A brief introduction to the inverse Ising problem and some algorithms to solve it

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Simplifications for this talk

- Ising variables $s_i = \pm 1$
- At most pairwise (two body) interactions.
  The most general Hamiltonian is

$$\mathcal{H}(\boldsymbol{s}|\boldsymbol{J},\boldsymbol{h}) = \sum J_{ij} s_i s_j + \sum_i h_i s_i$$

with corresponding measure

$$P(s_1,\ldots,s_N) = \frac{1}{Z(\boldsymbol{J},\boldsymbol{h})} \exp\left[\sum_{i\neq j} J_{ij} s_i s_j + \sum_i h_i s_i\right]$$

The direct problem
(main pb. in stat. mech.)

- Given the Hamiltonian, compute the free energy

$$F(\boldsymbol{J},\boldsymbol{h}) = \log Z(\boldsymbol{J},\boldsymbol{h}) = \log \sum_{\{s_i\}} \exp\left(\sum J_{ij} s_i s_j + \sum_i h_i s_i\right)$$

and average values

$$\langle \mathcal{O} \rangle = \sum_{\boldsymbol{s}} \mathcal{O}(\boldsymbol{s}) P(\boldsymbol{s})$$

The sum is over exponentially many terms

The inverse Ising problem

- Given data generated according to

$$P(s_1, \ldots, s_N) = \frac{1}{Z(\boldsymbol{J}, \boldsymbol{h})} \exp \left[\sum_{i \neq j} J_{ij} s_i s_j + \sum_i h_i s_i \right]$$

  which may be

  - either M configurations of spins
  - either magnetizations and correlations

$$m_i = \langle s_i \rangle \qquad C_{ij} = \langle s_i s_j \rangle - m_i m_j$$

- GOAL: estimate couplings and fields $(\boldsymbol{J}, \boldsymbol{h})$

The "exact" solution

Maximize the log-likelihood

$$L(\boldsymbol{J},\boldsymbol{h}|\boldsymbol{s}) = \frac{1}{M}\log\prod_{k=1}^{M} P(\boldsymbol{s}^{(k)}|\boldsymbol{J},\boldsymbol{h}) =$$

$$= \sum_i h_i \langle s_i \rangle + \sum_{ij} J_{ij} \langle s_i s_j \rangle - \log Z(\boldsymbol{J},\boldsymbol{h})$$

$$= \sum_i h_i m_i + \sum_{ij} J_{ij}(C_{ij} + m_i m_j) + F(\boldsymbol{J},\boldsymbol{h})$$

Taking the derivatives

$$m_i + \partial_{h_i} F(\boldsymbol{J},\boldsymbol{h}) = 0 \implies \boxed{m_i(\mathrm{DATA}) = m_i(\boldsymbol{J},\boldsymbol{h})}$$

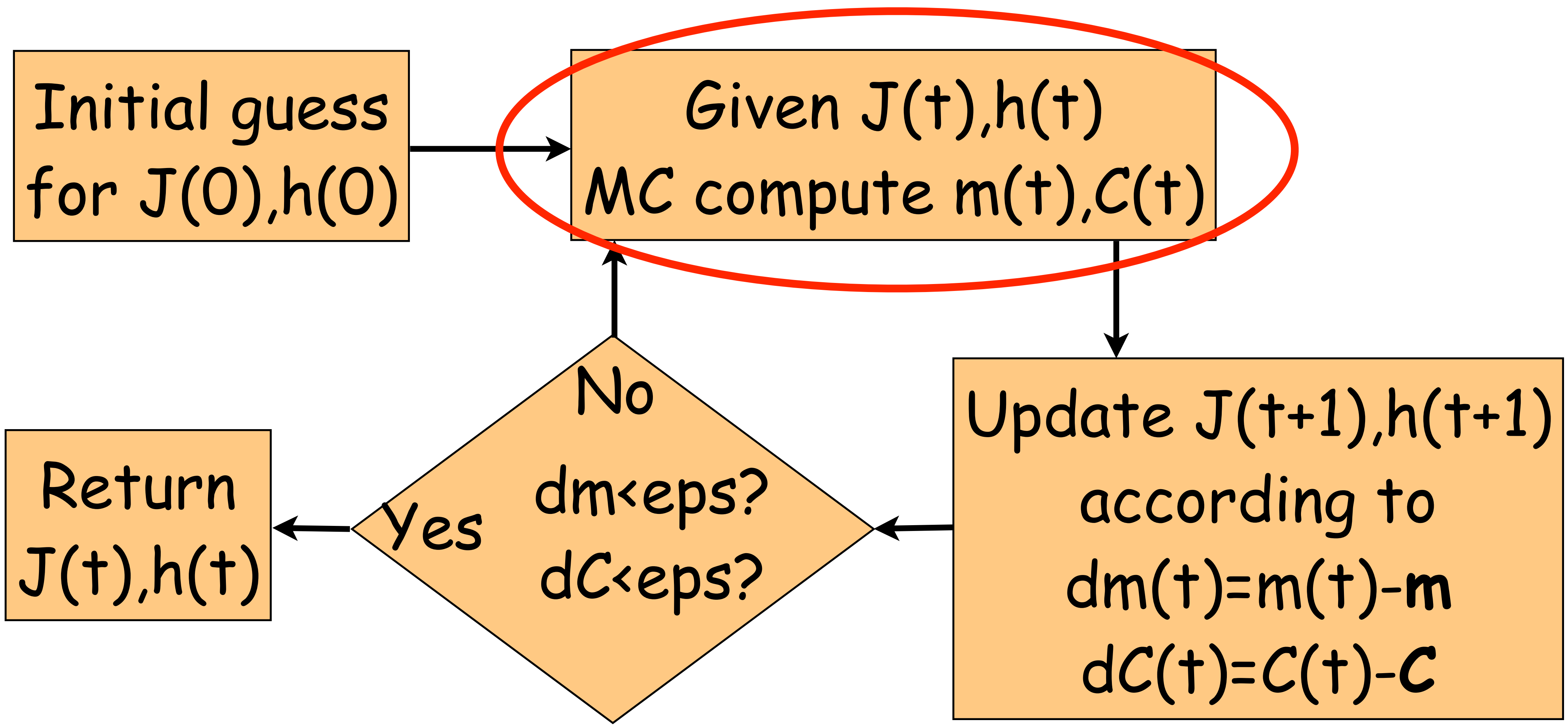
$$C_{ij} + m_i m_j + \partial_{J_{ij}} F(\boldsymbol{J},\boldsymbol{h}) = 0 \implies \boxed{C_{ij}(\mathrm{DATA}) = C_{ij}(\boldsymbol{J},\boldsymbol{h})}$$

Input data: Magnetizations and Correlations

- Less information than having configurations
- If only
$$m_i = \langle s_i \rangle \qquad C_{ij} = \langle s_i s_j \rangle - m_i m_j$$
are given then **maximum entropy principle** implies Hamiltonian contains only single-body and two-body interactions
$$\mathcal{H}(\boldsymbol{s}|\boldsymbol{J},\boldsymbol{h}) = \sum J_{ij} s_i s_j + \sum_i h_i s_i$$

Brute force solution by Monte Carlo

Monte Carlo -> unbiased solution ...but it is slow!



Mean field approximations (MFA)

Log-likelihood $L(\boldsymbol{J},\boldsymbol{h}|\boldsymbol{s}) = \frac{1}{M}\log\prod_{k=1}^{M} P(\boldsymbol{s}^{(k)}|\boldsymbol{J},\boldsymbol{h}) =$

$$= \sum_i h_i m_i + \sum_{ij} J_{ij}(C_{ij} + m_i m_j) - \log Z(\boldsymbol{J},\boldsymbol{h})$$

$$\downarrow$$

$$F_{\mathrm{MFA}}(\boldsymbol{J},\boldsymbol{h})$$

$$m_i^{\mathrm{MFA}} = -\partial_{h_i} F_{\mathrm{MFA}}(\boldsymbol{J},\boldsymbol{h})$$

$$m_i^{\mathrm{MFA}}(\boldsymbol{J},\boldsymbol{h}) = m_i(\mathrm{DATA})$$

$$C_{ij}^{\mathrm{MFA}}(\boldsymbol{J},\boldsymbol{h}) = C_{ij}(\mathrm{DATA})$$

MFA to the free-energy

- naive mean-field (nMF)

$$P(\boldsymbol{s}) = \prod_i P_i(s_i)$$

$$F_{\mathrm{nMF}} = \sum_i \left[H\left(\frac{1+m_i}{2}\right) + H\left(\frac{1-m_i}{2}\right)\right] + \sum_i h_i m_i + \sum_{i \neq j} J_{ij} m_i m_j$$

$$H(x) \equiv -x \ln(x)$$

$$\frac{\partial F_{\mathrm{nMF}}}{\partial m_i} = \sum_j J_{ij} m_j + h_i - \mathrm{atanh}(m_i) = 0$$

$$m_i = \tanh\left[h_i + \sum_j J_{ij} m_j \right]$$

MFA to the free-energy

- nMF + Onsager reaction term (TAP)

$$F_{\mathrm{TAP}} = \sum_i \left[H\left(\frac{1+m_i}{2}\right) + H\left(\frac{1-m_i}{2}\right)\right] + \\ + \sum_i h_i m_i + \sum_{i \neq j} \left(J_{ij} m_i m_j + \frac{1}{2} J_{ij}^2 (1-m_i^2)(1-m_j^2) \right)$$

$$m_i = \tanh \left[h_i + \sum_j J_{ij} \left(m_j - J_{ij}(1-m_j^2) m_i \right) \right]$$

reaction term

MFA to the free-energy

- Plefka expansion in small J

$$F_{\mathrm{nMF}} = \sum_i \left[H\left(\frac{1+m_i}{2}\right) + H\left(\frac{1-m_i}{2}\right)\right] + \sum_i h_i m_i + \sum_{i \neq j} J_{ij} m_i m_j$$

$$F_{\mathrm{TAP}} = \sum_i \left[H\left(\frac{1+m_i}{2}\right) + H\left(\frac{1-m_i}{2}\right)\right] + \\ + \sum_i h_i m_i + \sum_{i \neq j} \left(J_{ij} m_i m_j + \frac{1}{2} J_{ij}^2 (1-m_i^2)(1-m_j^2) \right)$$

MFA to the free-energy

- Bethe approximation (BA)
  - tries to include any correlations between n.n. spins
  - in principle no small J required
    (but beware to phase transitions)
  - factorization over links

$$P(\boldsymbol{s}) = \prod_i P_i(s_i) \prod_{ij} \frac{P_{ij}(s_i, s_j)}{P_i(s_i) P_j(s_j)}$$

