Some recent results on the inverse Ising problem

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Outline of the talk

- Bethe approx. for inverse Ising problem
- Comparison among several mean-field approximations (IP, nMF, TAP, SM, Bethe...)
- Correlations normalization trick
- Major limitation in using TAP and Bethe in frustrated models with a field
- New method: pseudo-likelihood + decimation (Aurelien DECELLE)

Inverse Ising problem

- M configurations of N Ising variables ($s_i = \pm 1$) extracted from

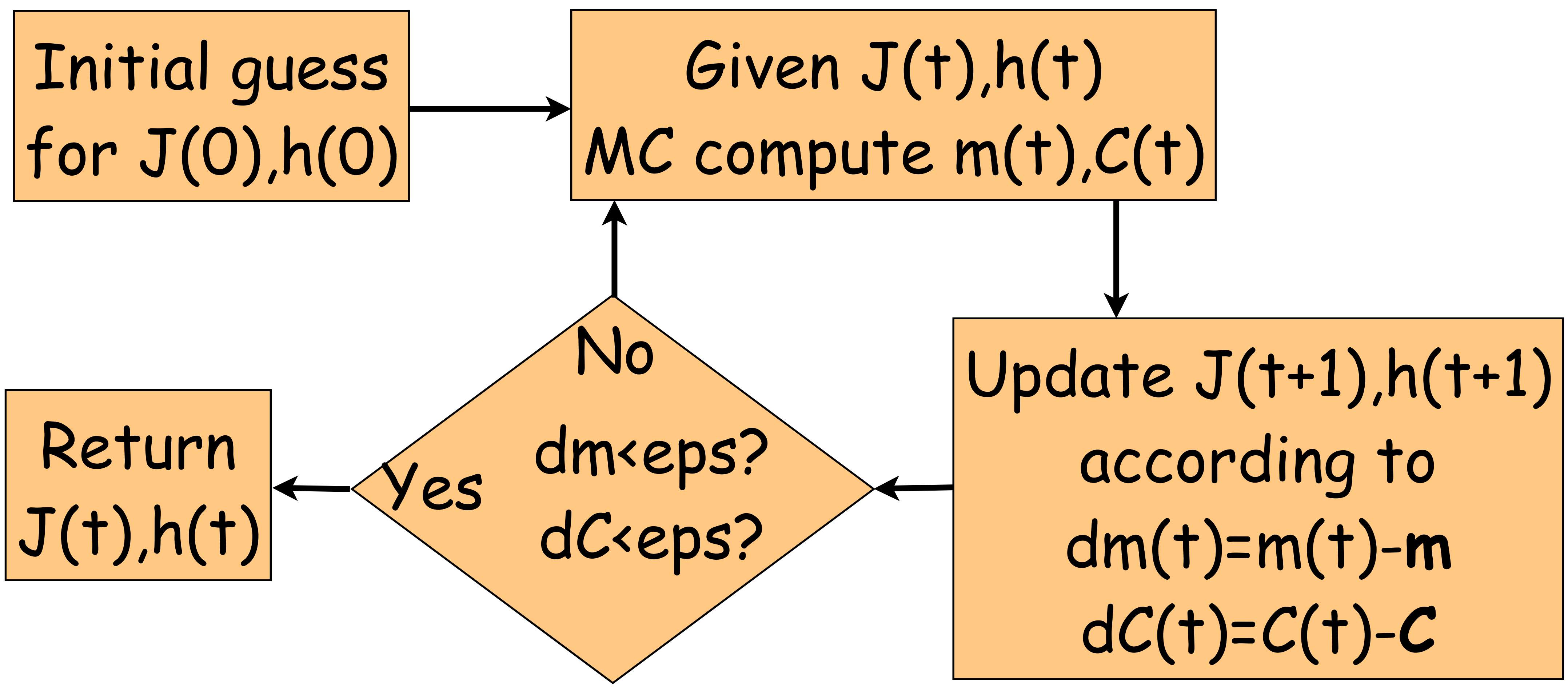
$$P(s_1, \ldots, s_N) = \frac{1}{Z(\boldsymbol{J}, \boldsymbol{h})} \exp \left[\sum_{i \neq j} J_{ij} s_i s_j + \sum_i h_i s_i \right]$$

[alternatively only magnetizations $m_i = \langle s_i \rangle$ and correlations $C_{ij} = \langle s_i s_j \rangle - m_i m_j$ are given]

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

Solving inverse Ising pb.

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



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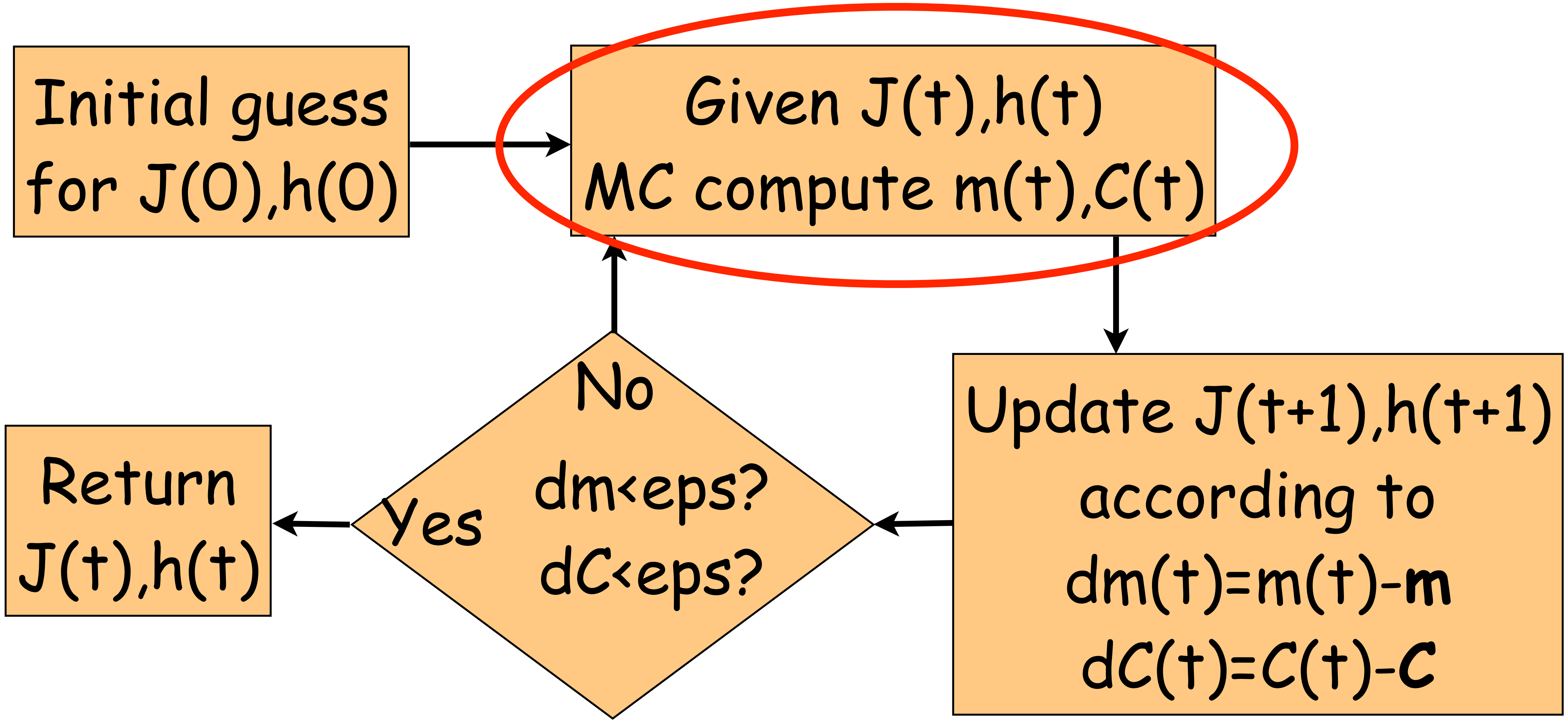

Solving inverse Ising pb.

Mean field approximations (MFA)

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

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

Solving inverse Ising pb.

Mean field approximations (MFA)

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

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

Solving inverse Ising pb.

Mean field approximations (MFA)

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

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

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

Solving inverse Ising pb.

