Rare events analysis of temperature chaos in the Sherrington–Kirkpatrick model

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Abstract. We investigate the question of temperature chaos in the Sherrington–Kirkpatrick spin glass model, applying a recently proposed rare events based data analysis method to existing Monte Carlo data. Thanks to this new method, temperature chaos is now observable for this model, even with the limited size systems that can currently be simulated.

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The phenomenon of temperature chaos for spin glasses is the extreme sensitivity of the infinite volume equilibrium state to the slightest change of temperature. In a system with $N$ spins, temperature chaos means that the equilibrium states at two different temperatures $T_1$ and $T_2$ (in the same quenched disorder sample) become uncorrelated for $N \gg N^*$, with some crossover $N^*$ that diverges as $T_1 - T_2 \to 0$. It was first predicted for finite dimensional spin glasses [1]–[4] using either scaling or Migdal–Kadanoff renormalization group type arguments. Some numerical evidence has been presented [5]–[10] for temperature chaos in the spin glass phase of the low dimensional Edwards–Anderson Ising model (EAI) by analyzing the finite size scaling behavior of the average (both thermal and disorder) overlap between two clones at different temperatures. The interpretation of these numerical results has been criticized recently in [11], where it was argued that the so-called chaos length and chaos exponents $\zeta$ are not related to temperature chaos, and that temperature chaos is present for rare disorder samples even in small volumes, stressing the need to consider individual disorder samples rather than disorder averaged data. A new rare events based analysis method was introduced in this paper as the proper method to analyze temperature chaos numerically in spin glasses, with the outcome that there is indeed temperature chaos in the 3D EAI model with binary distributed quenched couplings, but it shows unexpected characteristics.

Concerning the Sherrington–Kirkpatrick (SK) model [12, 13], the infinite range version of the Edwards–Anderson model for which the mean field approximation is exact, no evidence for temperature chaos has been found numerically despite heroic efforts [14, 15], although the small excess observed in [15] at low $q$ in the overlap probability distribution $P(q_{T_1,T_2})$ for the largest system simulated could be interpreted as the onset of temperature chaos. It was later shown analytically [16, 17] that there is indeed temperature chaos in mean field spin glasses by computing, using Parisi replica techniques, the free energy cost paid in order to constrain two clones, at temperatures $T_1$ and $T_2$ respectively, to have a given non-zero overlap (namely to be correlated), and finding a non-zero solution. However, the effect is extremely weak in the case of the Sherrington–Kirkpatrick model, due to some accidental cancellations (for earlier analytical work on temperature chaos in the Sherrington–Kirkpatrick model see [18]–[20]). It has been argued that this weakness explains the negative results of [14, 15], and that it is hopeless to observe chaos numerically for the Sherrington–Kirkpatrick model.

Our aim in this paper is to challenge this pessimistic opinion and reinvestigate the question of temperature chaos in the Sherrington–Kirkpatrick model numerically, using the rare events method of [11]. It is indeed important to observe temperature chaos in the Sherrington–Kirkpatrick model numerically, since the current analytical methods are neither straightforward nor fully rigorous. We follow [11] closely to analyze the probability density function (pdf) of the reduced chaos overlap $X^J_{T_1,T_2}$ between two clones at temperatures $T_1$ and $T_2$ respectively, defined as

$$X^J_{T_1,T_2} = \frac{\langle q^2_{T_1,T_2} \rangle_J}{\left( \langle q_{T_1,T_2} \rangle_J \langle q^2_{T_2,T_2} \rangle_J \right)^{1/2}},$$

(1)

where $J$ is a quenched disorder sample and $q_{T_1,T_2}$ is the overlap between two independent spin configurations with the same disorder sample $J$ (two real replicas, a.k.a. clones) and temperatures $T_1$ and $T_2$ respectively. Namely, we study the fluctuations of $X^J_{T_1,T_2}$ with
respect to the quenched disorder $J$. Clearly, $0 \leq X^J_{T_1, T_2} \leq 1$. We use the data of [15] for the Sherrington–Kirkpatrick model with binary distributed quenched couplings, and system sizes $N = 256, 512, \ldots, 4096$. With the parallel tempering algorithm used in [14, 15] we have data for many couples of values of $T_1$ and $T_2$, but we concentrate our analysis on the values $T_1 = 0.4$ and $T_2 = 0.6$, in order to compare with the 3D EAI results of [11]. Indeed, on the one hand, it has been argued in [21] that for binary distributed quenched couplings the value $T = 0.4$ for the SK model is equivalent to the value $T = 0.703$ for the 3D EAI model (used in [11]). On the other hand, the ratio $(T_c - T_1)/(T_c - T_2)$ is the same in both situations. The value $T_1 = 0.4$ is anyway the lowest temperature in our parallel tempering data, and the value $T_2 = 0.6$ is a good compromise between accuracy (which decreases dramatically as $T_2$ decreases towards $T_1$) and the need to stay away from the critical point $T_c = 1$.

In figure 1 we show the histogram of $X^J_{0.4, 0.6}$ for $N = 256$ and 4096. If temperature chaos holds, this histogram should be concentrated at the origin ($X^J = 0$) for $N \to \infty$. At first glance the data show just the opposite, with a histogram that is peaked at a large value, $X^J \approx 0.9$, in both cases. There is, however, a remarkable broadening of the histogram as $N$ increases from $N = 256$ to 4096, with the appearance of a long low $X^J$ tail. Such a broadening is quite unusual in statistical physics, and can be interpreted as the onset of temperature chaos, as the following large deviation analysis shows.

