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LETTER TO THE EDITOR

Statistical mechanics of the knapsack problem

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Abstract. The knapsack problem is an NP-complete combinatorial optimization problem with inequality constraints. Using the replica method of statistical physics, we study the space of its solutions for a large problem size. It turns out that this problem is closely related to the theory of the binary perceptron.

Statistical physics provides interesting tools for the analysis of the complex energy landscapes which appear in combinatorial optimization problems. Based on the replica approach of disorder physics, the ground state properties of models like the *travelling salesman problem* [1], the *matching problem* [2] and the *graph partitioning problem* [3] have been investigated analytically in recent years. In these cases, the cost functions which have to be optimized, can be mapped onto classical spin Hamiltonians with competing interactions, well known from spin-glass physics.

In this letter, we study the so-called 'knapsack problem', which maps onto a rather different type of statistical physics model. Here, the cost function is much simpler than in the aforementioned cases, and does not lead to any frustration effects. The problem becomes complex by an additional set of inequality constraints which have to be satisfied by the optimal solution. Like many other combinatorial optimization problems, 'knapsack' belongs to the NP-complete class [6]. Thus, one expects that in the worst case, optimal solutions require a number of computational time steps that increase exponentially with the size of the problem. Nevertheless, solutions that are close to the optimum can be found in polynomial time. Recently, an algorithm, developed by Ohlsson, Peterson and Söderberg [7], which is based on mean-field (MF) annealing, was found to work very efficiently for large, random knapsack problems.

Inspired by this work we analyse the knapsack model for large problem sizes within the statistical mechanics framework. We show the close correspondence of the present problem to the binary perceptron model that was introduced by Gardner and Derrida [4] and solved by Krauth and Mézard [5]. The knapsack problem is defined in the following way:

One has N items i with utilities c_i and loads a_{ki}. The aim is to fill a 'knapsack' in such a way that the total utility

$$U(s) = \sum_{i=1}^{N} c_i s_i \tag{1}$$

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is maximized subject to a set of K additional constraints:

$$\sum_{i=1}^{N} a_{ki} s_i \leqslant b_k \qquad k = 1, \ldots, K. \tag{2}$$

The s_i binary decision variables that take the values +1 when the item i goes into the knapsack and 0 otherwise. The variables a_{ki}, c_i and b_k are real and non-negative. To get an insight into the typical behaviour of the problem, we will investigate the case where the a_{ki} are independent random numbers equally distributed in the unit interval. For simplicity, we will set c_i equal to the constant $\frac{1}{2}$. In this case the utility is proportional to the number of items used. Finally, we also specify the variables b_k fixed to a common value b.

We are interested in the scaling of the problem, when $N \to \infty$. An interesting limit is obtained when K, the number of constraints scales like N, i.e., when we set $K = \alpha \cdot N$, with α finite. It is convenient to convert the decision variables $s_i = (1, 0)$ into spin variables $\hat{s}_i = (1, -1)$, using the transformation $\hat{s} = 2(s - \frac{1}{2})$. Likewise, we set

$$a_{ki} = \tfrac{1}{2} + \xi_{ki} \tag{3}$$

where the random part ξ_{ki} has zero mean and variance $\sigma^2 = \frac{1}{12}$. Hence, up to a constant, the utility

$$U = \frac{N}{4} + \frac{1}{4} \sum_{i=1}^{N} \hat{s}_i \tag{4}$$

is given by the total 'magnetization' of the spins $\hat{s}_i$, and the inequalities (2) read

$$\sum_i a_{ki} s_i - b = \frac{1}{2} \sum_{i=1}^{N} (1 + \hat{s}_i) \xi_{ki} + \frac{1}{4} \sum_{i=1}^{N} \hat{s}_i + \frac{N}{4} - b \leqslant 0. \tag{5}$$

