Rotation invariant spin glass models and a matrix integral

Yoshiyuki Kabashima

Institute for Physics of Intelligence,
The University of Tokyo, Japan

Outline

- Background, motivation, and purpose
- Replica analysis in rotationally invariant (RI) models
- Expectation propagation (EP) in RI models
- Summary

Background

- Sherrington-Kirkpatrick (SK) model (1975)
  - Originally: ``Solvable'' model of spin glass
  - Later: Also handled as "prototype" model of inference problem

$$H(S) = -\sum_{i<j} J_{ij} S_i S_j - h \sum_{i=1}^{N} S_i$$

$$S_i \in \{+1, -1\}$$

$$\begin{cases} J_{ij} \sim_{\text{i.i.d.}} \mathcal{N}\left(0, N^{-1} J^2\right), \\ h: \text{ external field} \end{cases}$$

Replica symmetric (RS) solution

$$\begin{cases} q = \int Dz \tanh^2\left(\beta\left(h + \sqrt{\hat{q}} z\right)\right) \\ \hat{q} = J^2 q \end{cases}$$

$$\left(\begin{array}{l} q = \dfrac{1}{N} \displaystyle\sum_{i=1}^{N} \left[\langle S_i \rangle_\beta^2 \right]_J, \\ \beta = T^{-1}: \text{ inverse temp.} \end{array} \right)$$

$$\left(Dz \triangleq \frac{dz \exp\left(-z^2/2\right)}{\sqrt{2\pi}} \right)$$

de Almeida-Thouless (AT) condition

Replica symmetry breaking (RSB) occurs and inference becomes difficult.

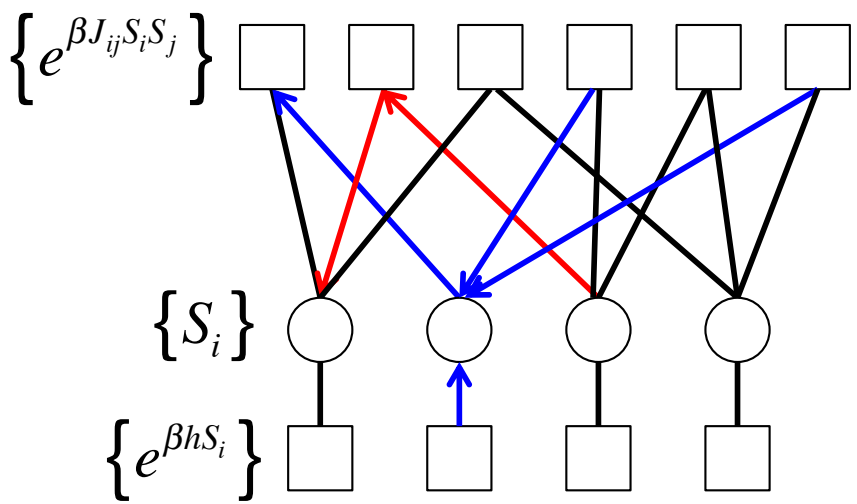
$$\beta^2 J^2 \int Dz \left(1 - \tanh^2\left(\beta\left(h + \sqrt{\hat{q}} z\right)\right)\right)^2 > 1$$

Consequences of "static" analysis by the replica method

Background

- YK (2003), Bolthausen (2014)
  - Employment of belief propagation (BP)(=AMP) for SK model

$$\begin{cases} m_i^t = \tanh\left(\beta\left(h+\gamma_i^t\right) - J^2\beta^2\left(1-q^{t-1}\right)m_i^{t-2}\right) \\ \gamma_i^{t+1} = \left[Jm^t\right]_i \end{cases}$$



Macro. dynamics (state evolution: SE)

$$\begin{cases} q^t = \int Dz \tanh^2\left(\beta\left(h+\sqrt{\hat{q}^t}z\right)\right) \\ \hat{q}^{t+1} = J^2 q^t \end{cases}$$

Micro. instability condition of the fixed point of AMP

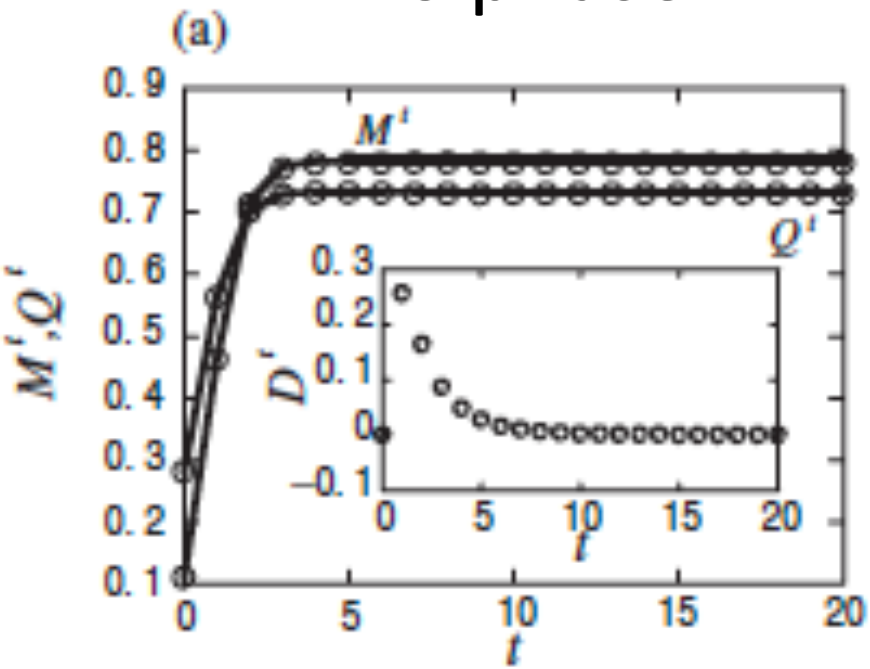
BP's fixed point is unstable ⇒ <u>Inference by BP fails</u>.

$$\beta^2 J^2 \int Dz\left(1-\tanh^2\left(\beta\left(h+\sqrt{\hat{q}}z\right)\right)\right)^2 > 1$$

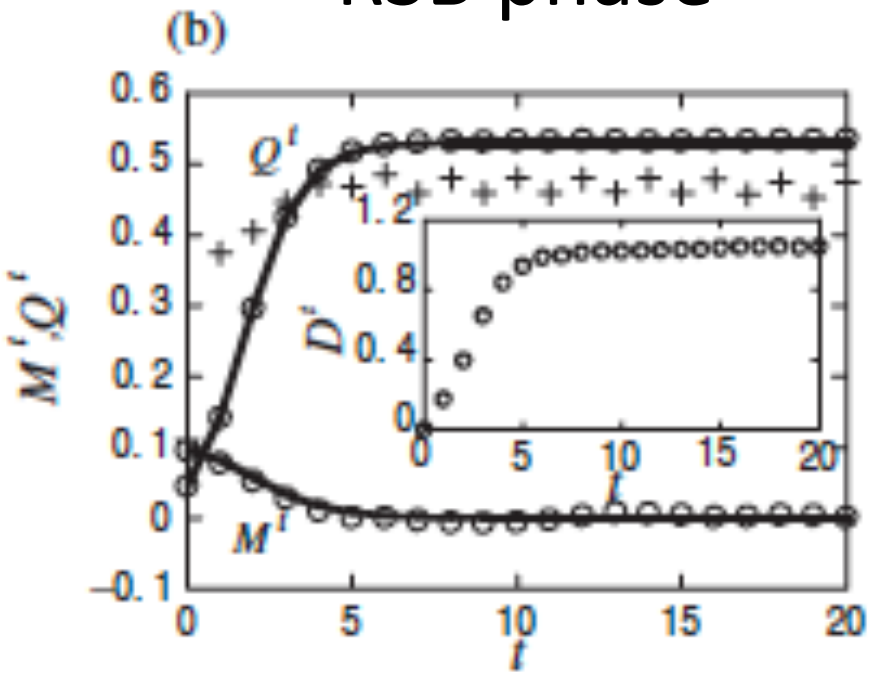
Consequences of "dynamical" analysis by AMP

