Exact Enumeration of Ground States in the Sherrington-Kirkpatrick Spin Glass

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Using the discrete $\pm J$ bond distribution for the Sherrington-Kirkpatrick spin glass, all ground states for the entire ensemble of the bond disorder are enumerated. Although the combinatorial complexity of the enumeration severely restricts attainable system sizes, here $N \leq 9$, some remarkably intricate patterns found in previous studies already emerge. The analysis of the exact ground state frequencies suggests a direct construction of their probability density function. Against expectations, the result suggests that its highly skewed appearance for finite $N$ evolves logarithmically slow towards a Gaussian distribution.

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The Sherrington-Kirkpatrick (SK) model\textsuperscript{1} of glassy behavior in magnetic materials has provided a conceptual framework for the effect of disorder and frustration that are observed in systems ranging from materials\textsuperscript{2} to combinatorial optimization and learning\textsuperscript{3}. It’s conceptual simplicity is expressed through the Hamiltonian

$$H = \frac{1}{\sqrt{N}} \sum_{i<j}^N J_{i,j} \sigma_i \sigma_j, \tag{1}$$

in which all pairs of binary Ising spin-variables $\sigma_i = \pm 1$ are mutually connected through a bond matrix $J_{i,j}$, which is symmetric and whose entries are random variables drawn from a distribution $P(J)$ of zero mean and unit variance. We note that this Hamiltonian possesses a local “gauge”-invariance under the transformation of

$$\sigma_i \rightarrow -\sigma_i \quad \text{and} \quad J_{i,j} \rightarrow -J_{i,j}, \tag{2}$$

at any site $i$ and the bonds to all its adjacent sites $j$\textsuperscript{4}.

The SK model has reached significant prominence because, despite of its apparent simplicity, its solution proved surprisingly difficult, revealing an amazing degree of complexity in its structure\textsuperscript{5}. While it is solvable in principle, many of its features have not been derived yet. One such feature concerns the probability density function (PDF) of its ground state energies. Being an extreme element of the energy spectrum, the distribution of $e_0$ is not necessarily normal but instead may follow a highly skewed “extreme-value statistics” as can be derived for the Random Energy Model\textsuperscript{6}. If the energies within that spectrum are uncorrelated, it can be shown that the PDF for $e_0$ is among one of only a few universal functions. This extreme-value statistics of the ground states has been pointed out in Ref.\textsuperscript{5} and has received considerable attention recently\textsuperscript{6,7,8,9}. For instance, if the sum for $H$ in Eq. (1) were over a large number of independent terms, $H$ would be Gaussian distributed. In such a spectrum, the probability of finding $H \rightarrow -\infty$ decays faster than any power, and ground states $e_0$ should be distributed according to a Gumbel PDF,\textsuperscript{5}

$$g_m(x) \propto \exp \{m \left( x - e^x \right) \} \tag{3}$$

with $m = 1$, here generalized to the case where $m$ refers to the $m$-th lowest extreme value\textsuperscript{10}.

In a spin glass the individual terms in Eq. (1) are not independent variables and deviations from any universal behavior may be expected. In particular, these deviations should become strongest when all spin variables are mutually interconnected such as here in the SK model, but may be less so for sparse graphs, such as low-dimensional lattices. (Although it should be noted that sparsely connected systems seem to have a Gaussian PDF, see Ref.\textsuperscript{5}, provably so finite-dimensional lattices\textsuperscript{5,12}. Indeed, in mean-field models Refs.\textsuperscript{6,7,9,11} find numerically a highly skewed PDF for $e_0$ which does not fit to the Gumbel distribution in Eq. (3) for an $m = 1$-lowest value. In Fig. 1 we plot the rescaled PDF of ground state energies in the SK obtained in Ref.\textsuperscript{5} for $\pm J$ bonds on systems of size $N = 127 - 511$ with the extremal optimization (EO) heuristic\textsuperscript{12}. The result resembles that of Ref.\textsuperscript{7} to a surprising degree. In fact, a naive fit of Eq. (3) for variable $m$ to the SK-data, as suggested by Ref.\textsuperscript{7}, yields virtually identical results, with $m \approx 5$.

