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Abstract

We establish asymptotic convergence of the standard simulated annealing algorithm - when used with a parameter dependent penalization - to the set of globally optimal solutions of the original combinatorial optimization problem. Precise and explicit asymptotic estimates are given. Moreover, we present an explicit description of the asymptotic behaviour of the expected cost, the variance of the cost and the entropy. We show that familiar properties like monotonicity of the expected cost and the entropy are no longer guaranteed in the penalized case and discuss the practical consequences of our results.

1 Introduction

An essential step in devising a simulated annealing scheme for a given combinatorial optimization problem is to equip the set of configurations with a convenient neighbourhood structure. For many problems of a less explicit nature this is quite cumbersome if not practically inexecutable.

One then resorts to a trick. The constraints defining the configuration space $\mathcal{S}$ are relaxed to such an extent that a manageable set of restrictions remains. Simulated annealing is now applied to the associated configuration space $\overline{\mathcal{S}}$. As the optimization process proceeds the elements of $\overline{\mathcal{S}} \setminus \mathcal{S}$ are increasingly penalized. From practical experience it is known that towards the end of the process only feasible solutions occur that are generally near optimal. In the literature, to the best of our knowledge, the only justification of the above penalization method is that it works in practice. Convergence proofs are not given.

In this paper we intend to fill this gap.
We start in section 2 with a terse survey of the simulated annealing algorithm. Next, in section 3 the penalization approach is introduced and examplified. In section 4 we introduce the concept of a parameter dependent penalization. This is in fact a very simple formalization of the penalty treatment found in the practical literature (cf. [2], [5]). We establish asymptotic

convergence of the standard annealing algorithm - when used with a parameter dependent penalization - to the set of globally optimal solutions of the original problem. Precise and explicit asymptotic estimates are given. Section 5 is devoted to the asymptotic analysis of some useful statistical quantities familiar from the unpenalized case. Specifically, we present an explicit description of the asymptotic behaviour of the expected cost, the variance of the cost and the entropy. Moreover, we show that familiar properties like monotonicity of the expected cost and the entropy are no longer guaranteed in the penalized case. Finally, in section 6 some practical consequences of our results are discussed.

2 Outline of the annealing algorithm.

Simulated annealing [3] is a versatile heuristic optimization technique based on the analogy between simulating the physical annealing process of solids and solving large-scale combinatorial optimization problems. For a detailed explanation of the method as well as the origin of our notation we refer to [1].

Quite generally, a combinatorial optimization problem may be characterized by a finite set $\mathcal{S}$ consisting of all system configurations and a cost function f assigning a real number to each configuration $i \in \mathcal{S}$. Here we choose the sign of the cost function in such a way that the lower the value the better the corresponding configuration.
The problem is to find an $i_{opt} \in \mathcal{S}$ satisfying

$$\forall i \in \mathcal{S}: \quad f(i_{opt}) \leq f(i). \tag{2.1}$$

Any such solution i_{opt} is called a (global) optimum. Throughout we shall write $f_{opt} = f(i_{opt})$ for the optimal cost and $\mathcal{S}_{opt}$ for the set of optimal solutions.

In its standard form, simulated annealing can be summarized as follows.
The algorithm starts off from an arbitrary initial configuration. In each iteration, by slightly perturbing the current configuration i, a new configuration j is generated. The difference in cost, given by

$$\Delta f = f(j) - f(i), \tag{2.2}$$

is compared with an acceptance criterion which accepts all improvements but also admits, in a limited way, deteriorations in cost.

Initially, the acceptance criterion is taken such that deteriorations are accepted with a high probability. As the optimization process proceeds the acceptance criterion is modified such that the probability for accepting deteriorations decreases. At the end of the process this probability tends to zero. In this way the optimization process may be prevented from getting stuck in a local optimum. The process comes to a halt when during a prescribed number of iterations no further improvement in the optimum value found so far occurs.

The simulated annealing process can be modeled mathematically in terms of a one-parameter family of homogeneous Markov chains (see [1]). The states of each Markov chain correspond with the configurations $i \in \mathcal{S}$. The transition probabilities depend on the value of the control parameter $c > 0$, the analog of the temperature in the physical annealing process. Thus, if c

is kept constant, the corresponding Markov chain is homogeneous and its transition matrix $P = P(c)$ can be defined as

$$P_{ij}(c) = \begin{cases} G_{ij}(c)A_{ij}(c) & \text{if } i \neq j \\ 1 - \sum_{s\in\mathcal{S}, s\neq i} P_{is}(c) & \text{if } i = j, \end{cases} \tag{2.3}$$

where $G_{ij}(c)$ denotes the generation probability, i.e. the probability of generating configuration j from configuration i, and $A_{ij}(c)$ denotes the acceptance probability, i.e. the probability of accepting configuration j, once it has been generated from i.

The standard choice for the acceptance matrix $A(c)$ corresponds to the Metropolis criterion [4] and is given by

$$A_{ij}(c) = \begin{cases} \exp\left(\frac{-\Delta f}{c}\right) & \text{if } \Delta f > 0 \\ 1 & \text{if } \Delta f \leq 0. \end{cases} \tag{2.4}$$

In addition, the generation matrix $G(c)$ is chosen such that

(*i*) G is symmetric, i.e. $\forall c > 0, \forall i, j \in \mathcal{S} : G_{ij}(c) = G_{ji}(c)$,

(*ii*) The Markov chain associated with G is irreducible.

