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# An asymptotical study of combinatorial optimization problems by means of statistical mechanics[☆]

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Dedicated to Jef L. Teugels on the occasion of his 65th birthday

## 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 show how a statistical mechanics formalism can be utilized to analyze the asymptotic behavior of combinatorial optimization problems with sum objective function and provide an alternative proof for the following result: Under a certain combinatorial condition and some natural probabilistic assumptions on the coefficients of the problem, the ratio between the optimal solution and an arbitrary feasible solution tends to one almost surely, as the size of the problem tends to infinity, so that the problem of optimization becomes trivial in some sense. Whereas this result can also be proven by purely probabilistic techniques, the above approach allows one to understand why the assumed combinatorial condition is essential for such a type of asymptotic behavior.


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## 1. Introduction

Large combinatorial optimization problems are often hard to solve. This is in particular the case for NP-hard problems implying that most probably the considered problem is not solvable by any polynomial time algorithm. In these situations an asymptotic analysis of the problem is needed, where in general the coefficients of the problem are assumed to be random variables and the behavior of the optimal solution is investigated as the problem size tends to infinity.

For a number of combinatorial optimization problems, asymptotic results are available in the literature, e.g., for the linear assignment problem (LAP), the quadratic assignment problem (QAP) and the traveling salesman problem (TSP). In the LAP of size *n*, an $n \times n$ matrix $C = (c_{ij})$ is given and one looks for a permutation $\phi$ of $1, 2, \ldots, n$ that minimizes $\sum_{i=1}^{n} c_{i\phi(i)}$. If the coefficients $c_{ij}$ are independent random variables uniformly distributed on $[0, 1]$, Aldous [3] proved that the optimal value of the LAP is given by $\pi^2/6 - \mathrm{o}(1)$, confirming a conjecture of Mézard and Parisi [15] (for earlier work on that problem, see [10,11,13,16]). Thus, for large *n*, the optimal value becomes independent of the size of the problem and, heuristically, the larger number of summands is exactly compensated by the larger set of available permutations.

A completely different asymptotic behavior is exhibited by the QAP: In the Koopmans–Beckmann QAP of size *n*, two $n \times n$ matrices $A = (a_{ij})$ and $B = (b_{ij})$ are given and one looks for a permutation $\phi$ of $1, 2, \ldots, n$ that minimizes $g(\phi) = \sum_{i,j=1}^{n} a_{\phi(i)\phi(j)} b_{ij}$. If the coefficients $a_{ij}$ and $b_{ij}$ are independent random variables uniformly distributed on $[0, 1]$, then the optimal value is given by $g(\phi^*) = \Theta(n^2)$ and thus depends on the size *n* of the problem. However, under certain probabilistic constraints on the coefficients, the value of the objective function for any feasible solution gets arbitrarily close to the optimal value as $n \to \infty$, and in that way the problem of optimization becomes in some sense trivial (although the QAP is NP-hard!). Specifically, Burkard and Fincke [5,6] showed that for the Koopmans–Beckmann QAP and the bottleneck QAP, the ratio of the worst and the optimal feasible solution tends to 1 in probability (for the QAP this was strengthened to almost sure convergence by Frenk et al. [12] under similar probabilistic constraints, see also [17,18]). In [7], Burkard and Fincke extended the above convergence in probability result to a whole class of combinatorial optimization problems (including graph-theoretic problems) characterized by a specific combinatorial condition, which was generalized to almost sure convergence by Szpankowski [20]. Sharp convergence rates of the relative difference between best and worst solutions of bottleneck problems in the above class have recently been obtained by Albrecher [2].

The above results are derived by purely probabilistic techniques and the characterizing combinatorial condition appears as a technical requirement. However, the condition itself is structural and since it describes a class of optimization problems for which any feasible solution is in some sense asymptotically optimal, this is of considerable relevance in applications and it would be nice to gain additional insight into the geometry of this condition. This can be achieved to some extent by reconsidering the problem using a statistical mechanics formalism, which is done in this paper.