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$$m_i = \partial F_{\mathrm{MFA}}(\boldsymbol{J}, \boldsymbol{h}) / \partial h_i$$

Mean-field approximations (MFA) to the free-energy

- naive mean-field (nMF)

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

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

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

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

MFA to the free-energy

- nMF + Onsager reaction term (TAP)

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

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

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$$

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\boxed{m_i \;=\; \tanh\left[h_i + \sum_j J_{ij} \Big(m_j \underbrace{- J_{ij}(1-m_j^2) m_i}_{\text{reaction term}} \Big) \right]}
$$

MFA to the free-energy

- Plefka expansion in small J

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

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

MFA to the free-energy

- Bethe approximation (BA)

$$F_{\mathrm{BA}} = \sum_{i \neq j} \left[H\left(\frac{(1+m_i)(1+m_j)+c_{ij}}{4} \right) + H\left(\frac{(1-m_i)(1-m_j)+c_{ij}}{4} \right) + \right.$$
$$\left. + H\left(\frac{(1+m_i)(1-m_j)-c_{ij}}{4} \right) + H\left(\frac{(1-m_i)(1+m_j)-c_{ij}}{4} \right) \right] +$$
$$+ \sum_i (1-d_i) \left[H\left(\frac{1+m_i}{2} \right) + H\left(\frac{1-m_i}{2} \right) \right] + \sum_i h_i m_i + \sum_{i \neq j} J_{ij}(c_{ij} + m_i m_j)$$

MFA to the free-energy

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$$\left. + H\left(\frac{(1+m_i)(1-m_j)-c_{ij}}{4} \right) + H\left(\frac{(1-m_i)(1+m_j)-c_{ij}}{4} \right) \right] +$$
$$+ \sum_i (1-d_i) \left[H\left(\frac{1+m_i}{2} \right) + H\left(\frac{1-m_i}{2} \right) \right] + \sum_i h_i m_i + \sum_{i \neq j} J_{ij}(c_{ij} + m_i m_j)$$

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

$$\Downarrow$$

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

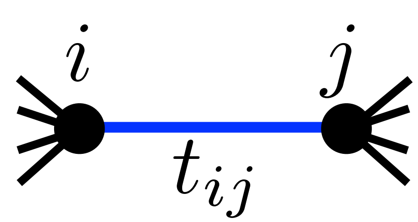
MFA to the free-energy

- Bethe approximation (BA) and cavity method

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

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

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



MFA to the free-energy

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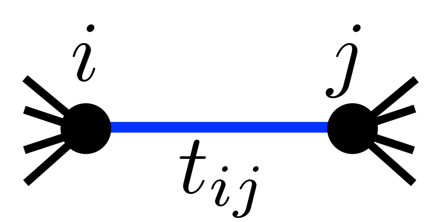

$$m_i^{(j)} = f(m_i, m_j, t_{ij}) \qquad m_j^{(i)} = f(m_j, m_i, t_{ij})$$

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

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

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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)

$$C_{ij} = \frac{\partial m_i}{\partial h_j} \,, \qquad (C^{-1})_{ij} = \frac{\partial h_i}{\partial m_j}$$

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$$C_{ij} = \frac{\partial m_i}{\partial h_j} \,, \qquad (C^{-1})_{ij} = \frac{\partial h_i}{\partial m_j}$$

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

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

Computing correlations by linear response in BA

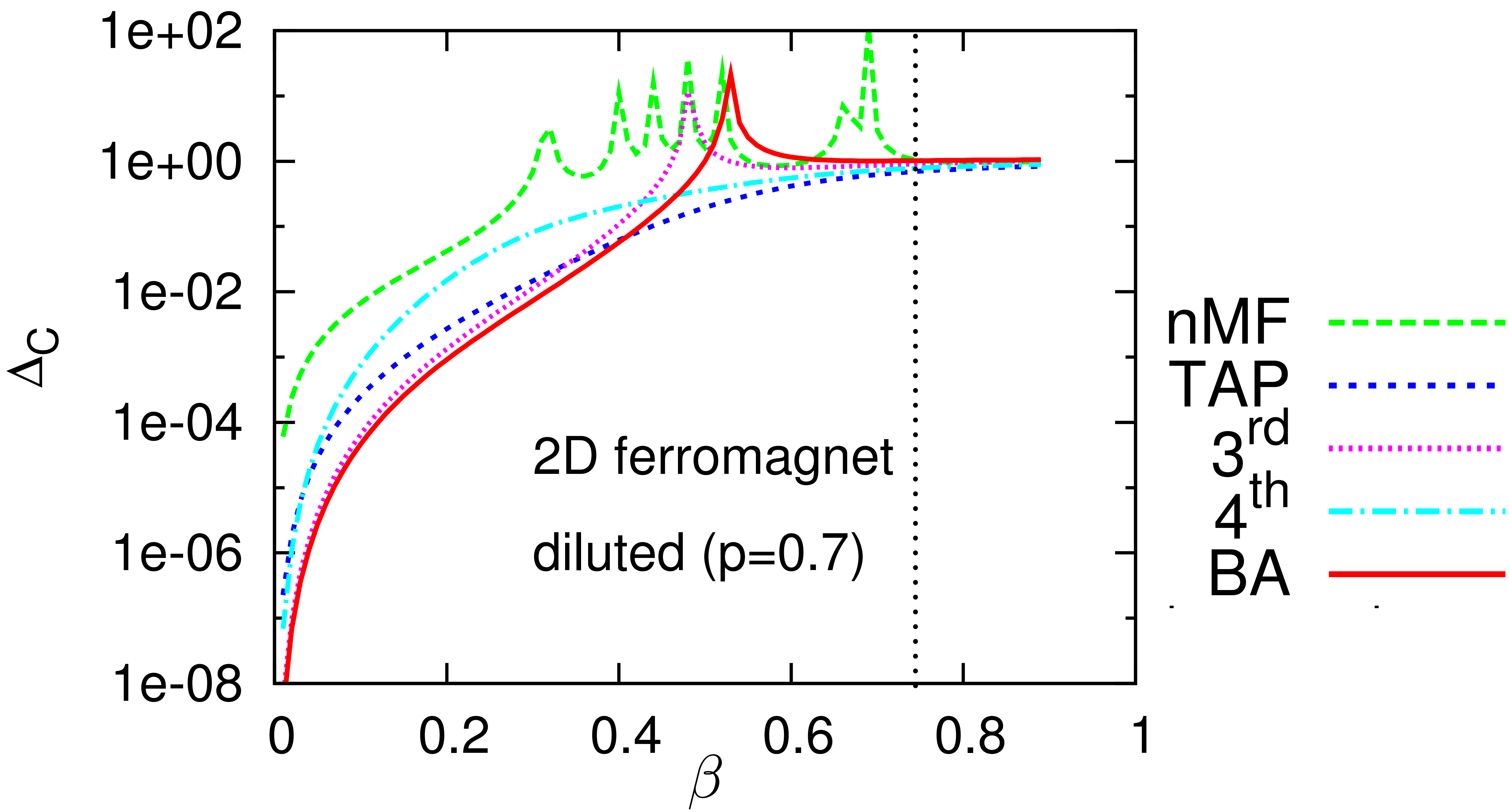
- Analytic expression for the correlations

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

- Coincide with the fixed point of Susceptibility Propagation
- No need to run any algorithm!

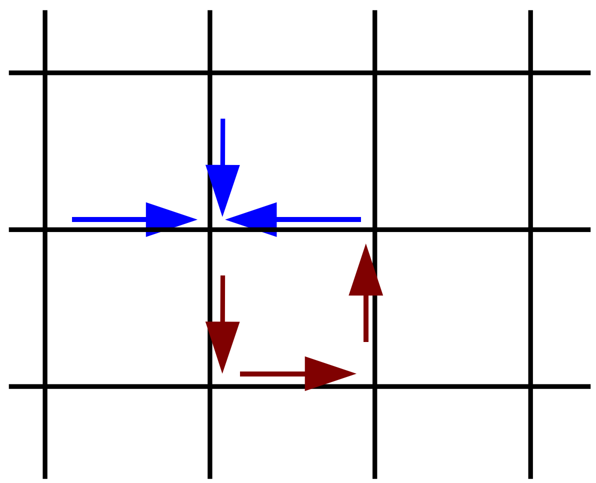
Numerical results on estimating correlations

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



Improving correlations by a normalization trick

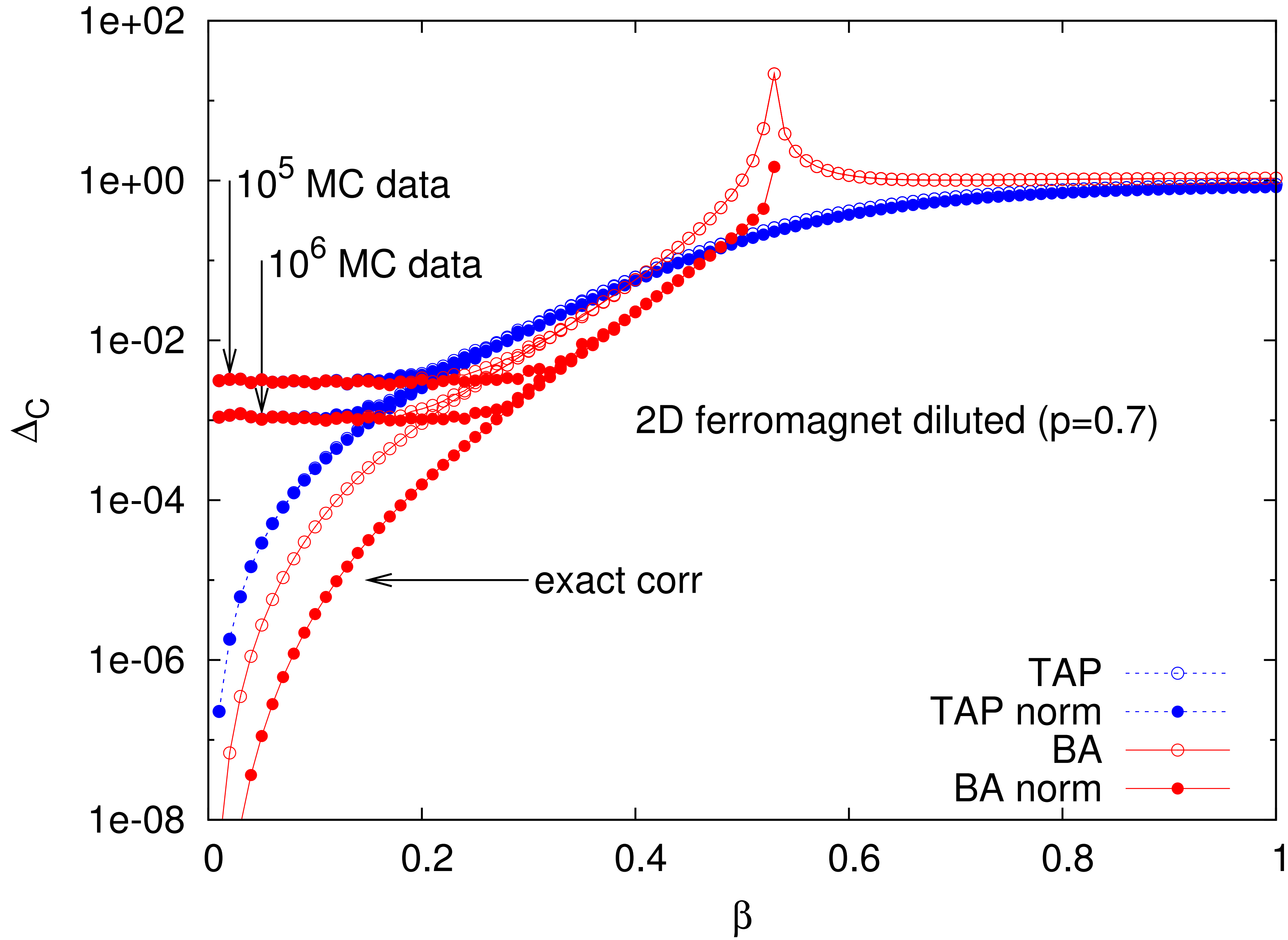
- In ferromagnetic models with loops, inferred correlations are too strong because of loops



