Mathematical Structures of Loopy Belief Propagation and Cluster Variation Method

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3. Interpretation of Adaptive TAP method by Cluster Variation Method
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5. Quantum Belief Propagation
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Abstract

We review of conventional generalized loopy belief propagation based on cluster variation method.
Some interpretations and extensions of the adaptive TAP method are given by using the cluster variation method.
Conventional formalisms and extensions of the quantum belief propagation are also summarized.

Belief Propagation

- **Belief Propagation (BP) has been proposed in order to achieve probabilistic inference systems (Pearl, 1988).**
- **It has been suggested that BP has a closed relationship to mean field methods in the statistical mechanics (Kabashima and Saad 1998).**
- **Generalizations of the BP have been proposed based on the cluster variation method which is one of the advanced mean field methods in the statistical mechanics (Yedidia, Freeman and Weiss, 2000).**

Cluster Variation Method

- **Cluster Variation Method for Classical System**

  R. Kikuchi: A theory of cooperative phenomena, Phys. Rev., 81 (1951).

  T. Morita: Cluster variation method of cooperative phenomena and its generalization I, J. Phys. Soc. Jpn, 12 (1957).

- **Cluster Variation Method for Quantum System**

  T. Morita: Cluster variation method of cooperative phenomena and its generalization II, Quantum Statistics, J. Phys. Soc. Jpn, 12 (1957).

Contents

Classical Spin System

Probability Distribution in the present talk

$$P(\boldsymbol{x}) \equiv \frac{1}{Z}\exp\left(-H(\boldsymbol{x})\right)$$

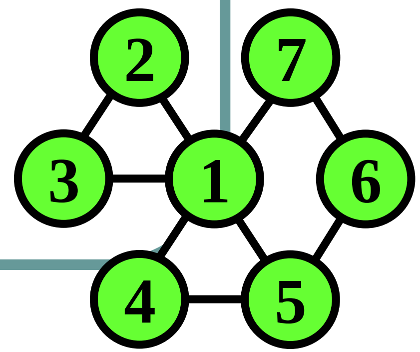
$$H(\boldsymbol{x}) \equiv -\vec{\theta}^{\mathrm{T}}\vec{x} - \frac{1}{2}\vec{x}^{\mathrm{T}}\boldsymbol{J}\vec{x} = -\sum_{i\in V}\theta_i x_i - \sum_{ij\in E} J x_i x_j$$

V: **Set of all the nodes** ***E***: **Set of all the edges**

State Variable $x_i \in \{+1,-1\}$

State Vector

$$\vec{x} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ x_6 \\ x_7 \end{pmatrix} \quad \vec{\theta} = \begin{pmatrix} \theta_1 \\ \theta_2 \\ \theta_3 \\ \theta_4 \\ \theta_5 \\ \theta_6 \\ \theta_7 \end{pmatrix} \quad \boldsymbol{J} = \begin{pmatrix} 0 & J & J & J & J & 0 & J \\ J & 0 & J & 0 & 0 & 0 & 0 \\ J & J & 0 & 0 & 0 & 0 & 0 \\ J & 0 & 0 & 0 & J & 0 & 0 \\ J & 0 & 0 & J & 0 & J & 0 \\ 0 & 0 & 0 & 0 & J & 0 & J \\ J & 0 & 0 & 0 & 0 & J & 0 \end{pmatrix}$$



Variational Principle of Free Energy Minimum

Gibbs distribution $P(\boldsymbol{x}) \equiv \frac{1}{Z}\exp\left(-H(\boldsymbol{x})\right)$

satisfies the minimization of free energy

$$\arg\min_{Q}\left\{F[Q]\middle|\sum_{\vec{x}}Q(\vec{x})=1\right\}=P(\boldsymbol{x})$$

$$F[Q]=\sum_{\boldsymbol{x}}\left(-H(\boldsymbol{x})+\ln Q(\boldsymbol{x})\right)Q(\boldsymbol{x})$$

Free Energy for Trial Probability $Q(\boldsymbol{x})$

$$L[Q]\equiv F[Q]-\lambda\left(\sum_{\vec{x}}Q(\vec{x})-1\right)=\sum_{\boldsymbol{x}}\left(-H(\boldsymbol{x})+\ln Q(\boldsymbol{x})\right)Q(\boldsymbol{x})-\lambda\left(\sum_{\vec{x}}Q(\vec{x})-1\right)$$

$$\rightarrow \frac{\delta L[Q]}{\delta Q(\vec{x})}=0 \rightarrow Q(\vec{x})=\exp(-\lambda)\exp\left(-H(\vec{x})\right)$$

Tractable Probabilistic Model

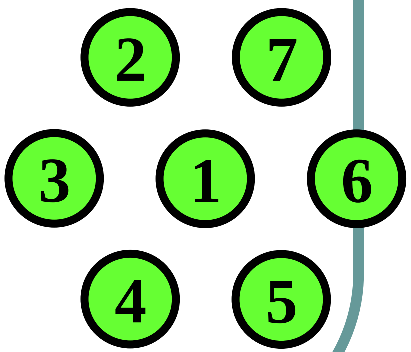
In the case of J=0 for all the edges ij

$$H(\boldsymbol{x}) \equiv -\sum_{i \in V} \theta_i x_i \quad \longrightarrow \quad P(\vec{x}) = \prod_{i \in V} \frac{\exp(\theta_i x_i)}{\sum_{x_i = \pm 1} \exp(\theta_i x_i)}$$

$$\langle x_i \rangle = \sum_{\vec{x}} x_i P(\vec{x}) = \tanh(\theta_i)$$

Factorizable Form

$$\langle x_i x_j \rangle = \sum_{\vec{x}} x_i x_j P(\vec{x}) = \tanh(\theta_i)\tanh(\theta_j)$$

