Spin glasses and algorithm benchmarks:
A one-dimensional view

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Abstract. Spin glasses are paradigmatic models that deliver concepts relevant for a variety of systems. However, rigorous analytical results are difficult to obtain for spin-glass models, in particular for realistic short-range models. Therefore large-scale numerical simulations are the tool of choice. Concepts and algorithms derived from the study of spin glasses have been applied to diverse fields in computer science and physics. In this work a one-dimensional long-range spin-glass model with power-law interactions is discussed. The model has the advantage over conventional systems in that by tuning the power-law exponent of the interactions the effective space dimension can be changed thus effectively allowing the study of large high-dimensional spin-glass systems to address questions as diverse as the existence of an Almeida-Thouless line, ultrametricity and chaos in short range spin glasses. Furthermore, because the range of interactions can be changed, the model is a formidable test-bed for optimization algorithms.

1. Introduction
Spin glasses pose formidable challenges not only theoretically, but also numerically [1]. Because analytically only the mean-field Sherrington-Kirkpatrick (SK) model [2] can be solved exactly, most of the research on realistic short-range systems—such as the Edwards-Anderson Ising spin glass [3]—is performed numerically. Due to diverging equilibration times in Monte Carlo simulations of spin glasses, as well as an extra overhead because of configurational averaging, only small systems can be studied. In order to probe the thermodynamic limit it is therefore of paramount importance to use fast algorithms, improved models, and large computer clusters.

Technological advances in the last decade have enabled the construction of powerful multiprocessor machines out of commodity components at low cost. Still, the numerical effort required to study conventional short-range spin glasses for low enough temperatures and large enough system sizes exceeds the CPU time delivered by an average computer cluster. Therefore, in addition to hardware advances, novel algorithms need to be developed and tested, and improved models have to be used.

In this work we emphasize the importance of the choice of model when studying spin glasses: the one-dimensional spin glass with power-law interactions allows the study of large systems for effectively high space dimensions. Furthermore, the model is an excellent algorithm benchmark to test and improve modern algorithms to study complex systems. The model has the advantage, in that by tuning the power-law exponent of the interactions the universality class (effective space

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dimension) as well as the complexity of the system can be changed. In what follows the model is introduced in detail. In addition, past applications to the nature of the spin-glass state [4, 5], ground-state energy distributions in spin glasses [6] and the existence of a spin-glass state in a field [7] are presented. Furthermore, new applications to field chaos and ultrametricity in spin glasses, as well as local-field distributions in spin glasses are presented. Finally, future applications of the model to answer problems in the physics of spin glasses are described, as well as applications to algorithm development and testing.

2. Model

The one-dimensional Ising spin glass with power-law interactions is given by the Hamiltonian [8, 9, 10, 4, 5, 6, 7]

\[ H = - \sum_{i<j} J_{ij} S_i S_j, \quad J_{ij} = c(\sigma) \epsilon_{ij} r_{ij}^\sigma, \quad r_{ij} = \frac{L}{\pi} \sin \left( \frac{\pi|\sigma|}{L} \right), \]

where \( S_i \in \{\pm 1\} \) are, for example, Ising spins and the sum ranges over all spins in the system. In equation (1) the \( \epsilon_{ij} \) are chosen from a Gaussian distribution of zero mean and standard deviation unity, and \( c(\sigma) \) is a constant which is chosen such that the model has a mean-field transition temperature \( T_{c,\text{MF}} = 1 \) (see reference [4] for details). To ensure periodic boundary conditions the spins are placed on a circular chain of circumference \( L \) and the distance \( r_{ij} \) between two spins \( i \) and \( j \) is thus given by the geometric distance on the circle topology. The model has a very rich phase diagram in the \( d-\sigma \) plane, see figure 1. Note that here we study the model in one space dimension, i.e., \( d = 1 \), which corresponds to the thick horizontal (white) line in the figure. By changing the power-law exponent \( \sigma \) the universality class as well as the range of the interactions of the model can be changed continuously for a large range of system sizes. This has the advantage that the model can be used to test the applicability of several theoretical predictions made for the mean-field SK model for finite-range systems. Furthermore, the scaling of different algorithms strongly depends on the interaction range between the spins. While the system is always fully connected, the range of the interactions and henceforth the effective space dimension of the model can be tuned as well. Therefore the model is an ideal benchmark for different optimization algorithms.

