Random Costs in Combinatorial Optimization

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The random cost problem is the problem of indentifying the minimum in a list of random numbers. By definition, this problem cannot be solved faster than by exhaustive search. It is shown that a classical *NP*-hard optimization problem, number partitioning, is essentially equivalent to the random cost problem. On the one hand this explains the bad performance of heuristic approaches to the number partitioning problem, but on the other hand it allows one to calculate the probability distributions of the optimum and suboptimum costs.

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Recent years have witnessed an increasing interaction among the disciplines of discrete mathematics, computer science, and statistical physics. Particularly the methods and concepts developed in spin glass theory have been applied successfully to problems from combinatorial optimization [1]. An optimization problem is defined by a set $\mathcal{X}$ (the domain) of feasible solutions $\sigma \in \mathcal{X}$ and a real valued function H on X. The minimization problem then is: Find that $\sigma \in \mathcal{X}$ which minimizes $H(\sigma)$. In combinatorial optimization $\mathcal{X}$ is always countable. For minimization problems, H is called the cost function; physicists call it Hamiltonian or energy.

The most interesting problems in combinatorial opimization are *NP*-hard [2], which means that no algorithm is known that solves the problem significantly faster than exhaustive search of the domain. Although it has not been proven, it is widely believed that for *NP*-hard problems faster algorithms do not exist [3,4]. A problem for which this can be proven is the *random cost problem:* Here the cost function is a table of random numbers and the role of σ is reduced to an index. It can be proven that one has to look at every number in the table to find the minimum [5]. Furthermore, it is obvious that there is no better heuristic than sequential lookup. In this sense the random cost problem is harder than many other *NP*-hard problems, for which much better heuristics do exist.

In this contribution it is shown that the random cost problem is not an artificial toy problem but a valid description of at least one classical problem from combinatorial optimization: the number partitioning problem.

Number partitioning (NPP) is one of Garey and Johnson's [3] six basic *NP*-complete problems that lie at the heart of the theory of *NP*-completeness. It is defined as follows: Given a set of positive numbers $\{a_1, a_2, \ldots, a_N\}$, find a partition, i.e., two disjoint subsets $\mathcal{A}_1$ and $\mathcal{A}_2$, such that the residue

$$E = \left| \sum_{a_j \in \mathcal{A}_1} a_j - \sum_{a_j \in \mathcal{A}_2} a_j \right| \tag{1}$$

is minimized. In the balanced number partioning problem, the optimization is restricted to partitions with $|\mathcal{A}_1| = |\mathcal{A}_2| = N/2$ (N even). A partition can be encoded by Ising spins $s_j = \pm 1$: $s_j = 1$ if $a_j \in \mathcal{A}_1$, $s_j = -1$ otherwise. The cost function then reads

$$E = \left| \sum_{j=1}^{N} a_j s_j \right|, \tag{2}$$

and the minimum partition is equivalent to the ground state of the Hamiltonian

$$H = E^2 = \sum_{i,j=1}^{N} s_i a_i a_j s_j \,. \tag{3}$$

In statistical mechanics, this is an infinite range Ising spin glass with Mattis-like, antiferromagnetic couplings $J_{ij} = -a_i a_j$ [6–9].

The computational complexity of the NPP depends on the number of bits needed to encode the numbers a_j. Numerical simulations show that for independent, identically distributed (i.i.d.) random b-bit numbers a_j, the solution time grows exponentially with N for $N \lesssim b$ and polynomially for $N \gtrsim b$ [10–12]. The transition from the "hard" to the computational "easy" phase has some features of a phase transition in physical systems. Phase transitions of this kind have been observed in numerous *NP*-complete problems [13–15] and can often be analyzed quantitatively in the framework of statistical mechanics. Compared to other problems, this analysis is surprisingly simple for the number partitioning problem [9].

Here we concentrate on the computationally hard regime $N \ll b$; i.e., we consider the a_j to be real numbers of "infinite" precision. For this case, Karmarkar *et al.* [16] have proven that the median value of the optimum residue E_1 is $\mathcal{O}(\sqrt{N}\,2^{-N})$ for the unconstrained and $\mathcal{O}(N2^{-N})$ for the balanced partitioning problem. Their proof yields no results on the distribution of E_1, however, or at least on its average value. Numerical simulations [7] indicate that the relative width of the distribution of E_1, defined as

$$r := \frac{\sqrt{\langle E_1^2 \rangle - \langle E_1 \rangle^2}}{\langle E_1 \rangle}, \tag{4}$$

where $\langle \cdot \rangle$ denotes the average over the a_j's, tends to 1 in the limit $N \to \infty$, for both the unconstrained and the balanced

partitioning problem. This means that the ground state energy is a non-self-averaging quantity.