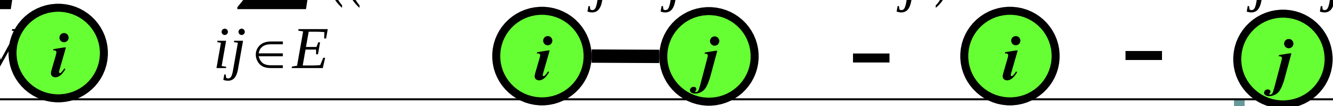


Conventional Loopy Belief Propagation

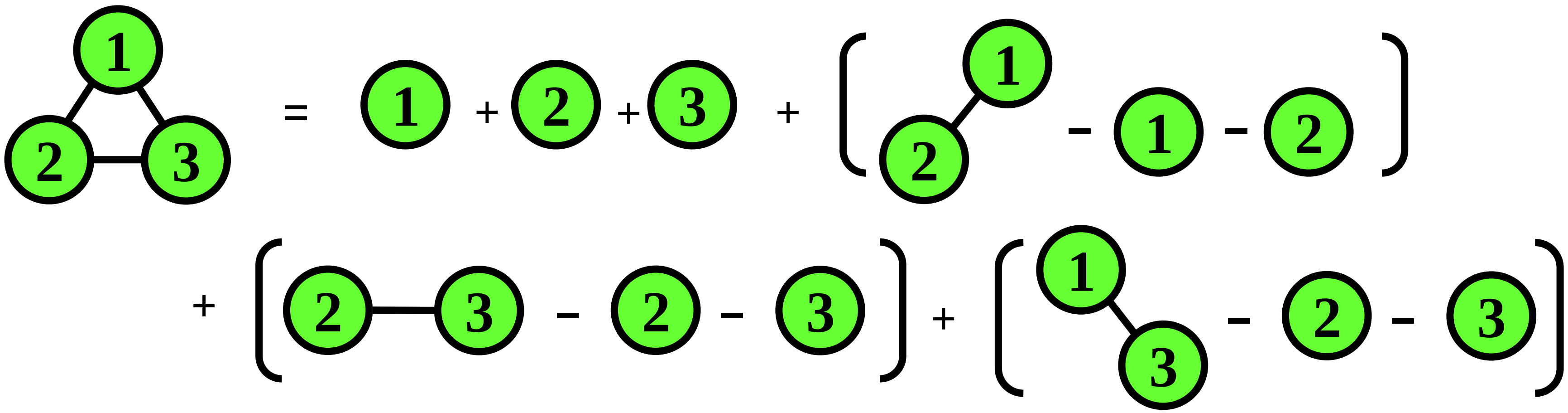
$$P(\boldsymbol{x}) = \frac{1}{Z}\exp\left(-H(\boldsymbol{x})\right) \qquad x_i \in \{+1,-1\}$$

$$H(\boldsymbol{x}) = -\sum_{i\in V}\theta_i x_i - \sum_{ij\in E} J x_i x_j$$

$$= -\sum_{i\in V}\theta_i x_i - \sum_{ij\in E}\left(\left(\theta_i x_i + \theta_j x_j + J x_i x_j\right) - \theta_i x_i - \theta_j x_j\right)$$



Example $V = \{1,2,3\}$ $E = \{12,23,13\}$



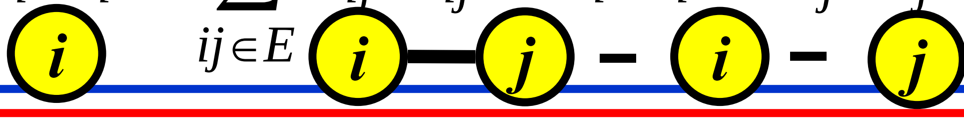
Conventional Loopy Belief Propagation

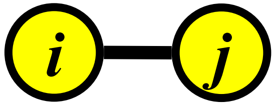
In the cluster variation method, the free energy is approximately expressed in terms of the free energies of all the edges and nodes.

$$F[Q]=\sum_{\boldsymbol{x}}\left(-H(\boldsymbol{x})+\ln Q(\boldsymbol{x})\right)Q(\boldsymbol{x})$$

Bethe Free Energy

$$F_{\mathrm{Bethe}}\left[\{Q_i,Q_{ij}\}\right]=\sum_{i\in V}F_i[Q_i]+\sum_{ij\in E}\left(F_{ij}[Q_{ij}]-F_i[Q_i]-F_j[Q_j]\right)$$





$$F_{ij}\left[Q_{ij}\right]=\sum_{x_i=\pm1}\sum_{x_j=\pm1}\left(-\theta_i x_i-\theta_j x_j-Jx_i x_j+\ln Q_{ij}(x_i,x_j)\right)Q_{ij}(x_i,x_j)$$

$$F_i\left[Q_i\right]=\sum_{x_i}\left(-\theta_i x_i+\ln Q_i(x_i)\right)Q_i(x_i)$$

$$Q_{ij}(x_i,x_j)\equiv\sum_{\boldsymbol{x}\backslash\{x_i,x_j\}}Q(\boldsymbol{x})$$

$$Q_i(x_i)\equiv\sum_{\boldsymbol{x}\backslash x_i}Q(\boldsymbol{x})$$

Conventional Loopy Belief Propagation

Marginal probabilities of edges and nodes are determined so as to minimize the Bethe free energy under some constraint conditions.