3. Application to spin-glass problems: past, present, and future

In what follows an overview over different problems in the field of spin glasses studied with the one-dimensional Ising chain are discussed, as well as current and future applications.

Nature of the spin-glass state

Traditionally, two main pictures have been used to describe the nature of the spin glass state: replica symmetry breaking (RSB) [11, 12, 13, 14] and the droplet picture [15, 16, 17, 10, 18]. Replica symmetry breaking predicts that droplet excitations involving a finite fraction of the spins cost only a finite energy in the thermodynamic limit. This can be tested by studying the distribution of the spin overlap \( P(q) \) at \( q = 0 \) [19, 20]. Scaling relations predict that \( P(q = 0) \sim L^{-\theta} \) with \( \theta = 0 \). Furthermore, the fractal dimension of the excitations is the same as the space dimension, i.e., \( d_s = d \). In contrast, for the droplet picture one expects \( \theta' \neq 0 \) and \( d - d_s < 0 \), i.e., excitation energies diverge as \( E \sim L^{\theta} \) in the thermodynamic limit and the surface of the excitations is fractal [16, 17, 10, 18]. Simulations of the one-dimensional Ising spin glass with power-law interactions have shown that, for system sizes \( L \) considerably larger than in higher-dimensional models [20], an intermediate scenario emerges [4, 5, 21]—known as TNT for “trivial–nontrivial”—where excitations cost a finite energy but their surfaces are fractal [22, 23] in the thermodynamic limit.
Figure 1.
Sketch of the phase diagram in the $d$-$\sigma$ plane of the long-range spin glass with power-law interactions. This work focuses only on $d = 1$, which corresponds to the horizontal white arrow. By tuning the power-law exponent $\sigma$, different universality classes can be probed: For $\sigma \leq 1/2$ ($d = 1$) the system is in the infinite-range SK universality class. For $1/2 < \sigma \leq 2/3$ the model exhibits a mean-field behavior corresponding to an effective space dimension $d_{\text{eff}} \geq 6$, where $d_{\text{eff}} \approx 2/(2\sigma - 1)$ for $1/2 \leq \sigma \leq 1$. The thick (red) line separates mean-field from non-mean-field behavior. For $2/3 < \sigma < 1$ the model is a long-range spin glass with a finite ordering temperature $T_c$, whereas for $1 \leq \sigma < 2$ the long-range spin glass has $T_c = 0$. When $\sigma \geq 2$ $[\sigma_c(d)]$ the model is short-ranged with zero transition temperature. Figure adapted from reference [4].

Ground-state energy distributions in spin glasses
There has been considerable work in understanding the behavior of ground-state energy distributions for the mean-field SK model [24, 25, 26, 27]. In particular, it has been shown that the ground-state energy distributions can possibly be fitted to modified Gumbel distributions [28, 29]. Work on short-range systems—only possible for small system sizes [30]—suggest Gaussian ground-state energy distributions in the thermodynamic limit. Thus the one-dimensional Ising chain offers itself as an ideal model to test the shape of the distributions when leaving the infinite-range universality class.

Results [6] have shown that for $\sigma \leq 0.5$, where the model exhibits infinite-range behavior, the skewness of the distributions tends to a constant in the thermodynamic limit, indicating that the data cannot be fitted properly with a Gaussian. For $\sigma > 0.5$, the skewness decays with a power law of the system size, indicating that outside the infinite-range region the ground-state energy distributions become Gaussian in the thermodynamic limit [31]. This shows that the infinite-range SK model shows a singular behavior in this respect [32].

Existence of an Almeida-Thouless line in short-range spin glasses
There has been an ongoing debate as to whether short-range spin glasses order in a field or not [33, 34, 35, 36, 37, 38, 39, 40, 41, 42]. Simulations of three-dimensional Ising spin glasses [41] suggest that the de Almeida-Thouless line [43], which exists for the mean-field SK model, does not exist for realistic short-range Ising spin glasses. While the aforementioned results found by studying the two-point correlation length [44] provide strong evidence that short-range spin glasses do not order in a field, there are some open questions. First, the system sizes simulated in reference [41] are not very large. Furthermore, it is unclear if short-range systems above the upper critical dimension order in a field or not because simulations of high-dimensional spin glasses are extremely difficult to perform, especially in an externally applied field.