It can be proven [1] that for $c > 0$ fixed the Markov chain associated with the above standard $P(c)$ has an equilibrium distribution $q(c)$, whose components are given by

$$q_i(c) = \frac{1}{N_0(c)} \exp\left(\frac{-f(i)}{c}\right) \tag{2.5}$$

with

$$N_0(c) = \sum_{j\in\mathcal{S}} \exp\left(\frac{-f(j)}{c}\right). \tag{2.6}$$

Thus, after a sufficiently large number of transitions at a fixed value of c the simulated annealing algorithm will find a solution $i \in \mathcal{S}$ with a probability approximately equal to $q_i(c)$.

From (2.5-6) one can derive

$$\lim_{c\downarrow 0} q_i(c) = \begin{cases} 0 & \text{if } i \notin \mathcal{S}_{opt} \\ \frac{1}{|\mathcal{S}_{opt}|} & \text{if } i \in \mathcal{S}_{opt}. \end{cases} \tag{2.7}$$

This result is very important, since it guarantees asymptotic convergence of the annealing algorithm to the set of globally optimal solutions under the condition that equilibrium is obtained at each value of c.

3 The penalization approach.

In practice, the following situation is frequently met.
It is difficult to define a generation mechanism on the set $\mathcal{S}$ itself, whereas $\mathcal{S}$ is contained in

a finite set $\overline{\mathcal{S}}$ that allows for a simple generation mechanism.
For example, let $\mathcal{S}$ consist of all 0\1 n-vectors satisfying a given set of restrictions. Then it may be hard to find a generation mechanism compatible with these restrictions. More so, it may even be problematic to find an explicit element of $\mathcal{S}$. On the other hand, in the space $\overline{\mathcal{S}} = \{0,1\}^n \supset \mathcal{S}$ it is extremely simple to define a generation mechanism, e.g. a new configuration may be generated from $\boldsymbol{x} \in \overline{\mathcal{S}}$ by randomly choosing one of its components and changing its value.
In the situation described above it is natural to choose $\overline{\mathcal{S}}$ as the configuration space and to extend the cost function f from $\mathcal{S}$ to $\overline{\mathcal{S}}$ in an appropriate way.
In problems of an explicit nature it is sometimes possible to find an extension $\overline{f}$ of f satisfying

$$\forall j \in \overline{\mathcal{S}} \setminus \mathcal{S}: \quad f(i_0) < \overline{f}(j), \tag{3.1}$$

where i_0 is some element of $\mathcal{S}$.
Clearly, in such a case the combinatorial optimization problems associated with the pairs $(\mathcal{S}, f)$ and $(\overline{\mathcal{S}}, \overline{f})$ have the same set of optimal solutions. Thus, theoretically, the simulated annealing algorithm, when applied to the pair $(\overline{\mathcal{S}}, \overline{f})$, converges asymptotically to the set of optimal solutions $\mathcal{S}_{opt}$ associated with the original pair $(\mathcal{S}, f)$. In practice, however, the convergence (to a near optimal solution) may be somewhat slow since extensions $\overline{f}$ constructed so as to satisfy (3.1) tend to be rather flat.
We shall call an extension $\overline{f}$ of f satisfying (3.1) a penalization of f, since it penalizes an element $j \in \overline{\mathcal{S}} \setminus \mathcal{S}$ for not belonging to $\mathcal{S}$.

As an illustration let us consider the integer programming problem

$$\begin{array}{lll} \mathcal{IP} & \text{minimize} & \boldsymbol{c}^T\boldsymbol{x} \\ & \text{subject to} & A\boldsymbol{x} \geq \boldsymbol{b}, \\ & & x_j = 0 \text{ or } 1, \;\; j = 1, 2, \ldots, n \end{array} \tag{3.2}$$

with $\boldsymbol{c}$ and $\boldsymbol{x}$ n-vectors, $\boldsymbol{b}$ an m-vector and A an $m \times n$-matrix. For convenience let us take $\boldsymbol{c} > \mathbf{o}$. Let us assume that the set

$$\mathcal{S} = \{\boldsymbol{x} \in \{0,1\}^n | A\boldsymbol{x} \geq \boldsymbol{b}\} \tag{3.3}$$

of feasible solutions is not empty.
Setting

$$\boldsymbol{y} = \boldsymbol{b} - A\boldsymbol{x} \tag{3.4}$$

$$y_{max} = \max\{y_i | i = 1, 2, \ldots, m\} \tag{3.5}$$

we may extend the cost function $f(\boldsymbol{x}) = \boldsymbol{c}^T\boldsymbol{x}$ from $\mathcal{S}$ to $\overline{\mathcal{S}} = \{0,1\}^n$ by putting

$$\overline{f}(\boldsymbol{x}) = \boldsymbol{c}^T\boldsymbol{x} + P(\boldsymbol{y}) \tag{3.6}$$

$$P(\boldsymbol{y}) = H(y_{max}) \left(\alpha + \sum_{i=1}^{m} H(y_i) r_i(y_i) \right). \tag{3.7}$$