For the special case of the QAP, an attempt in that direction can be found in Bonomi and Lutton [4]. There, however, an invalid convexity argument was applied to exchange the limit and the derivative for a sequence of functions over $[0, +\infty)$ (see [4], equalities (13) and (14)[1]), the exchange step being crucial for the whole proof.

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

In this paper we correct their proof and show more generally that the statistical mechanics approach can be applied to analyze the asymptotic behavior of a whole class of combinatorial optimization problems including the QAP.

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 the main asymptotic result, which is proved in Section 4. The proof involves six lemmata and parts of it are quite technical. Finally, in Section 5 we discuss the importance of the conditions imposed on the problems we deal with, and formulate some open questions.

## 2. Thermodynamics and combinatorial optimization

In combinatorial optimization one is interested in choosing a solution that minimizes (maximizes, respectively) the value of a certain objective function 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* $f: E \to \mathbb{R}^+$ be given. A *feasible solution* $S$ is a subset of the ground set $E$ and the set of feasible solutions is denoted by $\mathscr{S}$. By means of the cost function $f$ we associate costs to the feasible solutions. One possibility is to define an objective function $F: \mathscr{S} \to \mathbb{R}^+$ through

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

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

$$\min_{S \in \mathscr{S}} F(S). \tag{2}$$

Let us now turn to thermodynamics. A thermodynamical system may exhibit different states which are characterized by different values of energy. In thermodynamics, one is often interested in low-energy-states of the considered system, just as one is 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 in state $i$ with energy $E_i$ at temperature $T$ is given by

$$\frac{1}{Q(T)} \exp\left(\frac{-E_i}{k_{\mathrm{B}} T}\right), \tag{3}$$

with $k_{\mathrm{B}}$ being a physical constant known as *Boltzmann constant*, and $Q(T)$ denoting the so-called *partition function* defined by

$$Q(T) := \sum_j \exp\left(\frac{-E_j}{k_{\mathrm{B}}T}\right), \tag{4}$$

where the summation extends over all possible states of the system.

The statistical mechanics formalism can now be used to investigate combinatorial optimization problems (for simulation issues, cf. [8,9]). 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 [4]. We will repair and generalize their approach to a generic combinatorial optimization problem as introduced in the beginning of this section.

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

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

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

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

Denote by $\langle F(S)\rangle(\mu)$ the expected value of the objective function $F(S)$ in the above probabilistic model, for fixed $\mu$. Then $\langle F(S)\rangle(\mu)$ is given by

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

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 $\mu$:

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

Furthermore, the variance $\Delta F(S)(\mu)$ of the objective function $F(S)$ (in the probabilistic model introduced above) can be expressed as

$$\Delta F(S)(\mu) = \langle [F(S) - \langle F(S)\rangle(\mu)]^2\rangle = (\ln Q(\mu))''. \tag{9}$$

## 3. The main result

In this section we formulate the main result concerning a specific asymptotic behavior of combinatorial optimization problems, and introduce the probabilistic and combinatorial conditions to be imposed on 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 $n$. The ground set, the set of feasible solutions, the cost function, and the sum objective function of problem $P_n$ are denoted by $E_n$, $\mathscr{S}_n$, $f_n$, and $F_n$, respectively. Denote by $F_n^*$, $S_n^*$, the optimal value and an optimal solution of problem $P_n$, respectively:

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

Assume that the combinatorial optimization problem has the following properties:

(P1) For each $n \in \mathbb{N}$, all feasible solutions $S \in \mathscr{S}_n$ have the same cardinality $s_n$.
(P2) For some fixed $n \in \mathbb{N}$, let $\eta_n(e)$ be the number of feasible solutions $S \in \mathscr{S}_n$ such that $e \in S$. We suppose that there exists a constant $\eta_n$ 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 $M > 0$, with expected value $E := \mathbb{E}(f_n(e))$ and variance $D := \mathrm{Var}(f_n(e))$.
(P4) The cardinality of the set of feasible solutions $|\mathscr{S}_n|$ and the size of a feasible solution $s_n$ tend to infinity as $n$ tends to infinity. Furthermore

$$\lim_{n\to\infty} \frac{\ln|\mathscr{S}_n|}{s_n} = 0. \tag{10}$$

(P5) The size of the feasible solutions $s_n$ grows monotonically in $n$, i.e. $s_{n+1} \geqslant s_n$ for all $n \in \mathbb{N}$, and

$$\lim_{n\to\infty} \frac{s_n}{\ln n} = \infty. \tag{11}$$

We are interested in the asymptotic behavior of $F_n^*$ as $n$ tends to infinity and we will show that under (P1)–(P5), the ratio of the optimal solution and an arbitrary solution tends to 1 almost surely (a.s.). For the ease of exposition, let us restate this behavior as follows: the ratio $F_n^*/|S_n^*|$ tends to $E$ as the size $n$ of the problem tends to infinity, a.s. with respect to the probability measure Pr defined as the product measure on the probability space $(\Omega, \mathscr{A}, \mathrm{Pr})$, where $\Omega$ is the cartesian product of the individual probability spaces on which the random variables $f_n(e)$ are defined, and $\mathscr{A}$ is the corresponding product $\sigma$-algebra (note that due to the strong law of large numbers this formulation is equivalent to the former one). Summarizing, the main result is given by the following theorem:

**Theorem 3.1.** *Let a combinatorial optimization problem be given by* (2) *and let the properties* (P1)–(P5) *be fulfilled. Then*

$$\Pr\left(\lim_{n\to\infty} \frac{F_n^*}{s_n} = E\right) = 1. \tag{12}$$

## 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, *we have*

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

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

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

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

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

From (P2) we have

$$|\mathscr{S}_n|\cdot s_n = |E_n|\cdot\eta_n \tag{14}$$

and by substitution we obtain:

$$\frac{\langle F_n(S)\rangle(0)}{s_n} = \frac{\sum_{e\in E_n} f_n(e)}{|E_n|}. \tag{15}$$

Due to the Chernoff–Hoëffding bound we have

$$\Pr\left(\left|\frac{1}{|E_n|}\sum_{e\in E_n} f_n(e) - E\right| > \varepsilon\right) \leqslant 2\,\exp\left(-\frac{2\varepsilon^2|E_n|}{M^2}\right),$$

and thus, by the Borel–Cantelli lemma, (13) follows, if the sum

$$\sum_{n=1}^{\infty}\exp\left(-\frac{2\varepsilon^2|E_n|}{M^2}\right)$$

converges for all $\varepsilon > 0$. But this is indeed the case, since from (11), (14) and $\eta_n \leqslant |\mathscr{S}_n|$ we have that $\lim_{n\to\infty}|E_n|/\ln n = \infty$. □

**Lemma 4.2.** *Under the conditions of Theorem* 3.1 *for each $\omega \in \Omega$ there exists a convergent subsequence $(F^*_{n_m}(\omega))/s_{n_m}$ of the sequence $(F^*_n(\omega))/s_n$ with limit $l(\omega)$.*

**Proof.** Since $|(F^*_n(\omega))/s_n| \leqslant (Ms_n)/s_n = M$, the sequence $(F^*_n(\omega))/s_n$ is bounded. Therefore, it has at least one cluster point, which we denote by $l(\omega)$, and a subsequence $(F^*_{n_m}(\omega))/s_{n_m}$ converging to it, so that

$$l(\omega) := \lim_{m\to\infty}\frac{F^*_{n_m}(\omega)}{s_{n_m}}. \qquad \square \tag{16}$$

If $S^*_n$ is an optimal solution of problem $P_n$, the following inequalities hold for the partition function $Q_n(\mu)$ for each $\omega \in \Omega$:

$$\exp(-F_n(S^*_n)\cdot\mu) \leqslant Q_n(\mu) \leqslant |\mathscr{S}_n|\cdot\exp(-F_n(S^*_n)\cdot\mu) \tag{17}$$

$$-F^*_n\cdot\mu \leqslant \ln Q_n(\mu) \leqslant \ln|\mathscr{S}_n| - F^*_n\cdot\mu. \tag{18}$$