- Usually $C_{ii}^{\mathrm{MFA}} > 1$ which is unphysical
- Trick: enforce $C_{ii}^{\mathrm{MFA}} = 1$ by a normalization

$$\widehat{C}_{ij} \equiv \frac{C_{ij}}{\sqrt{C_{ii} C_{jj}}}$$

More numerical results on estimating correlations



MFA for the inverse Ising problem

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\end{aligned}
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MFA for the inverse Ising problem

$$(C^{-1}_{\mathrm{nMF}})_{ij} \;=\; \cancel{\frac{\delta_{ij}}{1-m_i^2}} - J_{ij}\;, \;\Longrightarrow\; \boxed{J_{ij}^{\mathrm{nMF}} = -(C^{-1})_{ij}}$$

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$$\Downarrow$$

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

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$$\Downarrow$$

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

$$\boxed{\begin{aligned} J_{ij}^{\mathrm{BA}} = -\mathrm{atanh}\Bigg[& \frac{1}{2(C^{-1})_{ij}} \sqrt{1+4(1-m_i^2)(1-m_j^2)(C^{-1})_{ij}^2} - m_i m_j - \\ & \frac{1}{2(C^{-1})_{ij}} \sqrt{\left(\sqrt{1+4(1-m_i^2)(1-m_j^2)(C^{-1})_{ij}^2} - 2m_i m_j (C^{-1})_{ij}\right)^2 - 4(C^{-1})_{ij}^2}\ \Bigg] \end{aligned}}$$

Normalization trick for the inverse Ising problem

TAP with m=0 $\quad J_{ij}^{\mathrm{TAP}} = -(C^{-1})_{ij}$

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TAP with m=0 $\quad J_{ij}^{\mathrm{TAP}} = -(C^{-1})_{ij}$

$$(C_{\mathrm{TAP}}^{-1})_{ij} = \left[1 + \sum_k (J_{ik}^{\mathrm{TAP}})^2\right] \delta_{ij} - J_{ij}^{\mathrm{TAP}} \quad \Longrightarrow \quad C_{\mathrm{TAP}} \neq C$$

Normalization trick for the inverse Ising problem

TAP with m=0 $\quad J_{ij}^{\mathrm{TAP}} = -(C^{-1})_{ij}$

$$(C_{\mathrm{TAP}}^{-1})_{ij} = \left[1 + \sum_k (J_{ik}^{\mathrm{TAP}})^2\right] \delta_{ij} - J_{ij}^{\mathrm{TAP}} \quad \Longrightarrow \quad C_{\mathrm{TAP}} \neq C$$

$$(\widehat{C}_{\mathrm{TAP}})_{ij} = \frac{(C_{\mathrm{TAP}})_{ij}}{\sqrt{(C_{\mathrm{TAP}})_{ii}(C_{\mathrm{TAP}})_{jj}}} = \lambda_i \lambda_j (C_{\mathrm{TAP}})_{ij}$$

λ_i are N new parameters to fix s.t. $\widehat{C}_{\mathrm{TAP}} = C$

More approximations 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

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

More approximations for the inverse Ising problem

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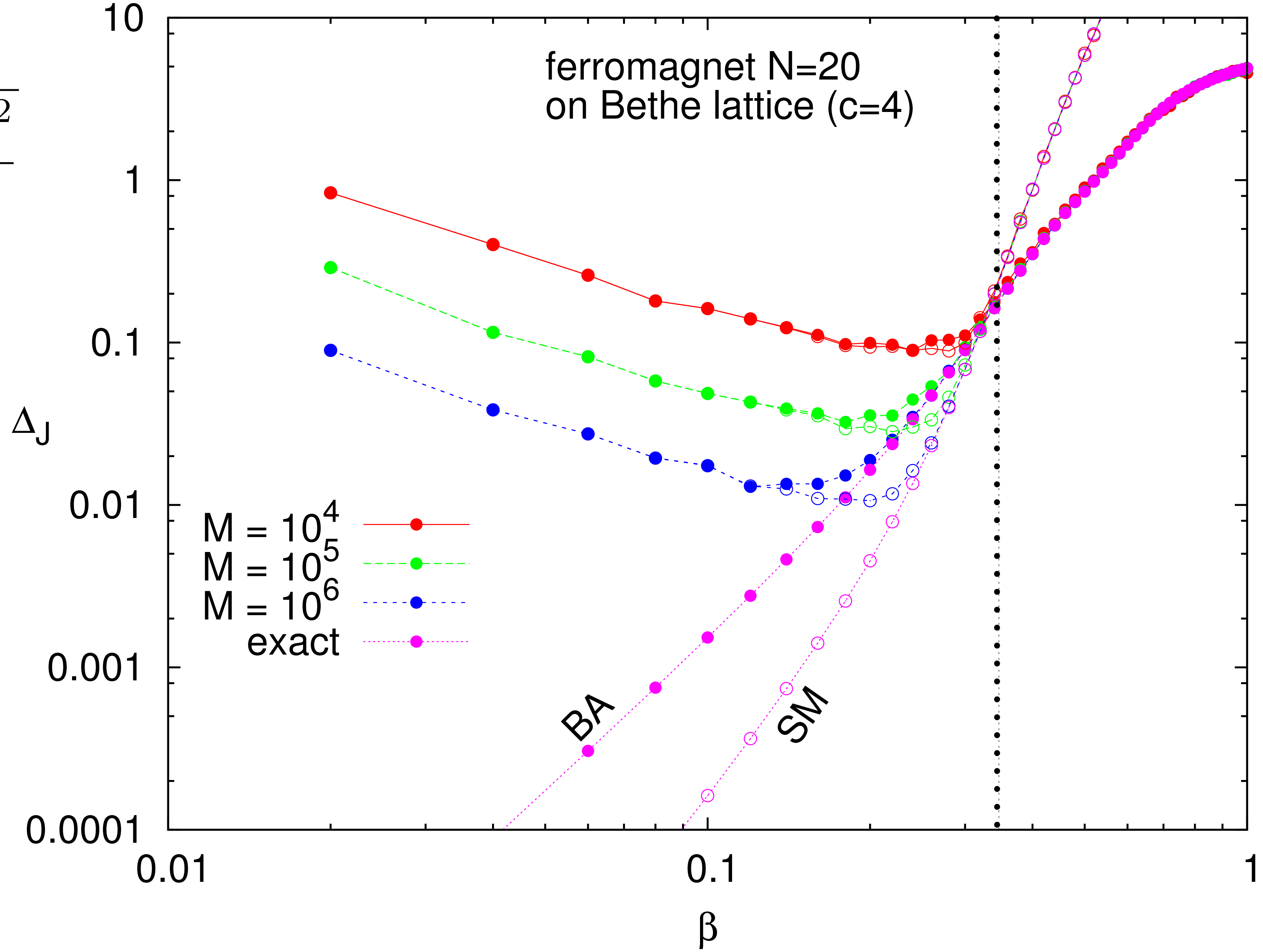
- Sessak-Monasson (SM) small correlation expansion

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

[for m=0 can be derived in 2 lines, ask me if interested]

