Extremal optimization for Sherrington-Kirkpatrick spin glasses

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Abstract. Extremal Optimization (EO), a new local search heuristic, is used to approximate ground states of the mean-field spin glass model introduced by Sherrington and Kirkpatrick. The implementation extends the applicability of EO to systems with highly connected variables. Approximate ground states of sufficient accuracy and with statistical significance are obtained for systems with more than $N = 1000$ variables using $\pm J$ bonds. The data reproduces the well-known Parisi solution for the average ground state energy of the model to about 0.01%, providing a high degree of confidence in the heuristic. The results support to less than 1% accuracy rational values of $\omega = 2/3$ for the finite-size correction exponent, and of $\rho = 3/4$ for the fluctuation exponent of the ground state energies, neither one of which has been obtained analytically yet. The probability density function for ground state energies is highly skewed and identical within numerical error to the one found for Gaussian bonds. But comparison with infinite-range models of finite connectivity shows that the skewness is connectivity-dependent.

1 Introduction

The Sherrington-Kirkpatrick (SK) model [1] has provided a rare analytic glimpse into the nature of frustrated spin glasses below the glass transition. It extends the notion of a spin glass on a finite-dimensional lattice introduced by Edwards and Anderson (EA) [2] to infinite dimensions, where all spin variables are infinitely connected and mean-field behavior emerges. In this limit, analytically intractable geometric properties of the lattice submerge. Consequently, the SK model simply establishes mutual bonds between *all* variables. Many features of this highly connected model have become analytically accessible with Parisi's replica symmetry breaking (RSB) scheme [3]. Only recently have RSB models with long-range but finite connectivity been analyzed successfully [4]. A comparable treatment of EA is still missing.

The SK model remains a topic of current research [5–7]. For one, its mathematical challenges, leaving certain scaling exponents as-of-now intractable, continue to inspire new theoretical approaches [8]. Furthermore, as scaling arguments [9,10] for EA suggest an entirely different picture, the fundamental question to the relevance of mean-field theory for any description of realistic systems at low temperature remains unanswered.

The challenge of the SK model is exemplified by the fact that it is an NP-hard problem to find the ground state of its instances [3]. Unlike in a spin model of ferromagnetism, in which couplings $J_{i,j} = 1$ always try to align neighboring spins, in a spin glass model like SK or EA, each spin is frustrated by a competition between randomly drawn, aligning and anti-aligning couplings (say, $J_{i,j} = \pm 1$) to its neighbors. As a result, its potential energy landscape is characterized by a hierarchy of valleys within valleys [11] with a number of local minima growing exponentially in the system size [3]. Since its low-energy landscape features prominently in its low-temperature properties, even numerical insights have been hard to come by. Some earlier work in this area has been focused on gradient descent [12,13] or Simulated Annealing algorithms [14], extrapolations to low temperatures from perturbative expansions near the glass transition [15], or on exact methods to enumerate low-lying energy values [16]. And even with the most sophisticated methods, like genetic algorithms (GA), accurate approximations have been limited to system size of $N \leq 300$ [5–7].

Here, we propose an alternative optimization procedure, based on the Extremal Optimization (EO) heuristic [17,18]. Our implementation of EO [19] is extremely simple and very effective, allowing to sample systems of sizes up to $N \approx 1000$ with sufficient accuracy and statistical significance. This approach produces results that not only verify previous studies by independent means, but also improve the accuracy. Previous studies [5,7] suggest that the fluctuation exponent of the ground state energies ρ is near to 3/4, excluding an earlier conjecture of

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5/6 [20,21]. Here, we double the size of the scaling regime to find $\rho = 0.750(3)$. These results strongly support analytical arguments by references [5,22] in favor of $\rho = 3/4$, assuming that such an exponent in a solvable model should be a simple rational number.