  - exact on trees

MFA to the free-energy

- Bethe approximation (BA)

$$F_{\mathrm{BA}} = \sum_{i\neq j}\left[H\left(\frac{(1+m_i)(1+m_j)+c_{ij}}{4}\right) + H\left(\frac{(1-m_i)(1-m_j)+c_{ij}}{4}\right) + \right.$$

$$\left. + H\left(\frac{(1+m_i)(1-m_j)-c_{ij}}{4}\right) + H\left(\frac{(1-m_i)(1+m_j)-c_{ij}}{4}\right)\right] +$$

$$+ \sum_i (1-d_i)\left[H\left(\frac{1+m_i}{2}\right) + H\left(\frac{1-m_i}{2}\right)\right] + \sum_i h_i m_i + \sum_{i\neq j} J_{ij}(c_{ij} + m_i m_j)$$

$$\partial F_{\mathrm{BA}}/\partial c_{ij} = 0 \qquad\qquad t_{ij} \;=\; \tanh(J_{ij})$$

$$\Downarrow$$

$$c_{ij}(m_i, m_j, t_{ij}) \;=\; \frac{1}{2t_{ij}}\left(1 + t_{ij}^2 - \sqrt{(1-t_{ij}^2)^2 - 4t_{ij}(m_i - t_{ij}m_j)(m_j - t_{ij}m_i)}\right) - m_i m_j$$

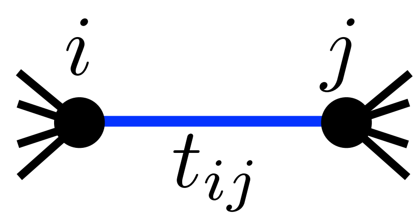
MFA to the free-energy

- Bethe approximation (BA) and cavity method

$$m_i = \frac{m_i^{(j)} + t_{ij}\, m_j^{(i)}}{1 + m_i^{(j)}\, t_{ij}\, m_j^{(i)}}$$

$m_i^{(j)}$: magnetization of i in absence of j

$$m_j = \frac{t_{ij}\, m_i^{(j)} + m_j^{(i)}}{1 + m_i^{(j)}\, t_{ij}\, m_j^{(i)}}$$



$$m_i^{(j)} = f(m_i, m_j, t_{ij}) \qquad m_j^{(i)} = f(m_j, m_i, t_{ij})$$

$$f(m_1, m_2, t) = \frac{1 - t^2 - \sqrt{(1-t^2)^2 - 4t(m_1 - m_2 t)(m_2 - m_1 t)}}{2t(m_2 - m_1 t)}$$

MFA to the free-energy

- Bethe approximation (BA) and cavity method

$$f(m_1, m_2, t) = \frac{1 - t^2 - \sqrt{(1-t^2)^2 - 4t(m_1 - m_2 t)(m_2 - m_1 t)}}{2t(m_2 - m_1 t)}$$

$$m_i = \tanh\left[h_i + \sum_j \operatorname{atanh}\Big(t_{ij} f(m_j, m_i, t_{ij})\Big)\right]$$

Small J expansion gives nMF, TAP, ...

$$h_i + \sum_j \operatorname{atanh}\Big(t_{ij} f(m_j, m_i, t_{ij})\Big) \simeq h_i + \sum_j \Big(J_{ij} m_j - J_{ij}^2 (1 - m_j^2) m_i + \dots\Big)$$

Computing correlations by linear response

- Correlations are trivial in MFA
  $C_{ij} = 0$ in nMF, TAP and BA (between distant spins)

- Non trivial correlations can be obtained by using the linear response (Kappen Rodriguez, 1998)

$$\chi_{ij} = \frac{\partial m_i}{\partial h_j} \qquad (\chi^{-1})_{ij} = \frac{\partial h_i}{\partial m_j}$$

$$(\chi^{-1}_{\mathrm{nMF}})_{ij} = \frac{\delta_{ij}}{1 - m_i^2} - J_{ij} \ ,$$

$$(\chi^{-1}_{\mathrm{TAP}})_{ij} = \left[\frac{1}{1 - m_i^2} + \sum_k J_{ik}^2 (1 - m_k^2)\right] \delta_{ij} - \left(J_{ij} + 2 J_{ij}^2 m_i m_j\right)$$

Computing correlations by linear response in BA

- Analytic expression for the linear responses in BA

$$(\chi_{\mathrm{BA}}^{-1})_{ij} = \left[\frac{1}{1-m_i^2} - \sum_k \frac{t_{ik} f_2(m_k, m_i, t_{ik})}{1 - t_{ik}^2 f(m_k, m_i, t_{ik})^2} \right] \delta_{ij} - \frac{t_{ij} f_1(m_j, m_i, t_{ij})}{1 - t_{ij}^2 f(m_j, m_i, t_{ij})^2}$$

- Coincide with the fixed point of Susceptibility Propagation

- No need to run any algorithm!

Solving the inverse problem by MFA

- Match measured magnetizations and correlations with MF approximated magnetizations and linear responses

$$m_i^{\mathrm{MFA}}(\boldsymbol{J},\boldsymbol{h}) = m_i(\mathrm{DATA})$$
$$\chi_{ij}^{\mathrm{MFA}}(\boldsymbol{J},\boldsymbol{h}) = C_{ij}(\mathrm{DATA})$$

- Under the Bethe approx. one could use either

c_{ij}^{BA} or χ_{ij}^{BA}

for n.n. correlations. Which one is better?

Zero field case is simpler

- If all field are zero, then magnetizations are null by symmetry, and expressions simplify to

$$\text{naive MF} \qquad (\chi'^{-1}_{\text{nMF}})_{ij} = \delta_{ij} - J_{ij},$$

$$\text{TAP} \qquad (\chi'^{-1}_{\text{TAP}})_{ij} = \left[1 + \sum_k J_{ik}^2\right] \delta_{ij} - J_{ij},$$

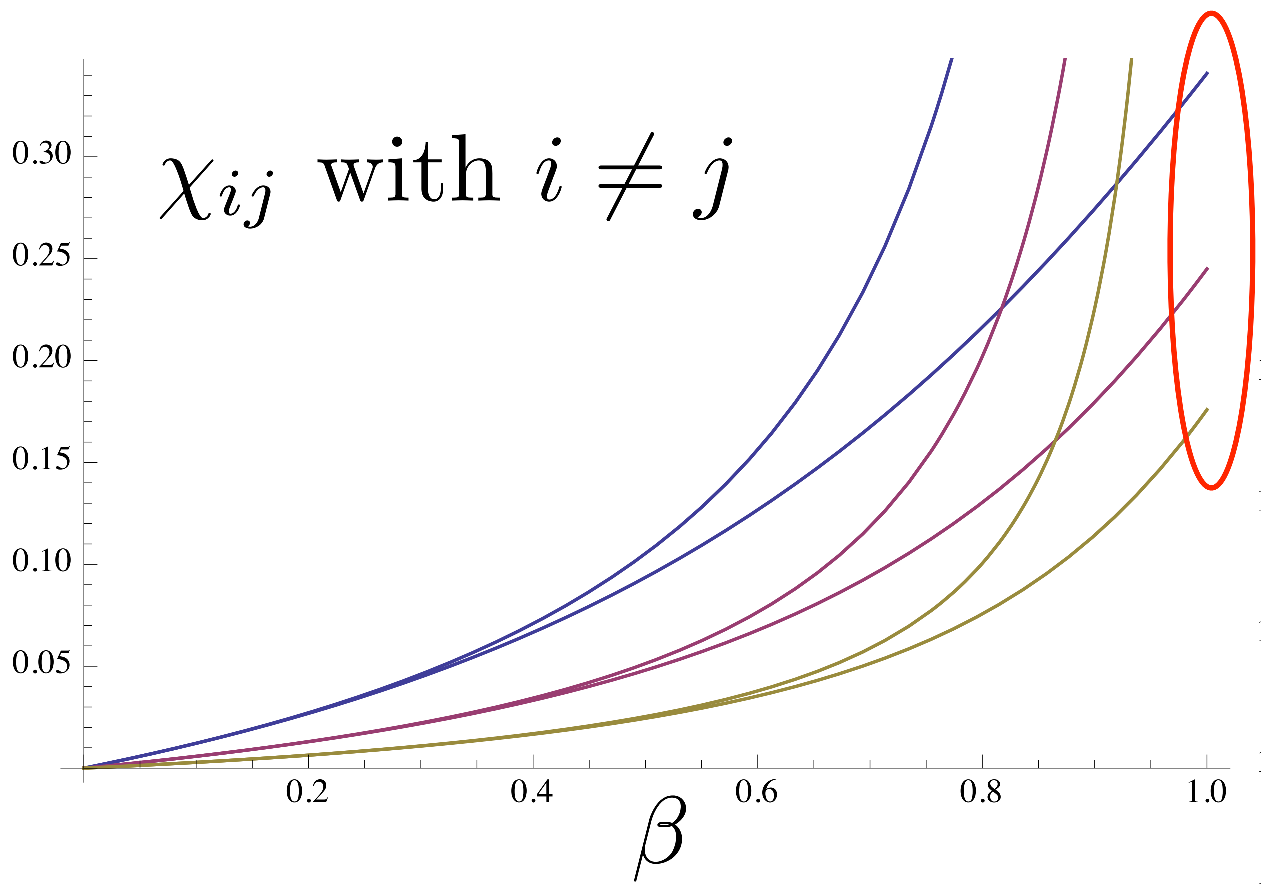
$$\text{Bethe} \qquad (\chi^{-1}_{\text{BA}})_{ij} = \left[1 + \sum_k \frac{t_{ik}^2}{1 - t_{ik}^2}\right] \delta_{ij} - \frac{t_{ij}}{1 - t_{ij}^2},$$