Numerical results for the inverse Ising problem

$$\Delta_J = \sqrt{\frac{\sum_{i<j}(J'_{ij} - J_{ij})^2}{\sum_{i<j} J_{ij}^2}}$$



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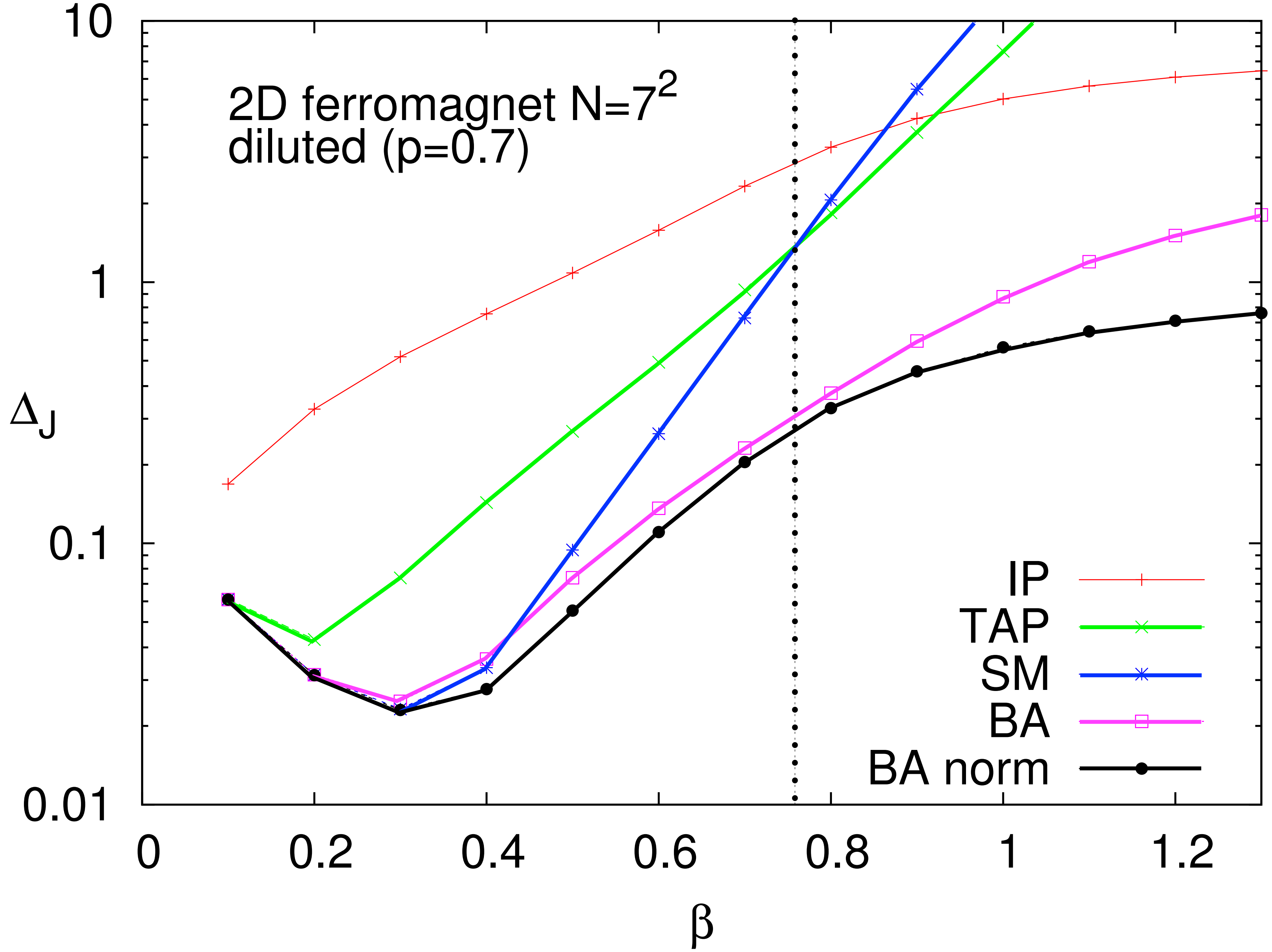


A major problem for frustrated models in a field

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

The resulting coupling is real only if

$$\Delta^{\mathrm{TAP}} \equiv 1 - 8m_i m_j (C^{-1})_{ij} \geq 0$$

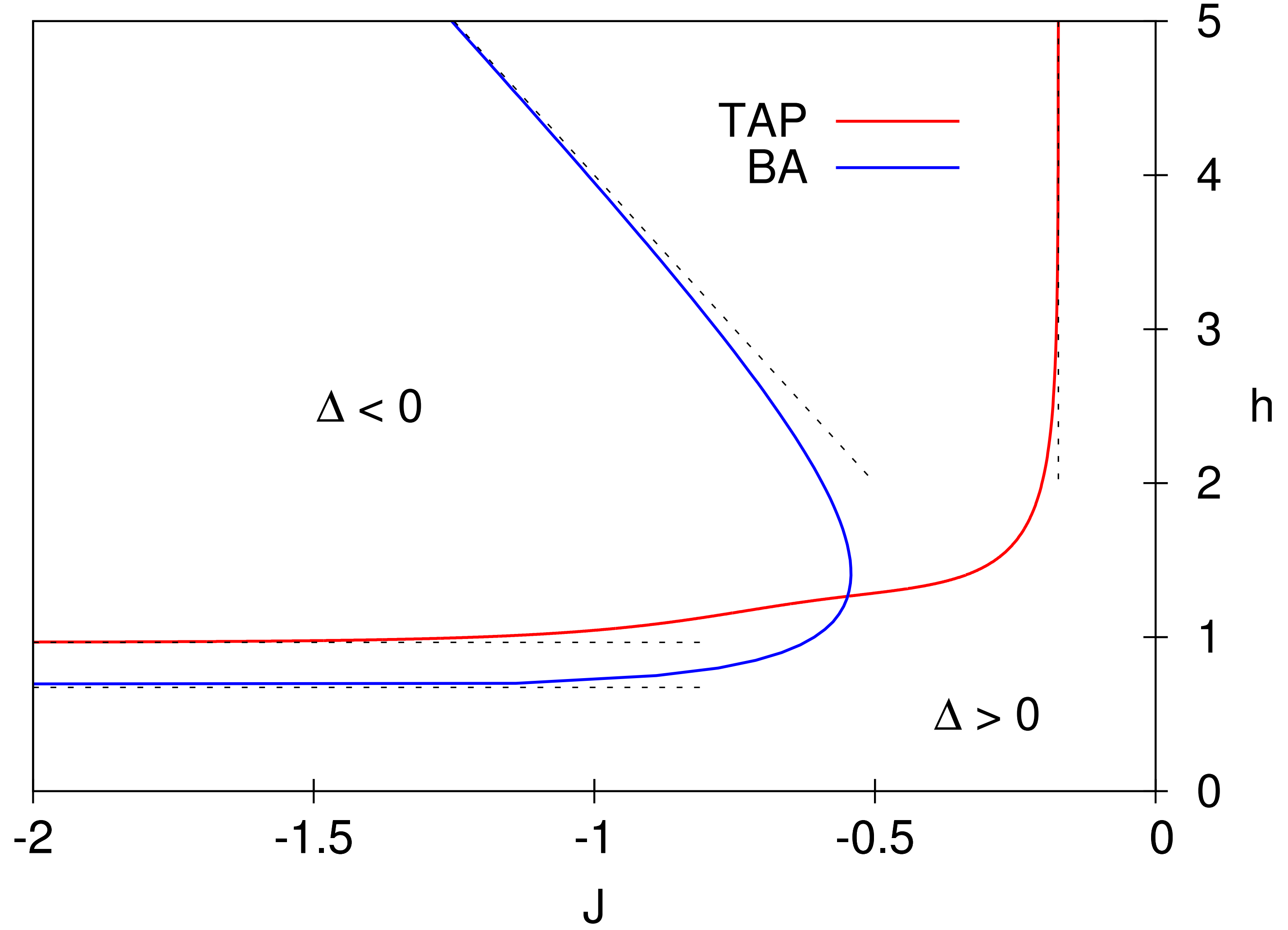
The same happens also within the BA

$$\Delta^{\mathrm{BA}} = \left(\sqrt{1 + 4(1 - m_i^2)(1 - m_j^2)(C^{-1})_{ij}^2} - 2m_i m_j (C^{-1})_{ij}\right)^2 - 4(C^{-1})_{ij}^2$$

A major problem for frustrated models in a field

Three spins interacting with a coupling J in a constant field h

$$P(s_1, s_2, s_3) \propto \exp[J(s_1 s_2 + s_2 s_3 + s_3 s_1) + h(s_1 + s_2 + s_3)]$$



Pseudo-likelihood method (PLM)

- Approximate $P(\boldsymbol{s}) \simeq \prod_i P_i(s_i|\boldsymbol{s}_{\setminus i})$
- Define the pseudo-log-likelihood as