Another surprising feature of the NPP is the bad performance of heuristic algorithms [17,18]. The best known heuristic, the differencing method [12,19], yields partitions with expected residue $\mathcal{O}(N^{-a\log N})$, $a > 0$ for a_j distributed uniformly between 0 and 1. This is still bad compared to $\mathcal{O}(\sqrt{N}\,2^{-N})$ for the true optimum.

In this contribution we show that all these features can be understood qualitatively and quantititavely by the observation that number partitioning is essentially equivalent to a random cost problem. Our line of reasoning closely follows Derrida [20,21], who introduces the random energy model (REM) in spin glass theory. The random cost problem is the optimization counterpart of the REM, with some modifications, as we will see below.

In the balanced NPP, the energies are distributed according to

$$P(E) = \binom{N}{N/2}^{-1} {\sum_{\{s_j\}}}' \left\langle \delta\left(E - \left|\sum_j a_j s_j\right|\right)\right\rangle, \quad (5)$$

where the primed sum runs over all spin configurations with $\sum s_j = 0$. The symmetry of the problem and our assumption of i.i.d. random variables a_j allow us to write

$$P(E) = 2\left\langle \delta\left(E - \sum_{j=1}^{N/2}(a_j - a_{N/2+j})\right)\right\rangle \Theta(E), \quad (6)$$

where Θ denotes the step function, $\Theta(x) = 1$ for $x \geq 0$ and $\Theta(x) = 0$ for $x < 0$. The symmetrization $a_{\rm sym}$ of a, i.e., the random variable distributed as the result of subtracting two independent variables $a_1 - a_2$, has mean 0 and variance $2\sigma^2$ with $\sigma^2 = \langle a^2\rangle - \langle a\rangle^2$. If g_k denotes the density of the kth partial sum of $a_{\rm sym}$ we can write $P(E) = 2g_{N/2}(E)\Theta(E)$, which according to the central limit theorem becomes

$$P(E) = \frac{2}{\sqrt{2\pi\sigma^2 N}} \exp\left(-\frac{E^2}{2\sigma^2 N}\right)\Theta(E) + \mathcal{O}(N^{-3/2}) \quad (7)$$

for large values of N. The energies in the unconstrained NPP follow the same distribution but with σ^2 replaced by $\langle a^2\rangle$.

The probability density of finding energies E_1 and E_2 is

$$P(E_1, E_2) = 4\Theta(E)\Theta(E')\binom{N}{N/2}^{-2} {\sum_{\{s_j\}}}' {\sum_{\{s'_j\}}}' \left\langle \delta\left(E_1 - \sum_j a_j s_j\right)\delta\left(E_2 - \sum_j a_j s'_j\right)\right\rangle \quad (8)$$

for the balanced NPP. Again we use the gauge invariance to state that each term in the above sum depends on $\{s_j\}$ and $\{s'_j\}$ only through the overlap

$$Q = \sum_{j=1}^{N} s_j s'_j. \quad (9)$$

Then

$$P(E_1, E_2) = \frac{4\Theta(E_1)\Theta(E_2)}{\binom{N}{N/2}} {\sum_{Q=-N}^{N}}' \binom{N/2}{\frac{N+Q}{4}}^2 P_Q(E_1, E_2), \quad (10)$$

where the primed sum denotes summation over $Q = -N, -N+4, \ldots, N-4, N$ and

$$P_Q(E_1, E_2) = \frac{1}{2}\, g_{(N+Q)/4}\left(\frac{E_1 + E_2}{2}\right) g_{(N-Q)/4}\left(\frac{E_1 - E_2}{2}\right). \quad (11)$$