RS SP eq. vs. AMP in SK model

RS phase



RSB phase



◯: trajectory of AMP

＋: trajectory of iterative substitution of TAP equation

Curves: trajectory of iterative substitution of RS saddle point equation

Insets: difference between $\boldsymbol{m}^{t+1}$ and $\boldsymbol{m}^{t}$

From YK, JPSJ 72, pp. 1645–1649 (2003)

Background

- Replica-BP correspondence in SK model

Replica method	Belief propagation (AMP)
RS saddle point equation	Macro. dynamics (state evolution: SE)

$$\begin{cases} q = \int Dz \tanh^2\left(\beta\left(h + \sqrt{\hat{q}}z\right)\right) \\ \hat{q} = J^2 q \end{cases}$$

$$\begin{cases} q^t = \int Dz \tanh^2\left(\beta\left(h + \sqrt{\hat{q}^t}z\right)\right) \\ \hat{q}^{t+1} = J^2 q^t \end{cases}$$

AT instability of RS solution

$$\beta^2 J^2 \int Dz \left(1 - \tanh^2\left(\beta\left(h + \sqrt{\hat{q}}z\right)\right)\right)^2 > 1$$

Instability of AMP's fixed point

$$\beta^2 J^2 \int Dz \left(1 - \tanh^2\left(\beta\left(h + \sqrt{\hat{q}}z\right)\right)\right)^2 > 1$$

✓ Similar correspondence also holds for CDMA/Hopfield/CS models.

Motivation

- Rotationally invariant (RI) models

$$H(S) = -\sum_{i<j} J_{ij} S_i S_j - h \sum_{i=1}^{N} S_i \qquad \begin{cases} J = O \times \mathrm{diag}(\lambda_i) \times O^\top \\ O \sim \text{uniform dist. on } O(N) \\ \lambda_i \sim \rho(\lambda) \end{cases}$$

  - Parisi-Potters (1994), Opper-Winther (2001), Takeda-Uda-YK (2006), …
  - Components of connection matrices are (weakly) correlated.
  - Exact analysis is still possible by the replica method using a characteristic function for matrix ensemble, which we here refer to as "matrix integral"

$$G(x) \triangleq \operatorname*{extr}_{\Lambda} \left\{ -\frac{1}{2} \int d\lambda \rho(\lambda) \ln(\Lambda - \lambda) + \frac{\Lambda x}{2} \right\} - \frac{1}{2} \ln x - \frac{1}{2}$$

  - BP-based analysis is also possible by the technique of "expectation-propagation" (EP), which was recently re-discovered as "vector approximate message passing (VAMP)"
    - Minka (2001), Opper-Winther (2005), Rangan et al (2017), …

How is the replica-BP correspondence generalized?

Purpose

- We here examine how the correspondence is generalized for the RI SG models using the matrix integral G(x).

Short course of replica method

- Random Hamiltonian → Necessity of <u>config. avg.</u> w.r.t. $\{J_{ij}\}$
  - Edwards and Anderson (1975)

Thermal average

$$\langle O \rangle = \mathrm{Tr}_{\mathbf{S}}\, O(\mathbf{S}) P_\beta(\mathbf{S}|\mathbf{J}) = \mathrm{Tr}_{\mathbf{S}} \frac{O(\mathbf{S}) e^{-\beta H(\mathbf{S}|\mathbf{J})}}{Z_\beta(\mathbf{J})}$$

Random variable depending on $\{J_{ij}\}$

Configurational (quenched) average

$$\left[\langle O \rangle^k\right] = \int \prod_{(ij)} dJ_{ij} P(J_{ij}) \left(\mathrm{Tr}_{\mathbf{S}}\, O(\mathbf{S}) P_\beta(\mathbf{S}|\mathbf{J})\right)^k \quad (k = 1, 2, \ldots)$$

All moments → Distribution of <*O*> → Full information about the system

Short course of replica method

- Unfortunately, assessment of the config. avg. is difficult

$$\left[\langle O\rangle^k\right]=\int\prod_{(ij)}dJ_{ij}P\left(J_{ij}\right)\left(\frac{\operatorname*{Tr}_{\mathbf{S}}O(\mathbf{S})e^{-\beta H(\mathbf{S}|\mathbf{J})}}{\operatorname*{Tr}_{\mathbf{S}}e^{-\beta H(\mathbf{S}|\mathbf{J})}}\right)^k \qquad Z_\beta(\mathbf{J})=\operatorname*{Tr}_{\mathbf{S}}e^{-\beta H(\mathbf{S}|\mathbf{J})}$$

Main source of difficulty

- This difficulty is resolved for ``extended'' avgs. for $n\geq k$

$$\left[\langle O\rangle^k\right]_n\triangleq\frac{\left[Z_\beta^n(J)\langle O\rangle^k\right]}{\left[Z_\beta^n(J)\right]}=\frac{\int\prod_{(ij)}dJ_{ij}P\left(J_{ij}\right)\left(\operatorname*{Tr}_{\mathbf{S}}e^{-\beta H(\mathbf{S}|\mathbf{J})}\right)^{n-k}\left(\operatorname*{Tr}_{\mathbf{S}}O(\mathbf{S})e^{-\beta H(\mathbf{S}|\mathbf{J})}\right)^k}{\int\prod_{(ij)}dJ_{ij}P\left(J_{ij}\right)\left(\operatorname*{Tr}_{\mathbf{S}}e^{-\beta H(\mathbf{S}|\mathbf{J})}\right)^n}$$

- No negative power of partition functions
- Can be assessed separately

Short course of replica method

- Key formula
  - For $n = 1,2,\ldots \in \mathrm{N}$

$$\left(\sum_{\mathbf{S}} e^{-\beta H(\mathbf{S}|\mathbf{J})}\right)^n = \sum_{\mathbf{S}^1,\mathbf{S}^2,\ldots,\mathbf{S}^n} e^{-\beta \sum_a H\left(\mathbf{S}^a\middle|\mathbf{J}\right)}$$

  - Note that this does not generally holds for real numbers $n \in \mathbb{R}$

- Spins $\mathbf{S}^1, \mathbf{S}^2, \ldots, \mathbf{S}^n$ are called *"replicas".*