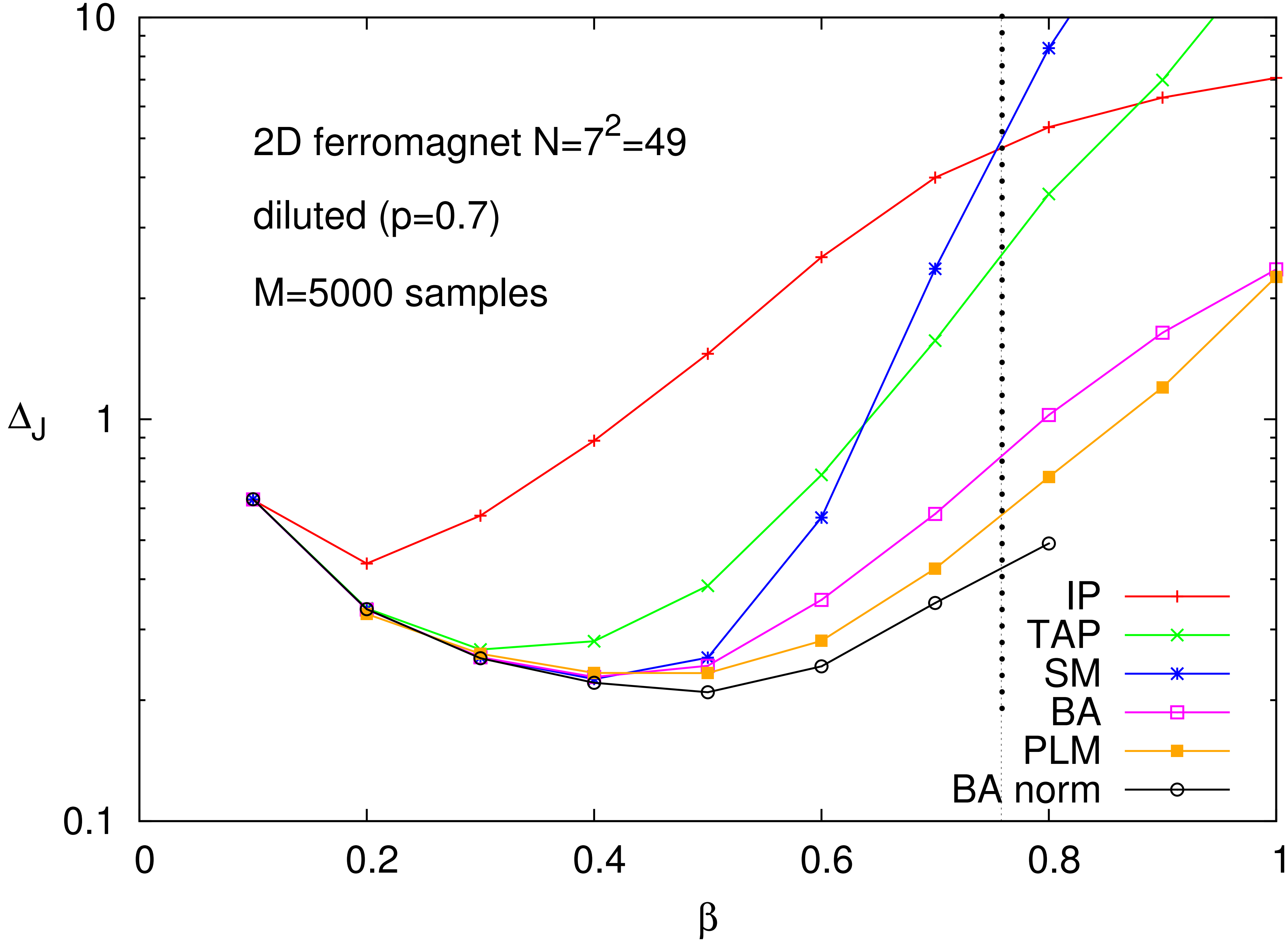
$$PL(\boldsymbol{h}, \boldsymbol{J}|\boldsymbol{s}) = \langle \log P(\boldsymbol{s}|\boldsymbol{h}, \boldsymbol{J}) \rangle = \sum_i \langle \log P_i(\boldsymbol{s}|h_i, \boldsymbol{J}_i) \rangle = \sum_i f_i$$

$$f_i = h_i m_i + \sum_j J_{ij}(C_{ij} + m_i m_j) - \langle \log 2 \cosh \big(s_i (h_i + \sum_j J_{ij} s_j) \big) \rangle$$

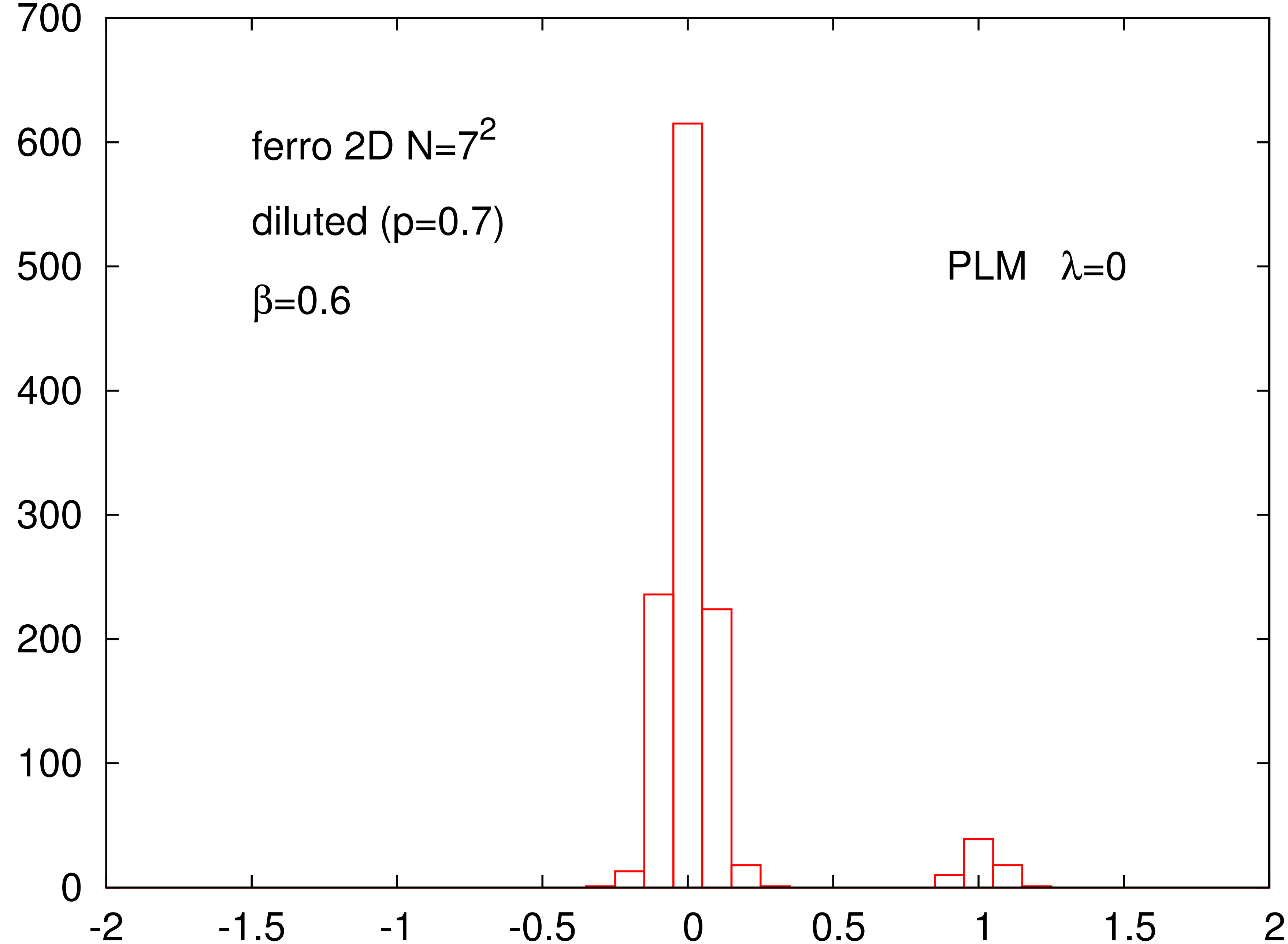
- Maximize f_i to estimate h_i and J_{ij}
- For sparse models use an L1 regularization and maximize

$$f_i - \lambda \sum_j |J_{ij}|$$

PLM vs. MFA


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

Couplings inferred by PLM



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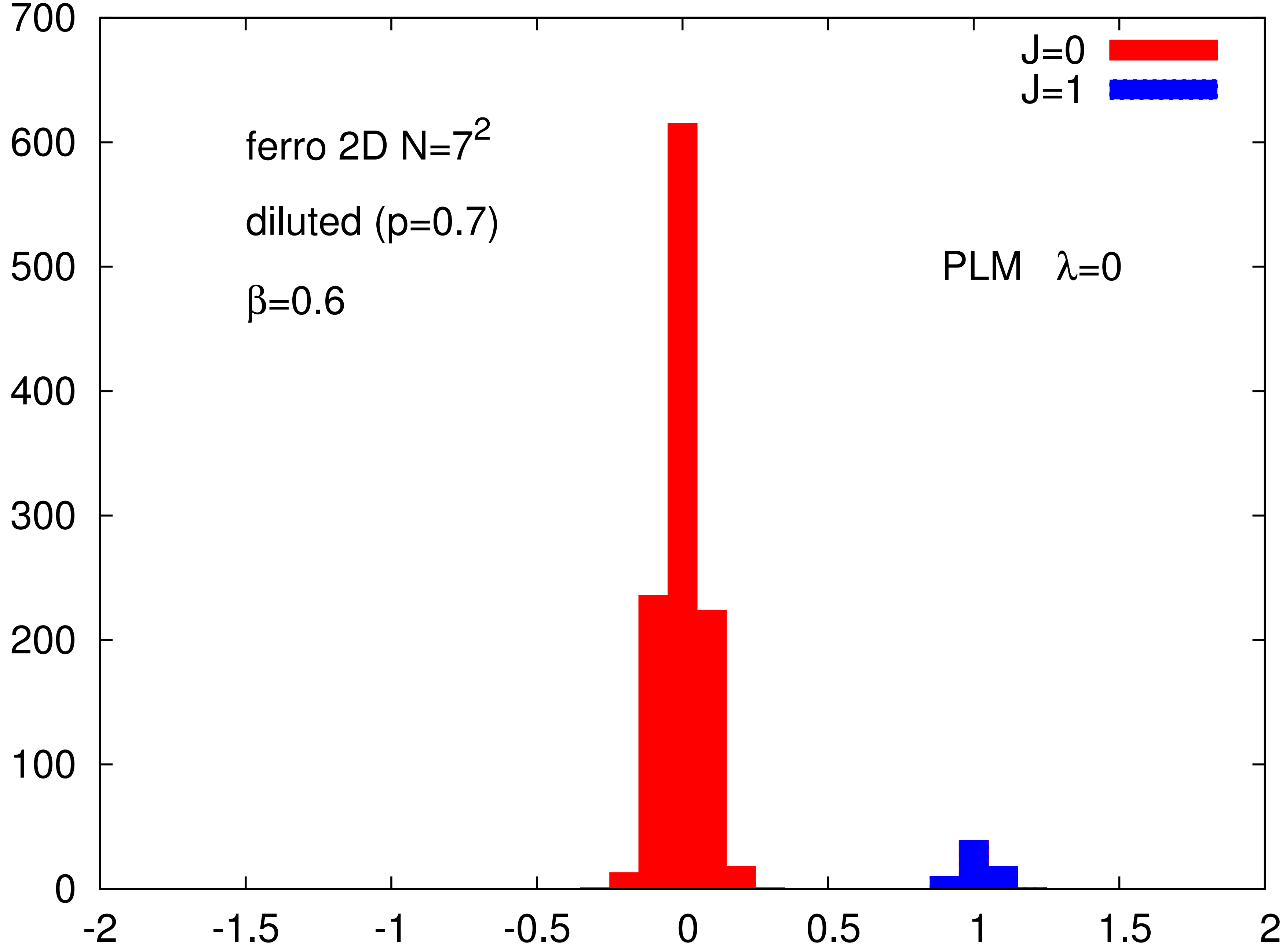

