Free-Energy Fluctuations and Chaos in the Sherrington-Kirkpatrick Model

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Sherrington-Kirkpatrick Model

1

Disordered model system governed by the mean-field spin glass Hamiltonian [1] for N Ising spins $\sigma_i = \pm 1$:

$$\mathcal{H}(\sigma) = -\frac{1}{\sqrt{N}} \sum_{i<j} J_{ij}\sigma_i\sigma_j$$

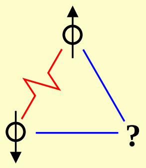
All spins are connected to one another.

Quenched disorder:

$J_{ij} > 0$:

$J_{ij} < 0$:

Bonds are normally distributed with zero mean und unit variance



Frustration

The mean-field model exhibits a phase transition at $T_c = 1$ that separates the glassy phase from the paramagnetic phase.

Objective

3

Calculate ΔF via Eq. (1) for different system sizes at fixed temperatures ($T < T_c$) to assess its scaling behavior.

In order to achieve this, four replicas have to be simulated by using parallel tempering Monte Carlo methods [3].

Parallel Tempering

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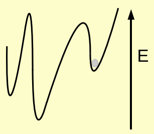
- common Monte-Carlo simulations get trapped in local energy basins in the glassy phase resulting in very long correlation and equilibration times



- remedy: perform Monte-Carlo simulations for many replicas at different temperatures
- swap configurations between these parallel-running simulations from time to time depending on a known probability
- simulations at high temperature assist simulations at lower temperature to overcome energy barriers

Free-energy Fluctuations and Chaos

2

- Chaos property of spin glasses:
  Infinitesimal change of the bond strengths leads to a complete change of the equilibrium state.
- Sample-to-sample Fluctuations of the free energy:
  Free energy depends on the realization of the disorder in finite systems

In order to derive a connection between energy fluctuations and chaos, the "Interpolating Hamiltonian" is introduced:

$$\mathcal{H}_t = -\sqrt{\frac{1-t}{N}} \sum_{i<j} J_{ij}\sigma_i\sigma_j - \sqrt{\frac{t}{N}} \sum_{i<j} J'_{ij}\sigma_i\sigma_j, \qquad 0 \le t \le 1$$

J_{ij} and J'_{ij} are independent Gaussian random numbers with unit variance.

Taking overlaps q_{ab} between independent replicas a, b with different interpolating parameters t and τ into account, the sample-to-sample fluctuations ΔF can be expressed as derived in [2]:

$$\begin{aligned}\beta^2 \Delta F^2 &= \frac{N^2\beta^4}{16} \int_0^\infty d\epsilon \, \frac{2\epsilon \log(1+\epsilon^2)}{(1+\epsilon^2)^2} E_J \langle (q_{13}^2(\epsilon) - q_{14}^2(\epsilon))(q_{13}^2(\epsilon) - q_{23}^2(\epsilon)) \rangle \\ &\quad + \frac{N\beta^2}{4} \int_0^\infty d\epsilon \, \frac{\epsilon \log(1+\epsilon^2)}{(1+\epsilon^2)^{3/2}} \left(E_J \langle q_{13}^2(\epsilon) \rangle - \frac{1}{N} \right) \qquad (1)\end{aligned}$$

where

$$q_{ab}(t,\tau) = \frac{1}{N} \sum_i \sigma_i^{a,t} \sigma_i^{b,\tau}, \qquad \frac{1}{\sqrt{1+\epsilon^2}} = \sqrt{1-t}\sqrt{1-\tau}.$$

$\langle \ldots \rangle$ denotes the thermal average, E_J the average over all coupling constants J_{ij} and J'_{ij} and β is the inverse temperature.

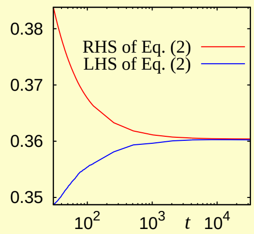
Results

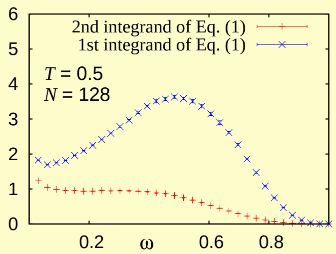
5

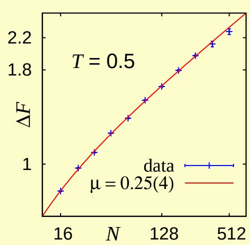
Spin glasses are equilibrated if Eq. (2) is satisfied [4]:

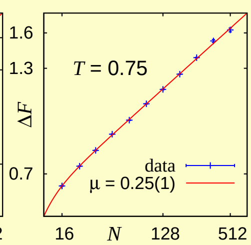
$$\frac{2}{N} \sum_{\langle i,j \rangle} \overline{J_{ij}^2 \langle \sigma_i \sigma_j \rangle^2} = 1 - \frac{2|U|}{\beta}, \quad (2)$$

where $U = -N^{-1} \sum_{\langle i,j \rangle} \overline{J_{ij} \langle \sigma_i \sigma_j \rangle}$.









- in order to render the bounds of integration in Eq. (1) more practical, the substitution $\omega = \exp(-\epsilon)$ has been excuted first
- overlaps for 33 different values of ω were calculated numerically to integrate Eq. (1)
- scaling behavior of ΔF is obtained by a best fit to $\Delta F \sim N^\mu (1 + a/N^b)$
- at $T = 0.5$ and $T = 0.75$ the fluctuations seem to increase with $\mu = 1/4$ for large systems

Bibliography

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[2] T. Aspelmeier, PRL 100 (2008) 117205

[3] M. E. J. Newman, G. T. Barkema, *Monte Carlo Methods in Stat. Physics*, (Oxford University Press, 2006)

[4] H. G. Katzgraber, A. P. Young, PRB 67 (2003) 134410

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