$$\underset{\{Q_i, Q_{ij}\}}{\arg\min}\left\{ F_{\mathrm{Bethe}}\left[\{Q_i, Q_{ij}\}\right] \middle| Q_i(\xi) = \sum_{\varsigma} Q_{ij}(\xi,\varsigma), \sum_{\xi} Q_i(\xi) = \sum_{\xi}\sum_{\varsigma} Q_{ij}(\xi,\varsigma) = 1 \right\}$$

Lagrange Multipliers to ensure the constraints

$$L_{\mathrm{Bethe}}\left[\{Q_i, Q_{ij}\}\right] \equiv F_{\mathrm{Bethe}}\left[\{Q_i, Q_{ij}\}\right] - \sum_{i\in V}\sum_{j\in\partial i}\sum_{\xi} \lambda_{i,j}(\xi)\left(Q_i(\xi) - \sum_{\varsigma} Q_{ij}(\xi,\varsigma)\right) - \sum_{i\in V} \nu_i \left(\sum_{\xi} Q_i(\xi) - 1\right) - \sum_{ij\in E} \nu_{ij}\left(\sum_{\xi}\sum_{\zeta} Q_{ij}(\xi,\zeta) - 1\right)$$

Conventional Loopy Belief Propagation

$$\frac{\partial}{\partial Q_i(x_i)} L_{\text{Bethe}}\left[\left\{Q_i, Q_{ij}\right\}\right] = 0$$

$$\frac{\partial}{\partial Q_{ij}(x_i, x_j)} L_{\text{Bethe}}\left[\left\{Q_i, Q_{ij}\right\}\right] = 0$$

Extremum Condition

Approximate Forms of Marginals

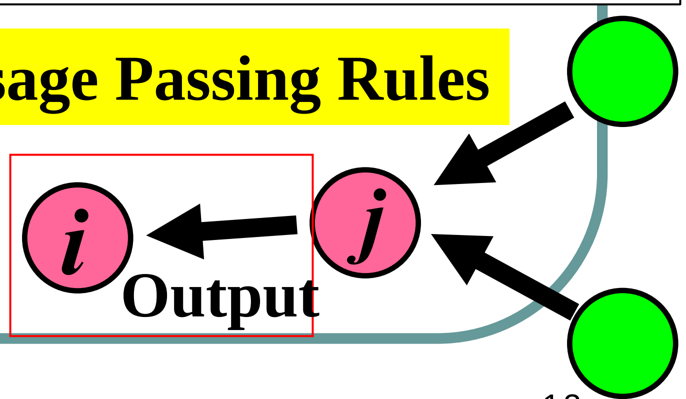
$$Q_i(x_i) = \frac{1}{Z_i}\left(\prod_{k\in\partial i} M_{k\to i}(x_i)\right) e^{\theta_i x_i}$$

$$Q_{ij}(x_i, x_j) = \frac{1}{Z_{ij}} \exp(\theta_i x_i + \theta_j x_j + J x_i x_j) \times \left(\prod_{k\in\partial i} M_{k\to i}(x_i)\right)\left(\prod_{l\in\partial j} M_{l\to j}(x_j)\right)$$

$$Q_i(x_i) = \sum_{x_j} Q_{ij}(x_i, x_j)$$

Reducibility Conditions

Message Passing Rules



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Tractable Probabilistic Model

Gaussian graphical model

Averages, variances and covariances are exactly calculated by using multidimensional Gaussian integral formulas.

$$\rho(\vec{x}) \equiv \frac{1}{Z_{\mathrm{f}}}\exp\left(-\frac{1}{2}\sum_{i\in V} D_i {x_i}^2 - H(\vec{x})\right)$$
$$= \frac{1}{Z_{\mathrm{f}}}\exp\left(\vec{\theta}^{\mathrm{T}}\vec{x} - \frac{1}{2}\vec{x}^{\mathrm{T}}(\boldsymbol{D}-\boldsymbol{J})\vec{x}\right)$$

$$\vec{m} = \langle \vec{x} \rangle = \int_{-\infty}^{+\infty} \vec{x}\rho(\vec{x})dx$$
$$= -(\boldsymbol{D}-\boldsymbol{J})^{-1}\vec{\theta}$$

$$H(\boldsymbol{x}) \equiv -\vec{\theta}^{\mathrm{T}}\vec{x} - \frac{1}{2}\vec{x}^{\mathrm{T}}\boldsymbol{J}\vec{x}$$
$$= -\sum_{i\in V}\theta_i x_i - \sum_{ij\in E} J x_i x_j$$

$$\left\langle (x_i - m_i)(x_j - m_j) \right\rangle = \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}(x_i - m_i)(x_j - m_j)\rho(\vec{x})d\vec{x}$$
$$= \left\langle i \left| (\boldsymbol{D}-\boldsymbol{J})^{-1} \right| j \right\rangle$$