Katzgraber and Young have simulated the one-dimensional Ising chain in a field for different values of the exponent $\sigma$ [7] and find that there is no de Almeida-Thouless line for the range
of the power-law exponent corresponding to a non-mean-field transition in zero field ($\sigma > 2/3$). This suggests that there is no de Almeida-Thouless line for short-range spin glasses below the upper critical dimension. In Figs. 2 and 3 data for a small external field $H_R = 0.10$ for $\sigma = 0.55$ (mean-field regime) and 0.75 (below the upper critical dimension), are shown. While the data for the correlation length—which scales as $\xi L/L = \tilde{X} (L^{1/\nu} (T - T_c(H_R)))$—cross for $\sigma = 0.55$ suggesting that there is a spin-glass state at finite fields, this is not the case for $\sigma = 0.75$ where simulations down to very low temperatures $|T T_c(H_R = 0)| \approx 0.69(1)$ have been performed. Data for $\sigma \approx 2/3$ where the one-dimensional Ising chain changes from the mean-field to the non-mean-field universality class show marginal behavior (not shown). Details about the simulation can be found in reference [7].

![Figure 2](image2.png)

**Figure 2.** Two-point correlation length at finite field for $\sigma = 0.55$. The data cross at $T_c \approx 0.95$ suggesting that there is a spin-glass state in a field. The system is in the mean-field yet not in the SK universality class. Figure adapted from reference [7].

![Figure 3](image3.png)

**Figure 3.** Two-point correlation length at finite fields for $\sigma = 0.75$. The data do not cross even for extremely low $T$ suggesting that there is no spin-glass state in a field. The system is in the non-mean-field universality class. Figure adapted from reference [7].

**Field chaos in spin glasses**

The chaotic response of spin glasses to small perturbations in the temperature, disorder, or externally applied field have been predicted a long time ago [45, 46] and analyzed on the basis of scaling arguments [16, 47]. Recently, Katzgraber and Krzakala have shown that temperature and disorder chaos in three-dimensional spin glasses can be observed using scaling laws [48] at low enough temperatures and that both perturbations seem to share the same scaling functions (although there was general consensus that disorder chaos is observable in spin glasses [49, 50, 51, 52, 53]).

We have studied the effects of small perturbations in the field [54, 55, 56] on the equilibrium state of the one-dimensional Ising spin chain at low but nonzero temperature. Following previous studies [54, 50, 51, 48, 55] we study field chaos when the field between two replicas of the system with the same disorder is shifted by an amount $\Delta H$. To study the effects of the perturbation
we compute the chaoticity parameter $Q$ given by

$$Q_{\Delta H} = \left[ \frac{\langle q_{00}^2 \Delta H \rangle}{\sqrt{\langle q_{00}^2 \rangle \langle q_{\Delta H, \Delta H}^2 \rangle}} \right]_{av} \sim \tilde{Q}[\Delta H/L^{\theta/d - 1/2}].$$

(2)

In equation (2) $q_{a,b} = L^{-1} \sum_i S_i^a S_i^b$ is the spin overlap between configurations $a$ and $b$ at different fields, $\langle \cdots \rangle$ represents a thermal average, and $[\cdots]_{av}$ a configurational average. Our results show that the data for the chaoticity parameter $Q$ can be scaled according to the scaling behavior presented in equation (2) with $d = 1$ and $\theta \approx 0$ for very low temperatures $T = 0.1 \ll T_c$. These preliminary results for small system sizes $L$ and few values of $\Delta H$ suggest that field chaos could be present in short-range as well as long-range spin glasses.

\begin{figure}
\centering
\includegraphics[width=0.5\textwidth]{chaoticity.png}
\caption{Chaoticity parameter $Q$ as a function of $\Delta H/L^{\sigma/4 - 1/2}$ for $\sigma = 0.00$ and 0.75 and (random) fields of strength $\Delta H = 0.01, 0.05, 0.07, 0.10, \text{ and } 0.15$ for $T = 0.10$ ($L = 16, 32, 64, \text{ and } 128$). The data for different fields collapse onto universal curves for the different values of $\sigma$ and $\theta \approx 0$. Note that for the SK model the data should collapse with $\Delta H/L^{3/8}$ [55]. This is not the case for the present results (work in progress [57]).}
\end{figure}

