

An asymptotical study of combinatorial optimization problems by means of statistical mechanics ^{*}

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Abstract. The analogy between combinatorial optimization and statistical mechanics has proven to be a fruitful object of study. Simulated annealing, a metaheuristic for combinatorial optimization problems, is based on this analogy.

In this paper we use the statistical mechanics formalism based on the above mentioned analogy to analyze the asymptotic behavior of a special class of combinatorial optimization problems characterized by a combinatorial conditions which is well known in the literature. Our result is analogous to results of other authors derived by purely probabilistic means: Under natural probabilistic conditions on the coefficients of the problem, the ratio between the optimal value and the size of a feasible solution approaches almost surely the expected value of the coefficients, as the size of the problem tends to infinity. Our proof shows clearly why the above mentioned combinatorial condition, which characterizes the class of investigated problems, is essential.

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1 Introduction

Large combinatorial optimization problems are often hard to solve. In most of the cases this coincides with the membership in the class of NP-hard problems which implies that most probably the considered problem is not solvable by any polynomial time algorithm. Such difficulties in solving large problems are one more reason why the asymptotic behavior is a topic of interest. Generally we are interested in the asymptotic behavior of the optimal value of a combinatorial optimization problem as its size tends to infinity, under the assumption that the coefficients of the problem are random variables and fulfill certain (probabilistic) conditions.

A number of results on the asymptotic behavior of different problems, e.g. the linear assignment problem (LAP), the quadratic assignment problem (QAP), the traveling

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salesman problem (TSP), are available in the literature. As illustrative examples we describe briefly some results on the LAP and the QAP, two problems which show a completely different asymptotic behavior. In the linear assignment problem of size n we are given an $n \times n$ matrix $C = (c_{ij})$ and look for a permutation ϕ of $1, 2, \dots, n$, which minimizes $\sum_{i=1}^n c_{i\phi(i)}$. A number of results on the asymptotic behavior of the LAP has been derived in the 80's and early 90's. In the case that the coefficients c_{ij} are independent random variables uniformly distributed on $[0, 1]$, Olin [14] and Karp [11], respectively, showed that the optimal value of the LAP is bounded and lies between 1.51 and 2. Aldous [2] recently proved that the optimal value is equal to $\frac{\pi^2}{6} - o(1) \approx \frac{\pi^2}{6} \approx 1.645$, which was already suggested by Mézard and Parisi [13] (see also [9]). Thus the optimal value is independent from the size of the problem.

A completely different asymptotic behavior is shown by the quadratic assignment problem (QAP). In the Koopmans-Beckman QAP of size n we are given two $n \times n$ matrices $A = (a_{ij})$ and $B = (b_{ij})$ and look for a permutation ϕ of $1, 2, \dots, n$ which minimizes $g(\phi) = \sum_{i,j=1}^n a_{\phi(i)\phi(j)} b_{ij}$. The optimal value $g(\phi^*)$ of the QAP depends on the size n of the problem: $g(\phi^*) = \Theta(n^2)$. Moreover, as the size of the problem approaches infinity, the value of the objective function yielded by any solution gets arbitrarily close to the optimal value. In 1982, Burkard and Fincke studied the asymptotic probabilistic behavior of quadratic (sum) assignment problems of the Koopmans-Beckmann form (see [4]). Under certain probabilistic constraints on the coefficients of the problem, they have shown the following result: **(BF1)** *The relative difference between the worst value and the optimal value of the objective function tends to zero with probability tending to one as the size of the problem tends to infinity.*

An analogous result holds for the bottleneck QAP, see Burkard and Fincke [5].

Under similar probabilistic constraints on the coefficients of the problem Frenk, Houweninge and Rinnooy Kan derived the following result for the QAP: **(FHR)** *The objective function value can almost surely be written asymptotically as a function of the size of the problem and of the expected value of the coefficients of the problem.* When applied to the QAP, FHR is stronger than BF1, since FHR implies the following property: **(BF1')** *The ratio between the worst value and the optimal value of the objective function approaches 1 almost surely as the size of the problem tends to infinity.*

Under weaker probabilistic constraints, Rhee derives an analogous but sharper result for the QAP (see [15]). In a later work, Rhee considers the difference between the objective function and the function which approximates it asymptotically and almost surely, as stated in FHR. She estimates the expected value of this difference (see [16]).

In 1985, Burkard and Fincke generalize and strengthen the results of [4] to a whole class of combinatorial optimization problems. Problems belonging to this class are among others quadratic assignment problems (either sum or bottleneck version) as well as certain combinatorial and graph theoretical optimization problems (see [6]). For such problems the following result holds: **(BF2)** *With probability tending to one the ratio between the worst value and the optimal value of the objective function approaches 1 as the size of the problem tends to infinity.*

Under slightly more restrictive probabilistic conditions Szpankowski [18] shows that the following property holds for a whole class of combinatorial optimization problems: **(S)** *The ratio between the best and the worst value of the objective function tends almost*

surely to 1 as the size of the problem approaches infinity. The class of problems considered by Szpankowski is characterized by the same combinatorial condition (cf. (10)) which characterizes the class of problems investigated by Burkard and Fincke [6].

It is remarkable that all results mentioned above are derived by using purely probabilistic techniques, although the class of problems to which these results apply is defined in terms of a combinatorial structural condition. Recall, for example, that the asymptotic behavior of the QAP and the LAP (or the TSP) are essentially different simply because of their different combinatorial structure (see e.g. [6]).

In 1986, Bonomi and Lutton used a statistical mechanics formalism to analyze the asymptotic behavior of the QAP (see [3]). Bonomi and Lutton applied, however, an invalid convexity argument to exchange the limit and the derivative for a sequence of functions over $[0, +\infty)$ (see [3], page 297, equalities (13) and (14)¹), the exchange step being crucial for the whole proof.

