]

\[
\langle X_1 \rangle_{12} = \langle X_1 \rangle_{125} \text{ for Binary State}
\]

Reducibility Conditions
Simplified Cluster Variation Method

\[ P_{125}(x_1, x_2, x_5) \propto W_{125}(x_1, x_2, x_5) \times M_{23 \to 1}(x_1)M_{13 \to 2}(x_2) \times M_{45 \to 1}(x_1)M_{14 \to 5}(x_5) \times M_{3 \to 1}(x_1)M_{4 \to 1}(x_1)M_{43 \to 1}(x_1) \]

\[ C = \{\{1,2,3\},\{1,3,4\},\{1,4,5\},\{1,2,5\}\} \]
\[ B = \{\{1,2\},\{1,3\},\{1,4\},\{1,5\}\} \]
\[ A = \{1\} \]
Simplified Cluster Variation Method

\[ P_{12}(x_1, x_2) \propto M_{23\rightarrow1}(x_1)M_{3\rightarrow12}(x_1, x_2) \]
\[ \times M_{25\rightarrow1}(x_1)M_{5\rightarrow12}(x_1, x_2) \]
\[ \times M_{3\rightarrow1}(x_1)M_{4\rightarrow1}(x_1)M_{5\rightarrow1}(x_1) \]
\[ \times M_{43\rightarrow1}(x_1)M_{45\rightarrow1}(x_1) \]

\[ C = \{\{1,2,3\},\{1,3,4\},\{1,4,5\},\{1,2,5\}\} \]
\[ B = \{\{1,2\},\{1,3\},\{1,4\},\{1,5\}\} \]
\[ A = \{1\} \]
Simplified Cluster Variation Method

\[ \sum_{X_1} \sum = \sum \sum_{X_1 X_5} \]

\[ \sum_{X_1} \sum = \sum \sum_{X_1 X_5} \]

\[ \sum_{X_1} \sum = \sum \sum_{X_1 X_5} \]
Simplified Cluster Variation Method

\[ P_1(X_1) = \sum_{X_2} P_{12}(X_1, X_2) \]

\[ P_1(X_1) = \sum_{X_2} \sum_{X_5} P_{125}(X_1, X_2, X_5) \]

\[ \sum_{X_1} P_{12}(X_1, X_2) \]

\[ = \sum_{X_1} \sum_{X_5} P_{125}(X_1, X_2, X_5) \]
Simplified Cluster Variation Method and Factor Graph

\[ C = \{\{1,2,3\}, \{1,3,4\}, \{1,4,5\}, \{1,2,5\}\} \]

\[ B = \{\{1,2\}, \{1,3\}, \{1,4\}, \{1,5\}\} \]

\[ A = \{1\} \]
Generalized Belief Propagation

\[ V = \{1,2,3,4,5\} \]

\[ C = \{ \gamma \mid \gamma = \{i,j,k\}, i \in V, j \in V, k \in V \} \]

\[ B = \{ \beta \mid \beta = \gamma \cap \gamma', \forall \gamma \in C, \forall \gamma' \in C \} \]

\[ A = \{ i \mid i = \beta \cap \beta', \forall \beta \in B, \forall \beta' \in B \} \]

\[ C = \{\{1,2,3\},\{1,3,4\},\{1,4,5\},\{1,2,5\}\} \]

\[ B = \{\{1,2\},\{1,3\},\{1,4\},\{1,5\}\} \]

\[ A = \{1\} \]
Generalized Belief Propagation

\[ V = \{1,2,3,4,5\} \]

\[ C = \{ \gamma \mid \gamma = \{i,j,k\}, i \in V, j \in V, k \in V \} \]

\[ B = \{ \beta \mid \beta = \gamma \cap \gamma', \forall \gamma \in C, \forall \gamma' \in C \} \]

\[ A = \{ i \mid i = \beta \cap \beta', \forall \beta \in B, \forall \beta' \in B \} \rightarrow V \]

\[ C = \{\{1,2,3\}, \{1,3,4\}, \{1,4,5\}, \{1,2,5\}\} \]

\[ B = \{\{1,2\}, \{1,3\}, \{1,4\}, \{1,5\}\} \]

\[ A = \{1\} \]

\[ V = \{1,2,3,4,5\} \]
Generalized Belief Propagation

Marginal Probabilities are determined so as to minimize the Kikuchi Free Energy under some Reducibility Conditions.