In this Communication, we derive the PDF in Eq. (3) \textit{analytically}, motivated from the study of exact enumerations of ground states in the SK for small $N$. We find an $N$-dependent parameter

$$m \sim \ln(N) \tag{4}$$

to leading order. As $m$ grows with $N$, the $g_m(x)$ ultimately develops a (symmetric) Gaussian form. Yet, $m$ grows sufficiently weakly to justify the highly skewed appearance of the PDF observed numerically over a wide range of sizes $N$, see Fig. 1.

Unlike for the Gaussian bond distribution, discrete bonds allow a complete enumeration of the ground-state
PDF for each possible bond structure at small system sizes \( N \). The motivation for such a study is provided by the hope to discern certain patterns in the solutions that may be extrapolated to the large-\( N \) limit. Looking at the PDF as a whole, we find at small \( N \) a highly skewed function. In Fig. 1 we show that the exact result for \( N = 9 \) compares quite well with the numerical sampling at larger \( N \), and with the Gumbel fit. A detailed analysis of the results at \( N \leq 9 \) suggests a direct construction of the PDF assuming only local gauge symmetry.

For the \( \pm J \) bond distribution, complete enumeration entails a generation of all possible symmetric \( N \times N \) bond matrices \( J_{i,j} \), filled with all combinations of \( J_{i,j} = +J \) or \( -J \). (Diagonal elements, corresponding to self-coupling terms, are zero.) For each instance, we then determine the ground state. Clearly, the combinatorial effort involved in merely generating all instances becomes prohibitive already for small \( N \), restricting us here to \( N \leq 9 \). For \( N = 9 \) the program runs for about 5h on a 2GHz computer. Larger \( N \) within reasonable CPU-time probably could have been reached with a more elaborate algorithm that recursively constructs from \( N - 1 \) to \( N \) only distinct instances by adding a new vertex with all possible bond combinations, and determines their ground state and their weight. We merely exploit the fact that we can always use Eq. 2 to gauge-transform to have one spin in any instance to, say, only possess \( J = +1 \) bonds, leaving us with \( (N-1)(N-2)/2 \) variable bonds or \( 2^{(N-1)(N-2)/2} \) instances at each \( N \).

In Tab. I we list the count \( n_{B}(N) \) for instances with \( B \) violated bonds, starting from the ferromagnetic (FM) instance with \( B = 0 \) to the totally anti-ferromagnetic (AFM) instance with

\[
B = B_{\text{max}} = \begin{cases} 
(N - 1)^2/4, & N \text{ odd}, \\
(N(N - 2))/4, & N \text{ even}. 
\end{cases}
\]

(5)

For instance, after accounting for the gauge symmetry, \( n_{0}(N) = 1 \) corresponds to the one instance with perfect ferromagnetic order, while on the bottom of each column we find the one perfect anti-ferromagnet with the largest number of violated bonds \( B_{\text{max}} \), which arises because the energy of the AFM is minimized when up and down spins divide as evenly as possible (still leaving about half of all \( \binom{N}{2} \) bonds violated). These numbers for \( N = 9 \), properly rescaled, are plotted in Fig. 1.

In an attempt to discern a pattern in the growth of these numbers, we found a few interesting facts. Starting for a given \( N \) at the FM instance \( (B = 0) \), we find

\[
n_{B}(N) = \left( \frac{\binom{N}{2}}{2} \right), \quad B < \left\lfloor \frac{N}{2} \right\rfloor,
\]

