Frustration: How it can be measured

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A misfit parameter is used to characterize the degree of frustration of ordered and disordered systems. It measures the increase of the ground-state energy due to frustration in comparison with that of a relevant reference state. The misfit parameter is calculated for various spin-glass models. It allows one to compare these models with each other. The extension of this concept to other combinatorial optimization problems with frustration, e.g., p-state Potts glasses, graph-partitioning problems, and coloring problems, is given.

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It is well established that two ingredients are necessary to characterize a spin glass: frustration (competition among the different interactions acting on a certain magnetic moment) and disorder; see [1, 2] for reviews. However, up to now the quantitative description of frustration seems to have been incomplete. Toulouse [3] has introduced the function $\Phi = \prod_{(c)} J_{ij}$, which measures the frustration effect in a local region of a lattice, where c indicates a closed contour along the $J_{ij} = +J$ or $-J$ bonds. However, this function cannot be simply generalized to other spin-glass models; in particular, it is not suited to models without underlying lattices. A nonlocal definition of frustration is given by Anderson [4]. That proposal contains the three following steps as subdividing the original sample into smaller blocks, determining the ground states of the blocks, and subsequent analyzing of the block coupling energy. Following that procedure one can distinguish between frustrated and nonfrustrated systems.

Frustration has an effect on ground-state energy and entropy. This can be easily seen starting from a (unfrustrated) ferromagnetic system by replacing $+J$ bonds by $-J$ bonds with increasing concentration p [5]. The ground-state energy increases up to a critical concentration p_c. Near p_c the ground-state entropy starts to increase. This reflects the fact that the problem to find the ground state becomes a problem of combinatorial optimization with a large number of optimal and nearly optimal solutions. The aim of this Brief Report is to use just the energy increase due to frustration as its global measure.

First, this concept was used to characterize the frustration effect in an amorphous Ising model with antiferromagnetic short-range interactions [6]. A misfit parameter

$$m = \frac{|E^{id}| - |E_0|}{|E^{id}|} \tag{1}$$

was introduced, where E_0 is the ground-state energy of the frustrated system and E^{id} is the ground-state energy of a relevant unfrustrated reference system. The latter can be obtained by replacing all negative bonds by positive ones. For the $\pm J$ spin glass the relation to Toulouse's frustration function can be seen by the expression given by Barahona [7]

$$E_0 = -\sum_{\langle ij \rangle} |J_{ij}| + 2 \sum_{\substack{\text{unsatisfied} \\ \text{edges}}} |J_{ij}|, \tag{2}$$

where the first term represents E^{id} and the second one the numerator of (1) having in mind that the restricted sum over unsatisfied edges is correlated to Toulouse's function by the total string length at minimal matching of elementary plaquettes with $\Phi = -1$.

The misfit parameter m of Eq. (1) is used to characterize the frustration in Ising zigzag chains dependent on the chain length [8] and in a neural network model [9]. It has been generalized to quantum systems [10, 11] and to define the local misfit and the misfit of a cluster of spins [11].

Now we introduce a modified misfit parameter. For a given state i of a system it is defined by

$$\mu_i = \mu(E_i) = \frac{E_i - E^{id}_{\min}}{E^{id}_{\max} - E^{id}_{\min}}, \tag{3}$$

where E_i is the energy of the state i. $E^{id}_{\min}$ and $E^{id}_{\max}$ describe the minimal and maximal ideally possible energy values, respectively, where "ideal" refers to the assumption that all local energies yield a minimal (maximal) contribution to the total energy. For spin glasses these energies have to be calculated assuming that all bonds are satisfied (nonsatisfied). Although, in general, $E^{id}_{\min}$ and $E^{id}_{\max}$ do not represent necessarily energies of a real system, they often can be identified with energies of a special reference system. In any case, they represent lower and upper bounds for the possible energy range of the considered frustrated system. Therefore μ_i is restricted to the interval between zero and unity. We define the misfit parameter for a system by the misfit of its ground state $\mu_0 = \mu(E_0)$.