Tractable Probabilistic Model

Gaussian graphical model

For the given probability distribution $P(x)$, we introduce the Gaussian graphical model so as to satisfy the following relations:

$$P(\vec{x}) = \frac{1}{Z}\exp\left(-H(\vec{x})\right)$$

Marginal Probability

$$\int_{-\infty}^{+\infty} x_i^2 \rho(\vec{x})d\vec{x} = 1$$

$$\sum_{x_i=\pm 1} x_i P_i(x_i) = \int_{-\infty}^{+\infty} x_i \rho(\vec{x})d\vec{x}$$

$$\rho(\vec{x}) \equiv \frac{1}{Z_{\mathrm{f}}}\exp\left(-\frac{1}{2}\sum_{i\in V} D_i x_i^2 + \sum_{i\in V}\mu_i x_i - H(\vec{x})\right)$$

Approximate form of $P_i(x_i)$ should be determined by using the cluster variation method.

Interpretation of Adaptive TAP

- **Adaptive TAP Free energy can be given in terms of the free energies of the Gaussian graphical model and of all the nodes in the present binary spin system as follows:**

$$F_{\mathrm{ATAP}}\left[\rho,\{Q_i,\rho_i\}\right]=F_{\mathrm{f}}[\rho]+\sum_{i\in V}\left(F_i[Q_i]-F_{i\mathrm{f}}[\rho_i]\right)$$

$$F_{\mathrm{f}}[\rho]=\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\cdots\int_{-\infty}^{+\infty}\left(H(\vec{x})+\ln\rho(\vec{x})\right)\rho(\vec{x})dx_1dx_2\cdots dx_N$$

$$F_{i\mathrm{f}}[\rho_i]=\int_{-\infty}^{+\infty}\left(-\theta_ix_i+\ln\rho_i(x_i)\right)\rho_i(x_i)dx_i$$

$$F_i[Q_i]=\sum_{x_i=\pm1}\left(-\theta_ix_i+\ln Q_i(x_i)\right)Q_i(x_i)$$

$$\rho(\vec{x})\equiv\frac{1}{Z_{\mathrm{f}}}\exp\left(-\frac{1}{2}\sum_{i\in V}D_i{x_i}^2+\sum_{i\in V}\mu_ix_i-H(\vec{x})\right)$$

Interpretation of Adaptive TAP

Marginal probabilities of edges and nodes are determined so as to minimize the adaptive TAP free energy under some constraint conditions.

$$L_{\mathrm{ATAP}}[\{\rho, \rho_i, Q_i\}] \equiv F_{\mathrm{ATAP}}[\{\rho, \rho_i, Q_i\}] - \sum_{i \in V} D_i \left(\int {x_i}^2 \rho(\vec{x}) d\vec{x} - 1 \right)$$

$$- \sum_{i \in V} h_i \left(\sum_{x_i} x_i Q_i(x_i) - \int x_i \rho(\vec{x}) d\vec{x} \right) - \sum_{i \in V} \nu_i \left(\sum_{x_i} Q_i(x_i) - 1 \right)$$

$$\rho(\vec{x}) \equiv \frac{1}{Z_{\mathrm{f}}} \exp\left(-\frac{1}{2} \sum_{i \in V} D_i {x_i}^2 + \sum_{i \in V} \mu_i x_i - H(\vec{x}) \right)$$

Interpretation of Adaptive TAP

- **By taking the first deviations of the adaptive TAP free energy, we derive the approximate form of marginal probabilities as follows:**

$$Q_i(x_i) \propto \exp\left(h_i x_i\right)$$

$$\rho(\vec{x}) \propto \exp\left((\vec{\mu} - \vec{\theta})\vec{x} - \frac{1}{2}\vec{x}^{\mathrm{T}}(\boldsymbol{D} - \boldsymbol{J})\vec{x} \right)$$

$$\begin{cases} \tanh(h_i) = (\vec{\mu} - \vec{\theta})(\boldsymbol{D} - \boldsymbol{J})^{-1}\left|i\right\rangle \\ 1 - \tanh^2(h_i) = \left\langle i\right|(\boldsymbol{D} - \boldsymbol{J})^{-1}\left|i\right\rangle \\ \left\langle i\right|\boldsymbol{D}\left|j\right\rangle = 0 \ \ (i \neq j) \end{cases}$$

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Extension of Adaptive TAP

- In the similar arguments, we can construct the following approximate free energy:

$$\rho(\vec{x}) \equiv \frac{1}{Z_{\mathrm{f}}} \exp\left(\frac{1}{2} \sum_{i \in V} D_i x_i^2 - H(\vec{x}) \right)$$

$$\rho_i(x_i) = \int \delta(x_i - z_i) \rho(\vec{z}) d\vec{z}$$

$$\rho_{ij}(x_i, x_j) = \int \delta(x_i - z_i) \delta(x_j - z_j) \rho(\vec{z}) d\vec{z}$$

$$F_{\mathrm{EATAP}}\left[\rho, \{Q_i, \rho_i, Q_{ij}, \rho_{ij}\}\right] = F_{\mathrm{f}}[\rho] + \sum_{i \in V} (F_i[Q_i] - F_{i\mathrm{f}}[\rho_i]) + \sum_{ij \in E} \Big((F_{ij}[Q_{ij}] - F_{ij\mathrm{f}}[\rho_{ij}]) - (F_i[Q_i] - F_{i\mathrm{f}}[\rho_i]) - (F_j[Q_j] - F_{j\mathrm{f}}[\rho_j]) \Big)$$