Here H denotes the Heaviside-function : $H(y) = 0$ if $y \leq 0$ and $H(y) = 1$ if $y > 0$. Furthermore, the functions $r_i : (0, \infty) \longrightarrow (0, \infty)$ are strictly increasing, but apart from that arbitrary. Finally, the constant α is chosen as follows. If a feasible solution $\boldsymbol{x}_o \in \mathcal{S}$ is known then $\alpha = \boldsymbol{c}^T \boldsymbol{x}_o$. Otherwise, we take

$$\alpha = \sum_{j=1}^{n} c_j. \tag{3.8}$$

Note that α as in (3.8) may be a large number. Thus the functions r_i must be chosen with due care so as to prevent $\overline{f}$ from being too flat. Alternatively, as soon as during the optimization process a feasible solution $\boldsymbol{x}_o$ is found we may use this to replace α with $\boldsymbol{c}^T \boldsymbol{x}_o$.

It is readily verified that $\overline{f}$ is indeed a penalization of f. In fact, $P(\boldsymbol{y})$ penalizes both the number of restrictions being violated as well as the magnitude of the individual violations.

Two remarks are in order here. Firstly, by the explicit form of the above problem it was relatively easy to construct a penalty function $P(\boldsymbol{y})$. When the problem is less explicit it is often hard to find the right weights to penalize with. Secondly, the penalization given by (3.6-7) stays the same during the whole optimization process. However, towards the end of the optimization process we experience a growing dislike of infeasible solutions. Therefore, it seems natural to penalize harder when the process proceeds.

Both these aspects can be taken into account by letting the penalization of f depend on the cooling parameter c, in such a way that as c tends to zero the elements of $\overline{\mathcal{S}} \setminus \mathcal{S}$ are increasingly penalized. In the next section we shall elaborate on this theme.

4 Parameter dependent penalizations

Consider an instance $(\mathcal{S}, f)$ of a combinatorial optimization problem. Throughout we assume that $\mathcal{S} \neq \mathcal{S}_{opt}$. Let $\overline{\mathcal{S}} \supset \mathcal{S}$ be finite and such that $\overline{\mathcal{S}}$ can conveniently be used as a configuration space for the standard annealing algorithm.
We shall call $\overline{f}_c$ a parameter dependent penalization of f with respect to $\overline{\mathcal{S}}$ if

$$(i) \quad \overline{f}_c : \overline{\mathcal{S}} \longrightarrow \mathcal{R} \text{ for } c > 0 \tag{4.1}$$

$$(ii) \quad \overline{f}_c(i) = f(i) \text{ for } i \in \mathcal{S} \tag{4.2}$$

$$(iii) \quad \lim_{c \downarrow 0} \overline{f}_c(i) = +\infty \text{ for } i \in \overline{\mathcal{S}} \setminus \mathcal{S}. \tag{4.3}$$

Thus the extension $\overline{f}_c$ of f has the property that the elements of $\overline{\mathcal{S}}$ that do not belong to the original configuration space $\mathcal{S}$ get punished more and more as c tends to zero.

To examplify the previous definition let us reconsider the integer programming problem introduced in (3.2). It is readily verified that for this problem a c-dependent penalization with respect to $\overline{\mathcal{S}} = \{0,1\}^n$ is given by

$$\overline{f}_c(\boldsymbol{x}) = \boldsymbol{c}^T \boldsymbol{x} + \sum_{i=1}^{m} H(y_i) R_i(y_i, c), \tag{4.4}$$

where the functions $R_i : (0,\infty) \times (0,\infty) \longrightarrow (0,\infty)$ are chosen such that for $c > 0$ fixed $y \longmapsto R_i(y,c)$ is strictly increasing, whereas for fixed $y > 0$

$$\lim_{c \downarrow 0} R_i(y,c) = +\infty. \tag{4.5}$$

Note that in choosing the functions R_i one has a great deal of freedom.

As an example with a less explicit structure let us consider the macro placement problem (see [2], [5]). In this problem it is required to place a given number of rectangles on a finite two-dimensional grid in such a way that they do not overlap and that the area of the enveloping rectangle is as small as possible. Clearly, a natural choice for the configuration space $\mathcal{S}$ is the collection of all placements in which the rectangles do not overlap. For the cost of each placement we may take the area of the enveloping rectangle. Suppose we generate a candidate configuration from the current one by a simple local rearrangement (e.g. a translation). Then it is quite difficult to do so without causing overlap. In fact, working directly with $\mathcal{S}$ is impracticable.
On the other hand, if we use the above generation mechanism in the space $\overline{\mathcal{S}}$ consisting of *all* placements - including those that exhibit overlap - there is no problem. We only have to punish the overlap. In practice this is done by choosing the following penalization:

$$\forall p \in \overline{\mathcal{S}}: \quad \overline{f}_c(p) = A(p) + \gamma \frac{O(p)}{c} \tag{4.6}$$

with $A(p)$ the area of the enveloping rectangle, $O(p)$ the total rectangle overlap and γ a scaling factor.