2 EO Algorithm

Our implementation of τ-EO proceeds as follows [17,18]: Assign to each spin variable $x_i(=\pm 1)$ a "fitness"

$$\lambda_i = x_i \sum_{j \neq i}^{N} J_{i,j} x_j, \qquad (1)$$

i.e. the (negative) local energy of each spin, so that

$$H = -\frac{1}{2\sqrt{N}} \sum_{i=1}^{N} \lambda_i \qquad (2)$$

is the familiar Hamiltonian of the SK model. For general bond matrices $J_{i,j}$, such as those drawing from a continuous Gaussian bond distribution with varying bond-weights attributed to different spins, more refined definitions of λ_i should be used [17,25]. Here it is conceptually and computationally most convenient to draw discrete bonds J from $\{-1, +1\}$ with equal probability, such that $\langle J \rangle = 0$ and $\langle J^2 \rangle = 1$.

A local search with EO [17] ideally requires the ranking of the fitnesses λ_i from worst to best before each update,

$$\lambda_{\Pi_1} \leq \lambda_{\Pi_2} \leq \ldots \leq \lambda_{\Pi_N}, \qquad (3)$$

where $i = \Pi_k$ indicates spin x_i as having the k-th ranked fitness. At each update, one spin of low fitness is forced to change *unconditionally*. Since EO does not converge to a specific configuration, it outputs the best-found after a certain number of updates.

Following reference [17], it is most expedient to *approximately* order the λ_i in equation (3) instead on a binary tree of depth $O(\log_2 N)$ with the least-fit spins ranking near the root. Unlike for sparse bond-matrices [18], flipping one spin also changes the fitness of *all* other spins, albeit by a small amount, $\Delta\lambda_i/\lambda_i = O(1/N)$. To avoid the cost of $O(\log N)$ for re-ordering the entire tree each update, a *dynamic* ordering scheme is used here: all λ_i are re-evaluated, but the tree is parsed only *once*, node-by-node, starting at the root. The fitness on the current node is only compared with its two sub-nodes and exchanged, iff its fitness is better. In this way, a newly improved fitness can be moved away from the root several times, but newly worse fitnesses move at most one step towards the root. Yet, a spin which suddenly attained a low fitness would move to the root at most within $O(\log_2 N)$ updates. Hence, re-ordering of fitnesses occurs faster than mis-orderings can escalate because $\Delta\lambda/\lambda \ll 1$.

In a τ-EO update, a spin is selected according to a scale-free probability distribution $P(k) \sim k^{-\tau}$ over the ranks $k \in \{1, \ldots, N\}$ in equation (3). Since the ranking
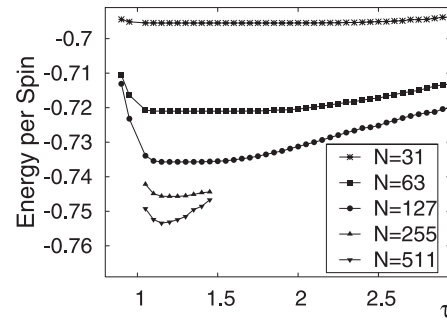

Fig. 1. Plot of the average best energy per spin found by EO as a function of the parameter τ. For each system size N, a set of test instances were created and optimized with τ-EO, each for N^3 update steps. Each data point represents the average over the best-found energies obtained with that τ. In accordance with Ref. [26], the optimal choice for τ within the given runtime moves closer to unity slowly with increasing system size. Within the range of N used here, a fixed $\tau \approx 1.2$ appears to be effective.

here is not linear as in equation (3) but on a tree, a level l, $0 \leq l \leq \lfloor \log_2(n) \rfloor$ is selected with probability $\sim 2^{-(\tau-1)l}$, and one randomly chosen spin on the lth level of the tree is updated [17]. In this manner of ranking and selecting from a binary tree, an ideal selection according to $P(k)$ is approximated while saving $O(N)$ in the computational cost. Tests show, in fact, that the τ-dependence for optimal performance of this algorithms follows the generic behavior described in reference [26], see Figure 1. EO at $\tau = 1.2$ finds consistently accurate energies using $O(N^3)$ update steps in each run, at least for $N \leq 1000$, verified by the fact that our data reproduces the exactly known energy of the SK to about 0.01%, see Figure 2. Including the linear cost of recalculating fitnesses and dynamic ordering, the algorithmic cost is $O(N^4)$. Runs take between ≈ 1 s for $N = 63$ to ≈ 20 h for $N = 1023$ on a 2 GHz Athlon CPU.