Ultrametricity in spin glasses

One of the cornerstones of the Parisi solution of the mean-field Sherrington-Kirkpatrick model is the concept of ultrametricity [58], but it is unclear if realistic short-range spin glasses exhibit this property in the low-temperature phase [59, 60]. Ultrametricity can be described as follows: Consider an equilibrium ensemble of states at $T < T_c$ and pick three, $\rho$, $\mu$ and $\nu$, at random. These indices are associated with the states $S_\rho$, $S_\mu$ and $S_\nu$. Order them so that the overlap $q_{\mu\nu} = L^{-1} \sum_i S_i^{\mu} S_i^{\nu}$ between them satisfies $q_{\mu\nu} \geq q_{\nu\rho} \geq q_{\mu\rho}$. Ultrametricity means that in the thermodynamic limit, we obtain $q_{\nu\rho} = q_{\mu\rho}$ with probability 1. Recent results on small three-dimensional systems suggest that short-range spin glasses do not possess this characteristic of the mean-field model [61], although opposing opinions [62] exist. Capitalizing on the success of the one-dimensional Ising spin glass with power-law interactions in elucidating different properties of spin glasses we have studied ultrametricity in spin glasses for different exponents $\sigma$.

In Figs. 5 and 6 we show preliminary sorted dendrograms using Ward’s method [63] for the SK model and the one-dimensional Ising chain for $\sigma = 0.75$ (data for $L = 512$, $T = 0.20$). Displayed are equilibrium states in configuration space. The distance between the states in the distance matrix is color coded (darker color corresponds to closer distances). The states are sorted linearly, where the order is determined from the hierarchical clustering [63] of the tree-structure of the underlying dendrogram (bottom panel in the figures). The clustering procedure starts with $L$ clusters which contain one state and the two closest lying clusters are merged (joining lines in the dendrogram). This procedure is repeated until one large cluster is obtained.
There is clearly structure in the dendrograms and a valid hierarchical clustering corresponds to an ultrametric structure of space [64]. Note that this is not the case for $T > T_c$ where the dendrograms show no structure at all (not shown). To further strengthen the aforementioned results, a finite-size scaling analysis of the data will be performed (work in progress [65]).

**Local-field distributions in spin glasses**

The distribution of local fields $P(h = \sum_j J_{ij} S_j, T)$ at a temperature $T$ has been of interest since the early days of spin glasses [66, 67, 68]. In particular, the behavior of the mean-field SK model is well understood [69, 70, 71, 72]. On the other hand, there has been little work for short-range Edwards-Anderson spin glasses since these can only be studied numerically.

It has been shown for the mean-field SK model that $P(h) \sim a|h|$ for $h \to 0$ and $T = 0$ in the thermodynamic limit. This suggests that spins with zero local field exist, i.e., domain walls can move freely at no energy cost in the system. Simulations for short-range finite-dimensional systems and intermediate system sizes have shown (unpublished work [73]) that $P(h) \sim c + a|h|$ for space dimensions $d \geq 2$ with possibly a finite value of $c$ in the thermodynamic limit. We have calculated the local field distribution for the one-dimensional Ising spin chain for different values of $\sigma$. Extrapolating the data to $T = 0$ we can study the behavior of $P(h = 0, T = 0) = c$ as a function of the system size $L$. Our results show that while for the SK model $c = 0.006(9)$, i.e., $P(h = 0, T = 0)|_{L \to \infty} \to 0$, for $0.5 < \sigma < \infty$ finite values of $c$ in the thermodynamic limit are obtained, e.g., for $\sigma = 0.75$ $c = 0.021(1)$. This again highlights the singular behavior of the
Future directions
So far the model has primarily been used to study properties of Ising spin glasses. A possible future direction would be to study versions of the model with different spin symmetries or dilution (which might allow the simulation of larger systems). For example, there has been considerable interest in the nature of the spin-glass state of the three-dimensional Heisenberg spin glass [74, 75, 76, 77]. In particular, it is unclear if spin and chirality degrees of freedom decouple. Recently, a one-dimensional Heisenberg chain with power-law interactions [78] has been studied in an attempt to answer this problem. There, simulations for $\sigma = 1.1$ where $T_c$ for the spin-glass sector is zero have been interpreted as a spin-chirality decoupling scenario since the chiralities showed a nonzero transition temperature. The model could also be extended to study XY spins. Furthermore, nonequilibrium properties in spin glasses [79] can also be studied for large system sizes. Finally, modifications of the Hamiltonian might be used to address problems in different fields, e.g., a $p$-spin version [80] of the one-dimensional Ising spin chain to study structural glasses (work in progress).