Let us now introduce the continuous and differentiable functions $G_n(\mu) = (\ln Q_n(\mu))/s_n$, defined on $[0, \infty)$, for all $n \in \mathbb{N}$ (note that $G_n(\mu)$ is a function of $\omega$ also, however in the sequel we do not explicitly indicate this dependence for the ease of notation). Dividing both sides of (18) by $s_n$ we get

$$-\mu \cdot \frac{F_n^*}{s_n} \leqslant G_n(\mu) \leqslant \frac{\ln |\mathscr{S}_n|}{s_n} - \mu \cdot \frac{F_n^*}{s_n}. \tag{19}$$

**Lemma 4.3.** *Under the conditions of Theorem* 3.1, *for each $\omega \in \Omega$ and $l(\omega)$ defined in* (16), *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 $[\alpha, \beta]$ for any $\alpha, \beta > 0$, and*

$$\lim_{k\to\infty} G_{n_k}(\mu) = -\mu \cdot l(\omega), \tag{20}$$

$$\lim_{k\to\infty} G'_{n_k}(\mu) = -l(\omega). \tag{21}$$

**Proof.** We apply the following classical result: Let a sequence of differentiable functions $G_{n_m}(\mu)$ be given, which are pointwise convergent on an interval $[\alpha, \beta]$ (here $\alpha > 0$, and $\beta$ is an arbitrarily large, but finite real number). Assume that the sequence of derivatives $G'_{n_m}(\mu)$ is equicontinuous and uniformly bounded on $[\alpha, \beta]$. 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 $[\alpha, \beta]$ (see, e.g., [19]).

Note that the pointwise convergence of $G_{n_m}(\mu)$ follows from Lemma 4.2, (10) and (19). 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 $[\alpha, \beta]$.

First, let us show that the sequence of derivatives $G'_n$ is uniformly bounded on $[\alpha, \beta]$. Note that $\forall S \in \mathscr{S}_n$, we have

$$F_n(S) = \sum_{e\in S} f_n(e) \leqslant M \cdot |S| = M \cdot s_n. \tag{22}$$

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

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

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

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

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

$$\begin{aligned} |G'_n(\mu_1) - G'_n(\mu_2)| &\leqslant \sum_{S\in\mathscr{S}_n} \frac{F_n(S)}{s_n} \cdot \left| \frac{\exp(-\mu_1 \cdot F_n(S))}{Q_n(\mu_1)} - \frac{\exp(-\mu_2 \cdot F_n(S))}{Q_n(\mu_2)} \right| \\ &\leqslant M \cdot \sum_{S\in\mathscr{S}_n} \frac{\exp(-\mu_1 \cdot F_n(S))}{Q_n(\mu_1)} \cdot \left| 1 - \frac{Q_n(\mu_1) \cdot \exp(-\mu_2 \cdot F_n(S))}{Q_n(\mu_2) \cdot \exp(-\mu_1 \cdot F_n(S))} \right|. \end{aligned} \tag{23}$$

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

$$\left|1-\frac{Q_n(\mu_1)\cdot\exp(\mu_1\cdot F_n(S_0))}{Q_n(\mu_2)\cdot\exp(\mu_2\cdot F_n(S_0))}\right| \leqslant T\cdot(\mu_2-\mu_1). \tag{24}$$

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

$$\begin{aligned}&\left|\sum_{S:F_n(S)>F_n(S_0)}\exp(\mu_2(F_n(S_0)-F_n(S)))-\sum_{S:F_n(S)>F_n(S_0)}\exp(\mu_1(F_n(S_0)-F_n(S)))\right|\\ &\quad\geqslant\left|\sum_{S:F_n(S)<F_n(S_0)}\exp(\mu_2(F_n(S_0)-F_n(S)))-\sum_{S:F_n(S)<F_n(S_0)}\exp(\mu_1(F_n(S_0)-F_n(S)))\right|.\end{aligned} \tag{25}$$