It is not at all obvious that EO would be successful in an environment where variables are highly connected. So far, EO has only obtained good results for systems where each variable is connected only to $O(1)$ other variables for $N \rightarrow \infty$. The update of a single variable hence impacts the extensive energy of the system only to subleading order, and only $O(1)$ variables need to rearrange their fitness. Applications of EO to highly connected systems, where each degree of freedom is coupled to most others over long-range interactions, proved unsatisfactory: for instance, in a continuum polymer model [27] with torsion angles between chain elements as variables, even a minute rotation leads to macroscopic changes in the total energy, and almost all moves are equally detrimental. In that case, criteria for move rejection are necessary, which are decidedly absent from EO so far. But for the SK in a update near E_0 we estimate $\Delta E/E = \sum_i \Delta\lambda_i / \sum_i \lambda_i \ll \sum_i(\Delta\lambda_i/\lambda_i) \sim 1/\sqrt{N}$, assuming a sum over terms with random signs. In fact, the ability to sustain roughly $\sqrt{N}$ perturbations to the system before altering the macroscopic state may be one of the advantages of EO.

Table 1. List of our computational results to approximate ground state energies e_0 of the SK model. For each system size N, we have averaged the energies over I instances and printed the rescaled energies $\langle e_0 \rangle$, followed by the deviation $\sigma(e_0)$ in equation (5). Given errors are exclusively statistical.

N	I	$\langle e_0 \rangle$	$\sigma(e_0)$
15	380 100	$-0.64445(9)$	0.0669(3)
31	380 100	$-0.69122(8)$	0.0405(2)
49	500 000	$-0.71051(6)$	0.0293(1)
63	389 100	$-0.71868(3)$	0.0246(1)
99	500 000	$-0.73039(3)$	0.01763(7)
127	380 407	$-0.73533(2)$	0.01468(7)
199	351 317	$-0.74268(2)$	0.01043(5)
255	218 473	$-0.74585(2)$	0.00862(5)
399	15 624	$-0.75029(5)$	0.0061(1)
511	25 762	$-0.75235(3)$	0.0051(1)
799	725	$-0.7551(1)$	0.0037(4)
1023	244	$-0.7563(2)$	0.0029(6)

3 Numerical results

Extensive computations to determine ground state energies per spin, e_0, of about $I = 5 \times 10^5$ instances for $N \leq 100$ to just $I \approx 250$ instances for $N = 1023$ have yielded the results listed in Table 1. Note that all values chosen for N are odd. Using $N = 2^i - 1$ was convenient to ensure a complete filling of all levels on the tree ranking the fitnesses in Section 2. Subsequently, we added data at intermediate values of N. For smaller N there was a minute but noticeable deviation in the behavior of $\langle e_0 \rangle$ between even and odd values of N, with even values leading to consistently lower $\langle e_0 \rangle$. Either set of data extrapolates to the same thermodynamic limit, with the same corrections-to-scaling exponent, but appears to differ in the amplitude of the scaling corrections. This behavior is consistent with the findings for even and odd-connectivity Bethe lattices [28]. (Note that even N here implies odd connectivity for each spin in the SK model, and vice versa.)

We have plotted $\langle e_0 \rangle$ vs. $1/N^{2/3}$ in Figure 2. The data points extrapolate to $-0.76324(5)$, very close to the best known Parisi energy of $-0.76321(3)$ [15]. All data shown in Fig. 2 fits to the asymptotic form $\langle e_0 \rangle_N = \langle e_0 \rangle_\infty + a/N^\omega$ with a goodness-of-fit $Q \approx 0.7$. The fit gives for the exponent for scaling corrections $\omega = 0.672(5)$, or $2/3$ within 1%. This is consistent with analytical results for scaling corrections obtained near T_g [29] and with numerical studies of ground state energies [5,7] for the SK model, but also with EO simulations of spin glasses on finite-connectivity Bethe lattices and ordinary random graphs [30].