From now on let us assume that the standard annealing algorithm is applied to the pair $(\overline{\mathcal{S}}, \overline{f}_c)$.
As a first property we have

Lemma 4.1 *There is a $c_0 > 0$ such that for $0 < c < c_0$*

$$\min_{i \in \mathcal{S}} f(i) = \min_{i \in \overline{\mathcal{S}}} \overline{f}_c(i). \tag{4.7}$$

Proof Let $i_0 \in \mathcal{S}$ be fixed. In view of (4.3) there exists for each $i \in \overline{\mathcal{S}} \setminus \mathcal{S}$ a $c(i) > 0$ such that $\overline{f}_c(i) > f(i_0)$ for $0 < c < c(i)$. Since $\overline{\mathcal{S}} \setminus \mathcal{S}$ is finite we can find an $i^* \in \overline{\mathcal{S}} \setminus \mathcal{S}$ satisfying

$$0 < c(i^*) = \min_{i \in \overline{\mathcal{S}} \setminus \mathcal{S}} c(i). \tag{4.8}$$

For $0 < c < c(i^*)$ we then have

$$\forall i \in \overline{\mathcal{S}} \setminus \mathcal{S}: \quad \overline{f}_c(i) > f(i_0) \tag{4.9}$$

and hence $\overline{f}_c$ assumes its minimum on $\mathcal{S}$. □

The preceding result shows that towards the end of the optimization process the optimal values corresponding to the pairs $(\mathcal{S}, f)$ and $(\overline{\mathcal{S}}, \overline{f}_c)$ coincide. On the other hand one has

$$\forall c > 0: \quad \min_{i \in \mathcal{S}} f(i) \geq \min_{i \in \overline{\mathcal{S}}} \overline{f}_c(i). \tag{4.10}$$

Thus, for each fixed value of $c > 0$, the minimum of $\overline{f}_c$ over $\overline{\mathcal{S}}$ constitutes a lower bound for the desired minimum of f over $\mathcal{S}$. This explains the practical phenomenon that when applying annealing with a penalty function the values one finds in the beginning of the optimization process are often lower than the eventual minimum f_{opt}.

Clearly, after a large number of transitions at fixed $c > 0$ the algorithm will find a solution $i \in \overline{\mathcal{S}}$ with a probability approximately equal to the corresponding component $\overline{q}_i(c)$ of the equilibrium distribution, which we can write as follows

$$\overline{q}_i(c) = \frac{A_i(c)}{M_0(c)} \tag{4.11}$$

with

$$M_0(c) = \sum_{j \in \overline{\mathcal{S}}} A_j(c) \tag{4.12}$$

$$A_i(c) = \exp\left(\frac{f_{opt} - \overline{f}_c(i)}{c}\right). \tag{4.13}$$

Let us discuss some characteristic properties of $\overline{q}(c)$.
First of all we clearly have

$$\forall i \in \mathcal{S} \;\; \forall j \in \overline{\mathcal{S}} \setminus \mathcal{S}: \quad \frac{\overline{q}_j(c)}{\overline{q}_i(c)} = \exp\left(\frac{f(i) - \overline{f}_c(j)}{c}\right) = o(1) \quad \text{as } c \downarrow 0, \tag{4.14}$$

so that for small c the probability of being in $\overline{\mathcal{S}} \setminus \mathcal{S}$ is negligible compared to that of being in $\mathcal{S}$.
Another property of a more graphical nature is the following.
For $i, j \in \mathcal{S}$ the curves representing $\overline{q}_i(c)$ and $\overline{q}_j(c)$ as a function of $c > 0$ either coincide or have no point in common, since obviously

$$\forall i, j \in \mathcal{S}: \quad f(i) < f(j) \Rightarrow [\forall c > 0: \quad \overline{q}_i(c) > \overline{q}_j(c)]. \tag{4.15}$$

Figure 4.1 on the next page shows the components of the equilibrium distribution in the penalized case as a function of the control parameter for a simple problem instance. As can be seen from this figure, a curve representing $\overline{q}_i(c)$ with $i \in \overline{\mathcal{S}} \setminus \mathcal{S}$ may well intersect other curves either corresponding to $j \in \mathcal{S}$ or to $j \in \overline{\mathcal{S}} \setminus \mathcal{S}$.
Note furthermore that

$$\forall i \in \mathcal{S}: \quad 0 < \overline{q}_i(c) < \frac{1}{|S_{opt}|}. \tag{4.16}$$

From figure 4.1 we see that (4.16) does not necessarily hold if we replace $\mathcal{S}$ by $\overline{\mathcal{S}}$.

It is interesting to compare the equilibrium distribution $q(c)$ given by (2.5), which is obtained by applying standard annealing directly on (S, f), with the equilibrium distribution $\overline{q}(c)$ resulting from the application of standard annealing on a penalizing pair $(\overline{S}, \overline{f}_c)$.
To do so it is convenient to write

$$\overline{q}_i(c) = \frac{\exp\left(\dfrac{-\overline{f}_c(i)}{c}\right)}{N_0(c) + N_1(c)} \tag{4.17}$$

with $N_0(c)$ as in (2.6) and

$$N_1(c) = \sum_{j \in \overline{\mathcal{S}} \setminus \mathcal{S}} \exp\left(\frac{-\overline{f}_c(j)}{c}\right). \tag{4.18}$$

