Random Costs in Combinatorial Optimization

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The random cost problem is the problem of finding the minimum in an exponentially long 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. This explains the bad performance of heuristic approaches to the number partitioning problem and allows us to calculate the probability distributions of the optimum and sub-optimum costs.

Number partitioning is one of Garey and Johnson’s six basic NP-complete problems that lie at the heart of the theory of NP-completeness. It is defined as follows: Given a set \{a_1, a_2, \ldots, a_N\} of positive numbers, find a partition, i.e. two disjoint subsets \(A_1\) and \(A_2\) such that the residue

\[
E = \left| \sum_{j \in A_1} a_j - \sum_{j \in A_2} a_j \right|
\]

is minimized. In the balanced number partitioning problem, the optimization is restricted to partitions with \(|A_1| = |A_2| = N/2\) (\(N\) even). A partition can be encoded by Ising spins \(s_j = \pm 1\): \(s_j = 1\) if \(a_j \in A_1\), \(s_j = -1\) otherwise. The cost function then reads

\[
E = \left| \sum_{j=1}^{N} a_j s_j \right|
\]

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

\[
H = E^2 = \sum_{i,j=1}^{N} s_i a_i a_j s_j.
\]

In statistical mechanics, this is an infinite range Ising spin glass with Mattis-like, antiferromagnetic couplings \(J_{ij} = -a_i a_j\).

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 \(N < b\) (roughly) and polynomially for \(N > b\). 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, 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.

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. have proven that the median value of the optimum residue \(E_1 = O(\sqrt{N} \cdot 2^{-N})\) for the unconstrained and \(O(N \cdot 2^{-N})\) 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
where \( \langle \cdot \rangle \) denotes the average over the \( a_j \)'s, tends to a finite value in the large \( N \) limit, more precisely: 
\[
\lim_{N \to \infty} r = 1, \quad \text{for both the unconstrained and the balanced partitioning problem. This means, that the ground state energy is a non self averaging quantity.}
\]

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

In this contribution we show that all these features can be understood qualitatively and quantitatively 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
\[
P(E) = \left( \frac{N}{N/2} \right)^{-1} \sum_{\{s_j\}} \left\langle \delta(E - \sum_j a_j s_j) \right\rangle, \tag{5}
\]
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
\[
P(E) = 2 \cdot \left\langle \delta(E - \sum_{j=1}^{N/2} (a_j - a_{N/2+j})) \right\rangle \cdot \Theta(E), \tag{6}
\]
where \( \Theta \) denotes the step-function, \( \Theta(x) = 1 \) for \( x \geq 0 \) and \( \Theta(x) = 0 \) for \( x < 0 \). The symmetrization \( a_{\text{sym}} \) 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 \( k \)-th partial sum of \( a_{\text{sym}} \) we can write \( P(E) = 2g_{N/2}(E)\Theta(E) \), which according to the central limit theorem becomes
\[
P(E) = \frac{2}{\sqrt{2\pi\sigma^2 N}} \exp \left( - \frac{E^2}{2\sigma^2 N} \right) \cdot \Theta(E) + \mathcal{O}(N^{-3/2}) \tag{7}
\]
for large values of \( N \). The energies in the unconstrained NPP follow the same distribution but with \( \sigma^2 \) replaced by \( \langle a^2 \rangle \).

The probability density of finding energies \( E_1 \) and \( E_2 \) is
\[
P(E_1, E_2) = 4 \cdot \Theta(E)\Theta(E') \left( \frac{N}{N/2} \right)^{-2} \cdot \sum_{\{s_j\}} \sum_{\{s'_j\}} \left\langle \delta(E_1 - \sum_j a_j s_j) \cdot \delta(E_2 - \sum_j a_j s'_j) \right\rangle \tag{8}
\]
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
\[
Q = \sum_{j=1}^N s_j s'_j. \tag{9}
\]