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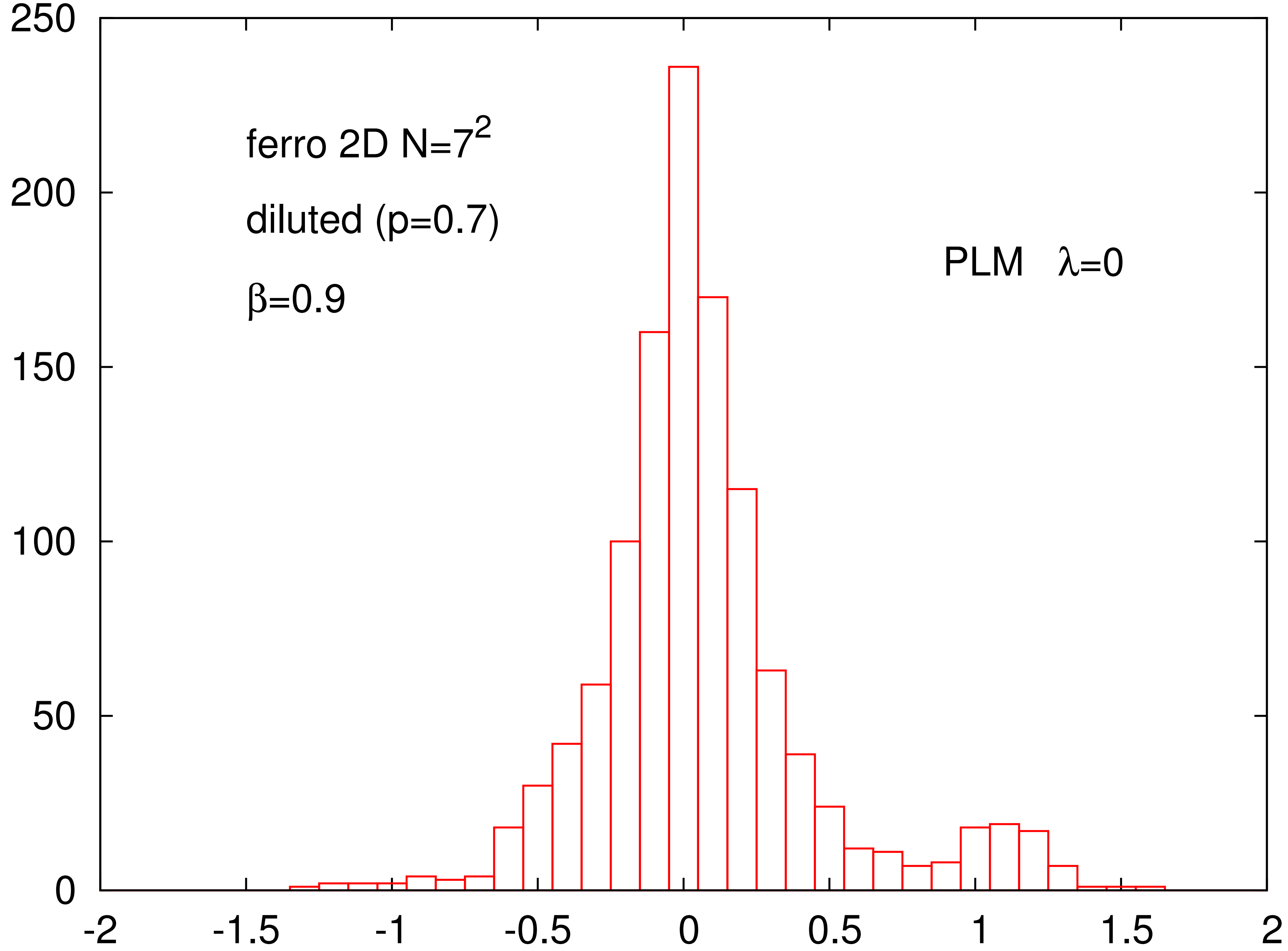
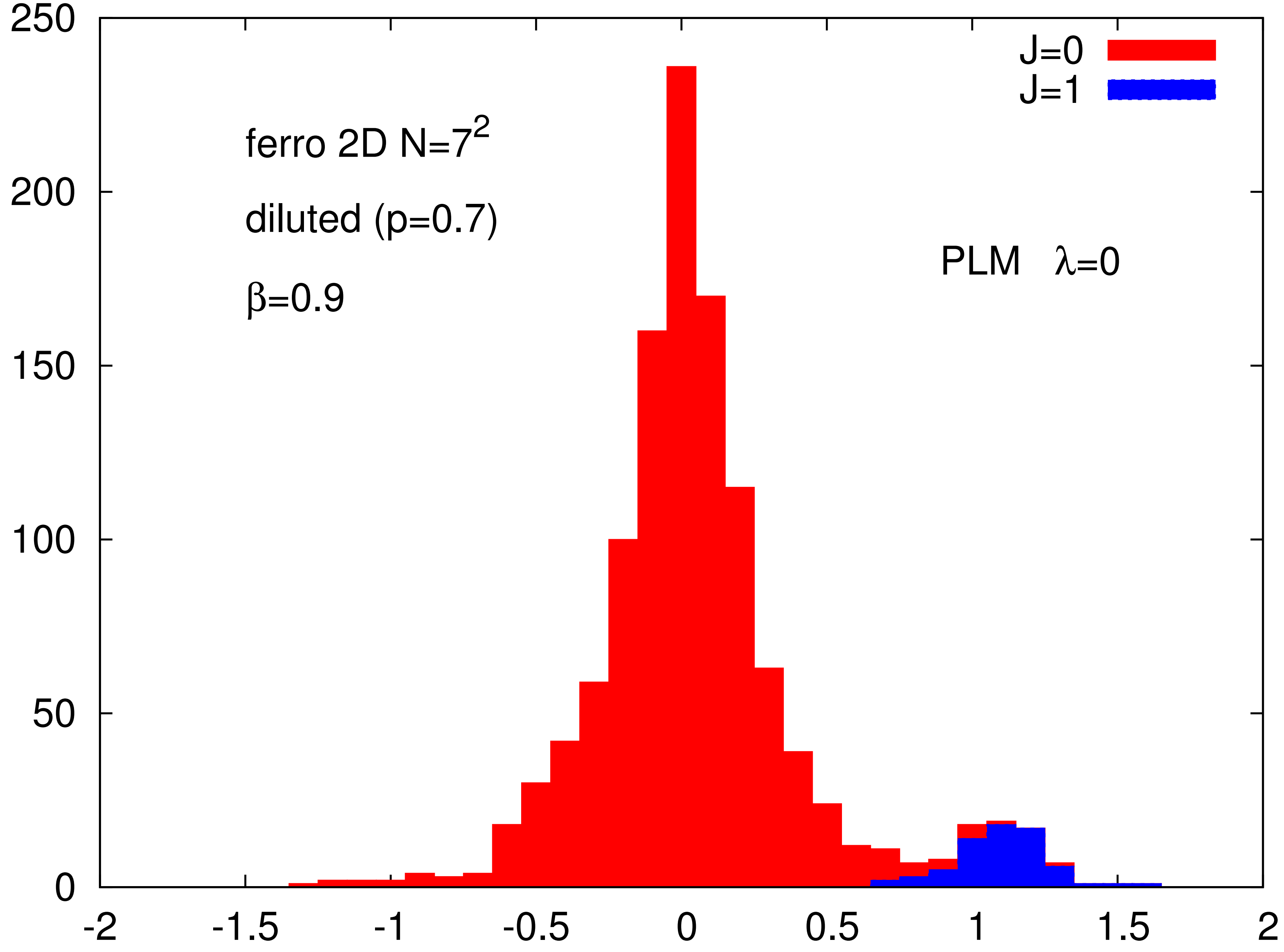