4. Algorithm benchmarking
The development (and testing) of algorithms to study systems with complex energy landscapes [81, 82] plays a crucial role in the field of statistical mechanics of disordered systems, as well as many interdisciplinary applications to other fields. We discuss some examples below.

In the past [21] we have used exchange Monte Carlo [83] to obtain ground-state energies for spin-glass systems [84]. In this technique, one simulates several copies of the system at different temperatures, and, in addition to the usual local Monte Carlo moves, one performs global moves in which the temperatures of two copies with adjacent temperatures are exchanged to overcome energy barriers in complex energy landscapes. By choosing a low enough minimal temperature, the ground state of the system can be probed. Interestingly, the algorithm works well for small values of the exponent $\sigma$, whereas for large $\sigma$ exchange Monte Carlo does not equilibrate in reasonable amounts of time—possibly because it is difficult to push domain walls out of the system. Conversely, the branch, cut & price algorithm [85, 86, 87] works best for large $\sigma$ values (see figure 7), i.e., in this case complementing exchange Monte Carlo.

Recently, the hysteretic [89] and extremal [90, 26] optimization methods have been introduced to heuristically estimate ground-state energies of spin glasses. Hysteretic optimization successively demagnetizes the system at zero temperature with some additional shake-ups until states close to the ground state are reached. In a recent project, Gonçalves and Böttcher [88] have studied the efficiency of hysteretic optimization when computing ground-state energies of the one-dimensional Ising chain as a function of the exponent $\sigma$. Their results clearly show that the method works best for infinite-range models ($\sigma \leq 0.5$) where avalanches in the hysteresis loops proliferate easily. Once the system is not infinite ranged, avalanche sizes are small and the algorithm is trapped (not shown). This shows that while hysteretic optimization is a fast method for fully-connected models such as the SK model or the traveling salesman problem, it is not efficient for short-range spin glasses.

5. Conclusions
By using a one-dimensional spin glass with power-law interactions we have been able to study a variety of open questions in the field of spin glasses. The model has two main advantages over conventional higher-dimensional models: larger system sizes can be studied and the universality class of the model can be tuned by changing the power-law exponent of the interactions. The different results obtained show that there is urgent need for a better theoretical description of short-range spin glasses. While the droplet model and replica symmetry breaking describe...
Figure 7. Mean CPU time in seconds ($t_{CPU}$) for determining a ground state of the one-dimensional Ising chain as a function of the chain length $L$ for different exponents $\sigma$ using the branch, cut & price algorithm. For $\sigma = 3.0$ (main panel) the CPU time increases $\sim L^{5.3}$, whereas for $\sigma \lesssim 2.0$ the CPU time increases exponentially (see inset for $\sigma = 1.0$). The dashed lines are guides to the eye. Figure adapted from reference [21].

Figure 8. Percentage error in the ground-state energies obtained with hysteretic optimization with respect to exact ground states obtained with other approaches as a function of the exponent $\sigma$ for different system sizes. The algorithm works relatively well for $\sigma \lesssim 0.5$ (vertical dashed line) whereas for larger values of $\sigma$, where the model is not infinite ranged the error increases considerably. Figure adapted from reference [88].

certain properties of spin glasses well, neither of both theories is able to deliver a full account of all properties of short-range systems.

Furthermore, the model serves as a strong benchmark for different optimization algorithms: Because the range of the interactions can be tuned, the applicability of algorithms to different models in different universality classes can be tested.

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