The large number of instances for which estimates of e_0 have been obtained allow a closer look at their distribution. The extreme statistics of the ground states has been pointed out in reference [31] and studied numerically in references [6,7]. Being an extreme element of the energy spectrum, the distribution of e_0 is not normal but follows a highly skewed "extremal statistics" [31]. If the energies within that spectrum are uncorrelated, it can be shown that the distribution for e_0 is among one of only
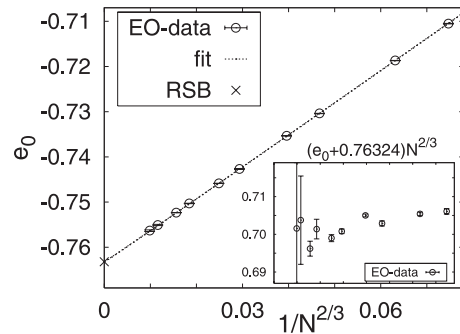

Fig. 2. Extrapolation of the data for $\langle e_0 \rangle$ in Table 1 for $N \to \infty$. The exact result of $-0.76321(3)$ ($\times$) is reproduced within 0.01% accuracy. The near-linear behavior of the fit yields a scaling-correction exponent of $\omega = 2/3$ to about 1%. The inset shows the same data, subtracted by -0.76324 and rescaled by $N^{2/3}$, which now extrapolates to the amplitude of the scaling corrections at $\approx 0.70(1)$. Despite "peeling off" layers of the asymptotic behavior, the data remains quite coherent, attesting to the accuracy of the EO heuristic.

a few universal functions. For instance, if the sum for H in equation (2) were over a large number of *uncorrelated* random variables λ_i, H would be Gaussian distributed. In such a spectrum, the probability of finding $H \to -\infty$ decays faster than any power, and ground states e_0 would be distributed according to a Gumbel distribution, [7,31]

$$g_m(x) = w \exp \left\{ m \frac{x-u}{v} - m \exp \left[\frac{x-u}{v} \right] \right\} \quad (4)$$

with $m = 1$, where m refers to the m th lowest extreme value.

Clearly, in a spin glass the local energies λ_i are not uncorrelated variables and deviations from the universal behavior may be expected. In particular, these deviations should become strongest when all spin variables are directly interconnected such as in the SK model, but may be less so for sparse graphs. Indeed, in the SK model with Gaussian bonds references [6,7] find numerically highly skewed distributions for e_0 which do not fit to the Gumbel distribution in equation (4) for $m = 1$. In Figure 3, we plot the rescaled distribution of ground state energies obtained here for $\pm J$ bonds. The result resembles those of reference [7] to a surprising degree. In fact, a naive fit of equation (4) for variable m to the SK-data, as suggested by reference [7], yields virtually identical results, with $m \approx 5$. This may indicate a high degree of universality with respect to the choice of bond distribution in the SK model, or a new universality class of extreme-value statistics for correlated variables. In Figure 3 we have also included data for $k + 1$-connected Bethe lattices from reference [28] for $k + 1 = 3$ and 25, which seem to suggest a smooth interpolation in k between a normal distribution and the SK result. Hence, while the distribution of e_0 seems to be universal with respect to bond distribution, its connectivity-dependence appears to disfavor the existence of a (unique) universal extreme-value statistic for correlated energies (see also reference [32]).
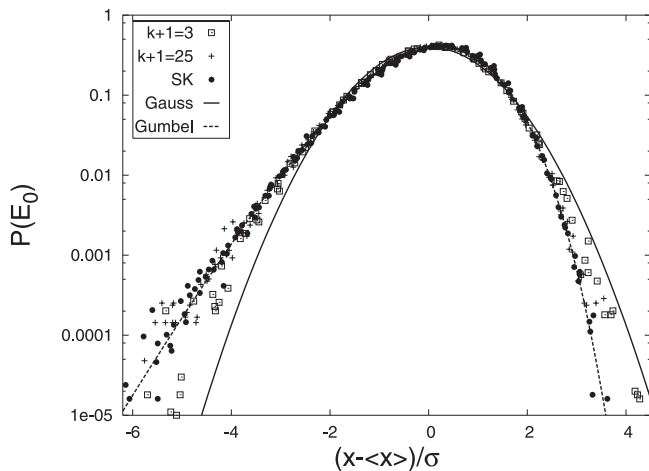
Fig. 3. Plot of the rescaled probability distribution of ground state energies using $\pm J$ bonds. Shown are the data for the SK model and for Bethe lattices of connectivity $k + 1 = 3$ and 25 from reference [28]. The data for increasing k seems to evolve away from a Gaussian (solid line) towards the SK data ($k = \infty$), the latter fitted by equation (4). The values obtained in the fit (dashed line) are $u = 0.26$, $v = 2.23$, $w = 90$, and $m = 5.4$.