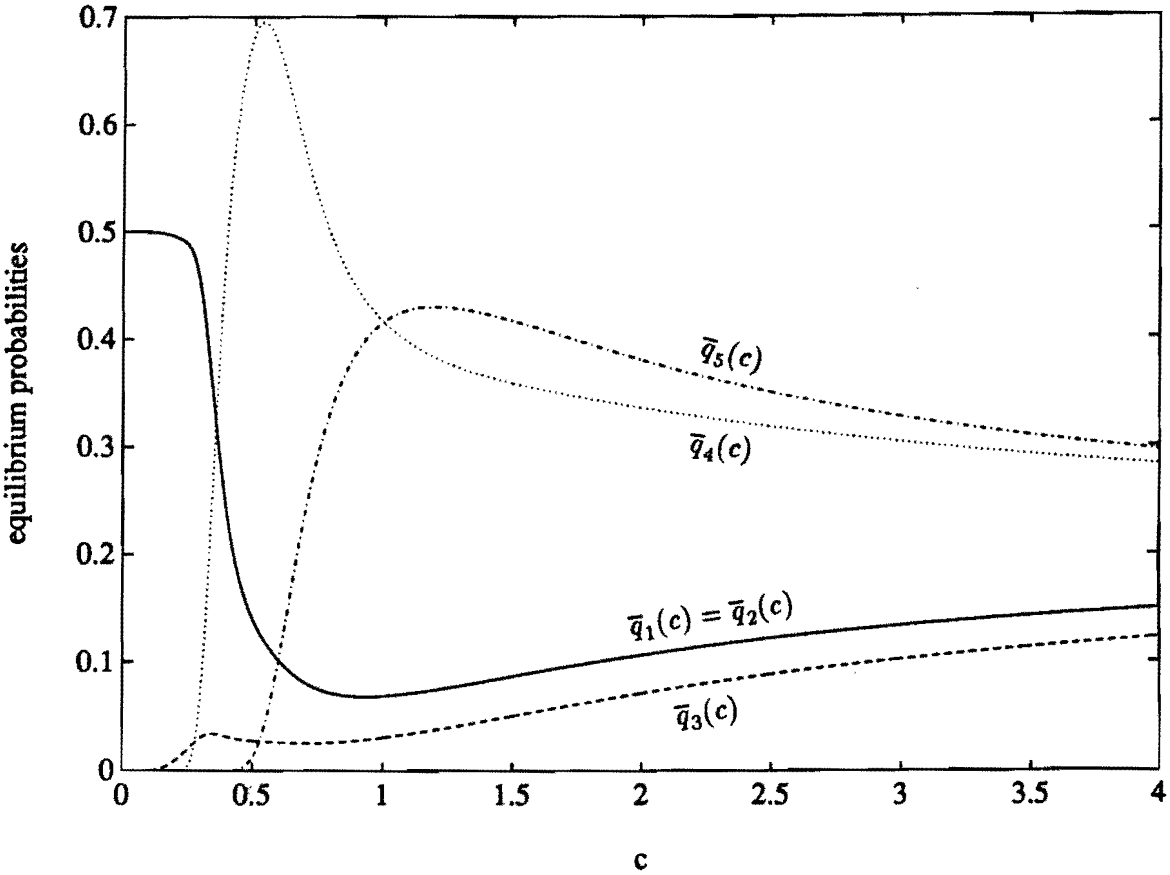

Figure 4.1: *The components of the equilibrium distribution in the penalized case as a function of c for the problem instance* $\mathcal{S} = \{1,2,3\}$, $f(1) = f(2) = 2.8$, $f(3) = 3.6$ *with the penalization* $\overline{\mathcal{S}} = \mathcal{S} \cup \{4,5\}$, $\overline{f}_c(4) = 1/c$, $\overline{f}_c(5) = 1/c^2$.

A direct comparison of (4.17) and (2.5) gives us

$$\forall i \in \mathcal{S} \;\; \forall c > 0: \quad \overline{q}_i(c) < q_i(c), \tag{4.19}$$

which is intuitively clear since in the penalized case the algorithm has more states to choose from.
Let us investigate the situation in the limit region as $c \downarrow 0$.
From (4.17) it is clear that

$$\forall i \in \mathcal{S} \;\; \forall c > 0: \quad 0 < 1 - \frac{\overline{q}_i(c)}{q_i(c)} = \frac{N_1(c)}{N_0(c) + N_1(c)} = \sum_{j \in \overline{\mathcal{S}} \setminus \mathcal{S}} \overline{q}_j(c) = o(1) \quad \text{as } c \downarrow 0, \tag{4.20}$$

where we used (4.14) in the last step.
Consequently, if $i \in \mathcal{S}$ then for small $c > 0$ the probabilities $\overline{q}_i(c)$ and $q_i(c)$ will be arbitrarily close.

Summarizing the above we may say that in the limit region as $c \downarrow 0$ the presence of infeasible states is barely felt, so that the probability of being in a state $i \in \mathcal{S}$ is effectively the same in the penalized as in the unpenalized case.
Of course this is exactly what one aims at in the first place.
As an immediate consequence we obtain asymptotic convergence in the sense that (2.7) is still valid if we replace $q_i(c)$ by $\overline{q}_i(c)$.