To clarify the term "ideal" energy, we will discuss the misfit parameter of a spin glass. As mentioned above, the minimal and maximal ideal energies correspond to a fictive state, where all interactions are satisfied and nonsatisfied, respectively,

$$E^{id}_{\min} = -E^{id}_{\max} = -\sum_{\langle ij \rangle} |J_{ij}|, \tag{4}$$

where the sum goes over all interactions. Obviously, $E_{\min}^{id}$ is the ground-state energy of an unfrustrated reference system, which can be obtained by replacing all J_{ij} by their absolute values. The misfit parameter can be calculated from Eqs. (3) and (4) as

$$\mu_0 = \frac{1}{2}\left(1 + \frac{E_0}{\sum_{\langle ij \rangle} |J_{ij}|}\right) . \tag{5}$$

TABLE I. Misfit parameter μ_0 for various spin-glass (SG) models and other combinatorial optimization problems in the ground state.

Model	μ_0	Remark (size, method)		Ref.
Mattis SG	0			[17]
SK model	0		mean field	[13]
	0.0217		replica solution	[15]
$2d$ Gaussian SG	0.090	square 16×16	transfer matrix	[18]
	0.0868	square 30 ×30	exact	[19]
$3d$ Gaussian SG	0.143	cubic 4 ×4 ×4	transfer matrix	[18]
	0.160	cubic 10 ×10 ×10	projected gradient method	[20]
$2d$ $\pm J$ SG	0.09	honeycomb 12 ×5	exact	[21]
	0.15	square 8 ×8	exact	[22]
	0.1515	square 48 ×48	multicanonical	[23]
	0.14975	square[a]	genetic	[24]
	0.22	triangular 6 ×6	exact	[22]
$3d$ $\pm J$ SG	0.211	cubic 4 ×4 ×4	exact	[25]
	0.201	cubic 12 ×12 ×12	multicanonical	[26]
	0.20233	cubic[a]	genetic	[24]
fully frustrated $\pm J$ systems	0.1667	diamond	exact	[28]
	0.25	d-dimensional hypercubic d = 2,3,4	exact	[27, 28]
	0.3125	$6d$ hypercubic	exact	[28]
	$0.5 - 1/(2\sqrt{d})$	$d \geq 8$ hypercubic	lower limit	[28]
	$0.5 - 1/\sqrt{2d\pi}$	$d \geq 8$ hypercubic	upper limit	[28]
	0.333	$2d$ triangular, $3d$ fcc	exact	[29, 30]
	0.417	$6d$ fcc	exact	[30]
	$0.5 - 1/(2d)$	d-dimensional fcc	exact	[30]
p partitioning ($\pm J$)		Bethe lattice	analytical approach	[31]
$p = 2$[b]	0.074	$z = 3$		
	0.230	$z = 8$		
	0.257	$z = 10$		
$p = 3$	0.105	$z = 3$		
	0.317	$z = 8$		
	0.354	$z = 10$		
p coloring ($\pm J$)		Bethe lattice	analytical approach	[31]
$p = 3$	0	$z = 3$		
	0.032	$z = 8$		
	0.058	$z = 10$		
p state $\pm J$ Potts glass		Bethe lattice		
$p = 2$	0.080	$z = 3$	MC and annealing	[32]
	0.134	$z = 4$		
	0.1975	$z = 6$		
	0.236	$z = 8$		
	0.265	$z = 10$		
$p = 3$	0.0068	$z = 3$	analytical approach	[31]
	0.172	$z = 8$		
	0.204	$z = 10$		
TSP	0.0134	$N = 32$		[33]

[a]Extrapolated from $1/N$ scaling.

[b]The misfit for the corresponding ($p = 2$)-coloring problem results in the same μ_0 values.

Compared to Eq. (1) we get $m = 2\mu_0$. For the $\pm J$ spin glass μ_0 is the fraction of nonsatisfied bonds in the ground state [12].

For the well-known Sherrington-Kirkpatrick (SK) model [13], the minimal ideal energy belongs to the ground-state energy of a reference system, in which the probability distribution of the interactions is a Gaussian one folded about zero [14]. In this case Eq. (4) gives

