Identification of Metastable States in Finite Temperature Simulations: A Self-Organization Approach

Yukito IBA*) and Koji HUKUSHIMA**)

*The Institute of Statistical Mathematics, 4-6-7 Minami Azabu, Minato-ku, Tokyo, 106-8569, Japan.

** Institute for Solid State Physics, Univ. of Tokyo, Roppongi, Minato-ku, Tokyo, 106-8666, Japan.

(Received)

How can we identify "metastable states" from a simulation of a *finite size* system at *finite temperatures*? Here we propose a self-organization approach to this problem based on a *finite mixture model* and *Expectation-Maximization (EM) algorithm* and apply it to the analysis of Monte Carlo simulation of Ising spin glass models.

In mean-field approximations, metastable states are often represented as saddle points of self-consistent equations. There seems, however, no established procedure to identify metastable states in *simulation data* at *finite temperatures*. Here we propose a method based on a *finite mixture model*[1)]. In the proposed method, we fit a mixture $P(y) = \sum_c w_c \cdot P_c(y|\lambda_c)$ of the distributions $\{P_c\}$ to a given set of data and regard each component P_c as a metastable state. The parameters $\{\lambda_c\}$ and weights $\{w_c\}$ ($\sum_c w_c$=1) of the components are estimated from the data by *EM algorithm*, which gives *maximum likelihood estimates* (MLE) of these parameters. In this algorithm, no auxiliary assumption for the assignment of each sample to the components is required. The classification of the data is automatically determined by the algorithm, once we give the number c_{max} of the component distributions.

In this paper, we apply this method to the analysis of binary patterns $\{\{d_i^j\}\}$ generated by the simulations of Ising spin glass models. Here and hereafter a suffix i is the index of a sample, while a suffix j is the index of an element in a sample (*e.g.*, the site of a spin). Our model is expressed as

$$P(\{\{d_i^j\}\}\,|\,\{\{m_c^j\}\},\{w_c\}) \;=\; \prod_i \left\{ \sum_c w_c \prod_j \frac{1+d_i^j m_c^j}{2} \right\} \tag{1}$$

where a set of *templates* $\{\{m_c^j\}\}$ of metastable states $\{c\}$ and their *weights* $\{w_c\}$ are parameters of the model. The value of m_c^j is interpreted as mean magnetization at a site j in a metastable state c. Note that each component $\prod_j \frac{1+d_i^j m_c^j}{2}$ is also written as $\exp(\sum_j x_c^j d_i^j)/\prod_{j'} 2\cosh x_c^{j'}$, where $x_c^j = \tanh^{-1} m_c^j$ is the mean field at a site j in a metastable state c.

The templates, weights and classification of the samples are simultaneously determined by the following version of EM algorithm. In E-step, we assign values

*) E-mail address: iba@ism.ac.jp

**) E-mail address: hukusima@chiral.issp.u-tokyo.ac.jp

$p_i(c)$, $c = 1, 2, .., c_{max}$, to each sample i, which represent the contribution of the sample i to the metastable state indexed by c:

$$p_i(c) := \frac{w_c \prod_j \frac{1+d_i^j m_c^j}{2}}{\sum_{c'} w_{c'} \prod_j \frac{1+d_i^j m_{c'}^j}{2}}. \tag{2}$$

When the value of $p_i(c)$ is ~ 1 for some c, the sample i is regarded as a member of the metastable state c. In M-step, templates of metastable states are updated as a weighted average of the samples that belong to the metastable states. The weights w_c is also updated (Here, the constant d_{max} indicates total number of the samples.):

$$m_c^j := \frac{\sum_i d_i^j \cdot p_i(c)}{\sum_i p_i(c)}, \qquad w_c := \frac{\sum_i p_i(c)}{d_{max}} . \tag{3}$$

Starting from random templates (or random classification of samples), templates and classification of samples are self-organized by the iteration of the E- and M- steps.

When the source of data is invariant under a transformation, templates of metastable states should also have the same symmetry. It is not difficult to incorporate such symmetry into a mixture model designed for the analysis of the data. For a set of data generated by Ising models without external fields, the model Eq. (1) is modified as

$$P(\{\{d_i^j\}\} \,|\, \{\{m_c^j\}\}, \{w_c^{\pm}\}) = \prod_i \left\{ \sum_c w_c^+ \prod_j \frac{1+d_i^j m_c^j}{2} + \sum_c w_c^- \prod_j \frac{1-d_i^j m_c^j}{2} \right\}, \tag{4}$$

which explicitly take account of the global ($+1 \leftrightarrow -1$) symmetry expected in the data. It is straightforward to derive an EM algorithm modified for this model.

A set of templates constructed from a simulation of the SK model without external fields (system size $N = 64$) are shown in Fig. 1. The model Eq. (1) with *four templates* are used for the analysis. The templates are grouped into two pairs (1,4) and (2,3). Members of each pair are approximately related by the ($+1 \leftrightarrow -1$) symmetry. Results with different number of templates and with the model Eq. (4) are also discussed at the conference, as well as results for the Hopfield model.

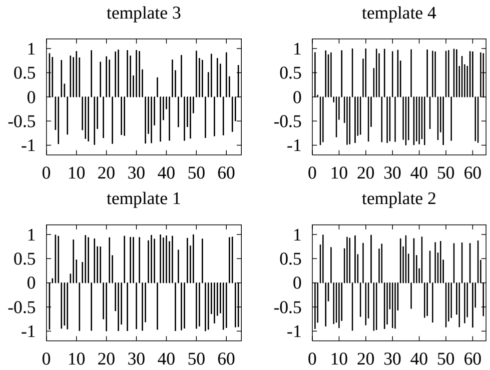

Fig. 1. An example of templates: For each template, the mean magnetization m_c^j at each site j ($j = 1, .., 64$) is shown.

References

1) D.M. Titterington, A.F.M. Smith, and U.E. Makov: *Statistical Analysis of Finite Mixture Distributions* (John Wiley and Sons, Chichester, 1985).