In this paper we show that the statistical mechanics approach can be applied to analyze the asymptotic behavior of a whole class of combinatorial optimization problems which contains QAP as an element. This class of problems is similar to the classes of problems investigated by Burkard and Fincke [6] and Szpankowski [18]. Its elements show the following asymptotic behavior: the ratio between the optimal value and the size of a feasible solution approaches the expected value of the coefficients of the problem almost surely, as the size of the problem tends to infinity. An interesting feature of this approach is that it makes clear the importance of a combinatorial condition which characterizes the investigated class of problems and is fulfilled by all problems which are currently known to show the above mentioned asymptotic behavior, e.g. the quadratic assignment problem. This condition says that the ratio between the logarithm of the number of feasible solutions and the cardinality of a feasible solution tends to 0 as the size of the problem tends to infinity.

The paper is organized as follows. In Section 2 the analogy between combinatorial optimization and statistical mechanics is described in some detail and the statistical mechanics formalism is introduced. In Section 3 we introduce the class of combinatorial optimization problems we are dealing with and formulate our main result. Then, in the next section the main result is proved. The proof involves six lemmata and parts of it are quite technical. Finally, in Section 5 we discuss the nature of the conditions imposed on the problems we deal with, and formulate some open questions and general remarks.

2 Thermodynamics and Combinatorial Optimization

In combinatorial optimization we are interested in choosing a solution which minimizes the value of a certain objective function (or maximizes it, in the case of a maximization problem) among a finite number of feasible solutions. More formally a generic combinatorial optimization problem P may be defined as follows. Let a *ground set* E and a *cost function* $f: E \rightarrow \mathbb{R}^+$ be given. A *feasible solution* S is a subset of the ground set E and the set of feasible solutions is denoted by \mathcal{S} . By means of the cost function f we associate costs to the feasible solutions. One possibility is to define an objective function

¹It is not difficult to give examples of sequences of real functions which are convex on $[0, +\infty)$, where the derivative and the limit can not be exchanged in a neighborhood of 0.

$F: \mathcal{S} \rightarrow \mathbb{R}^+$, where $F(S)$ is given by

$$F(S) = \sum_{e \in S} f(e) \quad (1)$$

for all $S \in \mathcal{S}$. Such an objective function is often called a *sum* objective function. The (sum) problem can then be formulated as the task of finding

$$\min_{S \in \mathcal{S}} F(S). \quad (2)$$

Let us turn now to thermodynamics. A thermodynamical system may show different states which are characterized by different values of energy. In thermodynamics we are often interested in low-energy-states of the considered system, just as we are interested in feasible solutions with a small value of the objective function in a minimization problem. More precisely, an analogy between combinatorial optimization and thermodynamics can be built along the following two lines:

- Feasible solutions of a combinatorial optimization problem are analogous to states of a physical system.
- The objective function value corresponding to a feasible solution is analogous to the energy of the corresponding state.

According to statistical mechanics the thermal equilibrium of a thermodynamical system is characterized by the so-called *Boltzmann distribution*, where the probability that the system is at a state i with energy E_i at temperature T is given by

$$\frac{1}{Q(T)} \exp\left(\frac{-E_i}{k_B \cdot T}\right), \quad (3)$$

with k_B being a physical constant known as *Boltzmann constant*, and $Q(T)$ being the so called *partition function* defined by

$$Q(T) := \sum_j \exp\left(\frac{-E_j}{k_B \cdot T}\right). \quad (4)$$

In the last equality the summation extends over all possible states of the system.

The statistical mechanics formalism can be used to investigate the asymptotic behavior of combinatorial optimization problems. The first authors who argued on the use of this formalism to analyze the asymptotic behavior of the quadratic assignment problem were Bonomi and Lutton [3]. We apply this approach to a generic combinatorial optimization problem as introduced in the beginning of this section.

Our probabilistic model looks as follows. A probability $Pr(S)$ is assigned to each feasible solution of the problem $S \in \mathcal{S}$ by

$$Pr(S) = \frac{\exp(-F(S) \cdot \mu)}{Q(\mu)}, \quad (5)$$

where μ is a parameter which simulates *the reciprocal of the temperature*, and $Q(\mu)$ is the partition function defined analogously as in the Boltzmann distribution by

$$Q(\mu) := \sum_{S \in \mathcal{S}} \exp(-F(S) \cdot \mu). \quad (6)$$

Denote by $\langle F(S) \rangle(\mu)$ the expected value of the objective function $F(S)$ in the above probabilistic model, for fixed reciprocal of the temperature equal to μ . $\langle F(S) \rangle(\mu)$ is given by the following equality:

$$\langle F(S) \rangle(\mu) = \frac{1}{Q(\mu)} \sum_{S \in \mathcal{S}} F(S) \exp(-F(S) \cdot \mu). \quad (7)$$

It can easily be seen that the right-hand side of the above equality is equal to the derivative of $-\ln Q(\mu)$ with respect to μ :

$$\langle F(S) \rangle(\mu) = -(\ln Q(\mu))'. \quad (8)$$

Further, it is well known and easily seen that the following relationship between the variance $\Delta F(S)(\mu)$ of the objective function $F(S)$ (in the probabilistic model introduced above) and the second derivative of $\ln Q(\mu)$ holds:

$$\Delta F(S)(\mu) = \left\langle [F(S) - \langle F(S) \rangle(\mu)]^2 \right\rangle = (\ln Q(\mu))''. \quad (9)$$

3 The main result

In this section we formulate our main result concerning a specific asymptotic behavior of combinatorial optimization problems, and introduce the probabilistic and combinatorial conditions to be imposed to the combinatorial problem so as to guarantee that specific behavior.