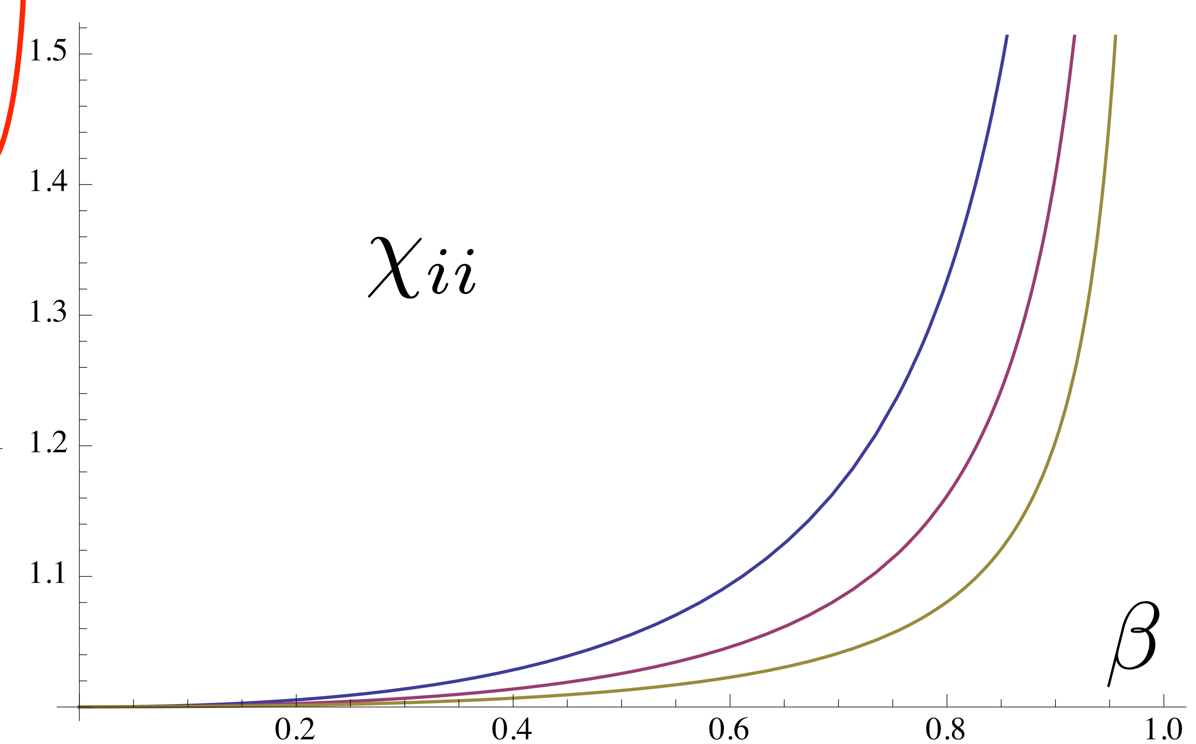
Exactly solvable case for the inverse Ising problem ?

- Curie-Weiss model, fully connected $J_{ij} = \beta/(N-1)$
  nMF approximation

N=10,20,40

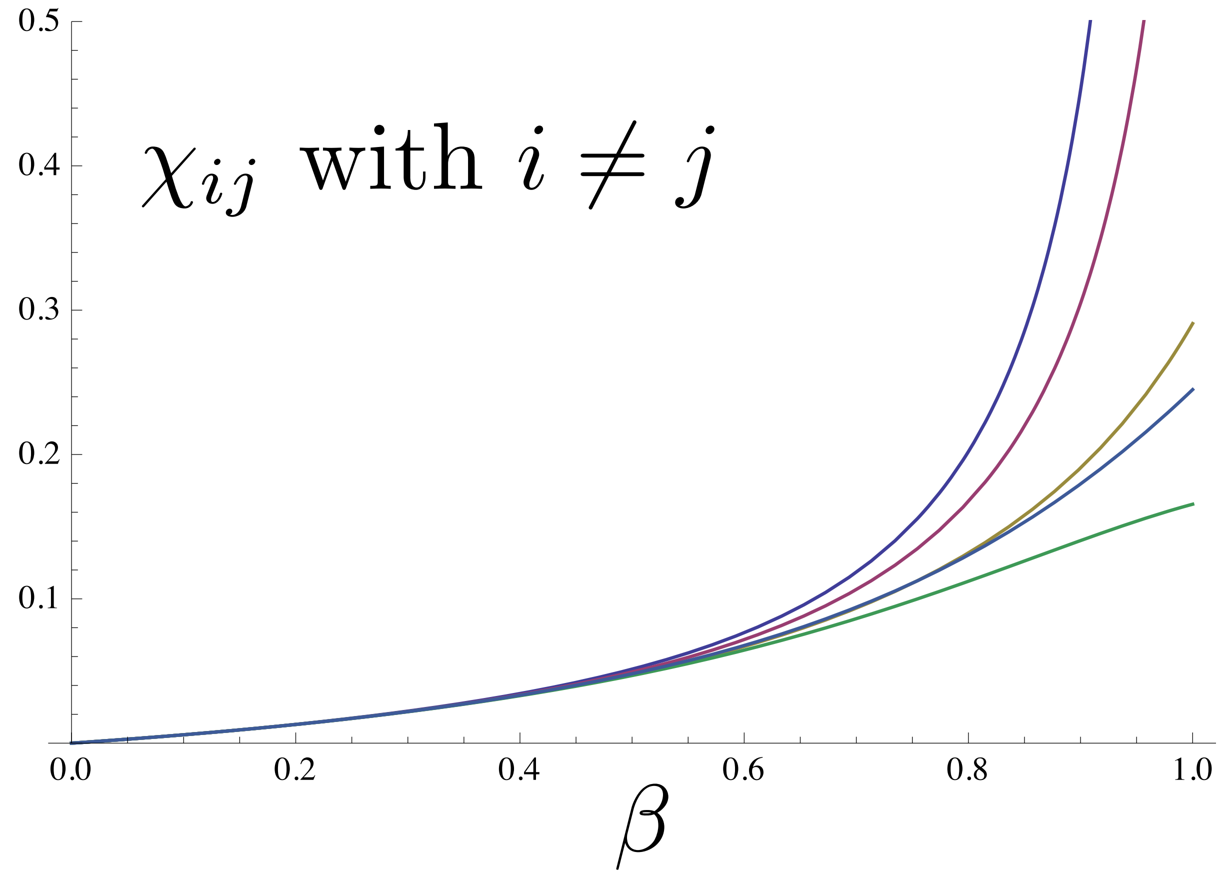
exact correlations

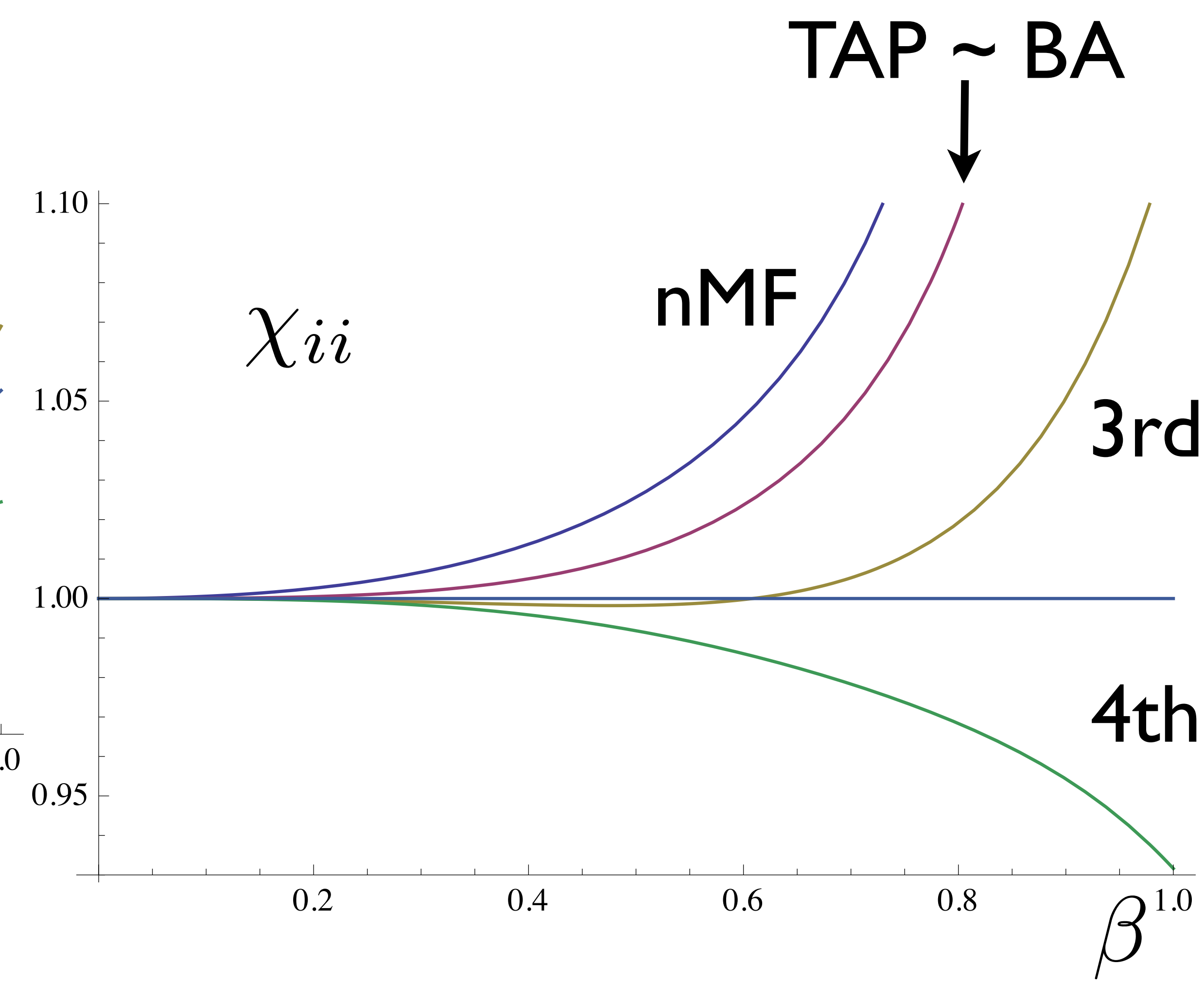




Exactly solvable case for the inverse Ising problem ?