$$E^{id}_{\min}/b = -E^{id}_{\max}/b = -\sqrt{2/\pi} \approx -0.798, \tag{6}$$

where b denotes the total number of bonds in the system. Equation (6) leads to $\mu_0 = 0$ for the mean-field solution in [13]. In other words, due to the mean-field approximation the frustration in the system vanishes and the resulting system is a Mattis-like spin glass. The misfit value μ_0 for Parisi's improved replica solution [15] is given in Table I together with a collection of data for various spin-glass models and related combinatorial optimization problems. Derrida [16] has considered the random-energy model (REM) as an approximation to spin-glass models and has calculated lower bounds for the ground-state energies in any dimension. For the $\pm J$ spin glass on a d-dimensional hypercubic lattice this approximation yields reasonable misfit values [$\mu_0 \geq 0.11$ and 0.17 for $d = 2$ and 3, respectively, and $\mu_0 \geq 0.5 - 1/\sqrt{2d/\ln 2}$ in the high-dimensional limit $d \to \infty$, which is lower than the lower limit of the fully frustrated $\pm J$ system (see Table I)]. Otherwise, for the symmetric Gaussian model on a square lattice the REM ground-state energy is lower than $E^{id}_{\min}$.

From Table I the various effects of dimension, coordination number, distribution and range of interactions, and number of states per spin variable on the frustration can be seen in a quantitative manner. At least for small coordination numbers and dimensions their increases result in additional constraints and therefore in increasing μ_0 values. The effect of different coordination numbers can be seen for the two-dimensional (2D) $\pm J$ Ising spin glasses with different lattice structures, for the p-state $\pm J$ Potts glass, for the p-partitioning problem, and for the p-coloring problem considering different z values. The influence of different dimensions can be studied by comparing the results for two and three dimensions. The comparison between two- and three-dimensional $\pm J$ spin glasses and spin glasses on a Bethe lattice with the same number of nearest neighbors z shows that μ_0 is more strongly influenced by the coordination number than by the spatial structure and dimension. However, it can also be seen that μ_0 is lower in the Bethe lattice than in higher netted lattices. Analytical expressions for $\mu_0(d)$ are given for hypercubic fully frustrated systems [28] and d-dimensional antiferromagnets with triangular plaquettes [30] at least in the high-dimensional limit. For finite d the results for fully frustrated systems are proved as upper bounds for systems with equal probability of $+J$ and $-J$ bonds.

In systems with a Gaussian distribution of interactions the energy can be decreased by choosing and frustrating the bond with the lowest strength in a plaquette. Therefore the misfit for such systems is smaller than for comparable systems with a $\pm J$ distribution.

Other relations between the parameters of a model and the resulting frustration can be investigated by using the p-state Potts glass, the p-partitioning problem, and the p-coloring problem. With an increasing number of colors p for the nearest neighbors of a site in a p-coloring problem, the chance to give all neighbors other colors increases and therefore the frustration in the system decreases. On the other hand, if the number p of subsets in the p-partitioning problem increases, the problem becomes more complicated and restricted, leading to an increase in frustration. In Potts glasses the number of possibilities to avoid frustration increases with the rising number p of states per spin and consequently μ_0 decreases. As outlined in [31], the p-state Potts glass can be understood approximately as an intermediate system between the p-partitioning and the p-coloring problem, which correspond to a ferromagnetic and an antiferromagnetic Potts glass with special magnetization constraints. Therefore, for the same p, the μ_0 values in the Potts glass are smaller than those of the partitioning problems but larger than those of the coloring problems. Small deviations for the case $p = 2$ are due to different methods.

Summarizing the results, we have introduced a global misfit parameter generalizing the fraction of unsatisfied bonds in the ground state of the short-range $\pm J$ spin glass to other spin glass models and to other systems with frustration. It measures the influence of frustration on the ground-state energy and it allows us to compare various spin-glass models quantitatively. It can be applied to systems without an underlying lattice structure. An advantage over the former parameter (1) is its invariance against any linear scaling of energies, which means, e.g., that additional self-energy terms leave the misfit unchanged.

The concept presented can be applied to other systems with frustration. For example, we have calculated μ_0 for a traveling salesman problem (TSP) with $N = 32$ cities using (3) (cf. Table I). The TSP can be transformed into an antiferromagnetic Potts model [2]. However, such a transformation is accompanied with additional global constraints for the cost function. We plan to focus on this topic in a forthcoming paper.

The misfit parameter refers only to the *energetic* aspect of frustration. It is an open question whether a similar parameter can be found for the *entropic* characterization of frustrated systems. A preliminary answer for the $\pm J$ models is given by Vogel *et al.* [22]. These authors have calculated the fraction of bonds, which are satisfied in *all* ground states. The difference between unity and this fraction can be used as a global entropic measure for frustration. Generalizations are under consideration.

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