Short course of replica method

- For $n = 1,2,\ldots \in \mathbb{N}$, extended avg. = Avg. w.r.t. joint dist. of "replicas" defined as

$$P_\beta\left(\mathbf{S}^1,\mathbf{S}^2,\ldots,\mathbf{S}^n\right) \triangleq \frac{\int \prod_{(ij)} dJ_{ij} P\left(J_{ij}\right) \exp\left(-\sum_{a=1}^{n} \beta H\left(\mathbf{S}^a \middle| \mathbf{J}\right)\right)}{\int \prod_{(ij)} dJ_{ij} P\left(J_{ij}\right) Z_\beta^n(\mathbf{J})}$$

$$\left[\langle O \rangle^k\right]_n = \operatorname*{Tr}_{\mathbf{S}^1,\mathbf{S}^2,\ldots,\mathbf{S}^n} P_\beta\left(\mathbf{S}^1,\mathbf{S}^2,\ldots,\mathbf{S}^n\right) O\left(\mathbf{S}^1\right) O\left(\mathbf{S}^2\right) \cdots O\left(\mathbf{S}^k\right)$$

- The joint dist. = Canonical dist. of "non-random" Hamiltonian

$$H\left(\mathbf{S}^1,\mathbf{S}^2,\ldots,\mathbf{S}^n\right) \triangleq -\frac{1}{\beta} \ln\left(\int \prod_{(ij)} dJ_{ij} P\left(J_{ij}\right) \underline{\exp\left(-\sum_{a=1}^{n} \beta H\left(\mathbf{S}^a \middle| \mathbf{J}\right)\right)}\right)$$

Randomness is averaged out

Standard stat. mech. techniques applicable

Short course of replica method

- Replica method
  - Evaluate the config. avgs. by the following procedures

1. For $n = 1,2,\ldots \in \mathbb{N}$, analytically evaluate the extended avgs. as a function of n.

$$\left[\langle O\rangle^k\right]_n = \operatorname*{Tr}_{\mathbf{S}^1,\mathbf{S}^2,\ldots,\mathbf{S}^n} P_\beta\left(\mathbf{S}^1,\mathbf{S}^2,\ldots,\mathbf{S}^n\right) O\left(\mathbf{S}^1\right) O\left(\mathbf{S}^2\right)\cdots O\left(\mathbf{S}^k\right)$$

2. Under appropriate assumptions, the obtained expression is likely to hold for real numbers $n \in \mathbb{R}$. So, we exploit the expression to assess the config. avgs. as

$$\left[\langle O\rangle^k\right]_n \triangleq \frac{\left[Z^n(J)\langle O\rangle^k\right]}{\left[Z^n(J)\right]} = \frac{\int\prod_{(ij)} dJ_{ij} P\left(J_{ij}\right)\left(\operatorname*{Tr}_{\mathbf{S}} e^{-\beta H(\mathbf{S}|\mathbf{J})}\right)^{n-k}\left(\operatorname*{Tr}_{\mathbf{S}} O(\mathbf{S}) e^{-\beta H(\mathbf{S}|\mathbf{J})}\right)^k}{\int\prod_{(ij)} dJ_{ij} P\left(J_{ij}\right)\left(\operatorname*{Tr}_{\mathbf{S}} e^{-\beta H(\mathbf{S}|\mathbf{J})}\right)^n}$$

$$\xrightarrow{n\to 0} \int\prod_{(ij)} dJ_{ij} P\left(J_{ij}\right)\left(\frac{\operatorname*{Tr}_{\mathbf{S}} O(\mathbf{S}) e^{-\beta H(\mathbf{S}|\mathbf{J})}}{\operatorname*{Tr}_{\mathbf{S}} e^{-\beta H(\mathbf{S}|\mathbf{J})}}\right)^k = \left[\langle O\rangle^k\right]$$

Short course of replica method

- In practice, the computation is reduced to the following procedures

1. For $n = 1,2,\ldots \in \mathbb{N}$, analytically evaluate $N^{-1}\ln\left[Z_\beta^n(J)\right]$ as a function of n (using the saddle point method in most cases).

$$\phi_\beta(n) \triangleq -\frac{1}{\beta N}\ln\left[Z_\beta^n(J)\right]$$

2. Under appropriate assumptions, the obtained expression is likely to hold for real $n \in \mathbb{R}$. So, we exploit the expression to assess the config. avg. of "free energy" as

$$\left[f(\beta)\right] \triangleq -\frac{1}{\beta N}\left[\ln Z_\beta(J)\right] = -\lim_{n\to 0}\frac{\partial}{\partial n}\frac{1}{\beta N}\ln\left[Z_\beta^n(J)\right] = \lim_{n\to 0}\frac{\partial}{\partial n}\phi_\beta(n)$$

Replica analysis in RI models

- Partition function

$$Z(\beta)=\sum_{\boldsymbol{S}}\exp\left(\beta\sum_{i<j}J_{ij}S_iS_j+\beta h\sum_i S_i\right)=\sum_{\boldsymbol{S}}\exp\left(\frac{1}{2}\mathrm{Tr}\left(\beta\boldsymbol{J}\boldsymbol{S}\boldsymbol{S}^{\top}\right)+\beta\boldsymbol{h}\cdot\boldsymbol{S}\right)$$

- Rotationally invariant matrix ensemble

$$\begin{cases} J=O\times\mathrm{diag}\left(\lambda_i\right)\times O^{\top} \\ O\sim\text{uniform dist. on } O(N) \\ \lambda_i\sim\rho\left(\lambda\right) \end{cases}$$

- Moments of partition function for $n\in\{1,2,\ldots\}$

$$\left[Z^n(\beta)\right]_J=\sum_{\boldsymbol{S}^1,\cdots,\boldsymbol{S}^n}\left[\exp\left(\frac{1}{2}\mathrm{Tr}\left(\beta\boldsymbol{J}\sum_{a=1}^{n}\boldsymbol{S}^a\left(\boldsymbol{S}^a\right)^{\top}\right)\right)\right]_J\times\prod_{a=1}^{n}e^{\beta\boldsymbol{h}\cdot\boldsymbol{S}^a}$$

Replica analysis in RI models

Rotational invariance assumption for the coupling matrix yields

$$\frac{1}{N}\ln\left[\exp\left(\frac{1}{2}\mathrm{Tr}\left(\beta \boldsymbol{J}\sum_{a=1}^{n}\boldsymbol{S}^a\left(\boldsymbol{S}^a\right)^\top\right)\right)\right]_J = G\left(\underline{\beta(1-q)+\beta nq}\right)+(n-1)G\left(\underline{\beta(1-q)}\right)$$