- Curie-Weiss model, fully connected $J_{ij} = \beta/(N-1)$
  more MFA (N=20)



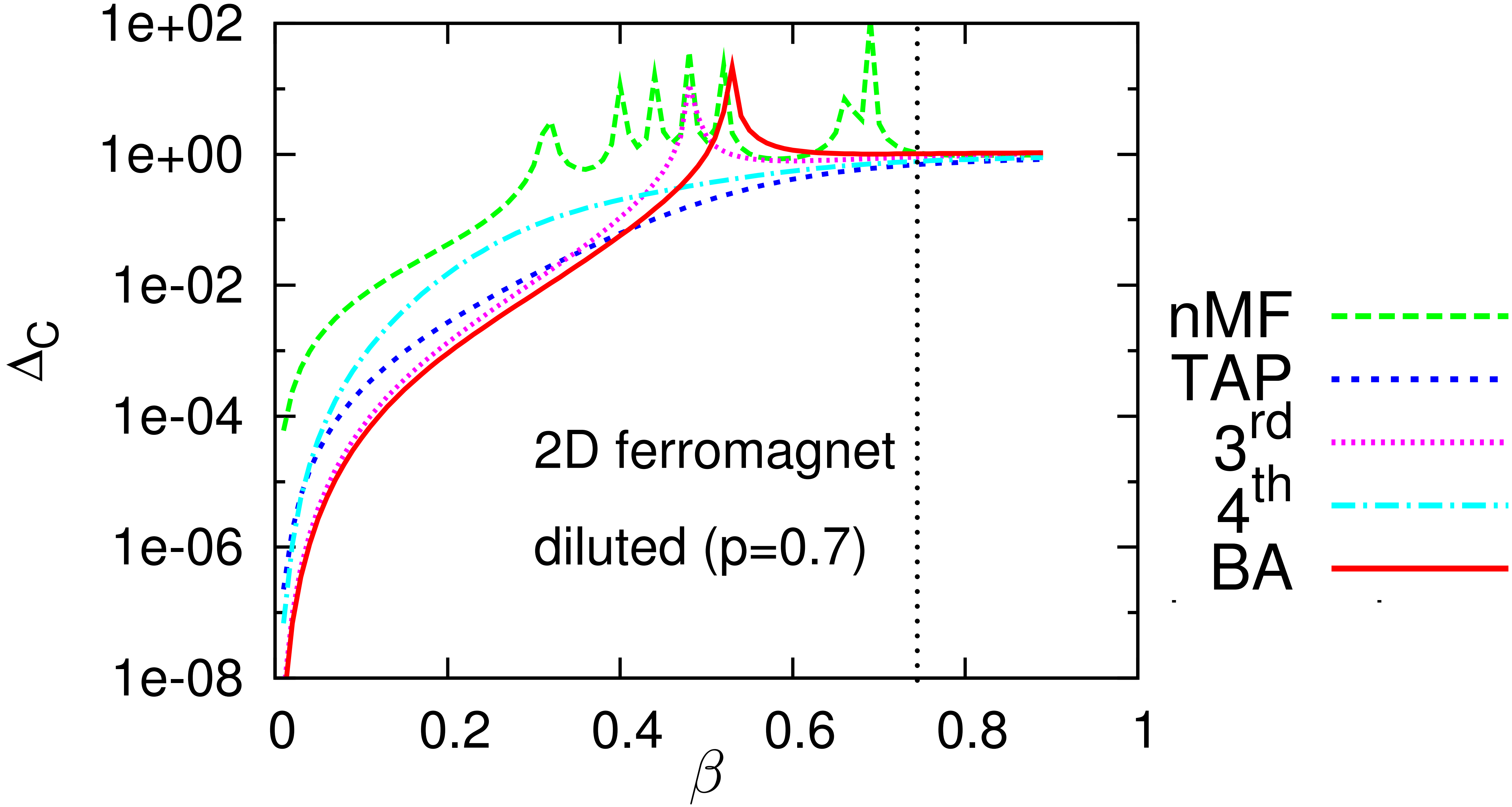


Exactly solvable case for the inverse Ising problem ?

- Bethe approximation on trees is ok
- Bethe approximation on random graph is ok only far from the critical point (as nMF for the Curie-Weiss model)
- How much the paramagnetic properties of a model on a finite size random graph are different from those of the same model defined on a tree?
    - see recent works on finite size corrections for models defined on random graphs (Lucibello and Morone)

Numerical results on estimating correlations

$$\Delta_C \equiv \sqrt{\frac{1}{N^2}\sum_{i,j}(\chi_{ij} - C^{\cdot}_{ij})^2}$$



Matching data and MF predictions

$$\begin{pmatrix} 1 & & C_{ij} \\ & \ddots & \\ C_{ij} & & 1 \end{pmatrix} \overset{?}{=} \begin{pmatrix} \chi_{11} & & \chi_{ij} \\ & \ddots & \\ \chi_{ij} & & \chi_{NN} \end{pmatrix}$$

- Usually only off-diagonal elements are used

$$J_{ij} = -(C^{-1})_{ij}$$

and diagonal elements are ignored...

MFA for the inverse Ising problem

$$(\chi^{-1}_{\text{nMF}})_{ij} = \frac{\delta_{ij}}{1-m_i^2} - J_{ij}\ , \Longrightarrow \boxed{J^{\text{nMF}}_{ij} = -(C^{-1})_{ij}}$$

$$(\chi^{-1}_{\text{TAP}})_{ij} = \left[\frac{1}{1-m_i^2} + \sum_k J_{ik}^2(1-m_k^2)\right]\delta_{ij} - \left(J_{ij} + 2J_{ij}^2 m_i m_j\right)$$

$$\Downarrow$$

$$\boxed{J^{\text{TAP}}_{ij} = \frac{\sqrt{1-8m_i m_j (C^{-1})_{ij}} - 1}{4 m_i m_j}}$$

equal for m=0

$$J^{\text{BA}}_{ij} = -\text{atanh}\left[\frac{1}{2(C^{-1})_{ij}}\sqrt{1+4(1-m_i^2)(1-m_j^2)(C^{-1})^2_{ij}} - m_i m_j - \frac{1}{2(C^{-1})_{ij}}\sqrt{\left(\sqrt{1+4(1-m_i^2)(1-m_j^2)(C^{-1})^2_{ij}} - 2m_i m_j (C^{-1})_{ij}\right)^2 - 4(C^{-1})^2_{ij}}\right]$$

More MFA for the inverse Ising problem

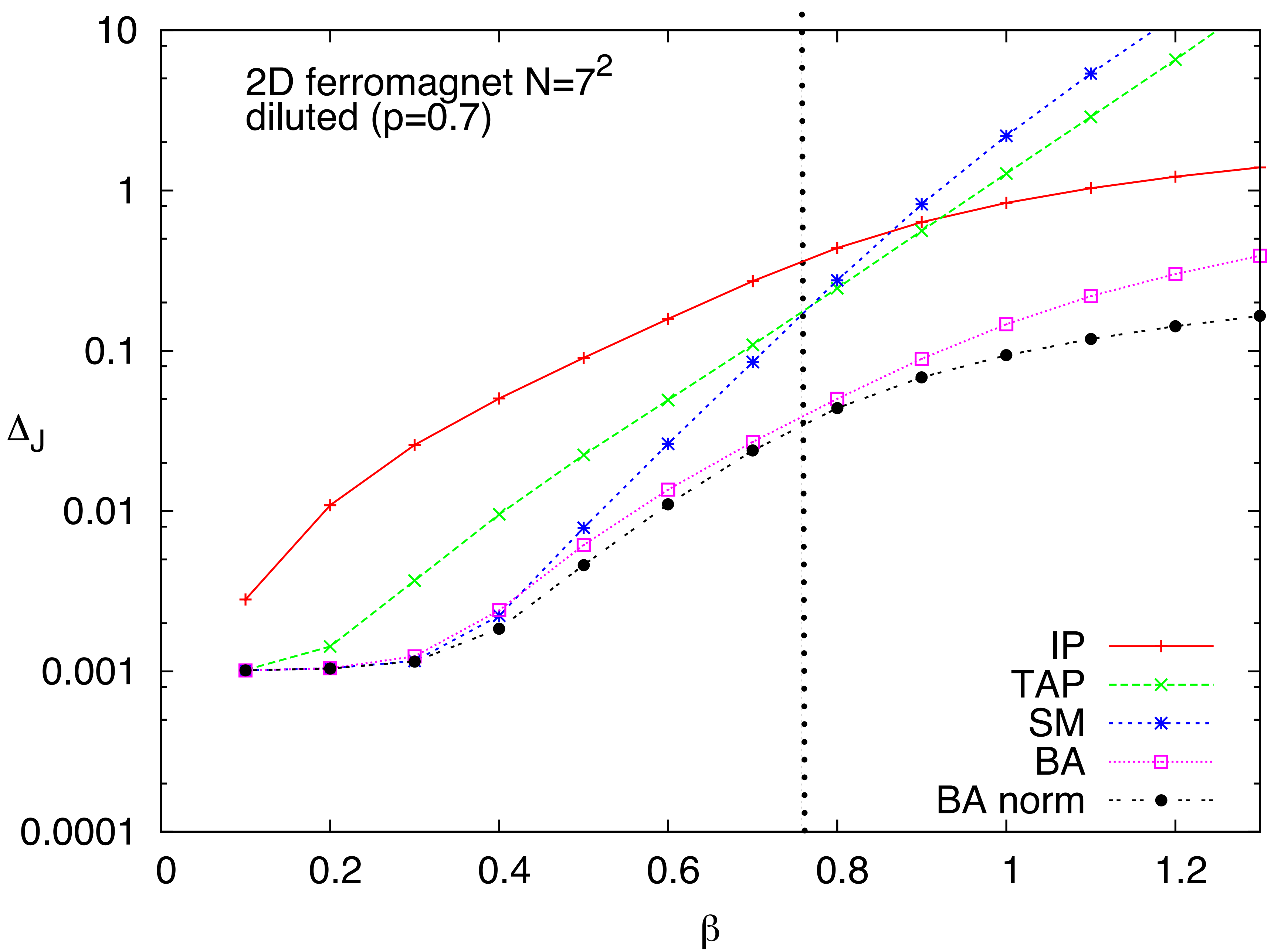
- Independent pair (IP) approximation

$$J_{ij}^{\mathrm{IP}} = \frac{1}{4}\ln\left(\frac{\Big((1+m_i)(1+m_j)+C_{ij}\Big)\Big((1-m_i)(1-m_j)+C_{ij}\Big)}{\Big((1+m_i)(1-m_j)-C_{ij}\Big)\Big((1-m_i)(1+m_j)-C_{ij}\Big)}\right)$$

- Sessak-Monasson (SM) small correlation expansion

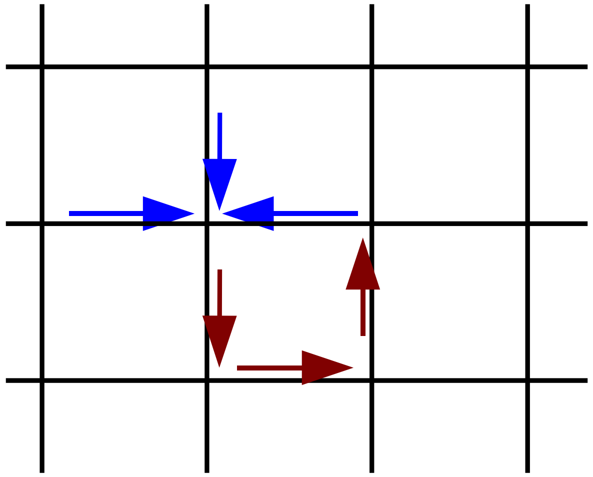
$$J_{ij}^{\mathrm{SM}} = -(C^{-1})_{ij} + J_{ij}^{\mathrm{IP}} - \frac{C_{ij}}{(1-m_i^2)(1-m_j^2)-(C_{ij})^2}$$