Consider a sequence P_n , $n \in \mathbb{N}$, of instances of a generic combinatorial optimization problem, where P_n is the instance of size n (whatever this means). The ground set, the set of feasible solutions, the cost function, and the objective function of problem P_n are denoted by E_n , \mathcal{S}_n , f_n , and F_n , respectively. Denote by F_n^* , S_n^* , the optimal value and an optimal solution of problem P_n , respectively:

$$F_n^* = \min_{S \in \mathcal{S}_n} F_n(S) = F_n(S_n^*).$$

We assume that the costs $f_n(e)$, $e \in E_n$, $n \in \mathbb{N}$, are random variables, and that we are interested in the asymptotic behavior of F_n^* as n tends to infinity. We will show that under certain combinatorial and probabilistic conditions formulated below, the ratio $F_n^*/|S_n^*|$ almost surely approaches the expected value of the cost coefficients $f_n(e)$ as the size n of the problem tends to infinity.

Assume that our combinatorial optimization problem has the following properties:

- (P1) For each $n \in \mathbb{N}$, all feasible solutions $S \in \mathcal{S}_n$ have the same cardinality s_n .
- (P2) For some fixed $n \in \mathbb{N}$, let $\eta_n(e)$ be the number of feasible solutions $S \in \mathcal{S}_n$ such that $e \in S$. We suppose that there exists a constant η_n such that $\eta_n(e) = \eta_n$ for all $e \in E_n$.

(P3) The costs $f_n(e)$, $n \in \mathbb{N}$, $e \in E_n$, are random variables identically and independently distributed on $[0, M]$, where $M > 0$.

(P4) The cardinality of the set of feasible solutions $|\mathcal{S}_n|$ and the cardinality of the feasible solutions s_n tend to infinity as n tends to infinity. Furthermore

$$\lim_{n \rightarrow \infty} \frac{\ln |\mathcal{S}_n|}{s_n} = 0. \quad (10)$$

Let us denote by $E := \mathbb{E}(f_n(e))$ and $D := \text{Var}(f_n(e))$ the (common) expected value and variance of the random variables $f_n(e)$, $n \in \mathbb{N}$, $e \in E_n$, respectively. We will show that $\lim_{n \rightarrow \infty} \frac{F_n^*}{s_n} = E$, almost surely. Summarizing, our main result is given by the following theorem:

Theorem 3.1 *Let a combinatorial optimization problem be given as in (2) and let the properties (P1)-(P4) be fulfilled. Then $\frac{F_n^*}{s_n}$ converges almost surely (briefly a.s.) to E as n tends to infinity, i.e.*

$$Pr \left(\lim_{n \rightarrow \infty} \frac{F_n^*}{s_n} = E \right) = 1. \quad (11)$$

4 Proof of the main result

The proof of Theorem 3.1 is based on the following lemmata:

Lemma 4.1 *Under the conditions of Theorem 3.1, the expected value of the objective function $F_n(S)$ for $\mu = 0$ (according to the distribution on \mathcal{S}_n defined by (5)) fulfills the following property*

$$\lim_{n \rightarrow \infty} \frac{\langle F_n(S) \rangle(0)}{s_n} = E \quad a.s.$$

Proof. By applying equality (7) for $\mu = 0$ we get

$$\langle F_n(S) \rangle(0) = \sum_{S \in \mathcal{S}_n} F_n(S) \cdot \frac{1}{|\mathcal{S}_n|}.$$

Considering property (P2), the last equality can be transformed as follows:

$$\langle F_n(S) \rangle(0) = \frac{1}{|\mathcal{S}_n|} \cdot \sum_{S \in \mathcal{S}_n} \sum_{e \in S} f_n(e) = \frac{1}{|\mathcal{S}_n|} \cdot \sum_{e \in E_n} \eta_n \cdot f_n(e) = \frac{\eta_n}{|\mathcal{S}_n|} \sum_{e \in E_n} f_n(e).$$

From (P2) we have $|\mathcal{S}_n| \cdot s_n = |E_n| \cdot \eta_n$, and by substitution we obtain:

$$\frac{\langle F_n(S) \rangle(0)}{s_n} = \frac{\sum_{e \in E_n} f_n(e)}{|E_n|}. \quad (12)$$

Since condition (P3) is satisfied, the variance D of the cost coefficients $f_n(e)$ is bounded, and the strong law of large numbers applies:

$$Pr \left(\lim_{n \rightarrow \infty} \frac{\langle F_n(S) \rangle(0)}{s_n} = E \right) = 1. \quad (13)$$

■

Lemma 4.2 *Under the conditions of Theorem 3.1, there exists a convergent subsequence $\frac{F_{n_m}^*}{s_{n_m}}$ of the sequence $\frac{F_n^*}{s_n}$ with limit equal to l .*

Proof. Since $\left| \frac{F_n(S_n^*)}{s_n} \right| \leq \frac{Ms_n}{s_n} = M$, the sequence $\frac{F_n^*}{s_n}$ is bounded. Therefore, it has at least one cluster point, which we denote by l , and a subsequence $\frac{F_{n_m}^*}{s_{n_m}}$ converging to l :

$$l := \lim_{m \rightarrow \infty} \frac{F_{n_m}^*}{s_{n_m}}. \quad (14)$$

■

If S_n^* is an optimal solution of problem P_n , the following inequalities hold for the partition function $Q_n(\mu)$:

$$\exp(-F_n(S_n^*) \cdot \mu) \leq Q_n(\mu) \leq |\mathcal{S}_n| \cdot \exp(-F_n(S_n^*) \cdot \mu) \quad (15)$$

$$-F_n^* \cdot \mu \leq \ln Q_n(\mu) \leq \ln |\mathcal{S}_n| - F_n^* \cdot \mu. \quad (16)$$

Let us now introduce the continuous and differentiable functions $G_n(\mu) = \frac{\ln Q_n(\mu)}{s_n}$, defined on $[0, \infty)$, for all $n \in \mathbb{N}$. Dividing both sides of (16) by s_n we get

$$-\mu \cdot \frac{F_n^*}{s_n} \leq G_n(\mu) \leq \frac{\ln |\mathcal{S}_n|}{s_n} - \mu \cdot \frac{F_n^*}{s_n}. \quad (17)$$