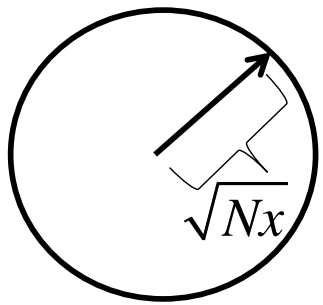
Eigenvalues of matrix $(\beta\sum_{a=1}^{n}S^a(S^a)^T)$

for replica spins of the replica symmetric (RS) configuration

$$\frac{1}{N}\boldsymbol{S}^a\cdot\boldsymbol{S}^b=\begin{cases}1 & (a=b)\\ q & (a\neq b)\end{cases}.$$

$$\boldsymbol{u}=\sqrt{x}O^\top\boldsymbol{1}$$

Here, the characteristic function is defined as



$$G(x)\triangleq\frac{1}{N}\ln\left[\exp\left(\frac{x}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}J_{ij}\right)\right]_J=\frac{1}{N}\ln\left[\exp\left(\frac{x}{2}\left(O^\top\mathbf{1}\right)^\top\mathrm{diag}(\lambda_i)\left(O^\top\mathbf{1}\right)\right)\right]_O$$

$$=\frac{1}{N}\ln\left[\frac{\int\exp\left(\frac{1}{2}\sum_{i=1}^{N}\lambda_i u_i^2\right)\delta\left(|\mathbf{u}|^2-Nx\right)d\mathbf{u}}{\int\delta\left(|\mathbf{u}|^2-Nx\right)d\mathbf{u}}\right]_O\simeq\underset{\Lambda}{\mathrm{extr}}\left\{-\frac{1}{2}\int\rho(\lambda)\ln(\Lambda-\lambda)d\lambda+\frac{\Lambda x}{2}\right\}-\frac{1}{2}\ln x-\frac{1}{2}$$

Cf) SK model

$$P_{\mathrm{SK}}\left(\left\{J_{ij}\right\}\right)=\prod_{i<j}\mathcal{N}\left(0,N^{-1}J^{2}\right)$$

$$G(x)\triangleq\frac{1}{N}\ln\left[\exp\left(\frac{x}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}J_{ij}\right)\right]_{J}$$

$$=\frac{1}{N}\ln\left\{\int\cdots\int\exp\left(\frac{x}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}J_{ij}\right)\frac{\exp\left(-\sum_{i<j}\frac{NJ_{ij}^{2}}{2J^{2}}\right)}{\left(\sqrt{2\pi N^{-1}J^{2}}\right)^{N(N-1)/2}}\prod_{i<j}dJ_{ij}\right\}$$

$$=\frac{1}{N}\ln\left\{\prod_{i<j}\sqrt{\frac{N}{2\pi J^{2}}}\int\exp\left(-\frac{NJ_{ij}^{2}}{2J^{2}}+xJ_{ij}\right)dJ_{ij}\right\}=\frac{1}{N}\ln\left\{\exp\left(\sum_{i<j}\frac{J^{2}x^{2}}{2N}\right)\right\}$$

$$=\frac{1}{N}\ln\left\{\exp\left(\frac{N(N-1)}{2}\times\frac{J^{2}x^{2}}{2N}\right)\right\}\xrightarrow{N\to\infty}\frac{J^{2}x^{2}}{4}$$

$$\therefore G_{\mathrm{SK}}(x)=\frac{J^{2}x^{2}}{4}\qquad\left(\left\{\begin{array}{l}G_{\mathrm{Hopfield}}(x)=-\frac{\alpha}{2}\ln(1-x)\\ G_{\mathrm{CDMA}}(x)=-\frac{\alpha}{2}\ln(1+x)\end{array}\right.\right)$$

Replica analysis in RI models

- This yields RS free entropy as

$$\frac{1}{N}\left[\ln Z(\beta)\right]_J = \lim_{n\to+0}\frac{\partial}{\partial n}\frac{1}{N}\ln\left[Z^n(\beta)\right]_J$$
$$= \underline{G(\beta(1-q)) + \beta q G'(\beta(1-q))} - \frac{\beta^2\hat{q}}{2}(1-q) + \int Dz \ln 2\cosh\left(\beta\left(h+\sqrt{\hat{q}}z\right)\right).$$

- Saddle point equation

$$\begin{cases} q = \int Dz \tanh^2\left(\beta\left(h+\sqrt{\hat{q}}z\right)\right) \\ \hat{q} = 2q\underline{G''(\beta(1-q))} \end{cases} \quad \left(\begin{array}{l} \beta(1-q) = \int \frac{d\lambda\rho(\lambda)}{\Lambda-\lambda} \\ 2G''(\beta(1-q)) = \frac{1}{\beta^2(1-q)^2} - \frac{1}{\int \frac{d\lambda\rho(\lambda)}{(\Lambda-\lambda)^2}} \end{array}\right)$$

- AT instability condition

$$2\beta^2\underline{G''(\beta(1-q))} \times \int Dz\left(1-\tanh^2\left(\beta\left(h+\sqrt{\hat{q}}z\right)\right)\right)^2 > 1.$$

Characterized by G(x)

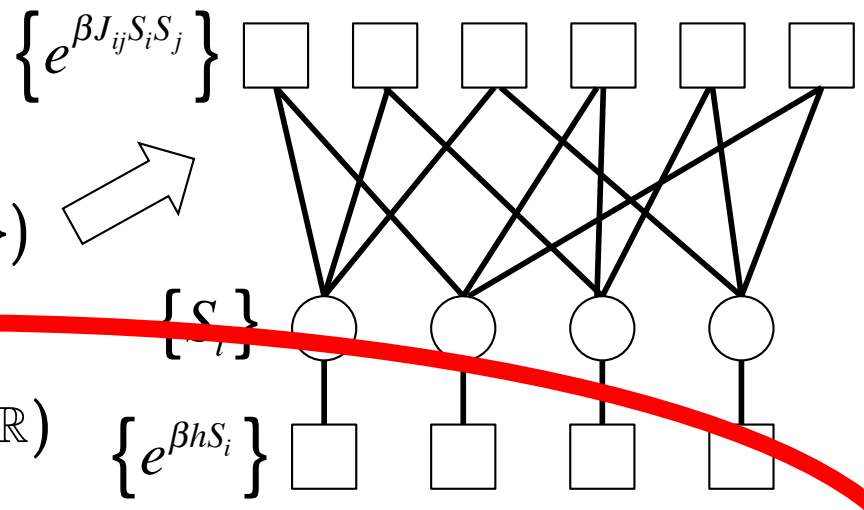
Expectation propagation

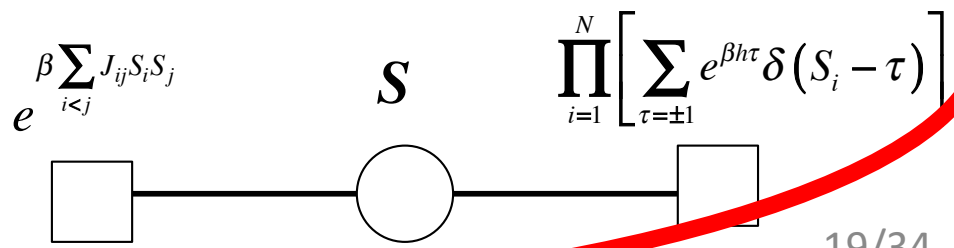
- Method of approximate inference proposed by Minka (2001)
  - Combination of BP and approximation by exponential family (mostly by Gaussians)
  - Can yield accurate inference *<u>even when couplings are statistically correlated</u>*