Numerical results for the inverse Ising problem



Improving correlations by a normalization trick

- In ferromagnetic models with loops, linear response correlations in BA are too strong because of loops, which are "unexpected" in SuscProp



- Leading to $\chi_{ii} > 1$ which is unphysical
- Trick: enforce $\chi_{ii} = 1$ by a normalization

$$\widehat{\chi}_{ij} = \frac{\chi_{ij}}{\sqrt{\chi_{ii}\chi_{jj}}}$$

Make MFA & LR consistent

"Consistency is more important than truth" (S. Ting)

Add Lagrange multipliers to your referred MF free-energy

$$F_{\mathrm{MFA}}(\{m_i\}, \{C_{ij}\}, \ldots)$$

to enforce consistency with linear response estimates

$$\chi_{ii} = 1 - m_i^2 \quad \chi_{ij} = C_{ij}$$

free energy minimum curvature

free energy minimum location

General framework (MFA + LR)

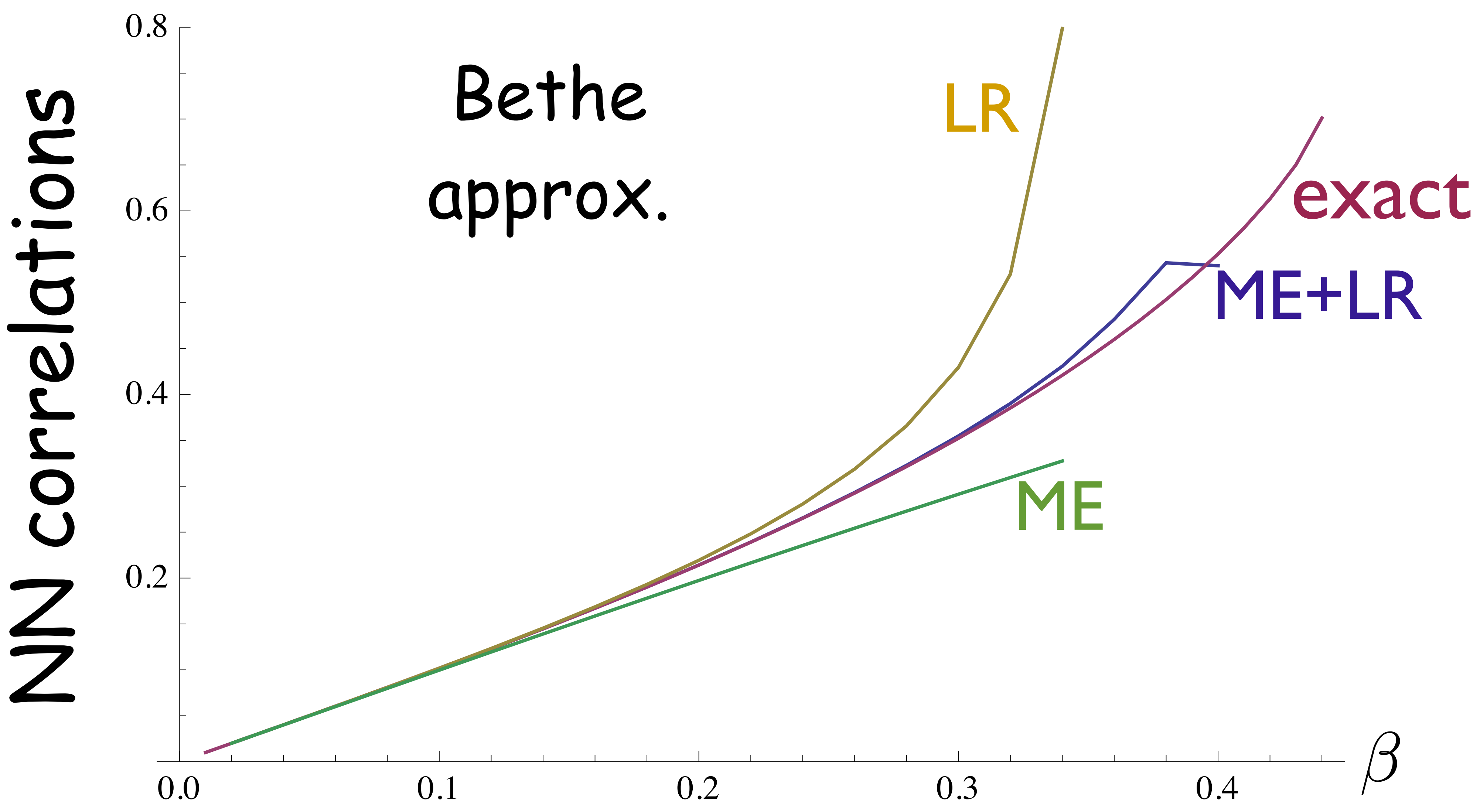
$$F_\lambda = F_{\mathrm{MFA}}(\{m_i\}, \{C_{ij}\}, \ldots) + \sum_i \lambda_i m_i^2 + \sum_{i<j} \lambda_{ij} C_{ij}$$

Your preferred MFA

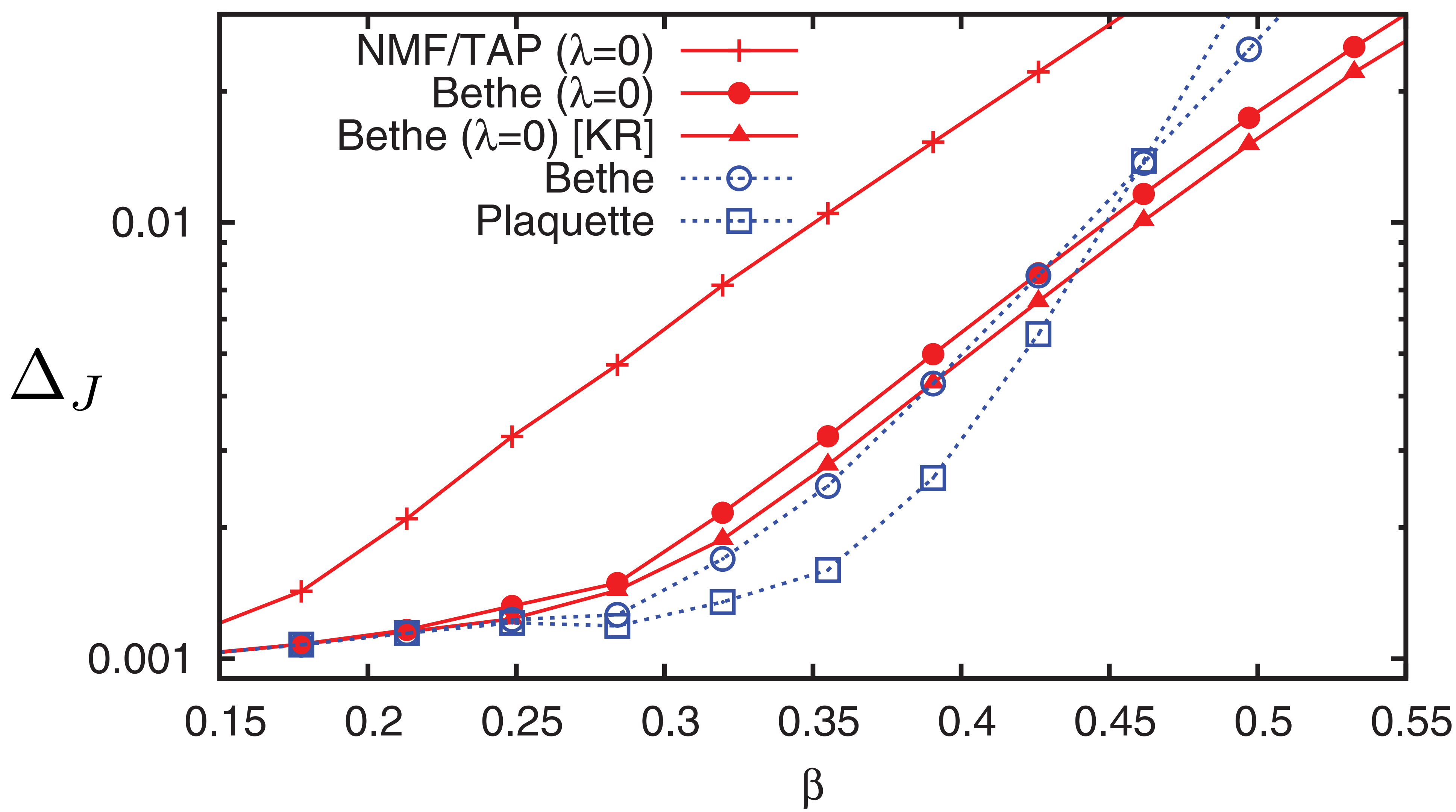
can be set to zero to recover known approx. or used to satisfy

$\chi_{ii} = 1 - m_i^2 \quad \chi_{ij} = C_{ij}$

Nearest-neighbor correlation (2D square lattice)