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

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

since the sign of $\exp(\mu_2(F_n(S_0)-F_n(S)))-\exp(\mu_1(F_n(S_0)-F_n(S)))$ depends on the sign of $F_n(S)-F_n(S_0)$ and together with (25) the above inequality holds. It follows that

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

We now show that

$$\begin{aligned}&\left|\sum_{S:F_n(S)>F_n(S_0)}[\exp((\mu_2-\mu_1)\cdot(F_n(S_0)-F_n(S)))-1]\right|\\ &\quad\leqslant\frac{1}{\alpha}\cdot(\mu_2-\mu_1)\cdot\sum_{S:F_n(S)>F_n(S_0)}\exp[\mu_2\cdot(F_n(S_0)-F_n(S))].\end{aligned} \tag{26}$$

Indeed, inequality (26) is a consequence of the following inequalities, which hold for all $S \in \mathscr{S}_n$ such that $F_n(S) \geqslant F_n(S_0)$:

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

and we obtain (24) with $T := 1/\alpha$. Returning to (23),

$$|G_n'(\mu_1)-G_n'(\mu_2)| \leqslant M\cdot\frac{1}{\alpha}\cdot(\mu_2-\mu_1)\cdot\sum_{S\in\mathscr{S}_n}\frac{\exp(-\mu_1\cdot F_n(S))}{Q_n(\mu_1)} = M\cdot\frac{1}{\alpha}\cdot(\mu_2-\mu_1),$$

from which the equicontinuity of $G_n'$ on $[\alpha, \beta]$ obviously follows.

Due to (10), (16) and (19) we have $\lim_{k\to\infty} G_{n_k}(\mu) = -\mu\, l(\omega)$. Then, uniform convergence of the above sequence together with the sequence of its derivatives implies

$$\lim_{k\to\infty} G_{n_k}'(\mu) = \left(\lim_{k\to\infty} G_{n_k}(\mu)\right)' = -l(\omega). \qquad \square$$

**Lemma 4.4.** *For almost all $\omega \in \Omega$ we have $l(\omega) \leqslant E$.*

**Proof.** Since for each $\omega \in \Omega$ and $n \in \mathbb{N}$ we have $F_n(S^*) \leqslant \langle F_n(S)\rangle(0)$, the assertion follows from Lemma 4.1. $\square$

For each $\omega \in \Omega$ and each cluster point $l(\omega)$ as defined in Lemma 4.2, there are now two possibilities: (i) either $l(\omega) = E$ and $E$ is the (unique) limit of $(F_n^*(\omega))/s_n$ or (ii) there exists a cluster point $l(\omega)$ of $(F_n^*(\omega))/s_n$ such that $l(\omega) < E$. If (i) is true for almost all $\omega \in \Omega$, the main result follows immediately. We show that the second case almost surely cannot happen:

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

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

for some $\mu_0 \in [0, \alpha]$. The last equality implies that $G_{n_{k_0}}''(\mu_0) \geqslant K$ and hence the second derivatives $G_{n_k}''(\mu)$ are unbounded as $k$ approaches infinity and $\mu$ approaches 0. We show that almost surely this cannot be the case, because: (a) The third derivative $G_{n_k}'''(\mu)$ is almost surely nonpositive for $\mu \geqslant 0$ 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 $G_n''(\mu) = (\Delta F_n(S)(\mu))/s_n$ (cf. (9)) for all $n \in \mathbb{N}$ and $\mu \geqslant 0$, 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 nonpositive for all $k \geqslant k_0$, $\mu \geqslant 0$, where $k_0$ is some fixed natural number.*