2 ways of bipartite graph expression

$$P(\boldsymbol{S}) = \frac{1}{Z(\beta)} \prod_{i<j} e^{\beta J_{ij} S_i S_j} \times \prod_{i=1}^{N} e^{\beta h S_i} \quad (S_i \in \{+1, -1\})$$

$$= \frac{1}{Z(\beta)} e^{\beta \sum_{i<j} J_{ij} S_i S_j} \times \prod_{i=1}^{N} \left[\sum_{\tau=\pm 1} e^{\beta h \tau} \delta(S_i - \tau) \right] \quad (S_i \in \mathbb{R})$$

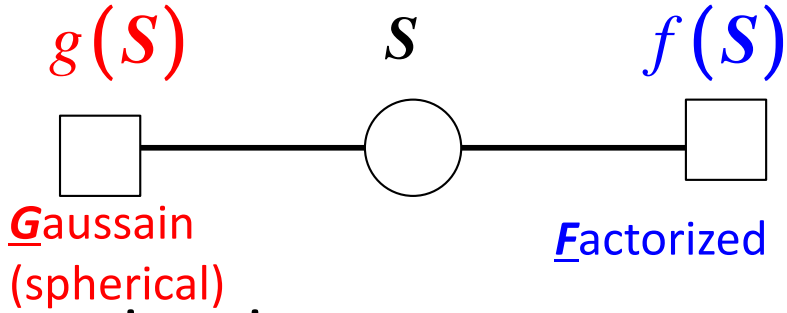




Each node represents collection of variables/factors

Expectation propagation

- "BP" on the right graph yields <u>exact results</u>, but comput. difficult.
- The comput. difficulties are resolved <u>by factorized Gaussian approximation.</u>



$$P(S) \propto \underbrace{e^{\beta \sum_{i<j} J_{ij} S_i S_j}}_{g(S)} \times \underbrace{\prod_{i=1}^{N} \left[\sum_{\tau=\pm 1} e^{\beta h \tau} \delta(S_i - \tau) \right]}_{f(S)}$$

$$\propto g(S) \exp\left(-\frac{\beta \Lambda_G}{2} \sum_{i=1}^{N} S_i^2 + \sum_{i=1}^{N} \beta \gamma_{G,i} S_i \right)$$ ⇦ Comput. feasible (Gaussian)

$$\propto \exp\left(-\frac{\beta \Lambda_F}{2} \sum_{i=1}^{N} S_i^2 + \sum_{i=1}^{N} \beta \gamma_{F,i} S_i \right) f(S)$$ ⇦ Comput. feasible (factorized)

$$\propto \exp\left(-\frac{\beta (\Lambda_G + \Lambda_F)}{2} \sum_{i=1}^{N} S_i^2 + \sum_{i=1}^{N} \beta (\gamma_{G,i} + \gamma_{F,i}) S_i \right)$$ ⇦ Comput. feasible (Gaussian/factorized)

※ $\begin{cases} \Lambda_{G,i} = \Lambda_G \\ \Lambda_{F,i} = \Lambda_F \end{cases}$ are assumed based on self-averaging property.

Nice property of Gaussians: Parameters ↔ Moments "analytically"

$$P\left(\boldsymbol{S}\middle|\boldsymbol{\gamma},\boldsymbol{\Lambda}\right) \propto \exp\left(-\frac{1}{2}\boldsymbol{S}^{\top}\boldsymbol{\Lambda}\boldsymbol{S}+\boldsymbol{\gamma}\cdot\boldsymbol{S}\right):\ \text{Gaussian}$$

Parameters: $\boldsymbol{\gamma}$, $\boldsymbol{\Lambda}$

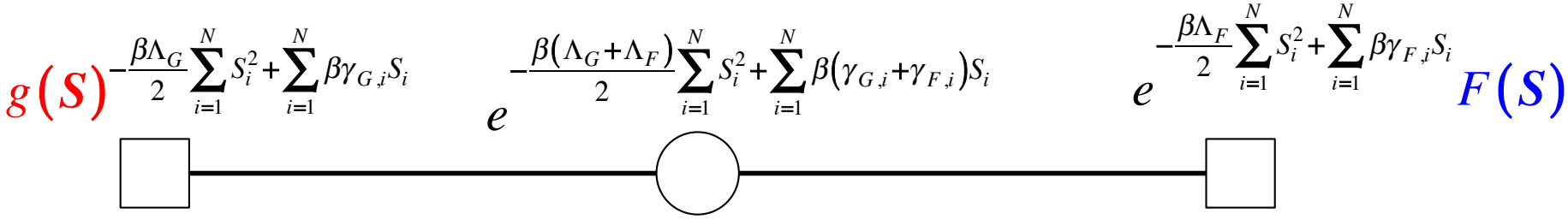
Moments: $\boldsymbol{m} \triangleq \langle \boldsymbol{S} \rangle$, $\boldsymbol{\Sigma} \triangleq \left(\left\langle \boldsymbol{S}\boldsymbol{S}^{\top} \right\rangle - \langle \boldsymbol{S} \rangle \left\langle \boldsymbol{S}^{\top} \right\rangle\right)$

In Gaussians, parameters and (1st and 2nd)moments are expressed <u>in closed forms</u> by each other.

$$\begin{cases} \boldsymbol{\gamma} = \boldsymbol{\Sigma}^{-1}\boldsymbol{m} \\ \boldsymbol{\Lambda} = \boldsymbol{\Sigma}^{-1} \end{cases} \Leftrightarrow \begin{cases} \boldsymbol{m} = \boldsymbol{\Lambda}^{-1}\boldsymbol{\gamma} \\ \boldsymbol{\Sigma} = \boldsymbol{\Lambda}^{-1} \end{cases}$$

Moment matching

- Parameters $\Lambda_G, \Lambda_F, \{\gamma_{G,i}\}, \{\gamma_{F,i}\}$ are determined by the consistency of moments up to the 2nd order



1st moments

$$m_i = \left[(\Lambda_G - J)^{-1} \gamma_G \right]_i \Leftrightarrow m_i = \frac{\gamma_{G,i} + \gamma_{F,i}}{\Lambda_G + \Lambda_F} \Leftrightarrow m_i = \tanh\left(\beta\left(h_i + \gamma_{F,i}\right)\right)$$

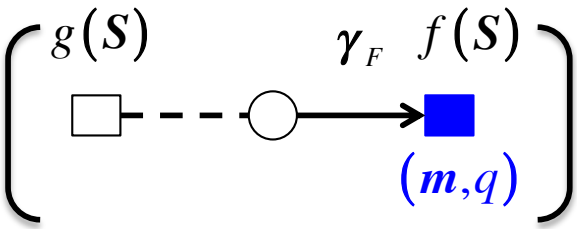
Macroscopic 2nd moments(**=spherical constraint**)

$$\sum_{i=1}^{N} m_i^2 + \underbrace{\beta^{-1}\mathrm{Tr}\left[(\Lambda_G - J)^{-1}\right]}_{\text{Macro. variance}} \Leftrightarrow \sum_{i=1}^{N} m_i^2 + \underbrace{\frac{N}{\beta(\Lambda_G + \Lambda_F)}}_{\text{Macro. variance}} \Leftrightarrow \underbrace{\sum_{i=1}^{N} S_i^2 = N}_{\textbf{Spherical const}}$$