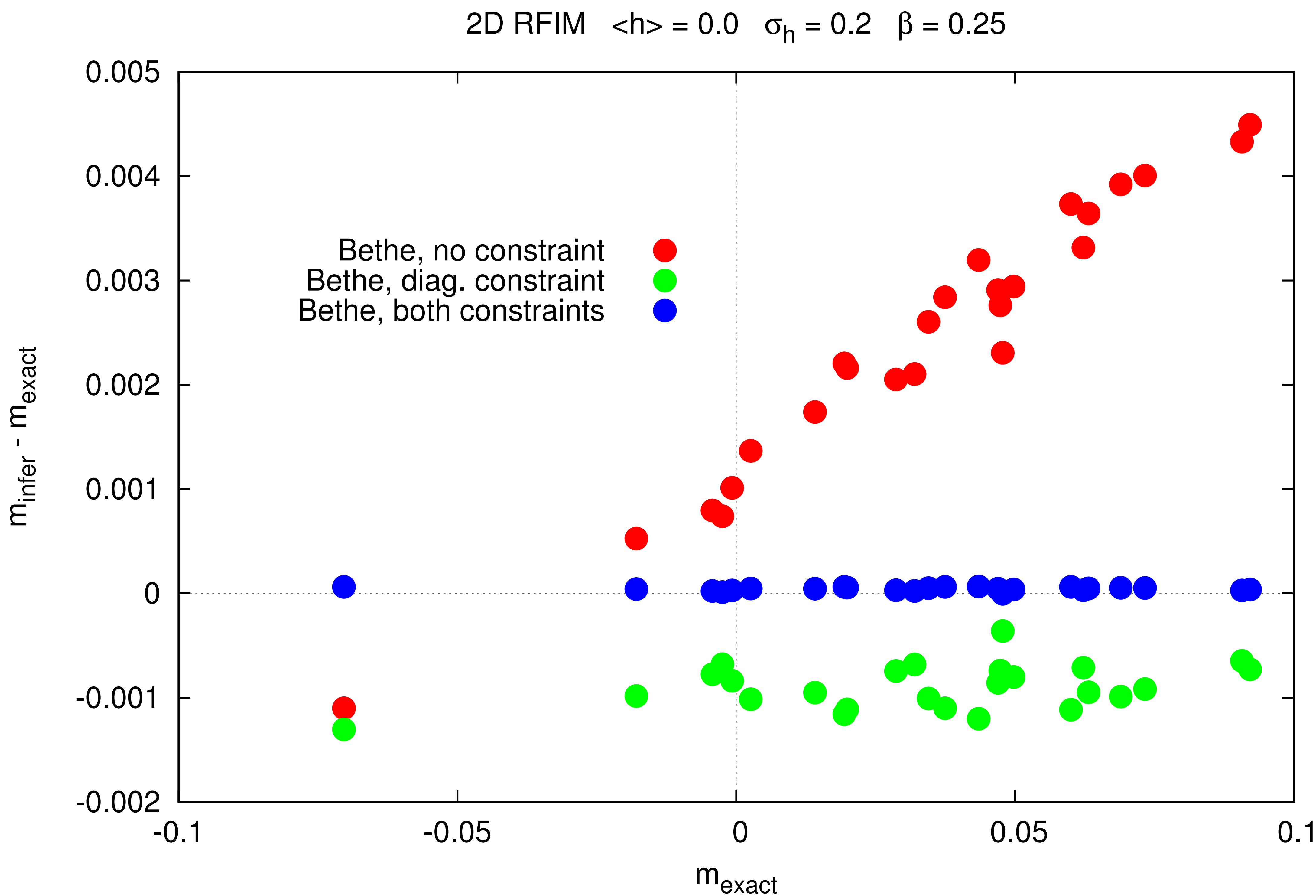


Off-diagonal constraint only

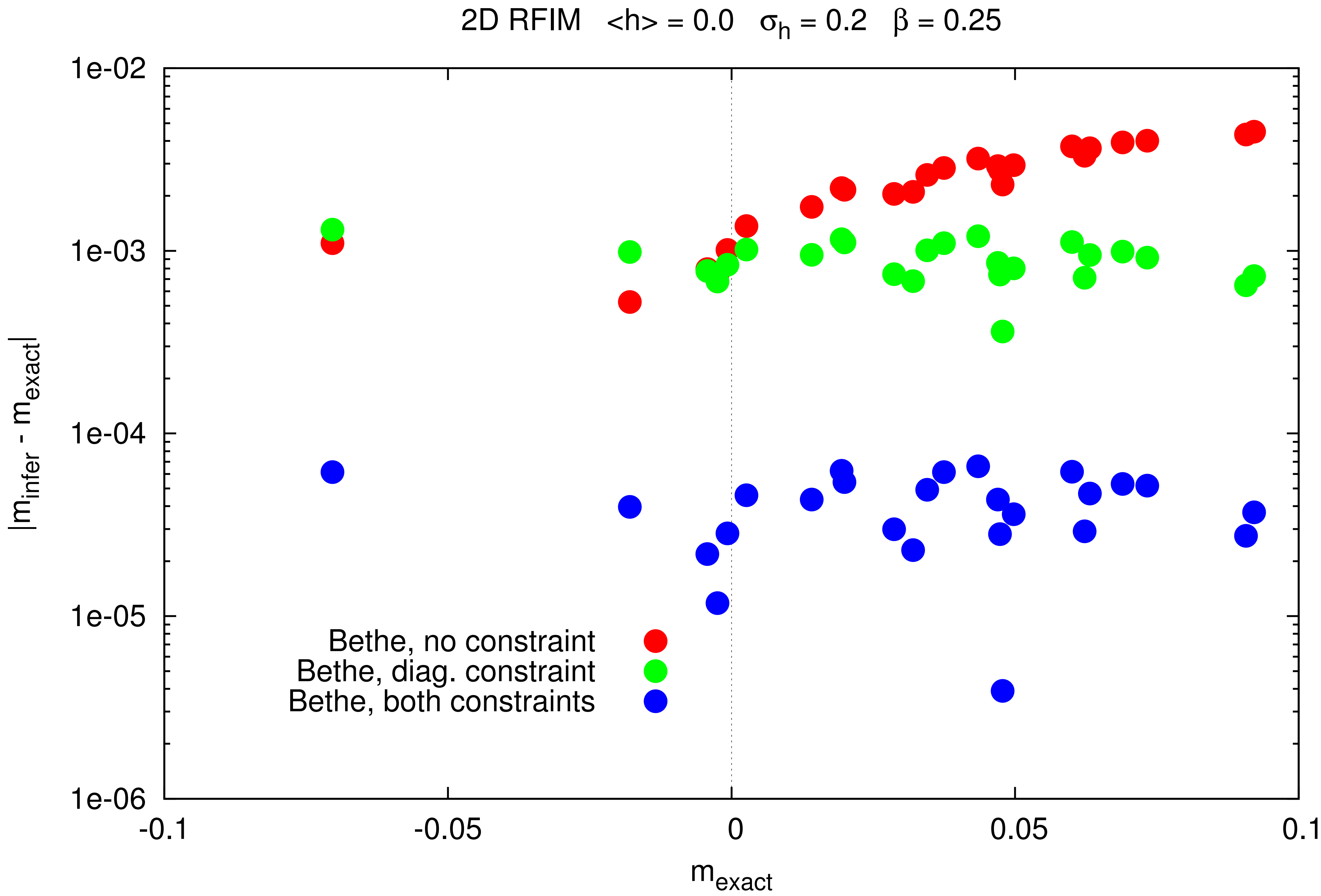


Bethe + off-diagonal constraints = SM

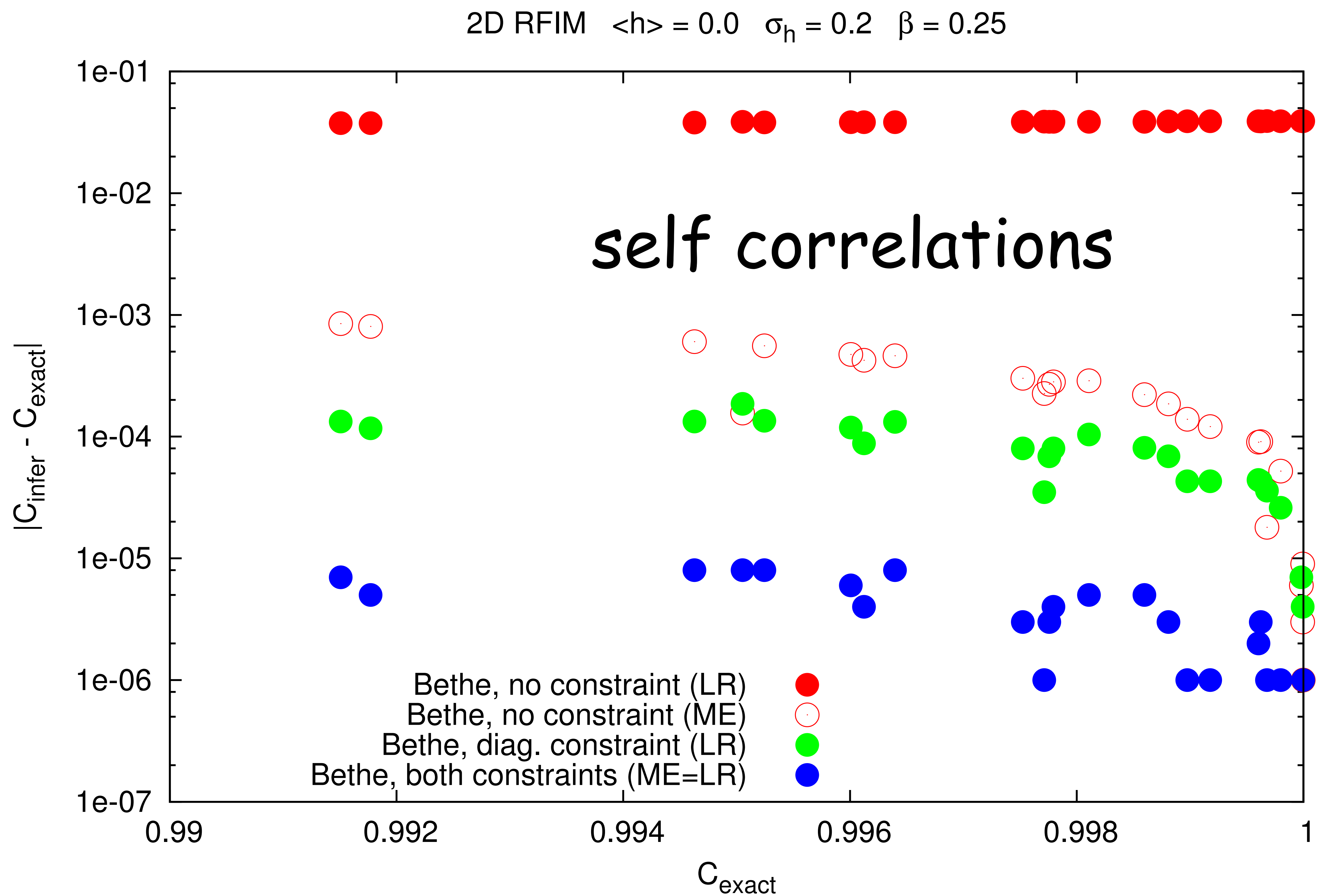
Random field Ising model
2D square lattice