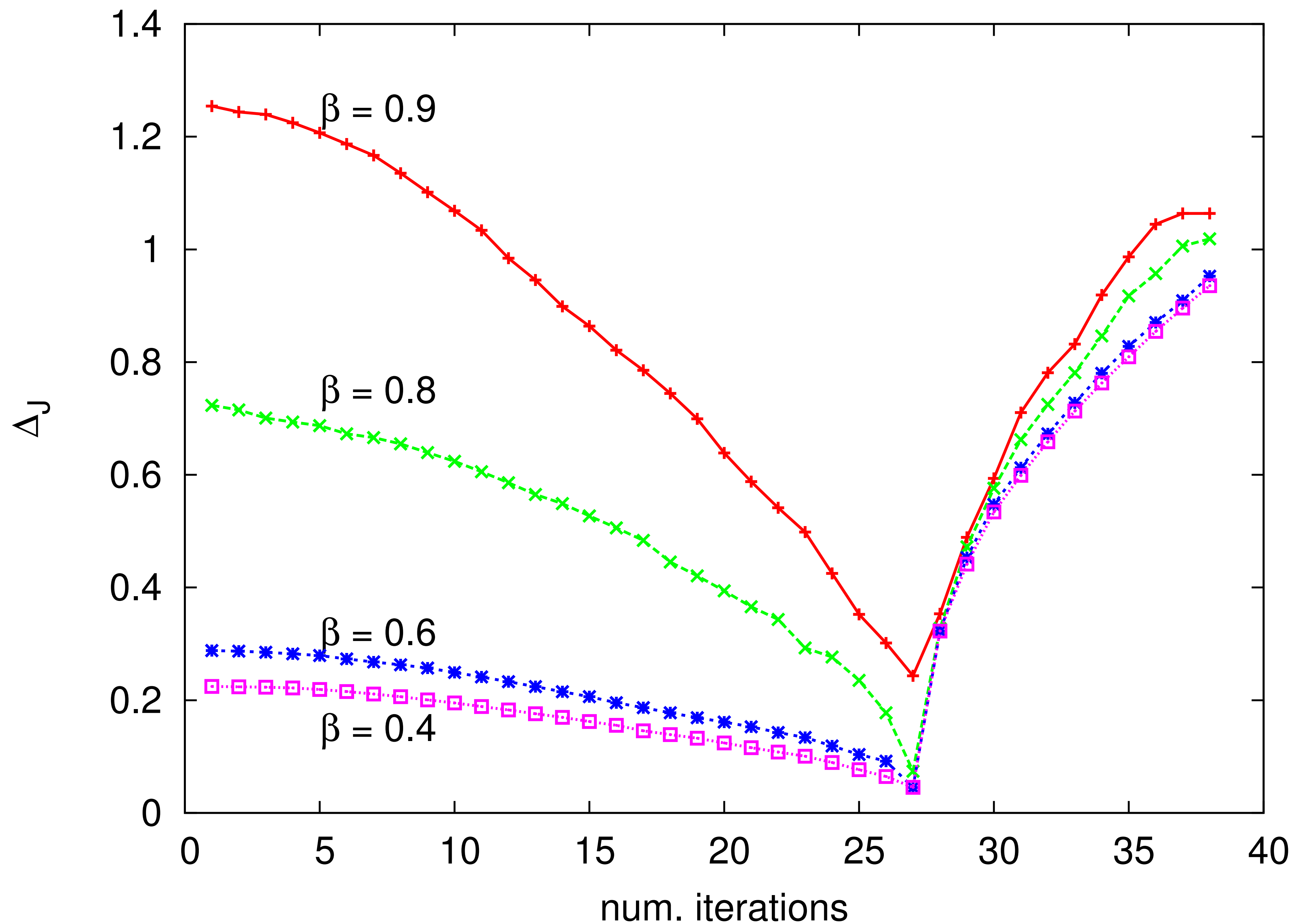
Couplings inferred by PLM



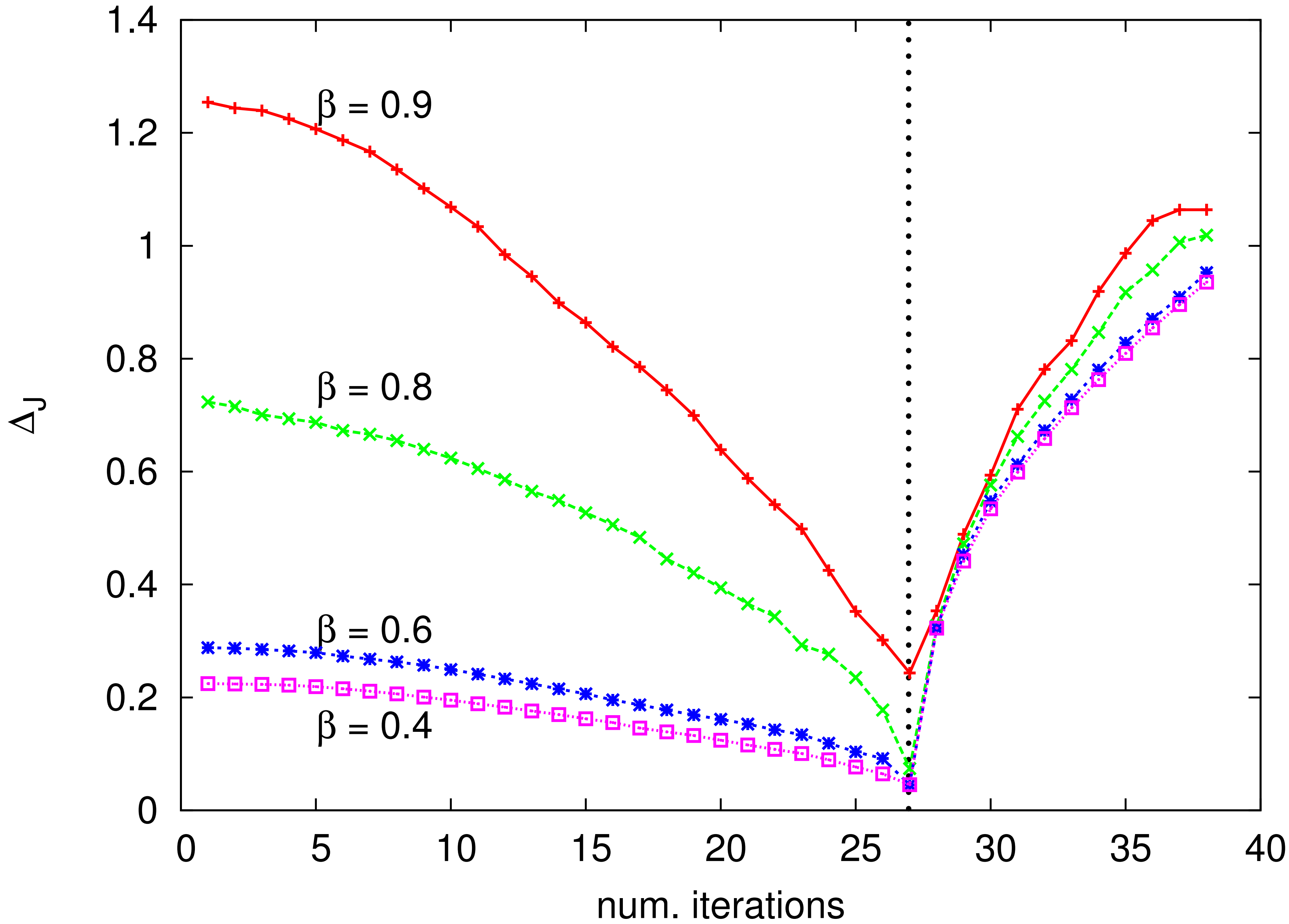
Decimation procedure

- Run PLM
- Set to zero a constant fraction of couplings (those inferred to be the smallest)
- Re-run PLM only on couplings not set to zero (this is impossible within a MFA)
- Iterate until...