For finite $\alpha = K/N$, we assume that for the optimal configuration the $\hat{s}_i$ are only weakly correlated to the a_{ki}, so that for large N, $\sum_i \xi_{ki} \hat{s}_i$ is of order $\sqrt{N}$. Thus, in order to satisfy (5), large magnetizations of $O(N)$ must be balanced by the remaining terms of the same order. Assuming b of $O(N)$, we get the condition $\frac{1}{4} \sum_{i=1}^{N} \hat{s}_i \simeq b - (N/4)$, so that the optimal utility satisfies

$$U_{\mathrm{opt}} \simeq b \cdot N. \tag{6}$$

For $b \gg N/4$, the inequalities (5) allow for a large positive magnetization, which corresponds to a solution where the knapsack can be filled with very many items. On the other hand, for $b \ll N/4$, the magnetization is negative, and only a few items are in the knapsack. In such extreme cases often good solutions to the optimization problem can be found from heuristics [7]. In the following, we will restrict ourselves to $b = N/4$, where about half of the items go into the knapsack, corresponding to zero magnetization. This is also the most complex case from the optimization point of view. A more detailed investigation of the parameter space will be given in a forthcoming paper.

Hence, for $b = N/4$, we set $U + (N/4) + (\sqrt{N}/4)M$, where

$$M(s) = \frac{1}{\sqrt{N}} \sum_i \hat{s}_i \tag{7}$$

describes the fluctuations of the magnetization around 0.

In the following, we calculate the $\sqrt{N}$ correction to the large N behaviour (6) of the utility using the Replica-method. For this problem it is convenient to work within the replica-symmetric (RS) scheme of the microcanonical ensemble.

In the microcanonical ensemble the averaged entropy of allowed configurations is defined via:

$$S(M) = \frac{1}{N}\langle\langle \ln \mathcal{N}(M)\rangle\rangle = \lim_{n\to 0}\frac{1}{Nn}\ln\langle\langle \mathcal{N}^n(M)\rangle\rangle \tag{8}$$

where the replica trick was utilized in the last equality. Here, $\mathcal{N}(M)$ is the number of configurations $\{\hat{s}_i\}$ which have a fixed M, implying also a fixed utility U. The quenched average $\langle\langle\ldots\rangle\rangle$ is taken over the distribution of the load variables a_{ki}. In this formalism, the *optimal utility* $U_{\rm opt}$ corresponds to the highest value of M, for which $S(M)$ is still positive. Explicitly, we have

$$\begin{aligned}\langle\langle \mathcal{N}^n(M)\rangle\rangle &= \left\langle\!\!\left\langle \prod_{a=1}^{n}\mathrm{Tr}_{s_i^a}\prod_{k=1}^{K}\Theta\left(-\left(\sum_i a_{ki}s_i^a - b\right)\right)\delta(M-M(s^a))\right\rangle\!\!\right\rangle \\ &= \left\langle\!\!\left\langle \prod_{a=1}^{n}\mathrm{Tr}_{\hat{s}_i^a}\prod_{k=1}^{K}\Theta\left(-\left(\sum_{i=1}^{N}\frac{(1+\hat{s}_i^a)\xi_{ki}}{\sqrt{N}}+\frac{M}{2}\right)\right)\delta\left(M-\frac{1}{\sqrt{N}}\sum_i \hat{s}_i^a\right)\right\rangle\!\!\right\rangle.\end{aligned} \tag{9}$$

In (9) the product of the Θ-functions accounts for the inequalities (2). Similar types of expressions appear in the problem of learning in neural networks of perceptron type. There, $-\xi_{ki}$ would correspond to an input pattern, which must be learnt by adjusting synaptic weights $\hat{s}_i$, such that K local fields $-\sum_{i=1}^{N}\xi_{ki}\hat{s}_i/\sqrt{N}$ are larger than some threshold. For the knapsack problem, this threshold contains the variable M, together with a random contribution and is not restricted to positive values.

The explicit evaluation of the entropy strongly resembles the corresponding calculation for the perceptron, and will only be sketched. To perform the quenched average, we use the fact that the variables $u_k^a = \sum_{i=1}^{N}(1+\hat{s}_i^a)\xi_{ki}/\sqrt{N}$, are jointly Gaussian distributed for $N\to\infty$, satisfying

$$\begin{aligned}\langle\langle u_k^a u_l^a\rangle\rangle &= \sigma^2\delta_{kl} \\ \langle\langle u_k^a u_l^b\rangle\rangle &= \sigma^2(1+q_{ab})\delta_{kl}.\end{aligned} \tag{10}$$

Here, the order parameters

$$q_{ab} = \frac{1}{N}\sum_i \hat{s}_i^a\hat{s}_i^b \tag{11}$$

measure the overlap between two random vectors that are consistent with all inequality constraints.