\[ = \sum X_5 \]

\[ = \sum \sum X_2 X_5 \]

Kikuchi Free Energy

Reducibility Conditions
Marginal probabilities are determined so as to minimize the Kikuchi Free Energy under some Reducibility Conditions.
Simplified Cluster Variation Method

\[ P_{125}(x_1, x_2, x_5) \propto W_{125}(x_1, x_2, x_5) \times M_{23\rightarrow 1}(x_1) M_{13\rightarrow 2}(x_2) \times M_{45\rightarrow 1}(x_1) M_{14\rightarrow 5}(x_5) \times M_{43\rightarrow 1}(x_1) \]

\[ C = \{1,2,3\}, \{1,3,4\}, \{1,4,5\}, \{1,2,5\} \]

\[ V = \{1,2,3,4,5\} \]
Simplified Cluster Variation Method

\[
P_1(X_1) = \sum_{X_2} \sum_{X_5} P_{125}(X_1, X_2, X_5)
\]

\[
= \sum_{X_2} \sum_{X_5}
\]

\[
P_2(X_2) = \sum_{X_1} \sum_{X_5} P_{125}(X_1, X_2, X_5)
\]

\[
= \sum_{X_1} \sum_{X_5}
\]
Simplified Cluster Variation Method and Factor Graph

\[ C = \{\{1,2,3\},\{1,3,4\},\{1,4,5\},\{1,2,5\}\} \]

\[ V = \{1,2,3,4,5\} \]
Selection of Basic Clusters and their Sub-Clusters in Generalized Belief Propagation on Square Grid

\[ P_V(\vec{X}) = \frac{1}{Z} \exp \left( \frac{J}{T} \sum_{\{i,j\} \in E} X_i X_j \right) \]

\[ X_i = \{+1, -1\} \]

The set of Basic Clusters

LBP (Bethe Approx.)

The Set of Basic Clusters and Their Sub-Clusters
Selection of Basic Clusters and their Sub-Clusters in Generalized Belief Propagation on Square Grid

\[ P_V(\tilde{X}) = \frac{1}{Z} \exp \left( \frac{J}{T} \sum_{\{i,j\} \in E} X_i X_j \right) \]

\[ X_i = \{+1, -1\} \]

GBP

\((\text{Square Approximation in CVM})\)
Critical Points for Ising Model

\[ P_V(\vec{X}) = \frac{1}{Z} \exp\left( \frac{J}{T} \sum_{\{i,j\} \in E} X_i X_j \right) \]

\[ X_i = \{+1, -1\} \]

\((V,E) =\) Square Lattice

<table>
<thead>
<tr>
<th>Method</th>
<th>(T_C/J)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Exact (Onsager)</td>
<td>2.2692</td>
</tr>
<tr>
<td>GBP</td>
<td>2.4257</td>
</tr>
<tr>
<td>SCVM</td>
<td>2.6253</td>
</tr>
<tr>
<td>Square Cactus CVM</td>
<td>2.7708</td>
</tr>
<tr>
<td>Bethe Approx.</td>
<td>2.8854</td>
</tr>
<tr>
<td>Factor Graph</td>
<td>3.4659</td>
</tr>
<tr>
<td>Mean Field Approx.</td>
<td>4.0000</td>
</tr>
</tbody>
</table>

\((V,E) =\) Cube Lattice

<table>
<thead>
<tr>
<th>Method</th>
<th>(T_C/J)</th>
</tr>
</thead>
<tbody>
<tr>
<td>High Temperature Series</td>
<td>4.5103</td>
</tr>
<tr>
<td>GBP</td>
<td>4.6097</td>
</tr>
<tr>
<td>SCVM</td>
<td>4.7611</td>
</tr>
<tr>
<td>Cube Cactus CVM</td>
<td>4.8396</td>
</tr>
<tr>
<td>Bethe Approx.</td>
<td>4.9326</td>
</tr>
<tr>
<td>Mean Field Approx.</td>
<td>6.0</td>
</tr>
<tr>
<td>Factor Graph</td>
<td>8.6181</td>
</tr>
</tbody>
</table>
Summary

We reviewed the generalized belief propagation based on cluster variation method. Some extensions of the generalized belief propagation have been given by using the simplified cluster variation method. The relationship between the factor graph and the present extensions by means of the simplified cluster variation method are clarified.