Inverse Ising via Pseudolikelihood Maximization

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What do we have?

- We observe a lot of states sampled from

$$P(\boldsymbol{\sigma}) = \frac{1}{Z}\exp(\beta\sum_i h_i\sigma_i + \beta\sum_{i<j} J_{ij}\sigma_i\sigma_j),$$

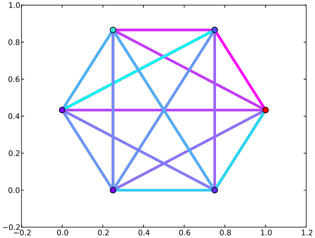
just like

$$\begin{aligned}
\boldsymbol{\sigma}^{(1)} &= \{+1, -1, +1, \cdots, +1\} \\
\boldsymbol{\sigma}^{(2)} &= \{-1, -1, +1, \cdots, -1\} \\
\boldsymbol{\sigma}^{(3)} &= \{-1, -1, +1, \cdots, -1\} \\
&\cdots \\
\boldsymbol{\sigma}^{(M)} &= \{+1, +1, +1, \cdots, +1\}
\end{aligned}$$

Without knowing the actual structure, we can only assume a *fully-connected* graph.

What do we have?

This is a *Sherrington-Kirkpatrick Model*.



Moments can be extracted from the observed data:

- Average magnetization of a site: $m_i = \langle \sigma_i \rangle$
- Correlation between a pair of sites: $c_{ij} = \langle \sigma_i \sigma_j \rangle - \langle \sigma_i \rangle \langle \sigma_j \rangle$

Maximum likelihood estimation

Probability of the observed samples (*strong assumption on independence!*)

$$P = \prod_k P(\boldsymbol{\sigma}^{(k)})$$

Rewrite and take the log,

$$\log(P) = \beta \sum_i \sum_k \sigma_i^{(k)} + \beta \sum_{i<j} J_{ij} \sum_k \sigma_i^{(k)} \sigma_j^{(k)} - M \log Z$$

$$l = \frac{1}{M} \log(P) = \beta \sum_i h_i m_i + \beta \sum_{i<j} J_{ij} (m_i m_j + c_{ij}) - \log Z$$

- Only the moments are found here!

$\{m_i\}$ *and* $\{c_{ij}\}$ *are sufficient statistics, and this is the standard formulation.*

Painful computability

$$\log(P) = \beta \sum_i \sum_k \sigma_i^{(k)} + \beta \sum_{i<j} J_{ij} \sum_k \sigma_i^{(k)} \sigma_j^{(k)} - M \log Z$$

Partition function Z *hinders computation*.
Approximate Z ?

Pseudolikelihood

(Erik Aurell and Magnus Ekeberg, *Inverse Ising Inference Using All the Data*, PRL (2012))

Can we write down a probability without Z ?

- Aha, how about the conditional probability?

$$P(\sigma_r = 1|\boldsymbol{\sigma}_{\setminus r}) = \frac{P(\boldsymbol{\sigma}|_{\sigma_r=1})}{P(\boldsymbol{\sigma}|_{\sigma_r=1}) + P(\boldsymbol{\sigma}|_{\sigma_r=-1}))},$$

and

$$P(\boldsymbol{\sigma}|_{\sigma_r=1}) = \frac{1}{Z}\exp(\beta(\sum_{i\neq r} h_i\sigma_i + h_r) + \beta(\sum_{i\neq r} J_{ir}\sigma_i + \frac{1}{2}\sum_{k,l\neq r} J_{kl}\sigma_k\sigma_l))$$

- So Z is gone!

$$P(\sigma_r|\boldsymbol{\sigma}_{\setminus r}) = \frac{1}{1 + \exp(-2\beta\sigma_r(h_r + \sum_{i\neq r} J_{ir}\sigma_i))}$$

Pseudolikelihood maximization

For the site r, we can maximize

$$P(\sigma_r|\boldsymbol{\sigma}_{\setminus r}) = \frac{1}{1+\exp(-2\beta\sigma_r(h_r+\sum_{i\neq r}J_{ir}\sigma_i))}$$

to estimate related parameters h_r and $\{J_{ir}\}$.

- Using all the samples, the objective function is simply

$$f_r = -\frac{1}{M}\sum_k \log(P(\sigma_r^{(k)}|\boldsymbol{\sigma}_{\setminus r}^{(k)}))$$

Parameters can be estimated by minimize this objective function.

How to compute?

We have N objective functions,

$$\{f_1, f_2, \cdots, f_N\}$$

Then how to minimize them simultaneously?

- Minimize — *Gradient descent*
- Multi-objective — *Working in-turn*

Rewriting

$$X_r^{(k)} = \sigma_r^{(k)} \sum_{i \neq r} J_{ir}^{\star} \sigma_i^{(k)}$$

$$P_r^{(k)} = \frac{1}{1 + \exp(-2\beta X_r^{(k)})}$$

How to compute?