**Proof.** We have

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

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

$$\begin{aligned} G_{n_k}'''(\mu) &= \frac{1}{s_{n_k}} \left[ \sum_{S \in \mathscr{S}_{n_k}} 2(F_{n_k}(S) - \langle F_{n_k}\rangle(\mu)) \frac{\mathrm{e}^{-F_{n_k}(S)\mu}}{Q_{n_k}(\mu)} \left( \frac{\langle F_{n_k}^2\rangle(\mu)}{Q_{n_k}(\mu)} - \langle F_{n_k}\rangle^2(\mu) \right) \right. \\ &\quad \left. + \sum_{S \in \mathscr{S}_{n_k}} [F_{n_k}(S) - \langle F_{n_k}\rangle(\mu)]^2 \left( -F_{n_k}(S) \frac{\mathrm{e}^{-F_{n_k}(S)\mu}}{Q_{n_k}(\mu)} + \langle F_{n_k}\rangle(\mu) \frac{\mathrm{e}^{-F_{n_k}(S)\mu}}{Q_{n_k}(\mu)} \right) \right] \\ &= \frac{1}{s_{n_k}} \left( 0 - \sum_{S \in \mathscr{S}_{n_k}} \left(F_{n_k}(S) - \langle F_{n_k}\rangle(\mu)\right)^3 \frac{\mathrm{e}^{-F_{n_k}(S)\mu}}{Q_{n_k}(\mu)} \right) = -\frac{\langle (F_{n_k} - \langle F_{n_k}\rangle(\mu))^3\rangle(\mu)}{s_{n_k}}. \end{aligned}$$

Hence it is enough to show that $F_{n_k}(S) - \langle F_{n_k}\rangle(\mu) \geqslant 0\ \forall \mu \geqslant 0$ for all $k \geqslant k_0$ almost surely. Indeed, for all $S \in \mathscr{S}_{n_k}$, $F_{n_k}(S) = \sum_{e \in S} f_{n_k}(e)$ is the sum of $s_{n_k}$ independent and identically distributed random variables with $\mathbb{E}(f_{n_k}(e)) = E$. The Chernoff–Hoëffding bound thus gives

$$\Pr\left( \left| \frac{F_{n_k}(S)}{s_{n_k}} - E \right| > \varepsilon \right) \leqslant 2 \exp\left( -\frac{2\varepsilon^2 s_{n_k}}{M^2} \right) \tag{27}$$

for all $\varepsilon > 0$, and by the Borel–Cantelli lemma we obtain

$$\Pr\left( \lim_{k \to \infty} \left| \frac{F_{n_k}(S)}{s_{n_k}} - E \right| = 0 \right) = 1, \tag{28}$$

since the growth rate (11) is in particular satisfied for any subsequence of $s_n$. Thus, for almost all $\omega \in \Omega$, $\lim_{k\to\infty} (F_{n_k}(S))/s_{n_k}(\omega) = E$. At the same time, we have from Lemma 4.3 that

$$\lim_{k\to\infty} \frac{\langle F_{n_k}\rangle(\mu)}{s_{n_k}}(\omega) = -\lim_{k\to\infty} G_{n_k}'(\mu) = l(\omega)$$

for all $\mu > 0$. The inequality $l(\omega) < E$, together with Lemma 4.1 for the case $\mu = 0$, thus implies that $F_{n_k}(S) - \langle F_{n_k}\rangle(\mu) \geqslant 0$ for all $k \geqslant k_0$ almost surely for all $\mu \geqslant 0$, as desired. □

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

**Proof.** Since $G''_n(0) = (\Delta F_n(S)(0))/s_n \geqslant 0$, we have by Markov's inequality

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

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

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

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

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

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

Summarizing, for almost all $\omega \in \Omega$, if $l(\omega) < E$, the second derivatives $G''_{n_k}(\mu)$ have to be bounded and unbounded at the same time. This implies that $l(\omega) < E$ almost surely cannot happen. Thus $l(\omega) = E$ a.s. and Theorem 3.1 holds.