The central limit theorem tells us that for large N

$$P_Q(E_1, E_2) = \frac{1}{2\pi\sigma^2 N\sqrt{1-q^2}}\, e^{-\frac{E_1^2 + E_2^2 - 2E_1E_2q}{2\sigma^2 N(1-q^2)}} \quad (12)$$

with $q = Q/N$. In the same limit we may apply Stirling's formula to the binomial coefficients and replace the sum over Q by an integral over q:

$$P(E_1, E_2) = \frac{2\Theta(E_1)\Theta(E_2)}{\pi^2\sigma^2 N}\sqrt{\frac{\pi N}{2}} \int \frac{dq}{1-q^2}\, e^{-\frac{E_1^2 + E_2^2 - 2E_1E_2q}{2\sigma^2 N(1-q^2)}}\, e^{-Nf(q)} \quad (13)$$

with

$$f(q) = \frac{1}{2}(1+q)\ln(1+q) + \frac{1}{2}(1-q)\ln(1-q). \quad (14)$$

The integral can be evaluated using the saddle point approximation. For E_1 and E_2 both $\mathcal{O}(\sqrt{N})$, the saddle point is at $q = 0$:

$$P(E_1, E_2) = \frac{2\Theta(E_1)\Theta(E_2)}{\pi\sigma^2 N} \exp\left(-\frac{E_1^2 + E_2^2}{2\sigma^2 N}\right); \quad (15)$$

i.e., $P(E_1, E_2) = P(E_1)P(E_2)$. A similar calculation shows that $P(E_1, E_2)$ factorizes for the unconstrained NPP, too. Note that for $E = \mathcal{O}(N)$ the saddle point is no longer at $q = 0$ and $P(E_1, E_2)$ does not factorize. This is plausible, since energies $\mathcal{O}(N)$ can be achieved only by putting a number $\mathcal{O}(N)$ of the lowest values a_j into one partition and a number $\mathcal{O}(N)$ of the largest values in the complement. The corresponding spin sequences then have an overlap $\mathcal{O}(N)$.

The two basic properties that lead to the factorization of $P(E, E')$ are the gauge invariance, i.e., the fact that $\langle\delta(E - \sum a_j s_j)\delta(E' - \sum a_j s'_j)\rangle$ depends only on the overlap q of the sequences, and the entropic dominance of the $q = 0$ contributions. Both properties persist if one considers the probability distributions of three or more levels, so we claim that $P(E_1, E_2, \ldots, E_k)$ factorizes as well. Instead of providing a formal derivation, we consider this as an assumption and discuss its consequences.

Motivated by the factorization of the distribution of energies, we may now specify our random cost problem: Given are $M = \mathcal{O}(2^N)$ random numbers E_i, *independently* drawn from the density $P(E)$, Eq. (7). Find the minimum of these numbers. The correspondence to the NPP requires $M = \frac{1}{2}\binom{N}{N/2}$ for the balanced and $M = 2^{N-1}$ for the unconstrained case.

Let E_k denote the kth lowest energy of an instance of our random cost problem. The independence of the E_i enables us to write

$$\rho_1(E_1) = MP(E_1)\left(1 - \int_0^{E_1} P(E')\,dE'\right)^{M-1} \quad (16)$$

for the probability density ρ_1 of the minimum energy. E_1 must be small to get a finite right-hand side in the large M limit. Hence we may write

$$\rho_1(E_1) \approx MP(0)[1 - E_1 P(0)]^{M-1} \approx MP(0)e^{-MP(0)E_1}.$$

This means that the probability density of the scaled minimal energy,

$$\varepsilon_1 = MP(0)E_1\,, \quad (17)$$

for large M converges to a simple exponential distribution

$$\rho_1(\varepsilon) = e^{-\varepsilon}\Theta(\varepsilon)\,. \quad (18)$$

Note that a rigorous derivation from Eq. (16) to Eq. (18) can be found in textbooks on extreme order statistics [22].

Along similar lines one can show that the density ρ_k of the kth lowest scaled energy is

$$\rho_k(\varepsilon) = \frac{\varepsilon^{k-1}}{(k-1)!}\,e^{-\varepsilon}\Theta(\varepsilon) \qquad k = 2, 3, \ldots. \quad (19)$$

Let us compare Eqs. (18) and (19) with other analytical and numerical results. From the moments of the exponential distribution Eq. (18), $\langle\varepsilon^n\rangle = n!$, we get

$$r = \frac{\sqrt{\langle E_1^2\rangle - \langle E_1\rangle^2}}{\langle E_1\rangle} = 1\,, \quad (20)$$

in perfect agreement with the numerical findings of Ferreira and Fontanari [7]. The average ground state energy is $\langle E_1\rangle = 1/[MP(0)]$, which gives

$$\langle E_1\rangle = \pi\sigma N 2^{-N} \quad (21)$$

for the balanced and

$$\langle E_1\rangle = \sqrt{2\pi\langle a^2\rangle}\,\sqrt{N}\,2^{-N} \quad (22)$$

for the unconstrained NPP. Again this is in very good agreement with numerical [7] and analytical [9] results.