Lemma 4.3 *Under the conditions of Theorem 3.1, for each l defined in (14), there exists a subsequence $G_{n_k}(\mu)$ of the sequence of functions $G_n(\mu)$, such that $G_{n_k}(\mu)$ and the sequence of its derivatives $G'_{n_k}(\mu)$ converge uniformly in $[\alpha, +\infty)$ for any $\alpha > 0$, and*

$$\lim_{k \rightarrow \infty} G_{n_k}(\mu) = -\mu \cdot l, \quad (18)$$

$$\lim_{k \rightarrow \infty} G'_{n_k}(\mu) = -l. \quad (19)$$

Proof. We apply the following well known result (see e.g. [17]). Let a sequence of differentiable functions G_{n_m} , pointwise convergent on an interval $[\alpha, +\infty)$, be given. Assume that the sequence of derivatives G'_{n_m} is equicontinuous and uniformly bounded on $[\alpha, \infty)$. Then, there exists a subsequence G_{n_k} of G_{n_m} such that both sequences G_{n_k} and G'_{n_k} are uniformly convergent on $[\alpha, \infty)$.

Note that the pointwise convergence of $G_{n_m}(\mu)$ follows from Lemma 4.2, (10) and (17). Thus, in order to prove the lemma it is sufficient to show that the sequence of functions G'_{n_m} is uniformly bounded and equicontinuous on $[\alpha, \infty)$.

First, let us show that the sequence of derivatives G'_n is *uniformly bounded* on $[\alpha, +\infty)$. Remark that $\forall S \in \mathcal{S}_n$ the following equality holds:

$$F_n(S) = \sum_{e \in S} f_n(e) \leq M \cdot |S| = M \cdot s_n. \quad (20)$$

The following inequalities show that $G'_n(\mu)$ is uniformly bounded:

$$|G'_n(\mu)| \leq \frac{\sum_{S \in \mathcal{S}_n} |F_n(S)| \cdot \exp(-\mu \cdot F_n(S))}{s_n \cdot Q_n(\mu)} \leq \frac{s_n \cdot M \cdot \sum_{S \in \mathcal{S}_n} \exp(-\mu \cdot F_n(S))}{s_n \cdot Q_n(\mu)} = M.$$

Secondly, we show that the sequence of functions G'_n is equicontinuous on $[\alpha, +\infty)$, i.e. $\forall \varepsilon > 0 \exists \delta > 0$, such that $\forall \mu_1, \mu_2 \in [\alpha, +\infty)$ and $\forall n \in \mathbb{N}$

$$|\mu_1 - \mu_2| < \delta \quad \Rightarrow \quad |G'_n(\mu_1) - G'_n(\mu_2)| \leq \varepsilon$$

holds.

Let us evaluate the difference $|G'_n(\mu_1) - G'_n(\mu_2)|$, for $\alpha \leq \mu_1 \leq \mu_2$ and $n \in \mathbb{N}$.

$$\begin{aligned} |G'_n(\mu_1) - G'_n(\mu_2)| &\leq \sum_{S \in \mathcal{S}_n} \frac{F_n(S)}{s_n} \cdot \left| \frac{\exp(-\mu_1 \cdot F_n(S))}{Q_n(\mu_1)} - \frac{\exp(-\mu_2 \cdot F_n(S))}{Q_n(\mu_2)} \right| \\ &\leq M \cdot \sum_{S \in \mathcal{S}_n} \frac{\exp(-\mu_1 \cdot F_n(S))}{Q_n(\mu_1)} \cdot \left| 1 - \frac{Q_n(\mu_1) \cdot \exp(-\mu_2 \cdot F_n(S))}{Q_n(\mu_2) \cdot \exp(-\mu_1 \cdot F_n(S))} \right|. \end{aligned} \quad (21)$$

Next, we show that there exists a $T > 0$ such that the following inequality holds for all $S_0 \in \mathcal{S}_n$ and for all $n \in \mathbb{N}$:

$$\left| 1 - \frac{Q_n(\mu_1) \cdot \exp(\mu_1 \cdot F_n(S_0))}{Q_n(\mu_2) \cdot \exp(\mu_2 \cdot F_n(S_0))} \right| \leq T \cdot (\mu_2 - \mu_1). \quad (22)$$

The following elementary transformations prove the existence of such a T . Assume w.l.o.g. that

$$\begin{aligned} &\left| \sum_{S: F_n(S) > F_n(S_0)} \exp(\mu_2(F_n(S_0) - F_n(S))) - \sum_{S: F_n(S) > F_n(S_0)} \exp(\mu_1(F_n(S_0) - F_n(S))) \right| \geq \\ &\left| \sum_{S: F_n(S) < F_n(S_0)} \exp(\mu_2(F_n(S_0) - F_n(S))) - \sum_{S: F_n(S) < F_n(S_0)} \exp(\mu_1(F_n(S_0) - F_n(S))) \right| \end{aligned}$$

(The other case can be handled analogously.) Then we have

$$\begin{aligned} \left| 1 - \frac{Q_n(\mu_1) \cdot \exp(\mu_1 \cdot F_n(S_0))}{Q_n(\mu_2) \cdot \exp(\mu_2 \cdot F_n(S_0))} \right| &= \left| 1 - \frac{1 + \sum_{S \in \mathcal{S}_n: S \neq S_0} \exp(\mu_1 \cdot (F_n(S_0) - F_n(S)))}{1 + \sum_{S \in \mathcal{S}_n: S \neq S_0} \exp(\mu_2 \cdot (F_n(S_0) - F_n(S)))} \right| \leq \\ &\frac{\left| \sum_{S: F_n(S) > F_n(S_0)} \left[\exp(\mu_2 \cdot (F_n(S_0) - F_n(S))) - \exp(\mu_1 \cdot (F_n(S_0) - F_n(S))) \right] \right|}{\sum_{S: F_n(S) > F_n(S_0)} \exp(\mu_2 \cdot (F_n(S_0) - F_n(S)))} = \end{aligned}$$