**Remark 1.** The proof technique can also be interpreted as follows: Since $(\langle F_n\rangle(\mu))/s_n = |G'_n(\mu)| \leqslant M$ is bounded, for each $\omega \in \Omega$ and for all $\mu \geqslant 0$ there exists a convergent subsequence such that $\lim_{k\to\infty}(\langle F_{n_k}\rangle(\mu))/s_{n_k} = l(\mu)$. In the proof it is shown that almost surely $l(\mu)$ does not depend on $\mu$ and $l = E$ a.s., from which it follows that

$$\lim_{n\to\infty}\frac{\langle F_n\rangle(\mu)}{s_n} = E \quad \text{almost surely for any } \mu \in [0, \beta]. \tag{29}$$

Recall that $\langle F_n\rangle(\mu)$ denotes the expectation of $F_n(S)$ w.r.t. the Boltzmann weight with parameter $\mu$ assigned to each admissible solution $S \in \mathscr{S}_n$. The right-hand side of (29) being independent of $\mu$, Theorem 3.1

can now be deduced for $\mu \to \infty$, since for any $S_0 \in \mathscr{S}_n$ we have (see, e.g., [1])

$$\lim_{\mu\to\infty} \Pr(S_0) = \lim_{\mu\to\infty} \frac{e^{-F_n(S_0)\mu}}{Q_n(\mu)} = \lim_{\mu\to\infty} \frac{e^{-F_n(S_0)\mu}}{\sum_{S\in\mathscr{S}_n} e^{-F_n(S)\mu}}$$

$$= \lim_{\mu\to\infty} \frac{e^{-\mu(F_n(S_0)-F_n^*)}}{|\mathscr{S}_n^*| + \sum_{S\in\mathscr{S}_n\backslash\mathscr{S}_n^*} e^{-\mu(F_n(S)-F_n^*)}} = \begin{cases} \dfrac{1}{|\mathscr{S}_n^*|} & \text{for } S_0 \in \mathscr{S}_n^*, \\ 0 & \text{for } S_0 \in \mathscr{S}_n\backslash\mathscr{S}_n^*, \end{cases}$$

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

**Remark 2.** As emphasized earlier, Theorem 3.1 can be proved in a much shorter way by using the following purely probabilistic argument: Under conditions (P1)–(P5), we have the Chernoff–Hoëffding bound (27) so that

$$\Pr\left(\sup_{S\in\mathscr{S}_n}\left|\frac{F_n(S)}{s_n} - E\right| > \varepsilon\right) \leqslant 2|\mathscr{S}_n| \exp\left(-\frac{2\varepsilon^2 s_n}{M^2}\right) \tag{30}$$

from which Theorem 3.1 can be deduced using the Borel–Cantelli lemma, since the right-hand side of (30) is summable for all $\varepsilon > 0$ provided that the growth condition (11) holds.

However, our alternative approach to prove Theorem 3.1 gives additional insight into the structure of the problem and the way the conditions (P1)–(P5) enter (see Section 5). In particular, the origin of the crucial growth condition (P4) receives a geometric interpretation in view of (19). Moreover the statistical mechanics formalism is of independent interest in view of applications such as simulated annealing (cf. [14]).

## 5. Discussion and open questions

Let us shortly discuss conditions (P1)–(P5). (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 explicitly shows the importance of condition (10). Note that (10) 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.

Condition (P5) is needed to guarantee the almost sure convergence of the result. If (11) is not fulfilled, then Lemmata 4.1, 4.4 and 4.5 hold in probability only, from which it follows that the main result holds only in probability, i.e.,

$$\lim_{n\to\infty} \Pr\left(\left|\frac{F_n^*}{s_n} - E\right| > \varepsilon\right) = 0 \quad \forall \varepsilon > 0.$$

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 stating 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 [20] 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 $|\mathscr{S}_{n+1}| \geqslant |\mathscr{S}_n|$ 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

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

feasible solutions

$$S_\phi = \{(i, j, \phi(i), \phi(j)) \colon 1 \leqslant i, j \leqslant n\}$$

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

$$\mathscr{S}_n = \{S_\phi \colon \phi \text{ is a permutation of } 1, 2, \ldots, n\},$$