(6)

where \( \left\lfloor x \right\rfloor \) refers to the next-smallest integer to \( x \). In this regime, the \( n_{B}(N) \) instances with \( B \) bond violations are due to all possible embeddings of \( B \) independent \( -J \) bonds in the fully connected graph of size \( N \). FM order is preserved and each new \( -J \) bond increments the number \( B \) of violations. At \( B = \lfloor N/2 \rfloor \), a few embeddings, where all \( B \) of such \( -J \) bonds are connected to the same spin, can be gauge-transformed into instances of lower \( (N \text{ even}) \) or equal \( (N \text{ odd}) \) number of violations, reducing the number of independent instances below the prediction Eq. 6. In general, for further increasing \( B \), more and more \( -J \) bonds can be gauge-transformed away.
at spins where \( -J \) bonds equal or outnumber \( +J \) bonds. A similar behavior is observed starting with the AFM instance: initially each \( +J \) bond added serves to decrement the number of violated bonds without changing the AFM order. This leads to \( n_{B_{\text{max}}}(N) \) just as given in Eq. \( 6 \), but only for \( i \leq [(N-5)/2] \). Instances with \( i = [(N-3)/2] \) fewer bond violations than the AFM are suddenly far more numerous, consisting not only of those with \( i \) embedded \( +J \) bonds, but also certain instances with \( i + 2 \) such bonds, in particular \((i+2)\)-gons and \(-t\)-trees. While in the AFM state for a given \( N \) half of the spins are up, the other half down, adding \( i + 2 \) to the \( (N + 1)/2 \) connected \(+J\) bonds must link oppositely oriented spins, which does not help to reduce violated bonds.

Finding a closed form expression for the number of instances with a certain number of bond violations beyond these limits near the FM and the AFM instances appears difficult. But we can venture to make some approximations to capture the noticeable asymmetry in the PDF visible in Fig. 1. As mentioned above, Eq. \( 6 \) breaks down for larger numbers of \(-J\) bonds because instances with any spins having equal or more than half their bonds being \(-J\) can be gauge-transformed and may have to be discounted. A conceivable approximation than is to only count instances in which no spin has more than \([(N - 1)/2]\) of \(-J\) bonds, rejecting instances that could be gauge-transformed into other instances satisfying this condition. This approximation reproduces Eq. \( 6 \) exactly, and it predicts exactly that there are no instances with more than \( B_{\text{max}} \) Violated bonds as given in Eq. \( 6 \).

Based on these arguments, we now construct an analytic expression for \( n_B(N) \) for \( N \to \infty \). As above, we consider embedding a random graph \( ^{13} \) of \(-J\) bonds in a fully-connected graph otherwise filled with \(+J\) bonds. With the above condition, we assume that in each instance the number of \(-J\) bonds corresponds to the number of violations \( B \), which is not generally true. An added bond gives each spin a probability of \( 2/N \) to be linked to it. Then, the probability of a single spin having a degree \( d \) of \(-J\) bonds is \( p_d = \left( B/N \right)^d \left( 1 - 2/N \right)^{-d} \). Hence, the probability for a single spin to have a degree \( d < B_{\text{max}} = [(N - 1)/2] \sim N/2 \) is

\[
p_d < B_{\text{max}} \sim \sum_{d=0}^{N/2} \left( B/N \right)^d \left( 1 - 2/N \right)^{-d}. \tag{7}
\]

Naively assuming that each spin can be treated independently, an instance as a whole has a probability of \( p_d < B_{\text{max}} \) to be counted. For the total number of instances with \( B \) violations, we obtain

\[
n_B(N) \approx \left( B/N \right)^{N/2} \left( 1 - 2/N \right)^{-N/2}. \tag{8}
\]

Asymptotic analysis for \( N \to \infty \) with \( B = N^2/4 + v \), \( v \ll 1 \), shows that \( \left( B/N \right)^{N/2} \sim \exp\left\{-N^2v^2/4 \right\} \) at its peak. An similar evaluation of \( p_d < B_{\text{max}} \) in Eq. \( 7 \) for \( 1 \ll N \ll B \leq N^2/2 \) yields an internal saddle point \( \tag{14} \)

at \( d \sim 2B/N \) for \( B \ll N^2/4 \) where \( p_d < B_{\text{max}} \) \( \sim 1 \) with exponentially small corrections, whereas for \( N^2/4 \leq B \leq N^2/2 \) the sum in Eq. \( 6 \) can be evaluated at its upper limit, \( d = N/2 \), to yield

\[
p_d < B_{\text{max}} \sim \exp\{\sum_{d=0}^{N/2} \left( B/N \right)^d \left( 1 - 2/N \right)^{-d} \} \sim \exp\left\{-N^2/4 + v - \ln(1 + v) \right\}. \tag{9}
\]