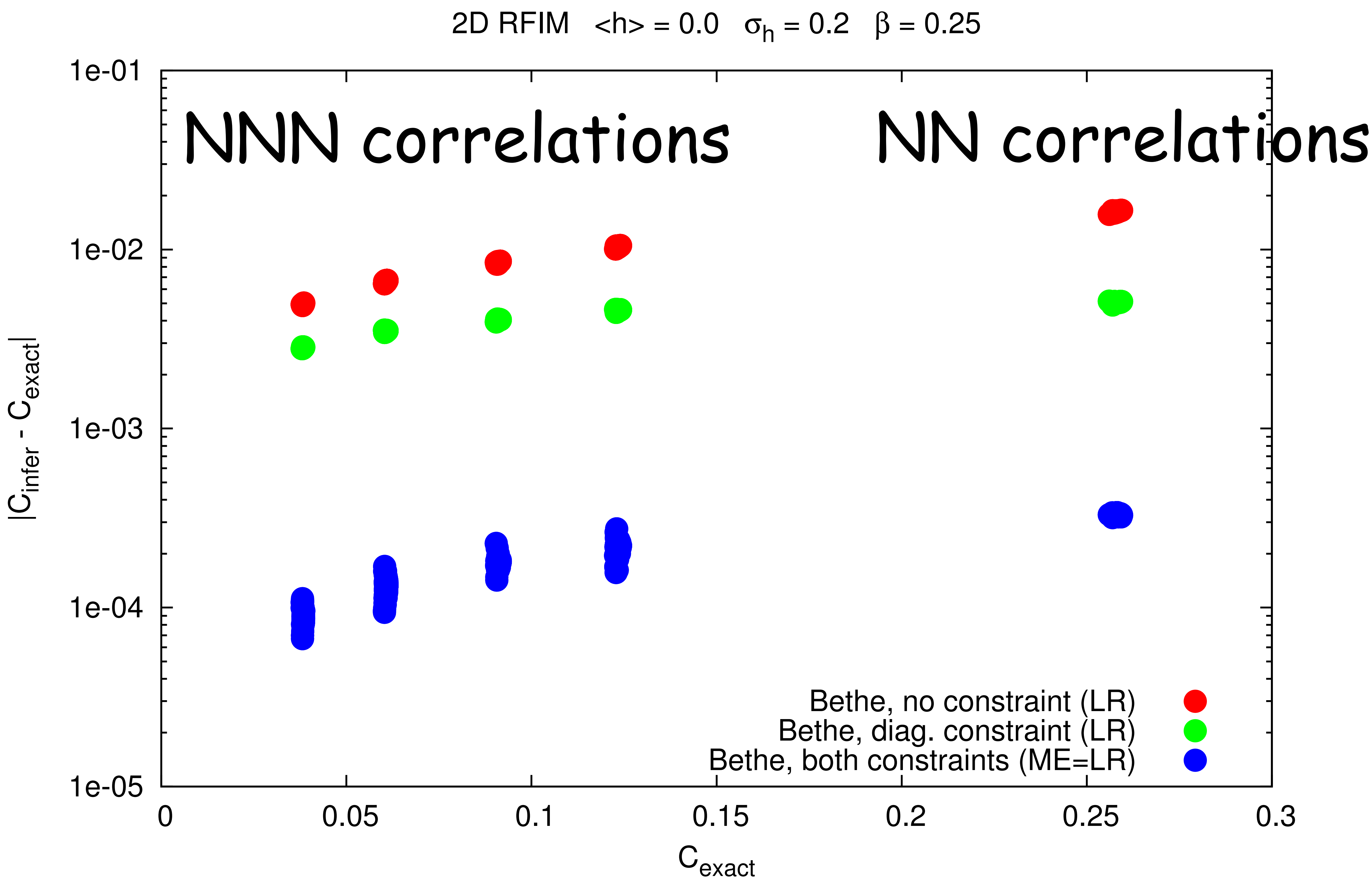
Random field Ising model
2D square lattice



Random field Ising model
2D square lattice



Random field Ising model
2D square lattice



Input data: Configurations

- More information than knowing only

$$m_i = \langle s_i \rangle \qquad C_{ij} = \langle s_i s_j \rangle - m_i m_j$$

- In principle one can access to all higher order correlations (but these are much more noisy)
- Many different inference algorithms. Among these:
  - Adaptive cluster expansion
  - cluster configurations & apply MFA within any state

Pseudo-likelihood method (PLM)

- For each variable define a conditional probability

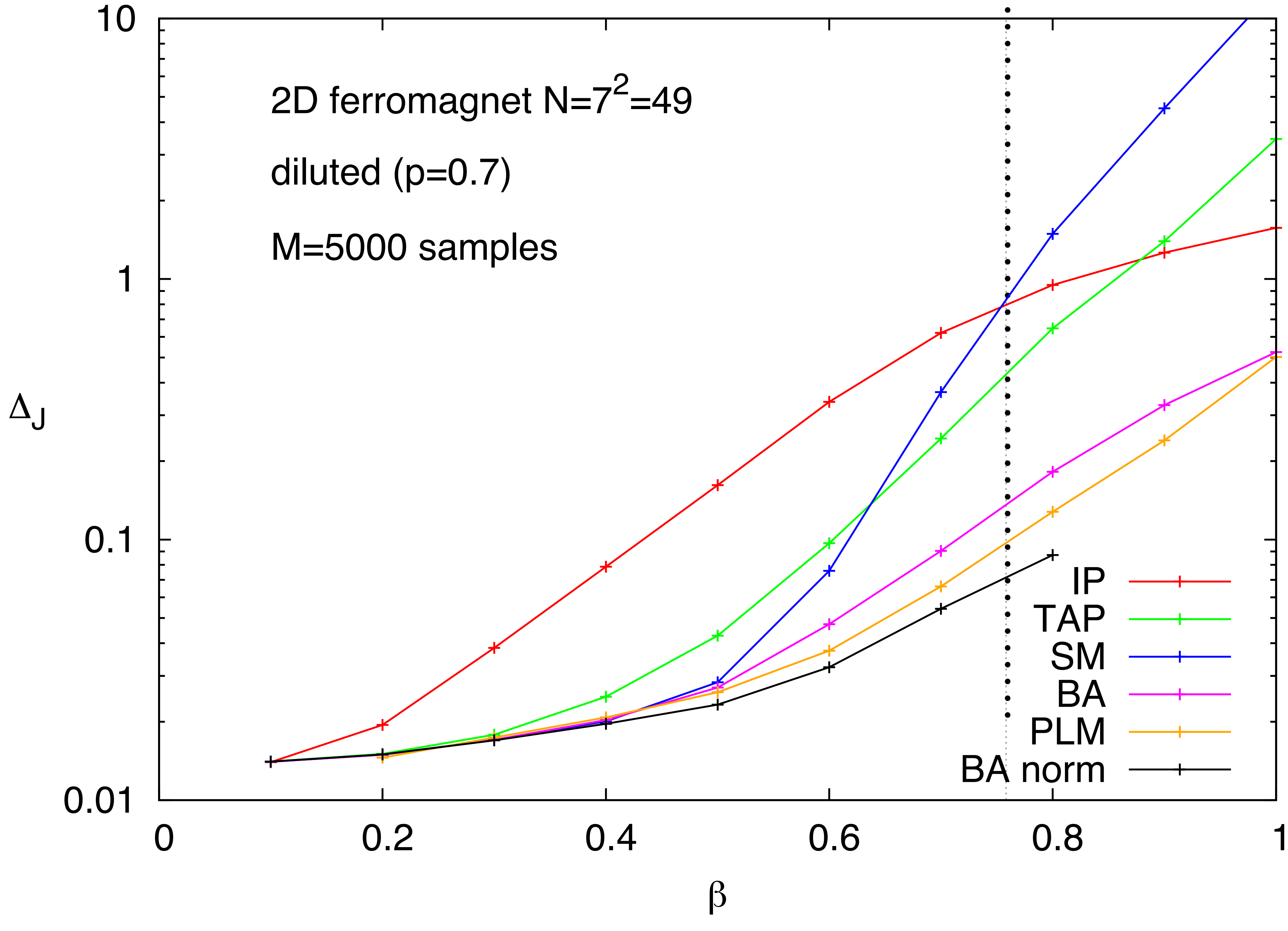
$$P_i(s_i|\boldsymbol{s}_{\setminus i}) = \frac{\exp[s_i(h_i + \sum_j J_{ij}s_j)]}{2\cosh(h_i + \sum_j J_{ij}s_j)}$$

- Maximize the local log-likelihood $L_i = \langle \log P_i(s_i|\boldsymbol{s}_{\setminus i})\rangle =$
$$h_i m_i + \sum_j J_{ij}(C_{ij} + m_i m_j) - \langle \log 2\cosh(h_i + \sum_j J_{ij}s_j)\rangle$$
to estimate h_i and J_{ij}

- Note that for each coupling J_{ij} PLM returns 2 estimates

- Better maximizing $PL(\boldsymbol{h}, \boldsymbol{J}) = \sum_i L_i$

PLM vs. MFA



2D ferromagnet N=7^2=49
diluted (p=0.7)
M=5000 samples
IP
TAP
SM
BA
PLM
BA norm
Δ_J
β
10
1
0.1
0.01
0
0.2
0.4
0.6
0.8
1