$$F_{\mathrm{f}}[\rho] = \int_{-\infty}^{+\infty} (H(\vec{z}) + \ln \rho(\vec{z})) \rho(\vec{z}) d\vec{z}$$

$$F_{i\mathrm{f}}[\rho_i] = \int_{-\infty}^{+\infty} (-\theta_i x_i + \ln \rho_i(x_i)) \rho_i(x_i) dx_i$$

$$F_{ij\mathrm{f}}[\rho_{ij}] = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} (-\theta_i x_i - \theta_j x_j - J_{ij} x_i x_j + \ln \rho_{ij}(x_i, x_j)) \rho_{ij}(x_i, x_j) dx_i dx_j$$

$$F[Q_i] = \sum_{x_i = \pm 1} (-\theta_i x_i + \ln Q_i(x_i)) Q_i(x_i)$$

$$F_{ij}[Q_{ij}] = \sum_{x_i = \pm 1} \sum_{x_j = \pm 1} (-\theta_i x_i - \theta_j x_j - J_{ij} x_i x_j + \ln Q_{ij}(x_i, x_j)) Q_{ij}(x_i, x_j)$$

Extension of Adaptive TAP

Approximate forms of marginal probabilities are derived by considering the following Lagrange multipliers for the constraint conditions.

$$
\begin{aligned}
L_{\mathrm{EATAP}}\left[\{\rho,\rho_i,\rho_{ij},Q_i,Q_{ij}\}\right] \equiv F_{\mathrm{EATAP}}\left[\{\rho,\rho_i,\rho_{ij},Q_i,Q_{ij}\}\right] &- \sum_{i\in V}\sum_{j\in\partial i} h_{i,ij}\left(\sum_{x_i} x_i Q_i(x_i) - \sum_{x_i}\sum_{x_j} x_i Q_i(x_i,x_j)\right) \\
&- \sum_{i\in V} h_i\left(\sum_{x_i} x_i Q_i(x_i) - \int x_i \rho(\boldsymbol{x})d\boldsymbol{x}\right) - \sum_{i\in E} h_{ij}\left(\sum_{x_i} x_i x_j Q_{ij}(x_i,x_j) - \int x_i x_j \rho(\boldsymbol{x})d\boldsymbol{x}\right) \\
&- \sum_{i\in V} D_i\left(\int x_i^2 \rho(\boldsymbol{x})d\boldsymbol{x} - 1\right) - \sum_{i\in V} \nu_i\left(\sum_{x_i} Q_i(x_i) - 1\right) - \sum_{ij\in E} \nu_{ij}\left(\sum_{x_i}\sum_{x_j} Q_{ij}(x_i,x_j) - 1\right)
\end{aligned}
$$

$$
\rho(\vec{x}) \equiv \frac{1}{Z_{\mathrm{f}}}\exp\left(\frac{1}{2}\sum_{i\in V} D_i x_i^2 - H(\vec{x})\right)
$$

$$
\rho_i(x_i) = \int \delta(x_i - z_i)\rho(\boldsymbol{z})d\boldsymbol{z} \qquad \rho_{ij}(x_i,x_j) = \int \delta(x_i - z_i)\delta(x_j - z_j)\rho(\boldsymbol{z})d\boldsymbol{z}
$$

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Density Matrix and Reduced Density Matrix

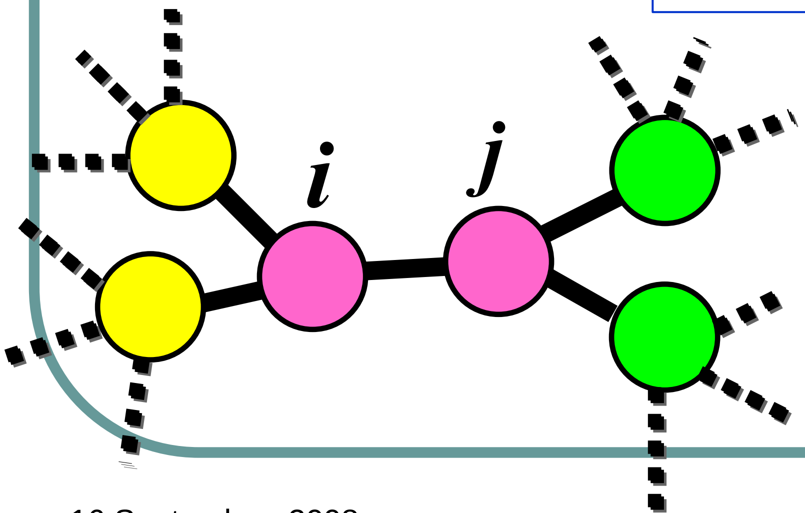
$$\boldsymbol{H} \equiv \sum_{ij \in E} \hat{\boldsymbol{H}}_{ij}$$