$$\begin{aligned} & \left| \frac{\sum_{S: F_n(S) > F_n(S_0)} \exp\left(\mu_1 \cdot (F_n(S_0) - F_n(S))\right) \left[\exp\left((\mu_2 - \mu_1) \cdot (F_n(S_0) - F_n(S))\right) - 1 \right]}{\sum_{S: F_n(S) > F_n(S_0)} \exp\left(\mu_2 \cdot (F_n(S_0) - F_n(S))\right)} \right| \leq \\ & \leq \frac{\left| \sum_{S: F_n(S) > F_n(S_0)} \left[\exp\left((\mu_2 - \mu_1) \cdot (F_n(S_0) - F_n(S))\right) - 1 \right] \right|}{\sum_{S: F_n(S) > F_n(S_0)} \exp\left(\mu_2 \cdot (F_n(S_0) - F_n(S))\right)}. \end{aligned}$$

We now show that

$$\begin{aligned} & \left| \sum_{S: F_n(S) > F_n(S_0)} \left[\exp\left((\mu_2 - \mu_1) \cdot (F_n(S_0) - F_n(S))\right) - 1 \right] \right| \leq \\ & \frac{1}{\alpha} \cdot (\mu_2 - \mu_1) \cdot \sum_{S: F_n(S) > F_n(S_0)} \exp\left[\mu_2 \cdot (F_n(S_0) - F_n(S))\right]. \end{aligned} \quad (23)$$

Indeed, inequality (23) follows from the following inequalities which hold for all $S \in \mathcal{S}_n$ such that $F_n(S) \geq F_n(S_0)$.

$$\begin{aligned} \left| \exp\left((\mu_2 - \mu_1) \cdot (F_n(S_0) - F_n(S))\right) - 1 \right| & \leq (\mu_2 - \mu_1) \cdot \sum_{i=1}^{\infty} \frac{(\mu_2 - \mu_1)^{i-1} \cdot (F_n(S) - F_n(S_0))^i}{i!} \\ & \leq (\mu_2 - \mu_1) \cdot \frac{1}{\alpha} \cdot \sum_{i=1}^{\infty} \frac{(\mu_2)^i \cdot (F_n(S) - F_n(S_0))^i}{i!} \\ & \leq (\mu_2 - \mu_1) \cdot \frac{1}{\alpha} \cdot \exp\left[\mu_2 \cdot (F_n(S) - F_n(S_0))\right]. \end{aligned}$$

By putting things together we get (22) with $T := \frac{1}{\alpha}$.

We return at (21) and obtain:

$$\left| G'_n(\mu_1) - G'_n(\mu_2) \right| \leq M \cdot \frac{1}{\alpha} \cdot (\mu_2 - \mu_1) \cdot \sum_{S \in \mathcal{S}_n} \frac{\exp(-\mu_1 \cdot F_n(S))}{Q_n(\mu_1)} = M \cdot \frac{1}{\alpha} \cdot (\mu_2 - \mu_1),$$

from which the equicontinuity of G'_n on $[\alpha, \infty)$ obviously follows.

Due to (10), (14) and (17) we have $\lim_{k \rightarrow \infty} G_{n_k}(\mu) = -\mu l$. Then, due to the uniform convergence of the above sequence together with the sequence of its derivatives we get

$$\lim_{k \rightarrow \infty} G'_{n_k}(\mu) = \left(\lim_{k \rightarrow \infty} G_{n_k}(\mu) \right)' = -l. \quad \blacksquare$$

Lemma 4.4 $E \geq l$, where E and l are defined above.

Proof. Consider the expected value $\mathbb{E}(F_n(S))$ of the objective function value of problem P_n , $S \in \mathcal{S}_n$ (with respect to the distribution of the random variables $f_n(e)$, $e \in E_n$). We have $\mathbb{E}(F_n(S)) = s_n E$ and hence $\mathbb{E}\left(\frac{F_n(S)}{s_n}\right) = E$. This implies that $\frac{F_n^*}{s_n} \leq E \quad \forall n \in \mathbb{N}$. Then, since l is defined as the limit of a subsequence of $\frac{F_n^*}{s_n}$, we have $l \leq E$. \blacksquare

At this point there are two possibilities: either $l = E$ and E is the (unique) limit of $\frac{F_n^*}{s_n}$, or there exists a cluster point l of $\frac{F_n^*}{s_n}$ such that $l < E$. In the first case the main result follows immediately. We show that the second case almost surely cannot happen.

Assume that $l < E$ throughout the rest of this section. Clearly, in this case the convergence of G_{n_k} and G'_{n_k} is not *uniform* over the whole $[0, \infty)$ (cf. Lemma 4.1). According to Lemma 4.3, however, $\lim_{k \rightarrow \infty} G'_{n_k}(\mu) = -l$ uniformly on $[\alpha, \infty)$ for each $\alpha > 0$, and $\lim_{k \rightarrow \infty} G'_{n_k}(0) = -E < -l$, due to Lemma 4.1. Under these conditions, for all $K > 0$ and for all $m \in \mathbb{N}$ there must be some $\mu_0 \geq 0$ and some $k_0 \in \mathbb{N}$, $k_0 > m$, such that $G''_{n_{k_0}}(\mu_0) \geq K$. Indeed, given a $K > 0$, we choose $\varepsilon = (E - l)/4$ and $\alpha = \frac{E-l}{2K}$, and apply the above mentioned convergence result on $[\alpha, \infty)$ and at $\mu = 0$. For k_0 large enough we have $G'_{n_{k_0}}(\alpha) > -l - \varepsilon$ and $G'_{n_{k_0}}(0) < -E + \varepsilon$. Thus, by the mean value theorem,

$$\alpha G''_{n_{k_0}}(\mu_0) = G'_{n_{k_0}}(\alpha) - G'_{n_{k_0}}(0) > E - l - 2\varepsilon = \frac{E - l}{2},$$

for some $\mu_0 \in [0, \alpha]$. The last equality implies that $G''_{n_{k_0}}(\mu_0) \geq K$. Thus the second derivatives $G''_{n_k}(\mu)$ are unbounded as k approaches infinity and μ approaches 0. We show that almost surely this cannot be the case, because: a) The third derivative $G'''_{n_k}(\mu)$ is almost surely non-positive for $\mu \geq 0$ and b) the sequence of second derivatives $G''_n(0)$ is almost surely bounded. Combining a) and b) with the nonnegativity of the second derivative $G''_n(\mu) = \frac{\Delta F_n(S)(\mu)}{s_n}$ (cf. (9)) for all $n \in \mathbb{N}$ and $\mu \geq 0$, yields the desired contradiction. The facts a) and b) are proven in the next two lemmata.