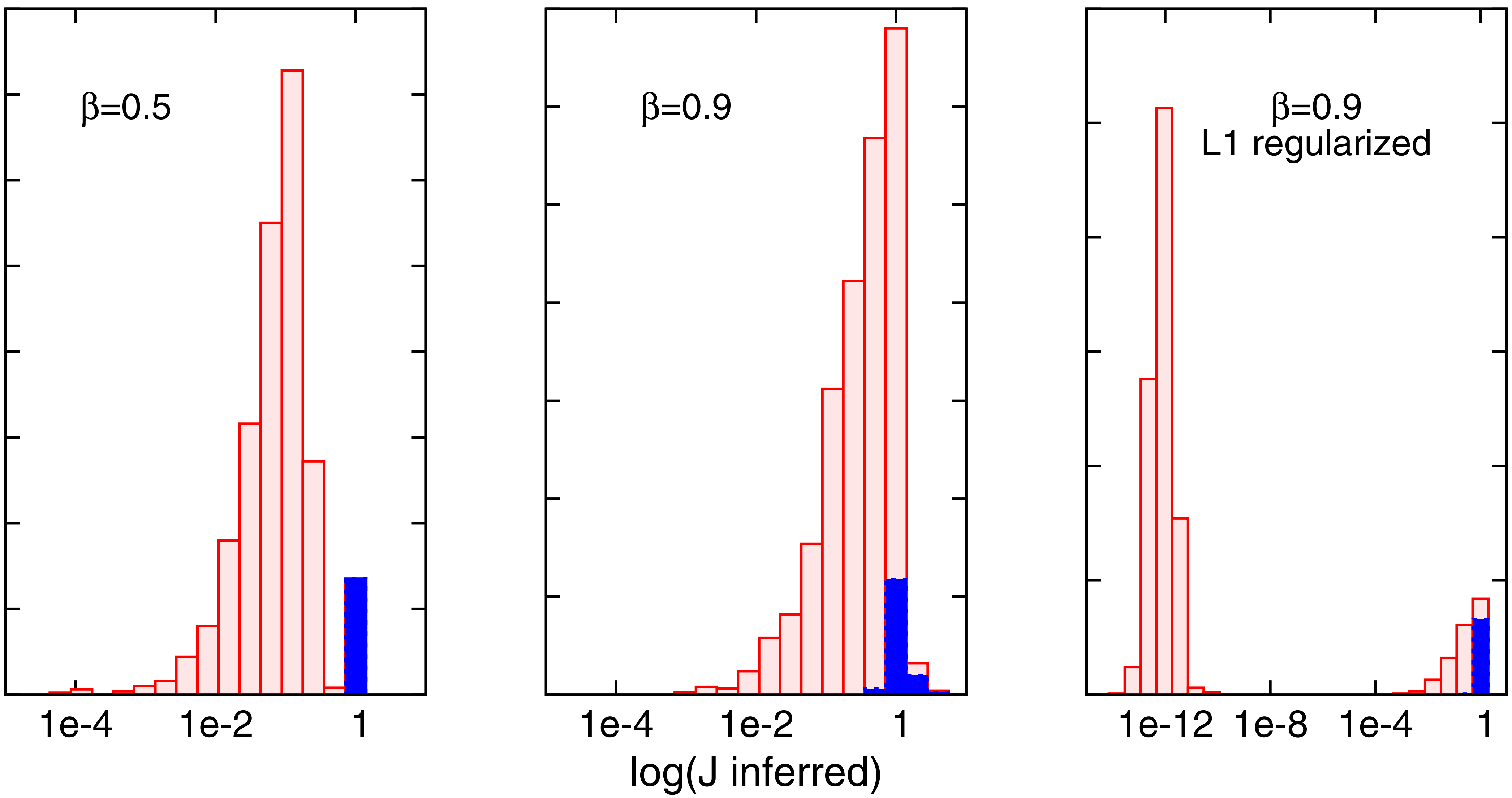
Inferring topology in sparse models

- For simplicity let's assume
  - $|J_{ij}| \in \{0, \beta\}$
  - non-zero couplings are sparse
- Maximize L1-regularized pseudo-likelihood

$$PL_\lambda(\boldsymbol{h}, \boldsymbol{J}) = \sum_i L_i - \lambda \sum_{ij} |J_{ij}|$$

- L1-regularization gives a bias to the estimates!

Couplings inferred by PLM

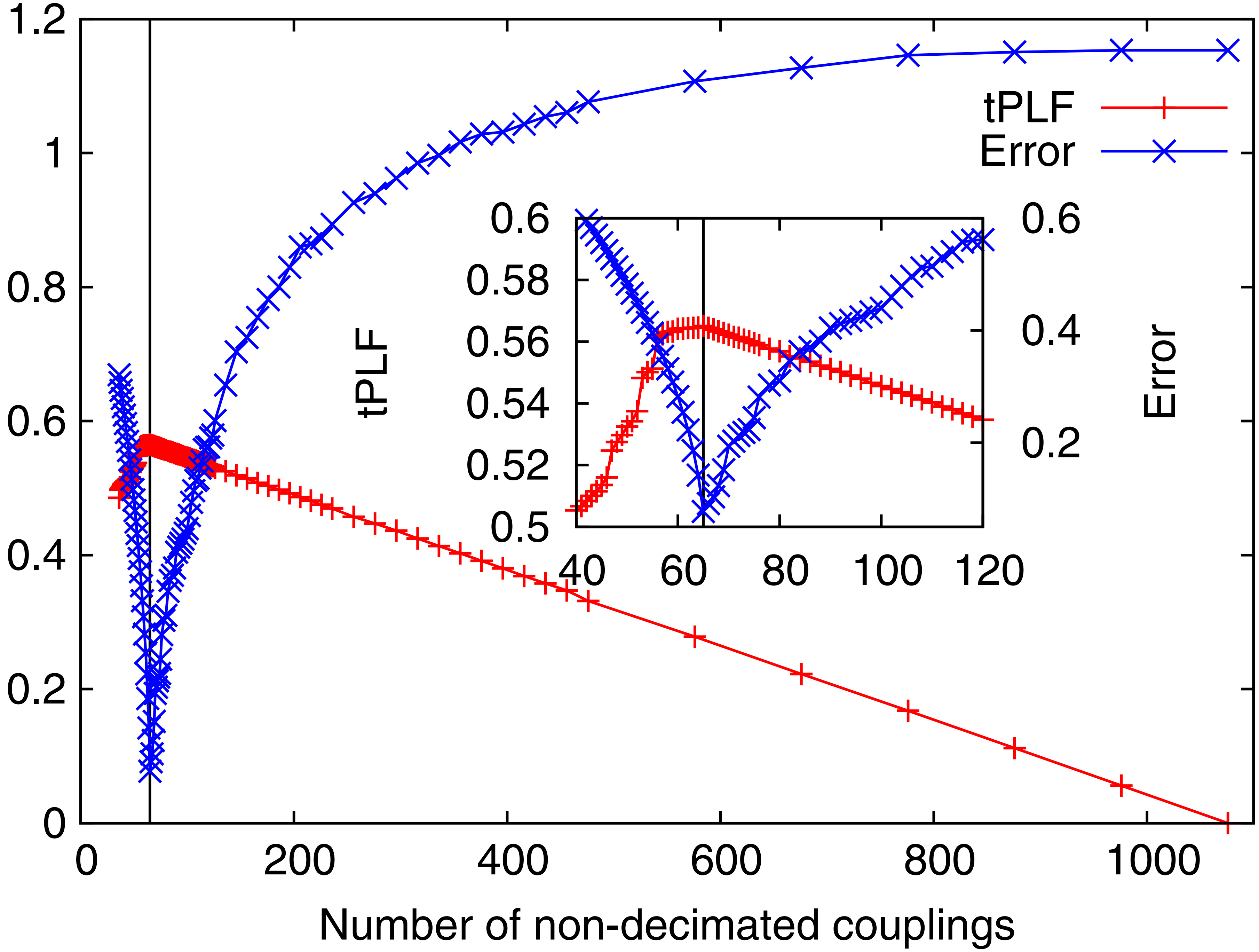


2D Ising model (30% dilution) M=4500

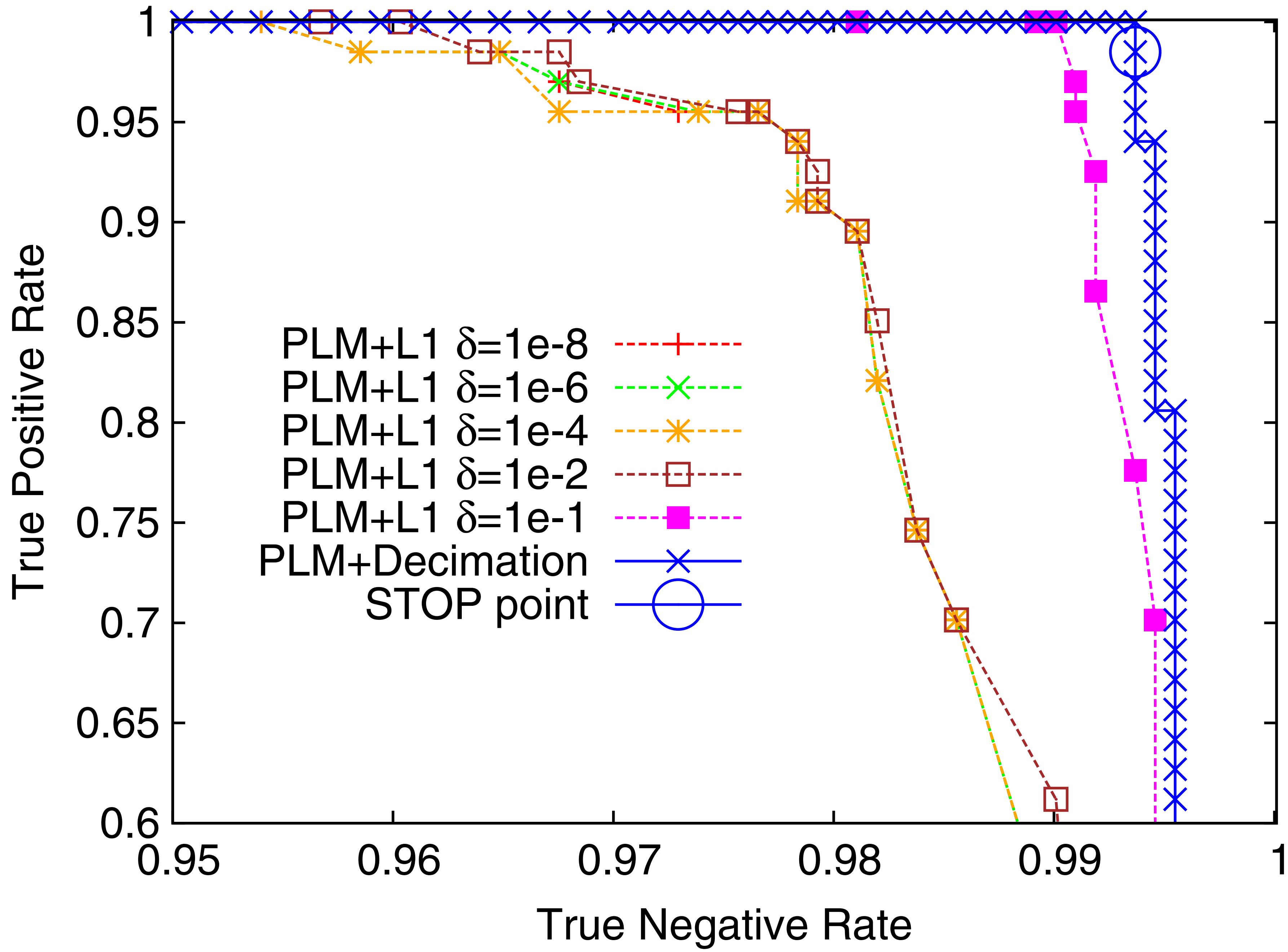
Decimation procedure

- No L1-regularizer -> no bias
- Maximize $PL(\boldsymbol{h}, \boldsymbol{J})$
- Set to zero a constant fraction of couplings (those inferred to be the smallest)
- Maximize again $PL(\boldsymbol{h}, \boldsymbol{J})$ only on couplings still not set to zero (this is impossible within a MFA)
- Iterate until maximum of $PL(\boldsymbol{h}, \boldsymbol{J})$ starts decreasing "sensibly"

PLM + decimation



PLM + decimation



Some conclusions

- Mean field approximations
  - Inverse problem harder than direct problem
  - Requires (at least) improvement in the direct problem
  - Fundamental problem of going beyond Bethe and trees...
- Pseudo-likelihood method
  - Better performances in general
  - Specially well suited for inferring topology in sparse models via L1-regularization, thresholding or decimation