$$\boldsymbol{\rho} \equiv \frac{1}{Z} \exp(-\boldsymbol{H})$$

Reduced Density Matrix

$$\boldsymbol{\rho}_i \equiv \mathrm{tr}_{\backslash i} \boldsymbol{\rho}$$

$$\boldsymbol{\rho}_{ij} \equiv \mathrm{tr}_{\backslash ij} \boldsymbol{\rho}$$

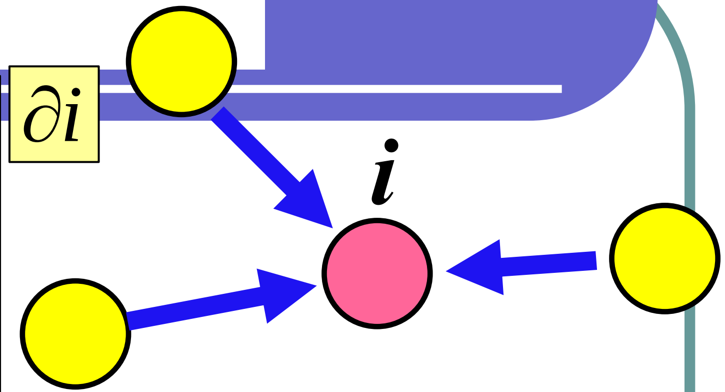


Reducibility Condition

$$\boldsymbol{\rho}_i \equiv \mathrm{tr}_{\backslash i} \boldsymbol{\rho}_{ij}$$

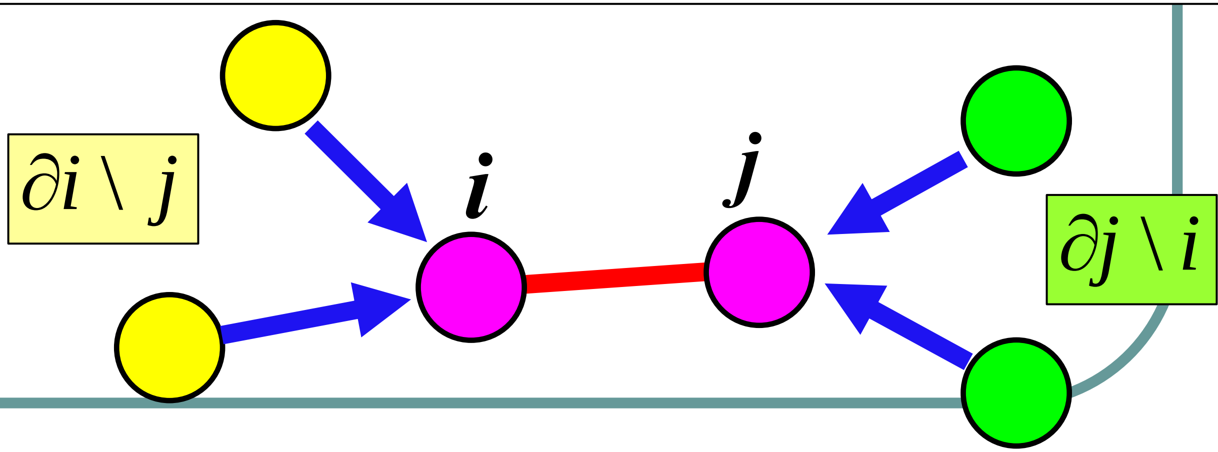
Reduced Density Matrix and Effective Fields

$$\rho_i \cong \frac{1}{Z_i}\exp\left(\sum_{k\in\partial i}\lambda_{k\to i}\right)$$



$$\rho_{ij} \cong \frac{1}{Z_{ij}}\exp\left(-H_{ij}+\sum_{k\in\partial i\setminus j}\lambda_{k\to i}\otimes I+\sum_{l\in\partial j\setminus i} I\otimes\lambda_{l\to j}\right)$$

All effective field are matrices

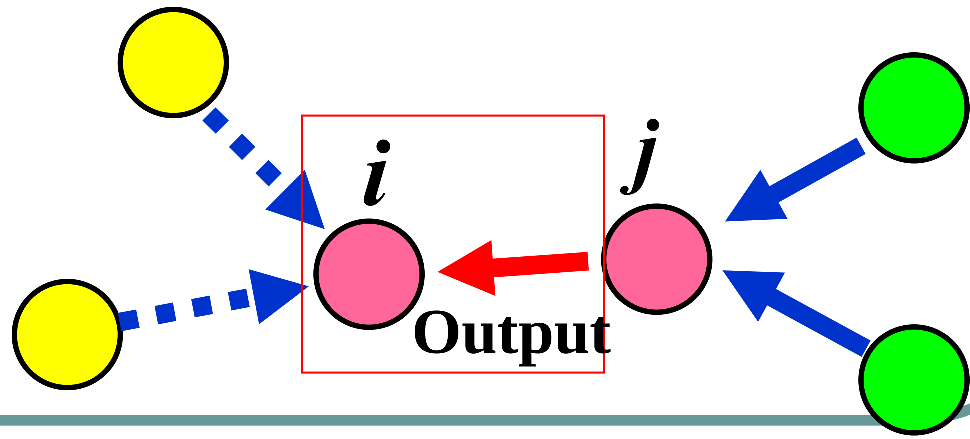


Conventional Belief Propagation for Quantum Statistical Systems

Propagating Rule of Effective Fields

$$\boldsymbol{\lambda}_{j\to i} = -\sum_{k\in\partial i\backslash j} \boldsymbol{\lambda}_{k\to i} + \log\left(\frac{Z_i}{Z_{ij}} \mathrm{tr}_{\backslash i}\left[\exp\left(-\boldsymbol{H}_{ij} + \sum_{k\in\partial i\backslash j} \boldsymbol{\lambda}_{k\to i}\otimes \boldsymbol{I} + \sum_{l\in\partial j\backslash i} \boldsymbol{I}\otimes\boldsymbol{\lambda}_{l\to j}\right)\right]\right)$$