Lemma 4.5 *The third derivative $G'''_{n_k}(\mu)$ is almost surely non-positive for $k \geq k_0$, $\mu \geq 0$, where k_0 is some fixed natural number.*

Proof. We have

$$G'''_{n_k}(\mu) = \frac{1}{s_{n_k}} [\Delta F_{n_k}(S)(\mu)]' = \frac{1}{s_{n_k}} \left[\sum_{S \in \mathcal{S}_{n_k}} [F_{n_k}(S) - \langle F_{n_k} \rangle(\mu)]^2 \frac{e^{-F_{n_k}(S)\mu}}{Q_{n_k}(\mu)} \right]',$$

where $\langle \cdot \rangle(\mu)$ denotes the expectation w.r.t. the Boltzmann distribution with parameter μ . It follows that

$$\begin{aligned} G'''_{n_k}(\mu) &= \frac{1}{s_{n_k}} \left[\sum_{S \in \mathcal{S}_{n_k}} 2 \left(F_{n_k}(S) - \langle F_{n_k} \rangle(\mu) \right) \frac{e^{-F_{n_k}(S)\mu}}{Q_{n_k}(\mu)} \left(\frac{\langle F_{n_k}^2 \rangle(\mu)}{Q_{n_k}(\mu)} - \langle F_{n_k} \rangle^2(\mu) \right) + \right. \\ &\quad \left. + \sum_{S \in \mathcal{S}_{n_k}} [F_{n_k}(S) - \langle F_{n_k} \rangle(\mu)]^2 \left(-F_{n_k}(S) \frac{e^{-F_{n_k}(S)\mu}}{Q_{n_k}(\mu)} + \langle F_{n_k} \rangle(\mu) \frac{e^{-F_{n_k}(S)\mu}}{Q_{n_k}(\mu)} \right) \right] = \end{aligned}$$

$$= \frac{1}{s_{n_k}} \left(0 - \sum_{S \in \mathcal{S}_{n_k}} \left(F_{n_k}(S) - \langle F_{n_k} \rangle(\mu) \right)^3 \frac{e^{-F_{n_k}(S)\mu}}{Q_{n_k}(\mu)} \right) = - \frac{\langle (F_{n_k} - \langle F_{n_k} \rangle(\mu))^3 \rangle(\mu)}{s_{n_k}}.$$

Hence it is enough to show that $F_{n_k}(S) - \langle F_{n_k} \rangle(\mu) \geq 0$, $\forall \mu \geq 0$, almost surely. Indeed, for all $S \in \mathcal{S}_{n_k}$, $F_{n_k}(S) = \sum_{e \in S} f_{n_k}(e)$ is the sum of s_{n_k} independent and identically distributed random variables with $\mathbb{E}(f_{n_k}(e)) = E$. Thus, according to the strong law of large numbers, we have

$$Pr \left(\lim_{k \rightarrow \infty} \left| \frac{F_{n_k}(S)}{s_{n_k}} - E \right| = 0 \right) = 1.$$

At the same time, we have for all $\mu > 0$

$$Pr \left(\lim_{k \rightarrow \infty} \left| \frac{\langle F_{n_k} \rangle(\mu)}{s_{n_k}} - l \right| = 0 \right) = 1,$$

due to the uniform convergence of $-G'_{n_k}(\mu) = \frac{\langle F_{n_k} \rangle(\mu)}{s_{n_k}}$ to l on any interval $[\alpha, \infty)$, $\alpha > 0$. The inequality $E > l$, together with Lemma 4.1 for the case $\mu = 0$, thus implies that $F_{n_k}(S) - \langle F_{n_k} \rangle(\mu) \geq 0$ *a.s.* for all $\mu \geq 0$, as desired. \blacksquare

Lemma 4.6 *The sequence of the second derivatives $G''_n(0)$ is almost surely bounded.*

Proof. Since $G''_n(0) = \frac{\Delta F_n(S)(0)}{s_n} \geq 0$, we have by Markov's inequality

$$Pr (G''_n(0) > K) \leq \frac{\mathbb{E}(G''_n(0))}{K}$$

for every $K > 0$, where \mathbb{E} denotes the expectation w.r.t. the distribution of the random variables $f_n(e)$, $e \in E_n$. Now we have

$$\begin{aligned} \mathbb{E}(G''_n(0)) &= \mathbb{E} \left(\frac{1}{s_n |\mathcal{S}_n|} \sum_{S \in \mathcal{S}_n} F_n^2(S) - \frac{1}{s_n |\mathcal{S}_n|^2} \left(\sum_{S \in \mathcal{S}_n} F_n(S) \right)^2 \right) \\ &= \frac{1}{s_n |\mathcal{S}_n|} \mathbb{E} \left(\sum_{S \in \mathcal{S}_n} \left(\sum_{e \in S} f_n(e) \right)^2 \right) - \frac{1}{s_n |\mathcal{S}_n|^2} \mathbb{E} \left(\sum_{S \in \mathcal{S}_n} \sum_{e \in S} f_n(e) \right)^2 \\ &= \frac{1}{s_n} \mathbb{E} \left(\sum_{e \in S} f_n(e) \right)^2 - \frac{\eta_n^2}{s_n |\mathcal{S}_n|^2} \mathbb{E} \left(\sum_{e \in E_n} f_n(e) \right)^2 \\ &= \frac{1}{s_n} (s_n D + s_n^2 E^2) - \frac{\eta_n^2}{s_n |\mathcal{S}_n|^2} (|E_n| D + |E_n|^2 E^2) \\ &= D \left(1 - \frac{s_n}{|E_n|} \right) \leq D, \end{aligned}$$

where we have used the equality $\eta_n |E_n| = s_n |\mathcal{S}_n|$. Thus, for any $K > 0$,

$$Pr (G''_n(0) > K) \leq \frac{D}{K}.$$

Since $D = \text{Var}(f_n(e))$ is finite, it follows that $G''_n(0)$ is almost surely bounded. \blacksquare