The following lemma establishes in a more direct way the asymptotic convergence of the standard annealing algorithm - when used on the pair $(\overline{\mathcal{S}}, \overline{f}_c)$ - to the set of globally optimal solutions of the original problem $(\mathcal{S}, f)$. The asymptotic behaviour is displayed in an explicit way.

Lemma 4.2 *The equilibrium distribution given by (4.11) satisfies*

$$\lim_{c\downarrow 0} \overline{q}_i(c) = \begin{cases} 0 & \text{if } i \in \overline{\mathcal{S}} \setminus \mathcal{S}_{opt} \\ \frac{1}{|\mathcal{S}_{opt}|} & \text{if } i \in \mathcal{S}_{opt}. \end{cases} \tag{4.21}$$

More precisely, there exists a $c_0 > 0$ such that for $0 < c < c_0$

$$0 < \frac{1}{|\mathcal{S}_{opt}|} - \overline{q}_i(c) < M_1 \exp\left(\frac{-\delta}{c}\right) \qquad \text{for } i \in \mathcal{S}_{opt} \tag{4.22}$$

$$0 < \overline{q}_i(c) < M_2 \exp\left(\frac{f_{opt} - \overline{f}_c(i)}{c}\right) \leq M_2 \exp\left(\frac{-\delta}{c}\right) \qquad \text{for } i \in \overline{\mathcal{S}} \setminus \mathcal{S}_{opt}, \tag{4.23}$$

where the positive constants M_1, M_2 and δ are given by

$$M_1 = (1 + |\mathcal{S}^*_{opt}|)/|\mathcal{S}_{opt}|^2 \tag{4.24}$$

$$M_2 = 1/|\mathcal{S}_{opt}| \tag{4.25}$$

$$\delta = f^*_{opt} - f_{opt} \tag{4.26}$$

$$f^*_{opt} = \min_{i \in \mathcal{S}\setminus\mathcal{S}_{opt}} f(i) \tag{4.27}$$

with

$$\mathcal{S}^*_{opt} = \left\{ i \in \mathcal{S} | f(i) = f^*_{opt} \right\}. \tag{4.28}$$

Proof Let us choose $c_1 > 0$ such that for $0 < c < c_1$

$$\forall i \in \overline{\mathcal{S}} \setminus \mathcal{S} : \quad \overline{f}_c(i) \geq f^*_{opt}. \tag{4.29}$$

By the definition of f^*_{opt} we then have

$$\forall i \in \overline{\mathcal{S}} \setminus \mathcal{S}_{opt} : \quad \overline{f}_c(i) \geq f^*_{opt} > f_{opt}, \tag{4.30}$$

so that

$$\forall i \in \overline{\mathcal{S}} \setminus \mathcal{S}_{opt} : \quad A_i(c) = \exp\left(\frac{f_{opt} - \overline{f}_c(i)}{c}\right) \leq \exp\left(\frac{-\delta}{c}\right). \tag{4.31}$$

Of course, for $i \in \mathcal{S}^*_{opt}$ the equality sign holds. On the other hand by (4.27) and (4.3) one has

$$\forall\, i \in \overline{\mathcal{S}} \setminus \mathcal{S}^*_{opt}: \qquad \lim_{c \downarrow 0} A_i(c) \exp\left(\frac{\delta}{c}\right) = \lim_{c \downarrow 0} \exp\left(\frac{f^*_{opt} - \overline{f}_c(i)}{c}\right) = 0. \tag{4.32}$$

Hence there exists a $0 < c_0 < c_1$ such that for $0 < c < c_0$

$$\sum_{j \in \overline{\mathcal{S}} \setminus \mathcal{S}_{opt}} A_j(c) < (1 + |\mathcal{S}^*_{opt}|) \exp\left(\frac{-\delta}{c}\right). \tag{4.33}$$

For $i \in \mathcal{S}_{opt}$ this yields

$$\begin{aligned} 0 < \frac{1}{|\mathcal{S}_{opt}|} - \overline{q}_i(c) &= \frac{\sum_{j \in \overline{\mathcal{S}} \setminus \mathcal{S}_{opt}} A_j(c)}{|\mathcal{S}_{opt}| \left(|\mathcal{S}_{opt}| + \sum_{j \in \overline{\mathcal{S}} \setminus \mathcal{S}_{opt}} A_j(c)\right)} \\ &< \frac{(1 + |\mathcal{S}^*_{opt}|)}{|\mathcal{S}_{opt}|^2} \exp\left(\frac{-\delta}{c}\right). \end{aligned} \tag{4.34}$$

For $i \in \overline{\mathcal{S}} \setminus \mathcal{S}_{opt}$ we obtain

$$0 < \overline{q}_i(c) = \frac{A_i(c)}{\sum_{j \in \overline{\mathcal{S}}} A_j(c)} < \frac{A_i(c)}{|\mathcal{S}_{opt}|} \le \frac{1}{|\mathcal{S}_{opt}|} \exp\left(\frac{-\delta}{c}\right), \tag{4.35}$$

which completes the proof. □

5 Equilibrium statistics for the penalized case

In the setting of the previous section let us investigate the asymptotic behaviour of some statistical quantities familiar from the unpenalized case (see [1]).