Expectation propagation for Ising spins

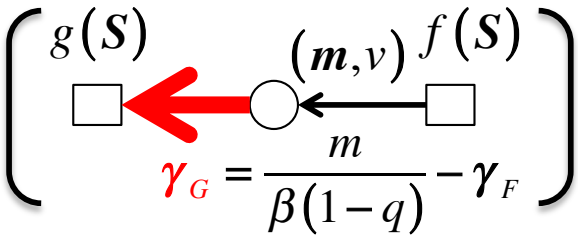
Initialization $\Lambda_F = 0,\ \boldsymbol{\gamma}_F = \boldsymbol{0}$

Main loop Repeat ①～④ until convergence

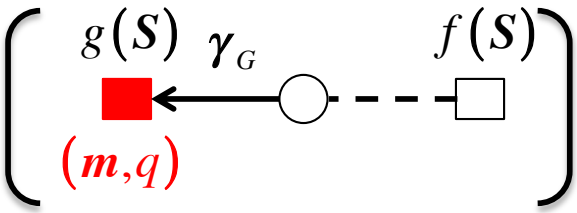


① $$m_i = \tanh\left(\beta\left(h+\gamma_{F,i}\right)\right),\ q = N^{-1}\sum_{i=1}^{N} m_i^2$$

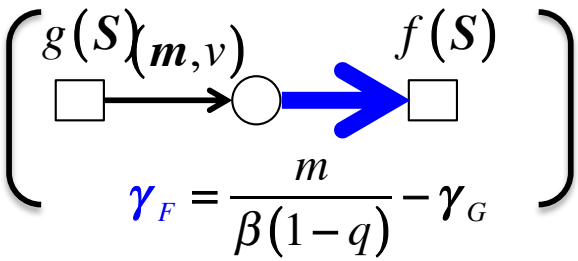
② $$\boldsymbol{\gamma}_G = \frac{\boldsymbol{m}}{\beta(1-q)} - \boldsymbol{\gamma}_F$$



③ $$\begin{cases} \text{Find } \Lambda_G \text{ s.t. } \boldsymbol{\gamma}_G^\top\left(\Lambda_G - J\right)^{-2}\boldsymbol{\gamma}_G^\top + \beta^{-1}\mathrm{Tr}\left(\Lambda_G - J\right)^{-1} = N, \\ \boldsymbol{m} = \left(\Lambda_G - J\right)^{-1}\boldsymbol{\gamma}_G,\ 1-q = N^{-1}\beta^{-1}\mathrm{Tr}\left(\Lambda_G - J\right)^{-1} \end{cases}$$



④ $$\boldsymbol{\gamma}_F = \frac{\boldsymbol{m}}{\beta(1-q)} - \boldsymbol{\gamma}_G$$



Output $\langle \boldsymbol{S} \rangle = \boldsymbol{m}$

Remark (I)

- The fixed point equation accords with the (constant diagonal) adaptive TAP equation by Opper and Winther (2001)

$$m_i = \tanh\left(\beta\left(h + \sum_{j\neq i} J_{ij} m_j - \underbrace{\left(\Lambda_G - \frac{1}{\beta(1-q)}\right)}_{2G'(\beta(1-q))} m_i\right)\right)$$

  - For SK model

$$\Lambda_G - \frac{1}{\beta(1-q)} = 2G'(\beta(1-q)) = \underbrace{J^2\beta(1-q)}_{\text{Reduction to the so-called TAP equation for SK model}}$$

Remark (II)

- Macroscopic dynamics for RI models

We suppose $\gamma_{F,i} = \sqrt{\hat{q}_F} z_i \ \left(z_i \sim_{\text{i.i.d.}} \mathcal{N}(0,1)\right),\ \gamma_{G,i} = \sqrt{\hat{q}_G} y_i \ \left(y_i \sim_{\text{i.i.d.}} \mathcal{N}(0,1)\right).$

State evolution

$$q = \int Dz \tanh^2\left(\beta\left(h + \sqrt{\hat{q}_F} z\right)\right) \longrightarrow \hat{q}_G = \frac{q}{\beta^2 (1-q)^2} - \hat{q}_F$$

$$\text{Find } \Lambda_G \text{ s.t. } 1 = \frac{1}{\beta}\int \frac{d\lambda \rho(\lambda)}{\Lambda_G - \lambda} + \hat{q}_G \int \frac{d\lambda \rho(\lambda)}{(\Lambda_G - \lambda)^2}$$

$$q = \hat{q}_G \int \frac{d\lambda \rho(\lambda)}{(\Lambda_G - \lambda)^2} \longrightarrow \hat{q}_F = \frac{q}{\beta^2 (1-q)^2} - \hat{q}_G$$

- The fixed point is shared with the corresponding RS SP eq.
- But, <u>the dynamics cannot be described by its iterative substitution</u>.

RS SP eq.

$$\begin{cases} q = \int Dz \tanh^2\left(\beta\left(h + \sqrt{\hat{q}_F} z\right)\right) \\ \text{Find } \Lambda_G \text{ s.t. } \beta(1-q) = \int \frac{d\lambda \rho(\lambda)}{\Lambda_G - \lambda} \\ \hat{q}_F = \frac{q}{\beta^2 (1-q)^2} - \frac{q}{\int \frac{d\lambda \rho(\lambda)}{(\Lambda_G - \lambda)}} = 2qG''(\beta(1-q)) \end{cases}$$

Ex) SK model

- Macro dynamics

State evolution of EP

$$q^t = \int Dz \tanh^2\left(\beta\left(h + \sqrt{\hat{q}_F^t}\, z\right)\right)$$

$$\hat{q}_G^t = \frac{q^t}{\beta^2\left(1 - q^t\right)^2} - \hat{q}_F^t$$

Consequence of

$$G_{SK}(x) = \frac{J^2 x^2}{4}$$

$$\text{Find } q^{t+1/2} \text{ s.t. } q^{t+1/2}\left(\beta^{-2}\left(1 - q^{t+1/2}\right)^{-2} - J^2\right) = \hat{q}_G^t$$

← Cubic equation（spherical const.）

$$\hat{q}_F^{t+1} = \frac{q^{t+1/2}}{\beta^2\left(1 - q^{t+1/2}\right)^2} - \hat{q}_G^t$$

State evolution of AMP

$$q^t = \int Dz \tanh^2\left(\beta\left(h + \sqrt{\hat{q}^t}\, z\right)\right)$$

$$\hat{q}^{t+1} = J^2 q^t$$

Remark (III)

- Stability of the fixed point of EP

$$\gamma_{F,i} = \gamma^*_{F,i} + \sqrt{\delta\hat{q}_F}\, z_i \quad \left(z_i \sim_{\text{i.i.d.}} \mathcal{N}(0,1)\right),$$
$$\gamma_{G,i} = \gamma^*_{G,i} + \sqrt{\delta\hat{q}_G}\, z_i \quad \left(z_i \sim_{\text{i.i.d.}} \mathcal{N}(0,1)\right),$$

Fixed point　　Small random perturbation

※No influence for macroscopic quantities such as $q = \frac{1}{N}\sum_{i=1}^{N} m_i^2$.