Summarizing, if $l < E$, the second derivatives G_{n_k}'' almost surely have to be bounded and unbounded at the same time. This implies that $l < E$ can not happen. Thus $l = E$ a.s. and Theorem 3.1 holds.

Remark: The proof technique can also be interpreted as follows: Since $\frac{\langle F_n \rangle(\mu)}{s_n} = |G_n'(\mu)| \leq M$ is bounded, for each $\mu \geq 0$ there exists a convergent subsequence such that $\lim_{k \rightarrow \infty} \frac{\langle F_{n_k} \rangle(\mu)}{s_{n_k}} = l(\mu)$. In the proof it is shown that $l(\mu)$ does not depend on μ and $l = E$ almost surely, from which it follows that

$$\lim_{n \rightarrow \infty} \frac{\langle F_n \rangle(\mu)}{s_n} = E \quad \text{almost surely for any } \mu \in [0, \infty). \quad (24)$$

Recall that $\langle F_n \rangle(\mu)$ denotes the expectation of $F_n(S)$ w.r.t. the Boltzmann weight with parameter μ assigned to each admissible solution $S \in \mathcal{S}_n$. The right hand side of (24) being independent of μ , Theorem 3.1 can now be deduced for $\mu \rightarrow \infty$, since for any $S_0 \in \mathcal{S}_n$ we have (see e.g. Aarts and Korst [1])

$$\begin{aligned} \lim_{\mu \rightarrow \infty} Pr(S_0) &= \lim_{\mu \rightarrow \infty} \frac{e^{-F_n(S_0)\mu}}{Q_n(\mu)} = \lim_{\mu \rightarrow \infty} \frac{e^{-F_n(S_0)\mu}}{\sum_{S \in \mathcal{S}_n} e^{-F_n(S)\mu}} \\ &= \lim_{\mu \rightarrow \infty} \frac{e^{-\mu(F_n(S_0) - F_n^*)}}{|S_n^*| + \sum_{S \in \mathcal{S}_n \setminus S_n^*} e^{-\mu(F_n(S) - F_n^*)}} = \begin{cases} \frac{1}{|S_n^*|} & \text{for } S_0 \in S_n^* \\ 0 & \text{for } S_0 \in \mathcal{S}_n \setminus S_n^* \end{cases} \end{aligned}$$

where $S_n^* \subset \mathcal{S}_n$ is the set of optimal solutions of problem P_n , and thus for all $n \in \mathbb{N}$ we have $\lim_{\mu \rightarrow \infty} \langle F_n \rangle(\mu) = F_n^*$.

5 Discussion and open questions

Let us shortly discuss conditions (P1)-(P4). (P3) is a probabilistic condition on the coefficients of the problem and we will come back to that later on. Condition (P4) is a crucial, purely combinatorial condition, which is used in Lemma 4.3 to show the pointwise convergence of $G_{n_k}(\mu)$ and this is the simplest kind of convergence which has to hold in order to get through with the other lemmata. A nice feature of our proof of the main result is that it shows explicitly the importance of condition (P4). Note that (P4) is essential for deriving any of the results existing in the literature on problems which show an asymptotic behavior similar to the one described by Theorem 3.1 (e.g. results BF1, BF2 and FHR).

Conditions (P1) and (P2) describe the combinatorial structure of the set of feasible solutions. (P1) characterizes the feasible solutions from a quantitative point of view saying that all feasible solutions have the same cardinality. (P2) describes the set of feasible solutions from a structural point of view showing how often an element of the ground set appears in some feasible solution. The fact that this frequency index is constant among different elements from the ground set means that the feasible solutions are distributed somehow uniformly in the ground set. It is an open question whether condition (P1) can be dropped or substituted by a weaker one. Szpankowski [18] showed in his purely probabilistic proof of Theorem 3.1, that (P2) can be dropped, if in addition F_n^* is a nonincreasing function of n and $|\mathcal{S}_{n+1}| \geq |\mathcal{S}_n|$ for all $n \in \mathbb{N}$.

Conditions (P1) and (P2) are fulfilled by many combinatorial optimization problems. (P4) is a more restrictive condition and it is essential for the correctness of the main result. As an illustrating example consider that the QAP fulfills all these conditions whereas the linear assignment problem (LAP) fulfills only (P1) and (P2) but not (P4). Indeed, the QAP of size n can be formulated as a general combinatorial optimization problem with a ground set

$$E_n = \{(i, j, k, l): 1 \leq i, j, k, l \leq n \text{ such that } i = j \text{ if and only if } k = l\},$$

feasible solutions

$$S_\phi = \{(i, j, \phi(i), \phi(j)): 1 \leq i, j \leq n\}$$

for ϕ being a permutation of $1, 2, \dots, n$, and the set of feasible solutions

$$S_n = \{S_\phi: \phi \text{ is a permutation of } 1, 2, \dots, n\},$$

(see also [6]). Clearly $|E_n| = O(n^4)$, $|S_\phi| = n^2$ for any permutation ϕ , $|S_n| = n!$, and condition (P4) is fulfilled, since $\frac{\ln(n!)}{n^2} = o(1)$. Each element (i, j, k, l) of the ground set appears in $(n-2)!$ feasible solutions, namely in all S_ϕ corresponding to some permutation ϕ for which $\phi(i) = k$, $\phi(j) = l$. Thus $\eta_n = (n-2)!$.