Assuming replica-symmetry, i.e. $q_{ab}=q$, the Gaussian fields u_k^a can be constructed via

$$u_k^a = \sigma(\sqrt{1+q}\,t_k + \sqrt{1-q}\,z_k^a) \tag{12}$$

where t_k, z_k^a are independent Gaussian random variables with zero mean and unit variance. Obviously, this ansatz satisfies the conditions (10). Finally, the trace $\mathrm{Tr}_{\hat{s}_i}$ is carried out using the saddle-point method. Then, the entropy is found by extremizing the expression

$$S(q,\hat{q},M) = \frac{\hat{q}(1-q)}{2} + \int Dt\,\ln 2\cosh(t\sqrt{-\hat{q}}) + \alpha\int Dt\,\ln H\left(\frac{M/2\sigma - \sqrt{1+q}\,t}{\sqrt{1-q}}\right) \tag{13}$$

with respect to q and $\hat{q}$, where $\hat{q}$ is the order parameter conjugate to q. As usual, the Gaussian measure Dt is

$$Dt \equiv \frac{dt \exp\left(-t^2/2\right)}{\sqrt{2\pi}}$$

and $H(x)$ is defined as

$$H(x) = \int_x^\infty Dt.$$

Due to the $\sqrt{N}$ scaling of (7), no order parameter conjugate to M is required [4].

At the maximal $M = M_{\mathrm{opt}}$, the number $\mathcal{N}(M)$ of configurations which satisfy all constraints is no longer exponential in N and the entropy vanishes. Solving the order parameter equations

$$\frac{\partial S}{\partial q} = \frac{\partial S}{\partial \hat{q}} = 0 \tag{14}$$

together with the *zero entropy condition* $S(M_{\mathrm{opt}}) = 0$, we obtain M_{opt} as a function of $\alpha = K/N$. The result is displayed in figure 1, together with a simple upper bound obtained from the annealed approximation $S_{\mathrm{ann}}(M) = (1/N)\ln\langle\langle\mathcal{N}(M)\rangle\rangle$. It becomes clear that by increasing the number of constraints (i.e. for a greater α), more and more of them must be satisfied trivially by setting $\hat{s}_i = -1$, or $s_i = 0$, i.e. by leaving items out of the knapsack. In this case, M becomes more and more negative and the total utility decreases.

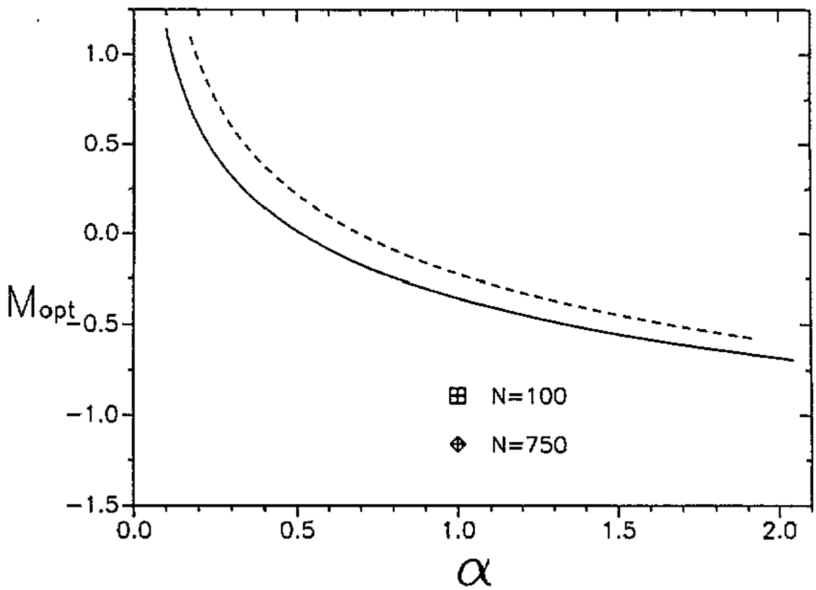

Figure 1. Optimal values M_{opt}. The full line represents the replica result and the dashed line is obtained from the annealed approximation. The two dots at $\alpha = 1$ are taken from simulations of [8] with $N = 100$ and $N = 750$ respectively.