Note that in the last exponential the linear term in \( v \) exactly cancels for \( v \ll 1 \). In that case, \( p_d < B_{\text{max}} \sim \exp\{\alpha vN/2 \} \) \( \sim \exp\{\alpha vN/2 \} \) provides an interpolation for both of its asymptotic regimes. Then, with \( v = 2w/N \), we obtain \( n_B(N) \propto e^{-w^2/(1 + \alpha w)^{1/2}} \) in Eq. \( 6 \). This result is indeed independent of \( N \) but a very poor (essentially Gaussian) fit of the data.

On the other hand, we may suppose that the cancellation is accidental, due to the neglect of nontrivial correlations in the above discussion, and assume that the more generic result in Eq. \( 10 \) is simple exponential, \( \exp\{\alpha vN/2 \} \) (with some \( \alpha > 0 \)), leading to an interpolation

\[
p_d < B_{\text{max}} \sim 1 + \exp\{\alpha vN/2 \}. \tag{11}
\]

With \( v = 2w/N \), we obtain

\[
n_B(N) \propto e^{-w^2/(1 + \alpha w)^{1/2}} \tag{12}
\]

This expression for \( N \to \infty \) has a moving saddle point \( \tag{14} \) at

\[
w_0 \sim -\frac{1}{\alpha} \left[ \ln \left( \frac{\alpha}{2} \right) - \ln \left( \frac{\alpha}{2} \right) + \frac{\ln \ln \left( \frac{\alpha N}{2} \right)}{\ln \left( \frac{\alpha N}{2} \right)} \right]. \tag{13}
\]

listing all orders in the expansion needed to facilitate a stationary saddle point. Transforming onto the saddle point by substituting \( w = w_0 + x/\alpha \) into Eq. \( 2 \) expanding in \( x \ll w_0 \) (i.e. \( x \ll \ln N \), so the \( x \)-domain spans the entire real line for \( N \to \infty \)), we finally obtain Eq. \( 3 \) with an \( N \)-dependent parameter \( m = -2w_0/\alpha \) which reduces to Eq. \( 4 \).

Finally, we can use the data in Tab. \( 1 \) also to consider the average number of violated bonds in the ground state. For each \( N \), this average is a rational number, the denominator being the total number of instances in the ensemble. Thus, the numerator provides a sequence of integers which is simply related to the average ground state energy. Tab. \( 1 \) shows the moments of the energy distribution. To retain integer numbers, we define

\[
\mathcal{E}_B(N) = 2B - \left( \frac{N}{2} \right), \tag{14}
\]

which is related to the true energy of an instance by \( E = \mathcal{E}_B(N)/\sqrt{N} \), according to Eq. \( 1 \). Then one would expect that \( \lim_{N \to \infty} \langle \mathcal{E}(N) \rangle / N^{3/2} \approx -0.7633 \), the Parisi solution for the ground state energy density of the SK model \( \tilde{\mathcal{E}}(N) \). Here, \( \langle \mathcal{E}(N) \rangle \) is the ratio of the value in the
TABLE II: List of the number of instances \( I \) and the first two moments (unnormalized) of the distributions listed in Tab. I for each \( N \). While the denominator is simply the number of instances, \( I = 2^\left(N - 1\right) \), the value in the third column is highly nontrivial with huge prime-factors. Even a partial identification of that sequence of numbers seems intractable.

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| \( N \) | \( I \) | \( \sum \beta E_{\beta n_B}(N) \) | \( \sum \beta^2 E_{\beta^2 n_B}(N) \) |
|-------|-----|----------------|----------------|
| 3     | 2   | -4             | 10             |
| 4     | 8   | -32            | 136            |
| 5     | 64  | -360           | 2176           |
| 6     | 1024| -8148          | 71664          |
| 7     | 32768| -338928       | 3645600        |
| 8     | 2097152| -28189776    | 388069088      |
| 9     | 268435456| -4294748800  | 70448532736    |

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