For the linear assignment problem of size n the ground set \bar{E}_n is given by $\bar{E}_n = \{(i, j): 1 \leq i, j \leq n\}$, the feasible solutions are given by $\bar{S}_\phi = \{(i, \phi(i)): 1 \leq i \leq n\}$, for some permutation ϕ of $1, 2, \dots, n$, and the set of feasible solutions \bar{S}_n is given as

$$\bar{S}_n = \{\bar{S}_\phi: \phi \text{ is a permutation of } 1, 2, \dots, n\}.$$

In this case we have $|\bar{S}_n| = n!$, $|\bar{S}_\phi| = n$ for all permutations ϕ , $|\bar{E}_n| = n^2$, and each pair (i, j) , belongs to $(n-1)!$ feasible solutions corresponding to permutations which assign i to j . Thus $\eta_n = (n-1)!$. Notice however, that condition (P4) is not fulfilled because $\frac{\ln n!}{n}$ tends to ∞ as n approaches infinity. It can be checked that the result of Theorem 3.1 does not hold in the case of the LAP. Indeed, consider an LAP with cost coefficients uniformly and independently distributed on $[0, 1]$. As shown by Karp [11], the expected optimal value of this problem $\mathbb{E}(F_n^*)$ is bounded from above by 2. Theorem 3.1 would now imply $Pr(\lim_{n \rightarrow \infty} \frac{F_n^*}{n} = \frac{1}{2}) = 1$, leading to

$$Pr\left(\exists n_0 \text{ such that } F_n^* \geq \frac{n}{4} \text{ for } n \geq n_0\right) = 1,$$

which contradicts the boundedness of F_n^* . Thus Theorem 3.1 cannot hold in this case.

Now let us turn to condition (P3). A standard assumption in the literature concerning the asymptotic behavior of combinatorial optimization problems is that the coefficients of the problem are independent random variables with a common distribution (and not necessarily bounded). Also the assumption of finite variance and higher order moments can be considered as a natural one (while being redundant in case of bounded cost coefficients). Szpankowski [18] showed that in such a case under additional monotonicity assumptions on F_n^* and $|S_n|$, Theorem 3.1 can be proved by purely probabilistic techniques. One can ask, however, what happens in our proof of the main theorem with our set of assumptions in case that the cost coefficients $f_n(e)$ are not bounded, but

distributed on $[0, +\infty)$, while fulfilling all other requirements in (P3). We can observe that the boundedness of the coefficients has only been exploited in the proofs of Lemma 4.2 and Lemma 4.3 to show that the sequences $\frac{F_n^*}{s_n}$ and $G_n'(\mu)$, $\mu \geq 0$, are bounded. Of course, if we drop the boundedness condition on $f_n(e)$, the boundedness of the above sequences cannot be guaranteed.

However, given that the first two moments of $f_n(e)$ are finite, the probability that $\frac{F_n(S)}{s_n}$ is bounded tends to 1 as the size n of the problem tends to infinity for any $S \in \mathcal{S}_n$. Indeed, recall that $\mathbb{E}(F_n(S)) = s_n E$, $\text{Var}(F_n(S)) = s_n D$, and therefore $\mathbb{E}\left(\frac{F_n(S)}{s_n}\right) = E$ and $\text{Var}\left(\frac{F_n(S)}{s_n}\right) = \frac{D}{s_n}$. By applying Chebyshev's inequality we get

$$\Pr\left(\frac{F_n(S)}{s_n} \geq K\right) \leq \Pr\left(\left|\frac{F_n(S)}{s_n} - E\right| \geq K - E\right) \leq \frac{D^2}{s_n^2(K - E)^2},$$

for any $K > E$. Since $s_n \rightarrow \infty$ as n approaches infinity, Lemma 4.2 and Lemma 4.3 hold in probability. This implies that also our main result holds in probability in the case that the coefficients of the problem are unbounded.

Corollary 5.1 *Let a combinatorial optimization problem be given as in (2). Assume that the costs $f_n(e)$, $n \in \mathbb{N}$, $e \in E_n$, are random variables identically and independently distributed on $[0, +\infty)$ with finite expectation and variance. Assume moreover that the properties (P1), (P2), and (P4) are fulfilled. Then $\frac{F_n^*}{s_n}$ converges in probability to E as the size n of the problem tends to infinity, i.e.*

$$\forall \epsilon > 0, \lim_{n \rightarrow \infty} \Pr\left(\left|\frac{F_n^*}{s_n} - E\right| < \epsilon\right) = 1. \quad (25)$$

It remains an open question whether the stronger convergence result for unbounded cost coefficients can be obtained through the statistical mechanics formalism. Another question of general interest arises when making an analogy with simulated annealing as another statistical mechanics approach in combinatorial optimization. Is there any class of problems which is well suited for simulated annealing? Is this class characterized by any combinatorial property? Clearly, this is a rather complex question and its complete answer seems to be currently out of sight.

Finally, let us briefly discuss the result presented in this paper in comparison to existing results on the asymptotic behavior of combinatorial optimization problems presented in [6, 18]. The “in probability” version of the result presented in this paper follows from the result of Burkard and Fincke [6], whereas the “almost sure” version does not. The stronger version of our result, the “almost sure” version, is the same as the result obtained by Szpankowski [18] under slightly different conditions. It is worthy to notice, however, that our proof technique is completely different from the purely probabilistic techniques applied in [6, 18] and provides a further application of the useful analogy between statistical mechanics and combinatorial optimization. Another nice feature of our proof is that it reveals the importance of the combinatorial condition (P4): The pointwise convergence of the expected value of the objective function can only be shown if that combinatorial condition is fulfilled.

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