Similar to the binary perceptron problem [5,4], the zero entropy condition does not correspond to the limit where the overlap q equals 1. In fact, from (13), it can be shown that for $q \to 1$, $S \to -\infty$. The critical overlap $q_c(M_{opt})$ is always below 1 (see figure 2). This means, that two solutions with utilities close to the optimum (within a relative deviation much less than $O(1/\sqrt{N})$) typically differ in a macroscopic number $O(N)$ of bits. As α, the relative number of constraints increases, q_c decreases. For $\alpha \to \infty$, two almost optimal solutions are uncorrelated.

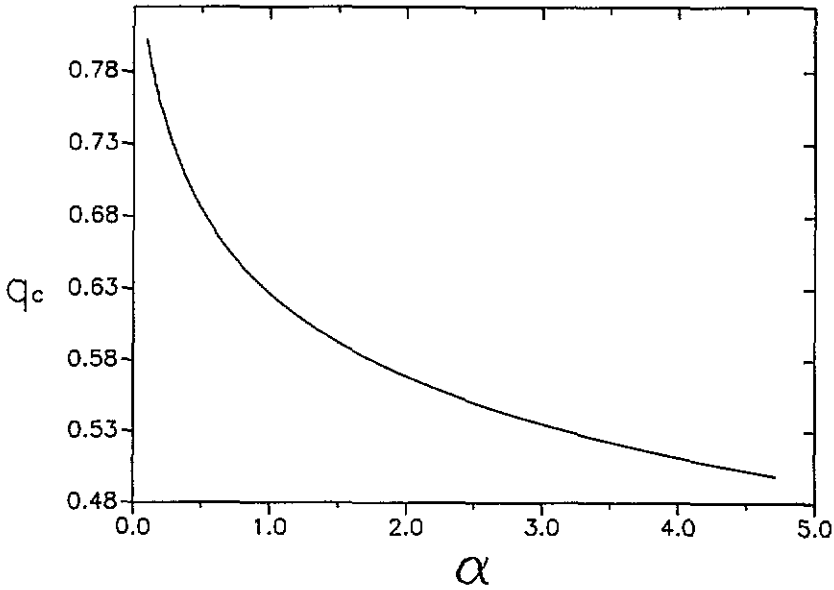

Figure 2. Overlap q_c of almost optimal solutions.

Our results are based on the assumption of replica symmetry. To check its validity, the stability of the RS-solution from the matrix of quadratic fluctuations of $q_{\alpha\beta}$ [9] must be calculated. This will be left to a forthcoming paper. Nevertheless, by the similarity of the knapsack problem with the binary perceptron, we strongly expect that replica symmetry is exact on the zero entropy line. In fact, for the binary perceptron, a careful analysis of the 1-step replica symmetry breaking solution [5] within a canonical ensemble (allowing for a violation of the inequality constraints) yields agreement with the RS calculations of the microcanonical ensemble [10].

We have compared our analytical result for M_{opt} with data [8] obtained from the MF-algorithm of [7] for $\alpha = 1$ (see the square and the diamond in figure 1). The difference ΔM of the data from the optimal value M_{opt} slightly increase with N. But the relative deviation from the maximal utility $\Delta U/U = \Delta M/(\sqrt{N} + M_{opt})$ is remarkably small and decreases from 0.055 for $N = 100$ to $\Delta U/U = 0.029$ at $N = 750$.

The validity of replica symmetry might give an explanation, why a MF-algorithm works so well for the knapsack problem. For such algorithm, the constraints of the problem are incorporated by a Hamiltonian that penalizes their violation. As for a simulated annealing method, the model is treated at finite temperature, which is slowly lowered to find nearly optimal solutions. However, for the mean-field algorithm, the temperature is not simulated by a stochastic process, but one derives approximate, deterministic equations [7] for the thermal averages of the decision variables $\{s_i\}$. An exact approach to such a type of mean-field theory has been developed for the Sherrington Kirkpatrick model of spin glasses by Thouless, Anderson and Palmer [11]. This so called TAP-approach and its relation to the replica theory has been analysed [12] in great detail. Assuming that a similar type of physics holds for the present problem, we suggest the following qualitative picture: When replica symmetry is exact, the phase space consists of a single ergodic component and we can expect that mean-field equations have only a single solution, which may be found without too many problems. The situation is worse for a broken replica symmetry. Here, exponentially (in N) many solutions would occur, and it would be hard to find one with a low free energy.

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