To check that the random cost ansatz does not only give the correct first and second moment of E_1, we calculated the distribution of E_1 and higher energies numerically. Figures 1 and 2 display the results for the balanced NPP. Equivalent plots for the unconstrained NPP look similar. The agreement between the numerical data and Eqs. (18) and (19) is convincing. The algorithm used to solve larger instances of the balanced NPP is described in [23].

All in all, the random cost problem seems to be a valid alternative formulation of the number partitioning problem. This correspondence not only provides new analytic results on the NPP but also has some consequences for the dynamics of algorithms: Any heuristic that

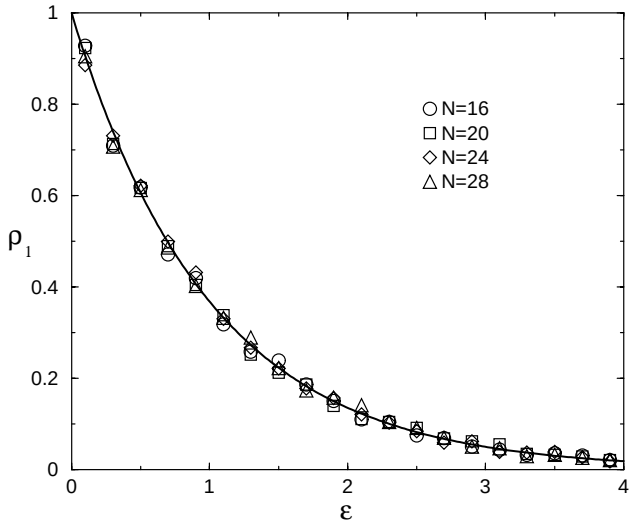

FIG. 1. Distribution of scaled ground state energies for the balanced number partioning problem. The solid line is given by Eq. (18); the symbols are averages over 10^4 random samples.

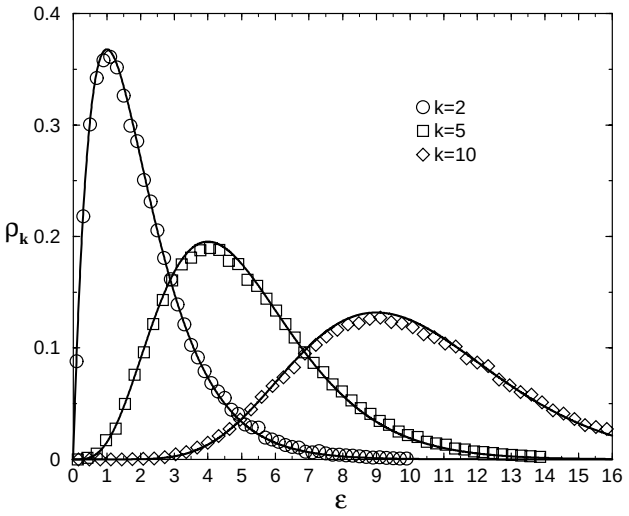

FIG. 2. Distribution of scaled kth lowest energy for the balanced number partioning problem. The solid lines are given by Eq. (19); the symbols are averages over 10^5 random samples of size $N = 24$.

exploits a fraction of the domain, generating and evaluating a series of feasible configurations, cannot be better than random search. The best solution found by random search is distributed according to Eq. (16), i.e., the average heuristic solution should approach the true optimum no faster than $\mathcal{O}(1/M)$, M being the number of configurations generated. Note that the best known heuristic, the complete Karmarkar-Karp differencing [12,23] converges slower, namely, like $\mathcal{O}(1/M^{\alpha})$ with $\alpha < 1$ to the true optimum. It would be interesting to check whether simple random search really converges faster. Beyond number partitioning, the dynamics of heuristic algorithms for other combinatorial optimization problems may be considered as a signature of a corresponding random cost problem, possibly with a differing $P(E)$.

With its focus on costs rather than configurations, our random cost problem is very similar to Derrida's random energy model from statistical mechanics [20,21], with an important difference: the $P(E)$ in Derrida's model is Gaussian; i.e., in principle, it allows arbitrary low energies. The random cost formulation of the NPP on the other hand leads to a strict lower bound for the energies. As a consequence, both models belong to different universality classes with respect to their asymptotic order statistics [22]. The replica method from statistical mechanics solves the Gaussian random energy model but fails for bounded distributions like the one encountered here [24]. It is an open problem how to modify the replica method in order to reproduce the statistical mechanics of the number partitioning problem [9].

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