Then
\[
P(E_1, E_2) = \frac{4\Theta(E_1)\Theta(E_2)}{(N/2)} \sum_{Q=-N}^{N} \left( \frac{N/2}{N+Q} \right)^2 P_Q(E_1, E_2), \tag{10}
\]
where the primed sum denotes summation over \( Q = -N, -N+4, \ldots, N-4, N \) and
\[
P_Q(E_1, E_2) = \frac{1}{2} \cdot g(N+Q)/4 \left( \frac{E_1 + E_2}{2} \right) \cdot g(N-Q)/4 \left( \frac{E_1 - E_2}{2} \right) \tag{11}
\]
(see above for a definition of \( g \)). For large values of \( N \), the central limit theorem tells us that
\[
P_Q(E_1, E_2) = \frac{1}{2\pi\sigma^2 N} \cdot e^{-\frac{E_1^2 + E_2^2 + 2E_1E_2q}{4\pi^2 N(1-q^2)}} \tag{12}
\]
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 \( q \):
\[
P(E_1, E_2) = \frac{2\Theta(E_1)\Theta(E_2)}{\pi^2\sigma^2 N} \sqrt{\frac{\pi N}{2}} \cdot \int dq \cdot \frac{e^{-\frac{E_1^2 + E_2^2 - 2E_1E_2q}{2\pi^2 N(1-q^2)}}}{1-q^2} e^{-Nf(q)} \tag{13}
\]
with
\[
f(q) = \frac{1}{2} (1+q) \ln(1+q) + \frac{1}{2}(1-q) \ln(1-q). \tag{14}
\]
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 \( q = 0 \):
\[
P(E_1, E_2) = \frac{2\Theta(E_1)\Theta(E_2)}{\pi^2\sigma^2 N} \exp \left( - \frac{E_1^2 + E_2^2}{2\sigma^2 N} \right) \tag{15}
\]
i.e. \( P(E_1, E_2) = P(E_1) \cdot P(E_2) \). 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 $O(N)$ can only be achieved by putting a number $O(N)$ of the lowest values $a_j$ into one partition and a number $O(N)$ of the largest values in the complement. The corresponding spin sequences then have an overlap $O(N)$.

The two basic properties that lead to the factorization of $P(E, E')$ are the gauge invariance, i.e. the fact that $\langle \delta(E - \sum a_j s_j) \delta(E' - \sum a_j s'_j) \rangle$ only depends 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 $M = O(2^N)$ random numbers $E_i$, independently drawn from the density $P(E)$. Find the minimum of these numbers. The correspondence to the NPP requires $M = \frac{1}{2}(\frac{N}{2})$ for the balanced and $M = 2^{N-1}$ for the unconstrained case.

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

$$\rho_1(E_1) = M \cdot P(E_1) \cdot \left(1 - \int_{0}^{E_1} P(E') dE'\right)^{M-1}$$

(16)

for the probability density $\rho_1$ of the minimum energy. $E_1$ must be small to get a finite r.h.s. in the large $M$ limit. Hence we may write

$$\rho_1(E_1) \approx M \cdot P(0) \cdot \left(1 - E_1 P(0)\right)^{M-1} \approx M \cdot P(0) \cdot e^{-M P(0) E_1}.$$  

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

$$\varepsilon_1 = M \cdot P(0) \cdot E_1$$

(17)

for large $M$ converges to a simple exponential distribution,

$$\rho_1(\varepsilon) = e^{-\varepsilon} \cdot \Theta(\varepsilon).$$

(18)

Note that a rigorous derivation from Eq. (16) to Eq. (18) can be found in any textbook on extreme order statistics [23]. Along similar lines one can show that the density $\rho_k$ of the $k$-th lowest scaled energy is

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

(19)

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

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

(20)

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

$$\langle E_1 \rangle = \pi \cdot \sigma \cdot N \cdot 2^{-N}$$

(21)

for the balanced and

$$\langle E_1 \rangle = \sqrt{2\pi \langle a^2 \rangle} \cdot \sqrt{N} \cdot 2^{-N}$$

(22)

for the unconstrained NPP. Again this is in very good agreement with numerical [1] and analytical [1] 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. Figs. (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 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. (18), i.e. the average heuristic solution should approach the true optimum no
faster than $O(1/M)$, $M$ being the number of configurations generated. Note that the best known heuristic, the complete Karmarkar-Karp differencing [12,23] converges slower, namely like $O(1/M^\alpha)$ 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 single cost distribution.

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 single energy distribution 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 [1].

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