Using the equilibrium distribution given by (4.11) we define the expected cost $\langle \overline{f}_c \rangle_c$, the variance of the cost $\overline{\sigma}^2_c$ and the entropy $\overline{S}_c$ - all taken at equilibrium - in the following way

$$\langle \overline{f}_c \rangle_c = \sum_{i \in \overline{\mathcal{S}}} \overline{f}_c(i)\, \overline{q}_i(c) \tag{5.1}$$

$$\overline{\sigma}^2_c = \sum_{i \in \overline{\mathcal{S}}} (\overline{f}_c(i) - \langle \overline{f}_c \rangle_c)^2\, \overline{q}_i(c) \tag{5.2}$$

$$\overline{S}_c = -\sum_{i \in \overline{\mathcal{S}}} \overline{q}_i(c) \ln \overline{q}_i(c). \tag{5.3}$$

The asymptotic behaviour of these quantities as c tends to zero is displayed in the next lemma.

Lemma 5.1 *Let the equilibrium distribution be given by (4.11). Then we have*

$$\lim_{c \downarrow 0} \langle \overline{f}_c \rangle_c = f_{opt}, \tag{5.4}$$

$$\lim_{c \downarrow 0} \overline{\sigma}^2_c = 0, \tag{5.5}$$

$$\lim_{c \downarrow 0} \overline{S}_c = \ln |\mathcal{S}_{opt}|. \tag{5.6}$$

More precisely, there exists a $c_0 > 0$ such that for $0 < c < c_0$

$$0 < \langle \overline{f}_c \rangle_c - f_{opt} < M\delta \exp\left(\frac{-\delta}{c}\right), \tag{5.7}$$

$$0 < \overline{\sigma}_c^2 < M\delta^2 \exp\left(\frac{-\delta}{c}\right), \tag{5.8}$$

$$0 < \overline{S}_c - \ln|\mathcal{S}_{opt}| < M\frac{\delta}{c} \exp\left(\frac{-\delta}{c}\right), \tag{5.9}$$

where the positive constants δ and M are given by (4.26) and

$$M = \frac{1 + |\mathcal{S}^*_{opt}|}{|\mathcal{S}_{opt}|} \tag{5.10}$$

with $\mathcal{S}^*_{opt}$ as in (4.28).
Furthermore, $\overline{\sigma}_c^2$ and $\overline{S}_c$ are positive for all $c > 0$.

Proof To prove (5.7) we recall from the proof of lemma 4.2 that there is a $c_1 > 0$ such that for $0 < c < c_1$

$$\overline{f}_c(i) \geq f^*_{opt} > f_{opt} \quad \forall i \in \overline{\mathcal{S}} \setminus \mathcal{S}_{opt}, \tag{5.11}$$

with f^*_{opt} as in (4.27).
Let us start by taking $0 < c < c_1$. Note that

$$\langle \overline{f}_c \rangle_c - f_{opt} = \sum_{i \in \overline{\mathcal{S}} \setminus \mathcal{S}_{opt}} \left(\overline{f}_c(i) - f_{opt}\right) \overline{q}_i(c) > 0. \tag{5.12}$$

As a first estimate we readily obtain

$$0 < \langle \overline{f}_c \rangle_c - f_{opt} < \frac{1}{|\mathcal{S}_{opt}|} \exp\left(\frac{-\delta}{c}\right) \sum_{i \in \overline{\mathcal{S}} \setminus \mathcal{S}_{opt}} \alpha_i(c) \tag{5.13}$$

with

$$\alpha_i(c) = (\overline{f}_c(i) - f_{opt}) A_i(c) \exp\left(\frac{\delta}{c}\right). \tag{5.14}$$

Let us examine $\alpha_i(c)$.
First, by (4.3)

$$\forall\, i \in \overline{\mathcal{S}} \setminus \mathcal{S}: \qquad \lim_{c \downarrow 0} \alpha_i(c) = \lim_{c \downarrow 0} (\overline{f}_c(i) - f_{opt}) \exp\left(\frac{f^*_{opt} - \overline{f}_c(i)}{c}\right) = 0. \tag{5.15}$$

Next, using (4.32) we find

$$\forall\, i \in \mathcal{S} \setminus \mathcal{S}^*_{opt}: \qquad \lim_{c \downarrow 0} \alpha_i(c) = \lim_{c \downarrow 0} (f(i) - f_{opt}) A_i(c) \exp\left(\frac{\delta}{c}\right) = 0. \tag{5.16}$$

Finally, we simply have

$$\forall\, i \in \mathcal{S}^*_{opt}: \qquad \alpha_i(c) = \delta. \tag{5.17}$$

Together (5.15), (5.16) and (5.17) imply the existence of a $0 < c_0 < c_1$ such that (5.7) holds for $0 < c < c_0$.

Next, let us show that $\overline{\sigma}_c^2$ is positive for all $c > 0$.
Suppose the contrary. Then, since $\overline{\sigma}_c^2$ is obviously nonnegative, there is a $\tilde{c} > 0$ such that $\overline{\sigma}_c^2$ vanishes for c equal to $\tilde{c}$. In view of the positivity of $\overline{q}_i(\tilde{c})$ this gives us $\overline{f}_{\tilde{c}}(i) = \langle \overline{f}_{\tilde{c}} \rangle_{\tilde{c}} = f_{opt}$ $\forall i \in \overline{S}$, which contradicts the fact that $\mathcal{S} \neq \mathcal{S}_{opt}$.