(see also [7]). Clearly $|E_n| = O(n^4)$, $|S_\phi| = n^2$ for any permutation $\phi$, $|\mathscr{S}_n| = n!$, and condition (P4) is fulfilled, since $(\ln(n!))/n^2 = \mathrm{o}(1)$. Each element $(i, j, k, l)$ of the ground set appears in $(n-2)!$ feasible solutions, namely in all $S_\phi$ corresponding to some permutation $\phi$ 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 $\bar{E}_n = \{(i, j) \colon 1 \leqslant i, j \leqslant n\}$, the feasible solutions are given by $\bar{S}_\phi = \{(i, \phi(i)) \colon 1 \leqslant i \leqslant n\}$, for some permutation $\phi$ of $1, 2, \ldots, n$, and the set of feasible solutions $\bar{\mathscr{S}}_n$ is given as

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

In this case we have $|\bar{\mathscr{S}}_n| = n!$, $|\bar{S}_\phi| = n$ for all permutations $\phi$, $|\bar{E}_n| = n^2$, and each pair $(i, j)$, belongs to $(n-1)!$ feasible solutions corresponding to permutations which assign $i$ to $j$. Thus $\eta_n = (n-1)!$. Note that here condition (P4) is not fulfilled because $(\ln n!)/n$ tends to $\infty$ as $n \to \infty$. 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 [13], the expected optimal value of this problem $\mathbb{E}(F_n^*)$ is bounded from above by 2. Theorem 3.1 would now imply $\Pr(\lim_{n\to\infty} F_n^*/n = \frac{1}{2}) = 1$, leading to

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

which contradicts the boundedness of $F_n^*$. Thus Theorem 3.1 cannot hold in this case. The fact that for any $\varepsilon > 0$, $\lim_{n\to\infty} (\ln n!)/n^{1+\varepsilon} = 0$ is another indication that condition (P4) is rather sharp.

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 and identically distributed random variables (not necessarily bounded). Also, the finiteness of variance and higher order moments is frequently assumed. Szpankowski [20] showed that in such a case under additional monotonicity assumptions on $F_n^*$ and $|\mathscr{S}_n|$, Theorem 3.1 can be proved by purely probabilistic techniques. One can ask, however, what happens in the proof of the main theorem with our set of assumptions in case that the cost coefficients $f_n(e)$ are not bounded, while fulfilling all other requirements in (P3). In this case, Chernoff–Hoëffding bounds for deviations from the mean are no longer available. In addition, the boundedness of the coefficients has been exploited in the proofs of Lemmas 4.2 and 4.3 to show that the sequences $(F_n^*)/s_n$ and $G_n'(\mu)$, $\mu \geqslant 0$, are bounded. If the boundedness condition on $f_n(e)$ is dropped, then 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 $(F_n(S))/s_n$ is bounded, tends to 1 for any $S \in \mathscr{S}_n$, as $n \to \infty$. Indeed, recall that $\mathbb{E}(F_n(S)) = s_n E$, $\mathrm{Var}(F_n(S)) = s_n D$, and therefore $\mathbb{E}((F_n(S))/s_n) = E$ and $\mathrm{Var}((F_n(S))/s_n) = D/s_n$. By applying Chebyshev's inequality, one obtains

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

for any $K > E$. Since $s_n \to \infty$ as $n$ approaches infinity, Lemma 4.2 holds in probability. Chebyshev's inequality shows that Lemma 4.1 also holds in probability and so do the remaining lemmata. This implies that Theorem 3.1 holds in probability in the case that the coefficients of the problem are unbounded.

It remains an open question whether an a.s. convergence result for unbounded cost coefficients can be obtained through the statistical mechanics formalism.

Another question of general interest arises in connection with simulated annealing as a statistical mechanics approach in combinatorial optimization. Is there any class of problems which is well suited for simulated annealing? Is this class characterized by a combinatorial property? Clearly, this is a rather complex question and its answer is left to future research.

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