Following [11] we consider the cumulative distribution function of the variable $X^J$, and introduce a large deviation (LD) potential $\Omega^N_{T_1, T_2}(\epsilon)$,

$$\text{Probability}[X^J_{T_1, T_2} < \epsilon] = 1 - e^{-N \Omega^N_{T_1, T_2}(\epsilon)}. \quad (2)$$

If this large deviation potential has a non-zero limit as $N \to \infty$ in some temperature interval around $T_1$ (obviously excluding $T_1$ itself), then temperature chaos holds, since $X^J_{T_1, T_2}$ vanishes in this limit (for any $J$).

We show in figure 2 the empirical large deviation potential $\Omega^N_{0.4, 0.6}(\epsilon)$, defined as $-1/N \ln(1 - \text{Probability}[X^J_{0.4, 0.6} < \epsilon])$, as a function of $\epsilon^2$. For small values of $\epsilon$, the data for our two larger systems $N = 2048$ and 4096 are compatible, making the case for a non-zero $N$ independent $\Omega^N_{0.4, 0.6}(\epsilon)$ for large $N$, and consequently for temperature chaos. We note that for small values of $\epsilon$ the finite size corrections make $\Omega^N_{0.4, 0.6}(\epsilon)$ smaller, strengthening the case for a non-zero $N \to \infty$ limit for $\Omega$. (For larger values of $\epsilon$, however, the finite size corrections make $\Omega$ larger.) A fit of the $N = 4096$ data for small values of $\epsilon$ shows that $\Omega^N_{0.4, 0.6}(\epsilon) \propto \epsilon^3$ with $\beta \approx 2.5$. The value $\beta \approx 1.7$ is reported in [11] for the 3D EAI model with binary couplings.

In a finite volume, temperature chaos weakens as $|T_2 - T_1|$ decreases, and the onset of chaos is pushed to higher and higher values of $N$. It has been suggested [11] that for

1 We have extended the statistics of [15] in order to have 1024 well thermalized disorder samples for each value of $N$. The number of parallel tempering sweeps (defined as a parallel tempering sweep per se plus a Metropolis sweep) is $10^6$ for measurements after $4 \times 10^5$ sweeps for equilibration, except for our largest system where these numbers are $2 \times 10^6$ and $8 \times 10^5$ respectively.

2 One should not confuse the large deviation potential $\Omega(\epsilon)$ with the coupled replica large deviation potential $\Delta F(q)$ of [16, 17]. The two objects are essentially different: the coupled replica potential describes events that are thermodynamically rare in typical samples, while the potential studied here describes thermodynamically typical events in rare samples. Nevertheless, the existence of a large deviation potential $\Omega(\epsilon)$ implies that typical samples are chaotic, as predicted by the non-zero $\Delta F(q)$ computed in [16].
Figure 1. Histograms of $X^J_{0.4,0.6}$ for $N = 256$ (left) and 4096 (right). Both histograms contain data for 1024 disorder samples. The histogram flattens as $N$ grows, with the appearance of a low $X$ tail that populates the whole allowed range.

Figure 2. The large deviation potential $\Omega^N_{0.4,0.6}(\epsilon)$ as a function of $\epsilon^2$ for system sizes $N = 256, 512, \ldots, 4096$. We use the standard Wald estimate for the statistical errors. Temperature chaos is absent for $N = 256$. For small values of $\epsilon$, the potential $\Omega^N_{0.4,0.6}$ increases as $N$ grows, reaching a limit (within statistical uncertainties) already for $N = 2048$. The solid line is a fit to the $N = 4096$ data. The data points with $\epsilon^2 \geq 0.2$ are excluded from this fit.

small $\epsilon$ and small temperature difference one has $\Omega^N_{0.4,0.6}(\epsilon) \propto \epsilon^\beta (T_2 - T_1)^b$ with $b \approx 1.8$ for the 3D EAI model. Our data for the SK model are compatible with such a scaling and a value $b \approx 3$, as shown in figure 3 for $N = 4096$. Due to large statistical errors in the small $\epsilon^\beta (T_2 - T_1)^b$ region where scaling holds, this is only a rough estimate. An extreme numerical effort would be needed in order to pinpoint precisely the value of the exponents $\beta$ and $b$. A method to either enrich the tail of the sample distribution corresponding to low values of $q_{T_1,T_2}$ or select the samples belonging to the tail before performing a lengthy Monte Carlo simulation would be of great help in this matter.

The analytical prediction [16, 17] for the SK model coupled replica large deviation potential $\Delta F(q)$ is that $\beta = 7/2$ and $b = 2$, but subleading terms are present which cause
transient effects in small volumes. This may explain the apparent discrepancy with our numerical results. Another possibility is that the exponents $\beta$ and $b$ are not the same for the potential $\Delta F(q)$ and the potential $\Omega(\epsilon)$ studied here.

In conclusion, we have reanalyzed our SK data using the new rare events based analysis method proposed in [11]. We find a clear signal for temperature chaos in the SK model, at the same evidence level as the results of [11] for the 3D EAI model. In both cases temperature chaos is best seen by analyzing individual quenched disorder samples: as $N$ grows, chaos first appears with rare samples that are very chaotic; chaotic samples are more numerous as $N$ keeps on growing; asymptotically, for values of $N$ far beyond numerical reach, all samples are chaotic. The finite size scaling of the distribution of chaotic samples is encoded in a large deviation potential that scales as a function of overlap squared, $\epsilon = q^2$, and temperature difference as $\Omega^N_{0.4,0.6}(\epsilon) \propto \epsilon^\beta(T_2 - T_1)^b$, and we give crude estimates of the values of the exponents $\beta$ and $b$.

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