$$\boldsymbol{\rho}_i \equiv \mathrm{tr}_{\backslash i}\boldsymbol{\rho}_{ij}$$



Quantum Heisenberg Model

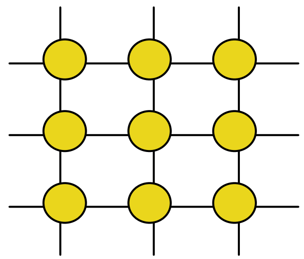
$$\boldsymbol{S}^{x} \equiv \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \boldsymbol{S}^{y} \equiv \frac{1}{2}\begin{pmatrix} 0 & -\mathrm{i} \\ -\mathrm{i} & 0 \end{pmatrix} \qquad \boldsymbol{S}^{z} \equiv \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\boldsymbol{S}_{\boldsymbol{i}}^{\nu} \equiv \overbrace{\boldsymbol{I} \otimes \boldsymbol{I} \otimes \cdots \otimes \boldsymbol{I} \otimes \underset{\substack{\Uparrow \\ \boldsymbol{i}}}{\boldsymbol{S}^{\nu}} \otimes \boldsymbol{I} \otimes \boldsymbol{I} \otimes \cdots \otimes \boldsymbol{I}}^{N} \quad (\nu = x, y, z)$$

$$\boldsymbol{H} \equiv -\sum_{ij \in E} J(\boldsymbol{S}_{\boldsymbol{i}}^{x}\boldsymbol{S}_{\boldsymbol{j}}^{x} + \boldsymbol{S}_{\boldsymbol{i}}^{y}\boldsymbol{S}_{\boldsymbol{j}}^{y} + \boldsymbol{S}_{\boldsymbol{i}}^{z}\boldsymbol{S}_{\boldsymbol{j}}^{z}) - \sum_{i \in V} h_i \boldsymbol{S}_{\boldsymbol{i}}^{z}$$

2^Nx2^N Matrix

$$\boldsymbol{\rho} \equiv \frac{\exp(-\beta \boldsymbol{H})}{\mathrm{tr}\left[\exp(-\beta \boldsymbol{H})\right]}$$



Ω

DEX-SMI

Statistical-Mechanical Approach to Probabilistic Information Processing

$$H \equiv -\sum_{ij \in E} J(S_i^x S_j^x + S_i^y S_j^y + S_i^z S_j^z)$$

Simple Cubic Lattice

High Temperature Expansion
+ Pade Approximation: 0.8387 (J>0)

$J > 0$

Approximation	Curie Point
Bethe	0.9102
Kikuchi	0.9108

$J < 0$

Approximation	Neel Point	Anti Neel Point
Bethe	1.0153	0.4298
Kikuchi	1.0232	0.2056

Ground state is always paramagnetic state in both Bethe and Kikuchi approximations.

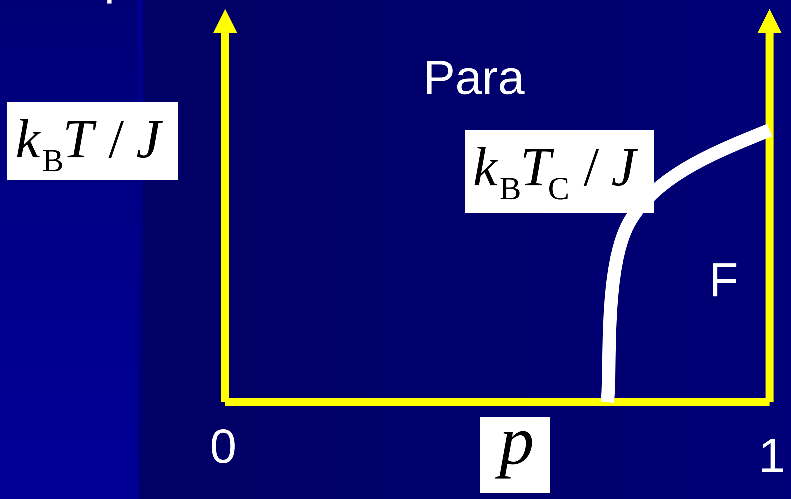
Random Heisenberg Magnets by using Bethe Approximation

$$H \equiv -\sum_{ij\in E} J_{ij}\left(S_i^x S_j^x + S_i^y S_j^y + S_i^z S_j^z\right)$$