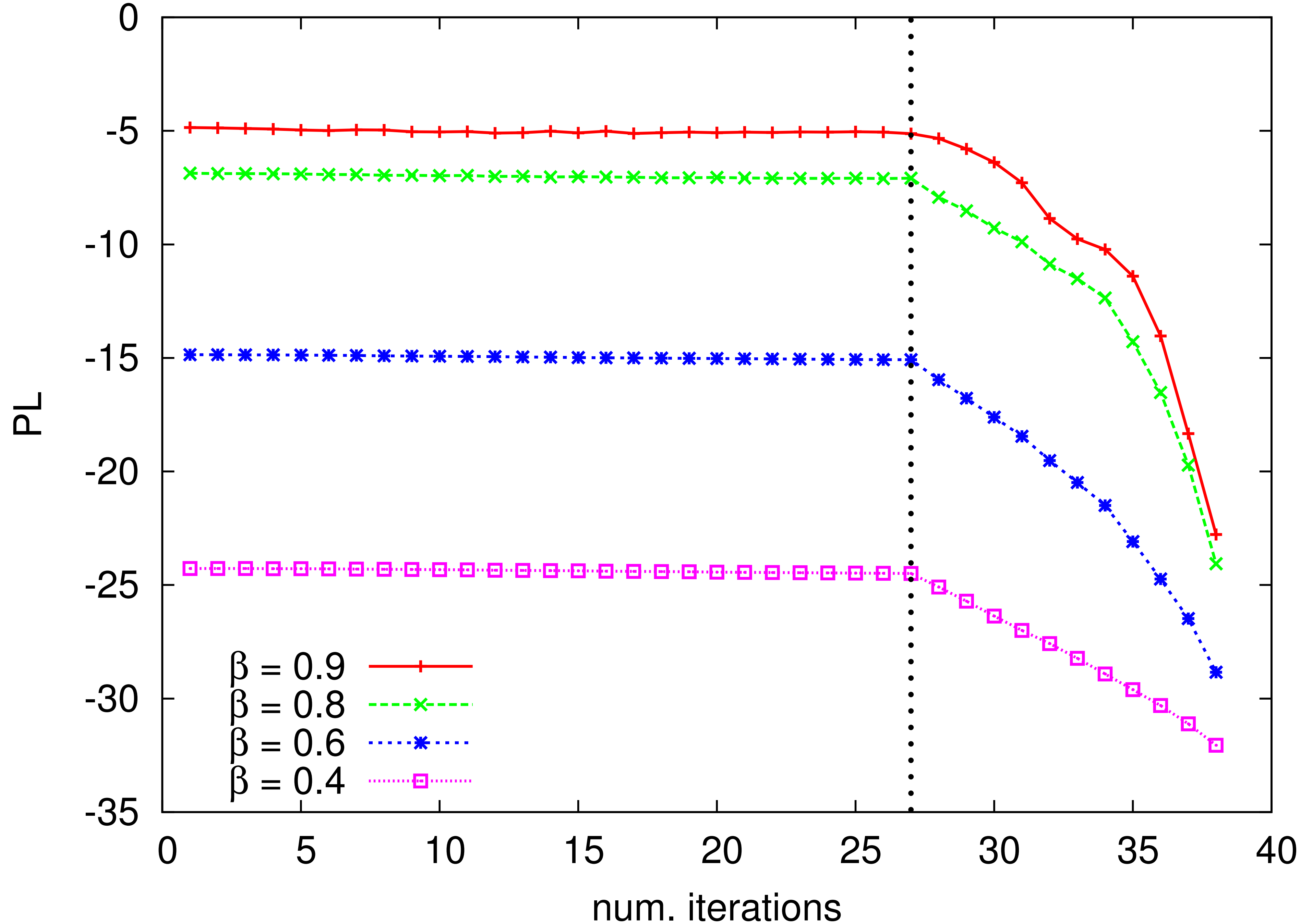
PLM + decimation



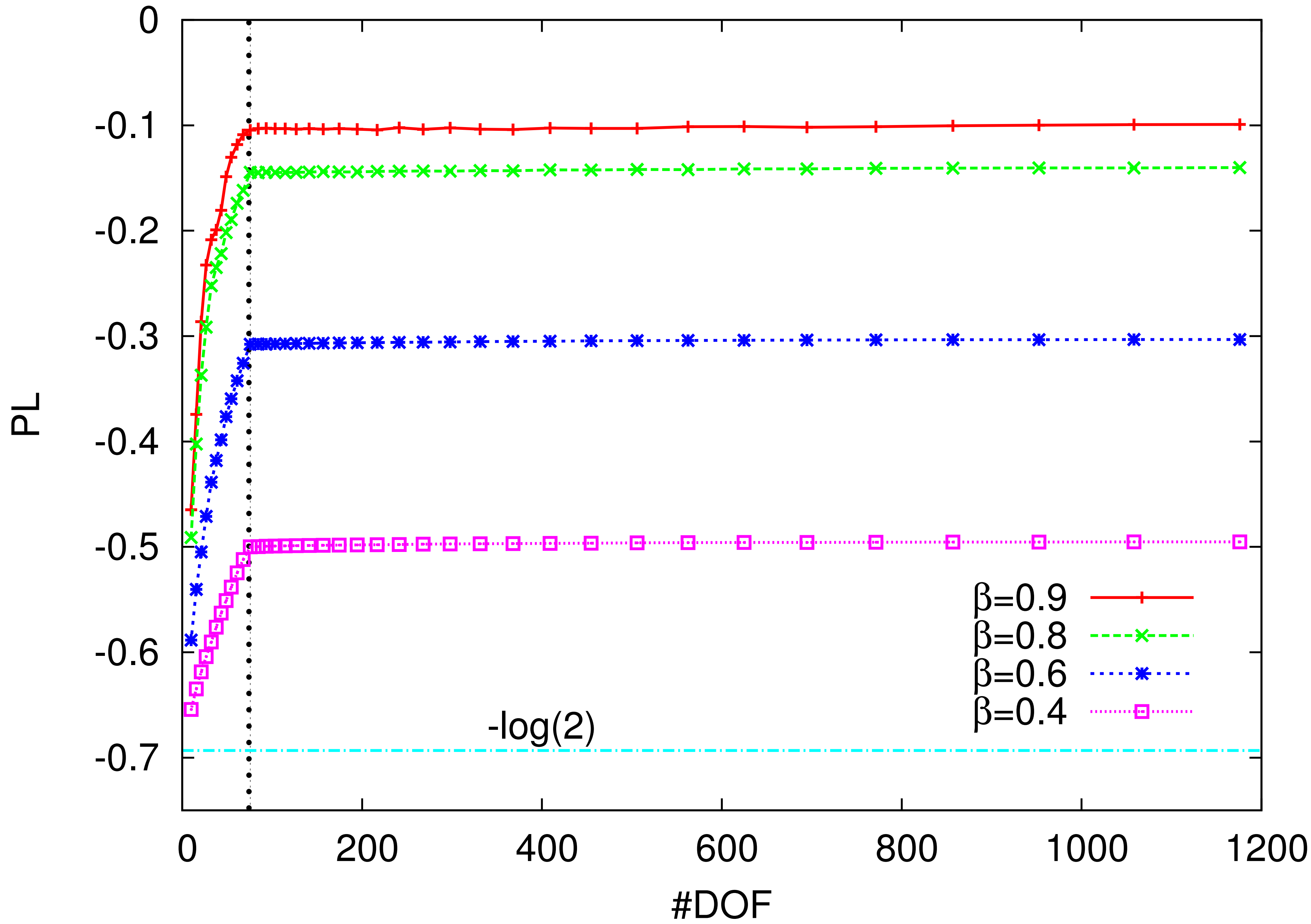
PLM + decimation



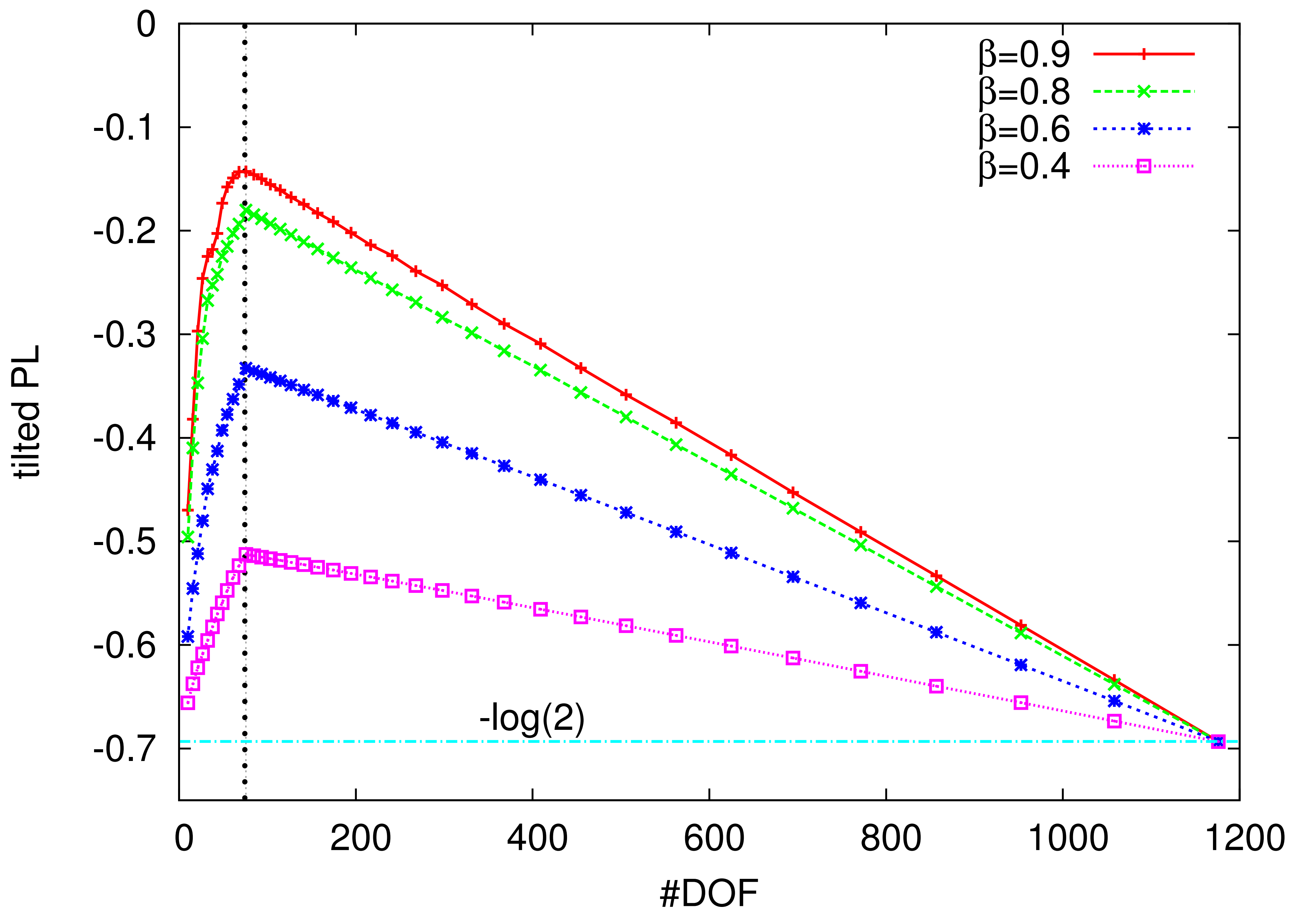
PLM + decimation



PLM + decimation



PLM + decimation



Summary of recent results about the inverse Ising pb.

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- Analytical expressions for the Bethe approx.
- Comparison of MFA in a wide temperature range
- Serious limitation of TAP and Bethe in a field
- Improvement in the inferred couplings by:
  - normalization trick (in weakly frustrated models)
  - PLM + decimation procedure