Gradient (going down the hill...)

$$\frac{\partial f_r}{\partial J_{ir}} = -\frac{1}{M}\sum_k \frac{1}{P_r^{(k)}} \frac{\partial P_r^{(k)}}{\partial J_i r}$$

$$\frac{\partial P_r^{(k)}}{\partial J_{ir}} = \frac{2\beta\sigma_r^{(k)}\sigma_i^{(k)}\exp(-2\beta X_r^{(k)})}{(1+\exp(-2\beta X_r^{(k)}))^2}$$

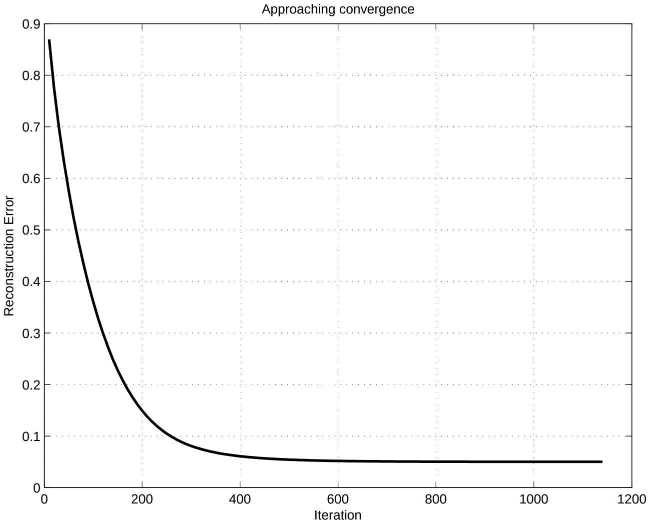
- *Formulating them in the form of matrix could make it better...*

Experiments and results

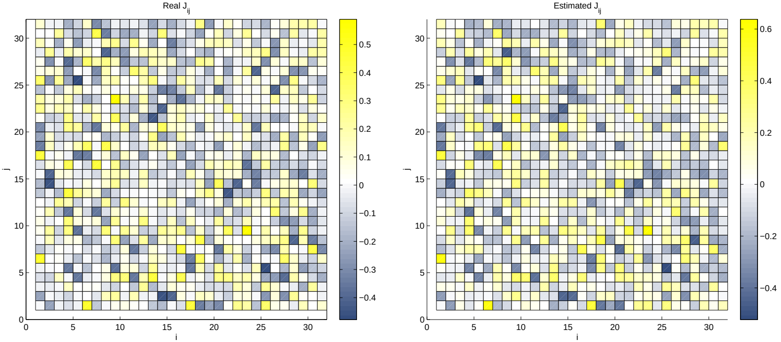
Experimental setup

- N $= 32$
- Zero external field $h_i = 0$
- J_{ij} sampled from a Gaussian $N(0, \frac{1}{pN})$
- Evaluated by *reconstruction error* $\Delta = \sqrt{\frac{\sum_{i<j}(J^{\star}_{ij} - J_{ij})^2}{N(N-1)/2}}$

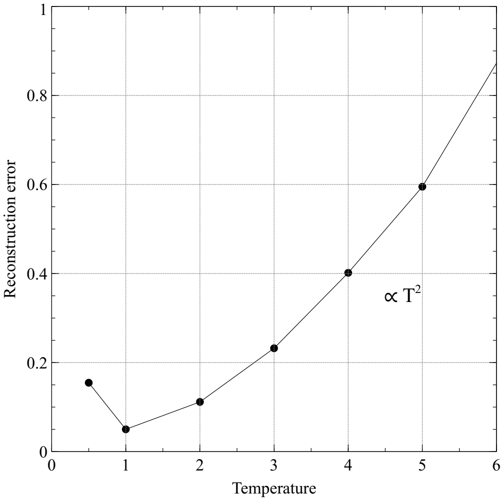
Effective minimization?



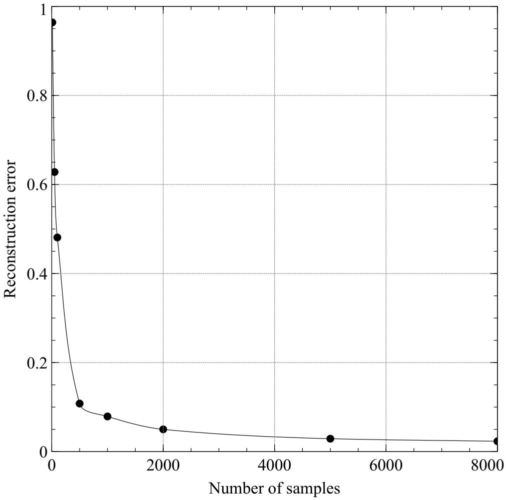
Coupling recovery



Error vs Temperature



Error vs Sample Number



Thank you!