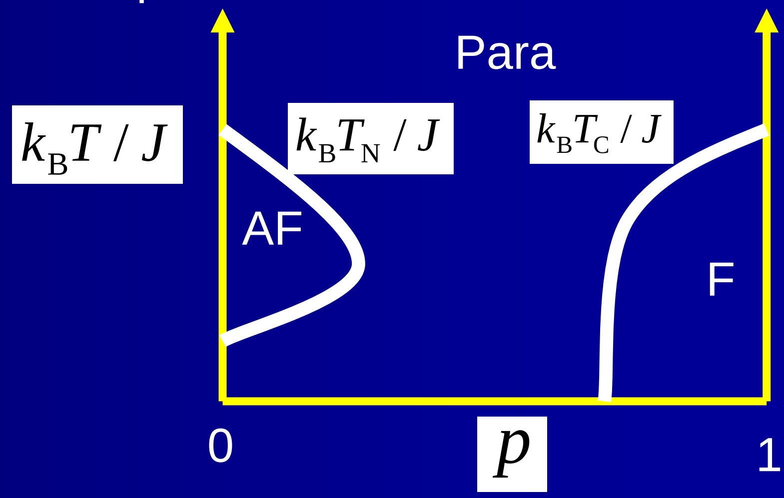
S. Katsura and K. Shimada: Phys. Stat. Sol. 97 (1980).

$$P\left(J_{ij}\right) = p\delta\left(J_{ij} - J\right) + \left(1-p\right)\delta\left(J_{ij} + J\right)$$

Square Lattice



Simple Cubic Lattice



Quantum Adaptive TAP approach

$$\boldsymbol{H} = -\mu \sum_{i \in V} \boldsymbol{a}_i^{+} \boldsymbol{a}_i - t \sum_{ij \in E} (\boldsymbol{a}_i^{+} \boldsymbol{a}_j + \boldsymbol{a}_j^{+} \boldsymbol{a}_i) + U \sum_{i \in V} \boldsymbol{a}_i^{+} \boldsymbol{a}_i^{+} \boldsymbol{a}_i \boldsymbol{a}_i$$

Bose Lattice Gas

Trial Reduced Density Matrices

$$\boldsymbol{\rho} \propto \exp\left(\sum_{i \in V} (\mu + h_{i,\mathrm{Vf}}) \boldsymbol{a}_i^{+} \boldsymbol{a}_i + t \sum_{ij \in E} (\boldsymbol{a}_i^{+} \boldsymbol{a}_j + \boldsymbol{a}_j^{+} \boldsymbol{a}_i) \right)$$

$$\boldsymbol{\rho}_i \propto \exp\left(h_{i,\mathrm{if}} \boldsymbol{a}_i^{+} \boldsymbol{a}_i \right) \qquad \boldsymbol{Q}_i \propto \exp\left(h_{i,\mathrm{if}} \boldsymbol{a}_i^{+} \boldsymbol{a}_i - U \boldsymbol{a}_i^{+} \boldsymbol{a}_i^{+} \boldsymbol{a}_i \boldsymbol{a}_i \right)$$

$$F_{\mathrm{QATAP}}\left[\boldsymbol{\rho}, \{\boldsymbol{Q}_i, \boldsymbol{\rho}_i\}\right] = F_{\mathrm{f}}[\boldsymbol{\rho}] + \sum_{i \in V} \left(F_i[\boldsymbol{Q}_i] - F_{i\mathrm{f}}[\boldsymbol{\rho}_i] \right)$$

$$\begin{cases} \mathrm{tr}\left[\boldsymbol{a}_i^{+} \boldsymbol{a}_i \boldsymbol{\rho}\right] = \mathrm{tr}\left[\boldsymbol{a}_i^{+} \boldsymbol{a}_i \boldsymbol{\rho}_i\right] = \mathrm{tr}\left[\boldsymbol{a}_i^{+} \boldsymbol{a}_i \boldsymbol{Q}_i\right] \\ \mathrm{tr}[\boldsymbol{\rho}] = \mathrm{tr}[\boldsymbol{\rho}_i] = \mathrm{tr}[\boldsymbol{Q}_i] = 1 \end{cases}$$

Quantum Heisenberg Model

$$H \equiv -\sum_{ij\in B} J\left(S_i^x S_j^x + S_i^y S_j^y + S_i^z S_j^z\right) - \sum_{i\in\Omega} h_i S_i^z \qquad (J>0)$$

Holstain-Primakof Transformation

Tractable Part

$$H \cong -\frac{J}{2}\sum_{ij\in B}\sum_{\sigma=\uparrow,\downarrow}\left(a_{i\sigma}^{+}a_{j\sigma} + a_{j\sigma}^{+}a_{i\sigma}\right) + \frac{J}{2}\sum_{i\in\Omega}\sum_{\sigma=\uparrow,\downarrow} a_{i\sigma}^{+}a_{i\sigma} - \sum_{i\in\Omega} h_i\left(a_{i\uparrow}^{+}a_{i\uparrow} - a_{i\downarrow}^{+}a_{i\downarrow}\right)$$
$$- J\sum_{ij\in B}\sum_{\sigma=\uparrow,\downarrow} a_{i\sigma}^{+}a_{j\sigma}^{+}a_{i\sigma}a_{j\sigma} - U\sum_{i\in\Omega}\sum_{\sigma=\uparrow,\downarrow} a_{i\sigma}^{+}a_{i\sigma}^{+}a_{i\sigma}a_{i\sigma}$$

Pair Approximation of QCVM

T. Morita: A Bose Lattice Gas Equivalent to Heisenberg Model and Its QCVM Study, Journal of the Physical Society of Japan, Vol.64, No.4, pp.1211-1216, 1995.

Contents

Summary

We reviewed the conventional loopy belief propagation based on cluster variation method.
Some interpretations and extensions of the adaptive TAP method have been given by using the cluster variation method.
Conventional formalisms and extensions of the quantum belief propagation have been also summarized.