$$\gamma_G = \frac{\boldsymbol{m}}{\beta(1-q)} - \gamma_F \Rightarrow \delta\hat{q}_G = \left(\frac{\int Dz \left(1 - \tanh^2\left(\beta\left(h + \sqrt{\hat{q}_F}\, z\right)\right)\right)^2}{(1-q)^2} - 1 \right) \delta\hat{q}_F$$

$$\gamma_F = \frac{\boldsymbol{m}}{\beta(1-q)} - \gamma_G \Rightarrow \delta\hat{q}_F = \left(\frac{\int \frac{d\lambda \rho(\lambda)}{(\Lambda_G - \lambda)^2}}{\beta^2 (1-q)^2} - 1 \right) \delta\hat{q}_G$$

Remark (III)

- Instability condition of the fixed point

$$\underbrace{\left(\frac{\int \frac{d\lambda\rho(\lambda)}{(\Lambda_G-\lambda)^2}}{\beta^2(1-q)^2}-1\right)\times\left(\frac{\int Dz\left(1-\tanh^2\left(\beta\left(h+\sqrt{\hat{q}_F}z\right)\right)\right)^2}{(1-q)^2}-1\right)}_{\text{Growth rate of variance}}>1$$

$$\underbrace{\beta^2\left(\frac{1}{\beta^2(1-q)^2}-\frac{1}{\int\frac{d\lambda\rho(\lambda)}{(\Lambda_G-\lambda)^2}}\right)}_{2\beta^2G''(\beta(1-q))}\times\int Dz\left(1-\tanh^2\left(\beta\left(h+\sqrt{\hat{q}_F}z\right)\right)\right)^2>1$$

$\Leftrightarrow$ <u>AT instability condition for RI models</u>

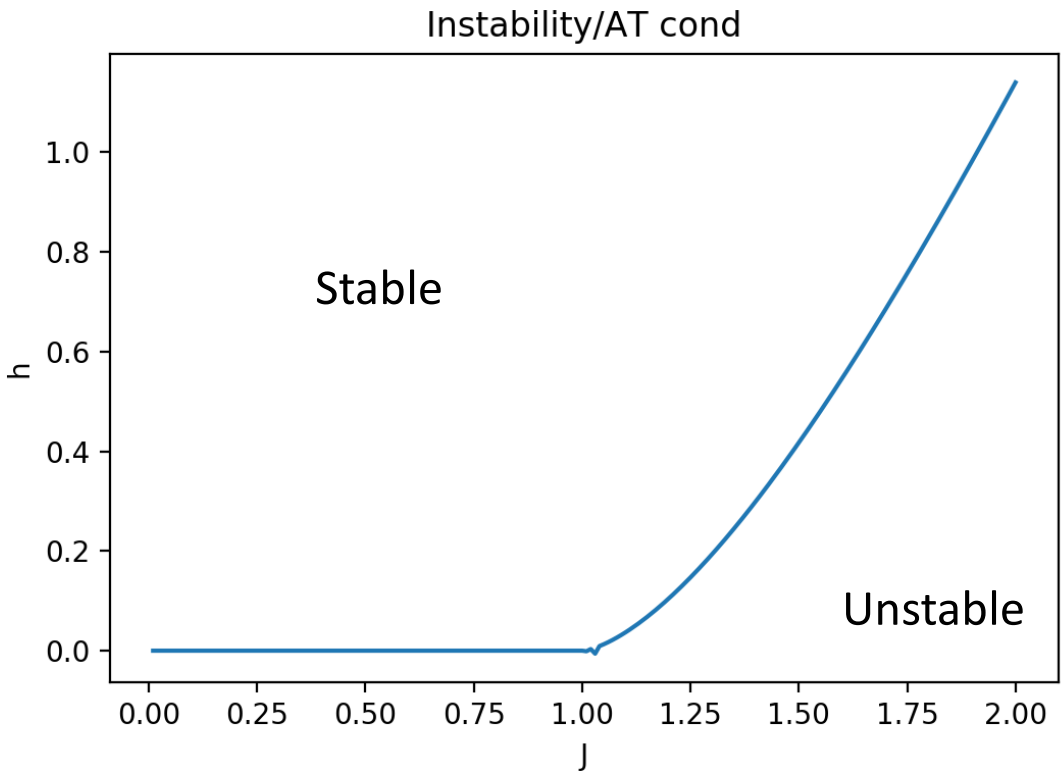
$$2\beta^2G''(\beta(1-q))\times\int Dz\left(1-\tanh^2\left(\beta\left(h+\sqrt{\hat{q}_F}z\right)\right)\right)^2>1$$