We now consider the scaling of the standard deviations in the distribution of e_0 with respect to system size,

$$\sigma(e_0) = \sqrt{\langle e_0^2 \rangle - \langle e_0 \rangle^2} \sim N^{-\rho}. \qquad (5)$$

where ρ is the fluctuation exponent. Similarly, the fluctuations of e_0 appear to be narrower than normal, with $\rho > 1/2$ in equation (5). Early theoretical work [20,21] suggested a value of $\rho = 5/6$. More recent numerical work [5,7] instead is pointing to a lower value. Reference [22] has advanced an alternative argument in favor of $\rho = 3/4$, based on corrections in the zero-mode of the propagator due to fluctuations.

In Figure 4 the numerical results for the standard deviations in the distribution of ground state energies e_0 is shown. The asymptotic scaling for $N \geq 63$ is certainly very close to $\rho = 3/4$. The crossover toward asymptotic behavior is similar to the results found for Gaussian bonds using a GA (see Fig. 1 in Ref. [7]), except that the EO data reaches about half a decade further into the asymptotic regime. A fit, weighted by the statistical error, to the data points in the scaling regime yields $\rho = 0.750(3)$, or 3/4 within 0.4%, with a goodness-of-fit $Q = 1$. As the inset of Figure 4 shows, any apparent trend towards a higher value [7] then $\rho = 3/4$ is easily explained in terms of scaling corrections, for instance, in powers of $1/N^{1/4}$.

4 Conclusions

We have shown that the extremal optimization heuristic can be extended successfully to highly connected systems. Results for the ground states of the SK model are consistent with previous studies while reaching assuringly
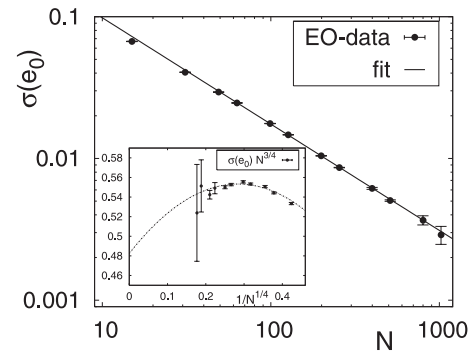

Fig. 4. Plot of the standard deviation in the distribution of ground state energies e_0 vs. the system size N. Asymptotic scaling sets in for $N \geq 63$, clearly favoring $N^{-3/4}$. A fit (full line) of these data points extrapolates to $\rho = 0.7500(29)$. The inset shows the same data reduced by the predicted asymptotic scaling, $\sigma(e_0)/N^{-3/4}$, as a function of $1/N^{1/4}$. Any deviation from $N^{-3/4}$-scaling would appear as divergent behavior for $N \to \infty$. Instead, the scaling corrections are well-captured, say, by a simple parabola in $1/N^{1/4}$.

larger systems sizes. These results provide more confidence into conjectures about as-of-yet unobtainable scaling exponents. Comparison with data for $k + 1$-connected mean-field spin glasses on Bethe lattices suggest a smooth interpolation in k for the extreme-value statistic of the ground-state energy between a Gaussian distribution for small k and a highly skewed Gumbel distribution with $m \approx 5$ for the SK model ($k \to \infty$).

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