Ex) SK model

- Instability condition of fixed point

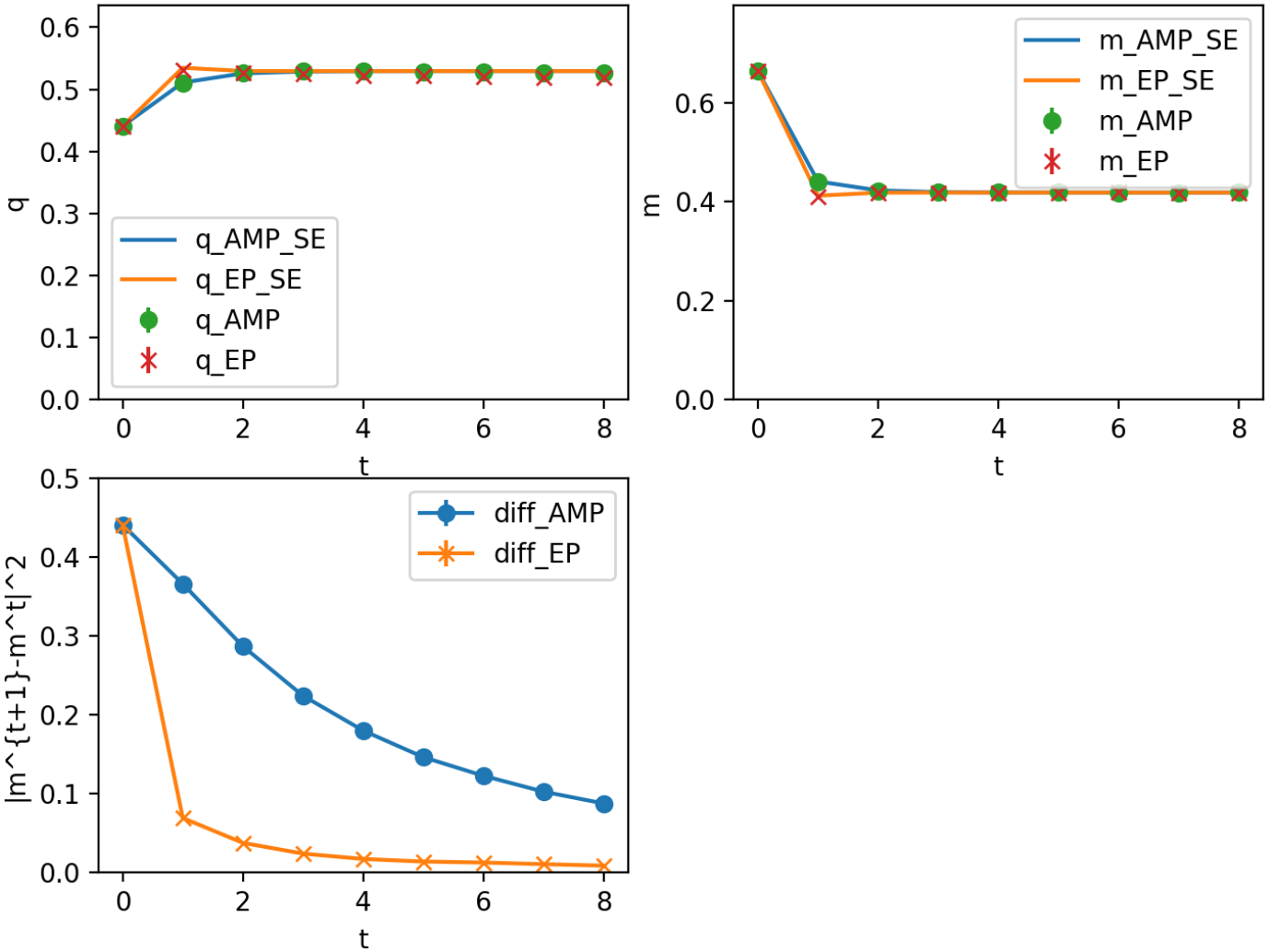
EP and AMP

$$\beta^2 J^2 \int Dz \left(1 - \tanh^2\left(\beta\left(h + \sqrt{\hat{q}_F}\, z\right)\right)\right)^2 > 1$$



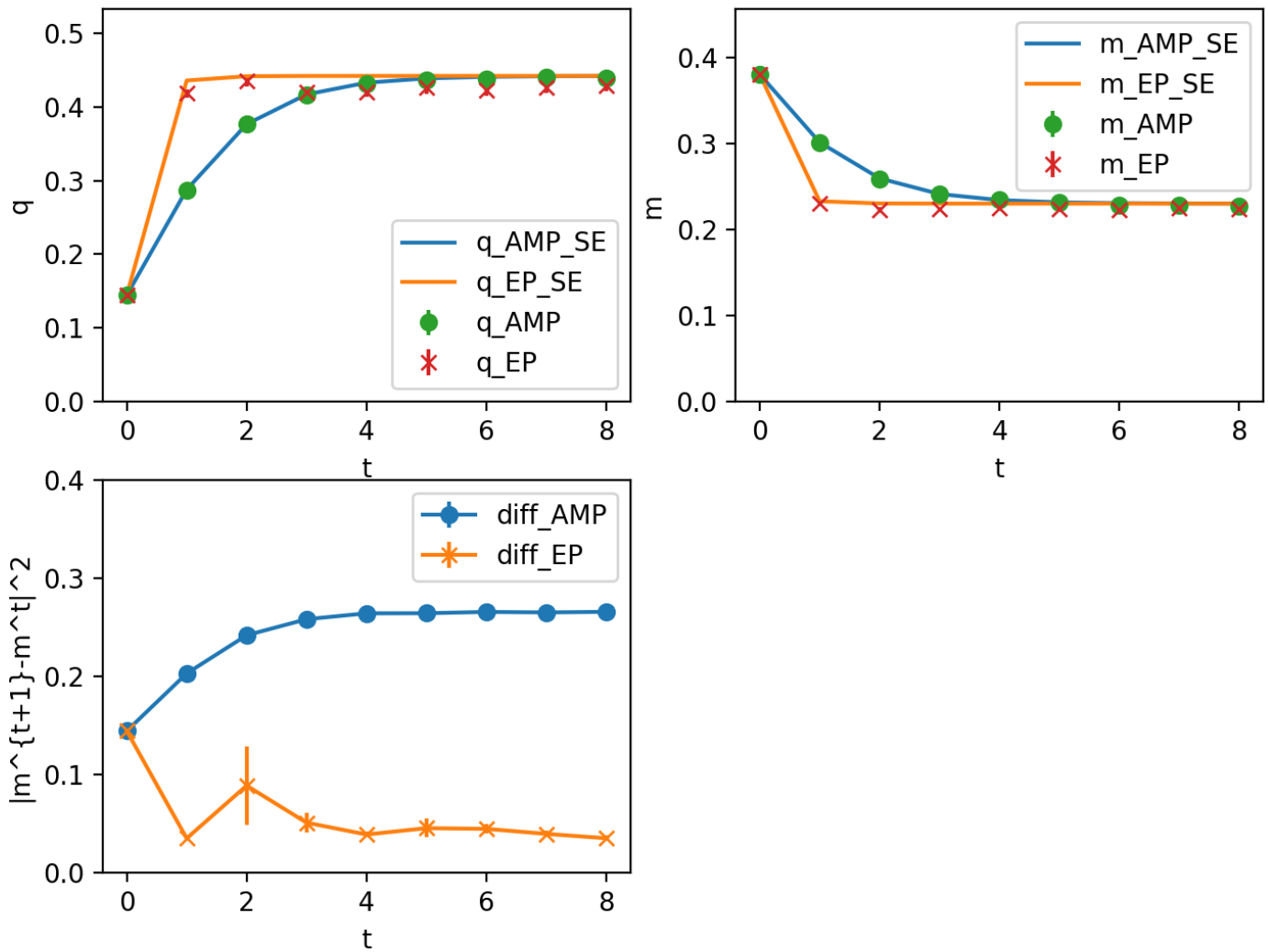
Numerical validation in SK model

- (J,h)=(1.6, 0.8) (stable case), N=1000, #experiments= 100



Numerical validation in SK model

- (J,h)=(1.6, 0.4) (unstable case), N=1000, #experiments= 100



Summary

- The replica saddle point equations of the RI SG models can be expressed using the matrix integral G(x).
  - Actually, G(x) is identical to the integral of R-transform.

- EP's fixed point of the RI SG models is macroscopically described by the replica symmetric solution using G(x).

- Instability condition of EP's fixed point is characterized using G(x) as well.

- However, macroscopic dynamics of EP cannot be described using G(x).

Comment

- The result can be further extended to rectangular RI models applied for generalized linear model (perceptron) (Takahashi and YK (2020a, 2020b))

Rectangular RI model

$$\begin{cases} X\left(\in \mathbb{R}^{M\times N}\right) = U \times \mathrm{diag}\left(\sigma_i\right) \times V^{\top} \\ U, V \sim \text{uniform dists. on } O(M), O(N) \\ \sigma_i \sim \rho(\sigma) \end{cases}$$

Generalized linear model

$$P\left(\mathbf{w}\middle|\mathbf{X},\mathbf{y}\right) = \frac{1}{Z} P(\mathbf{w}) \prod_{\mu=1}^{M} P\left(y_\mu \middle| \mathbf{w}\cdot\mathbf{x}_\mu\right)$$

Thank you for your attention

- References
  - YK, JPSJ 72, 1645 (2003)
  - YK, JPA 36, 11111 (2003)
  - T. Takahashi and YK, in Proc. ISIT2020, 1409 (2020) (arXiv:2001.02824)
  - T. Takahashi and YK, JSTAT (2020) 093402