As a first bound for $\overline{\sigma}_c^2$ we clearly have

$$\overline{\sigma}_c^2 < \frac{1}{|\mathcal{S}_{opt}|} \exp\left(\frac{-\delta}{c}\right) \sum_{i \in \overline{S}} \beta_i(c) \tag{5.18}$$

with

$$\beta_i(c) = (\overline{f}_c(i) - \langle \overline{f}_c \rangle_c)^2 A_i(c) \exp\left(\frac{\delta}{c}\right). \tag{5.19}$$

By (5.7) one has for $c > 0$ small enough

$$\forall i \in \mathcal{S}_{opt} : \quad \beta_i(c) < M^2 \delta^2 \exp\left(\frac{-\delta}{c}\right), \tag{5.20}$$

so that in the limit as c tends to zero $\mathcal{S}_{opt}$ does not contribute to the summation.
Using (5.4) an almost exact copy of the reasoning yielding (5.15), (5.16) and (5.17) now produces

$$\lim_{c \downarrow 0} \sum_{i \in \overline{S} \setminus \mathcal{S}_{opt}} \beta_i(c) = \delta^2 |\mathcal{S}_{opt}^*|. \tag{5.21}$$

By combining (5.18), (5.20) and (5.21) the proof of (5.8) is completed.

To conclude with let us consider the entropy $\overline{S}_c$, which can conveniently be rewritten as

$$\begin{aligned} \overline{S}_c &= -\sum_{i \in \overline{S}} \overline{q}_i(c) \ln\left(\frac{A_i(c)}{M_0(c)}\right) \\ &= \sum_{i \in \overline{S}} \overline{q}_i(c) \frac{\overline{f}_c(i) - f_{opt}}{c} + \sum_{i \in \overline{S}} \overline{q}_i(c) \ln M_0(c) \\ &= \frac{\langle \overline{f}_c \rangle_c - f_{opt}}{c} + \ln M_0(c). \end{aligned} \tag{5.22}$$

Consequently

$$\overline{S}_c - \ln|\mathcal{S}_{opt}| = \frac{\langle \overline{f}_c \rangle_c - f_{opt}}{c} + \ln\left(1 + \frac{1}{|\mathcal{S}_{opt}|} \sum_{j \in \overline{S} \setminus \mathcal{S}_{opt}} A_j(c)\right). \tag{5.23}$$

As for the first term, notice that because of (5.7) one has for $c > 0$ sufficiently small

$$0 < \frac{\langle \overline{f}_c \rangle_c - f_{opt}}{c} < M \frac{\delta}{c} \exp\left(\frac{-\delta}{c}\right). \tag{5.24}$$

Estimating the second term we obtain

$$0 < \ln\left(1 + \frac{1}{|\mathcal{S}_{opt}|} \sum_{j \in \overline{S} \setminus \mathcal{S}_{opt}} A_j(c)\right) \leq \frac{1}{|\mathcal{S}_{opt}|} \sum_{j \in \overline{S} \setminus \mathcal{S}_{opt}} A_j(c). \tag{5.25}$$

Clearly, by (4.32)

$$\forall i \in \overline{\mathcal{S}} \setminus \mathcal{S}_{opt}: \quad \lim_{c \downarrow 0} A_i(c) c \exp\left(\frac{\delta}{c}\right) = 0. \tag{5.26}$$

From (5.24), (5.25) and (5.26) it follows that for $c > 0$ small enough

$$0 < (\overline{S}_c - \ln |\mathcal{S}_{opt}|) c \exp\left(\frac{\delta}{c}\right) < M\delta, \tag{5.27}$$

which proves (5.9).
Since

$$\overline{S}_c = \sum_{i \in \overline{\mathcal{S}}} \overline{q}_i(c) \ln\left(\frac{1}{\overline{q}_i(c)}\right), \tag{5.28}$$

the positivity of $\overline{S}_c$ is a direct consequence of the fact that
$\forall c > 0 \;\; \forall i \in \overline{\mathcal{S}}: \quad 0 < \overline{q}_i(c) < 1.$ □

It is wellknown (see [1]) that in the unpenalized case both the entropy S_c as well as the expected cost $\langle f \rangle_c$ are strictly increasing on $c > 0$, so that $S_c > \ln |\mathcal{S}_{opt}|$ and $\langle f \rangle_c > f_{opt}$ for all $c > 0$.
In the penalized case there is no guarantee for this. Even worse, given any compact interval contained in $c > 0$ one can construct a penalization such that on that interval the expected cost $\langle \overline{f}_c \rangle_c$ is as far below f_{opt} as desired, while at the same time the entropy $\overline{S}_c$ is arbitrarily close to zero. Clearly, the latter implies non-monotonicity of $\overline{S}_c$ if $|\mathcal{S}_{opt}| > 1$.
The proof of the following lemma provides us with an explicit example of such a penalization.

Lemma 5.2 *Consider an instance $(\mathcal{S}, f)$ of a combinatorial optimization problem (as always such that $\mathcal{S} \neq \mathcal{S}_{opt}$).*
Given $\varepsilon > 0, R > 0$ and any interval $[c_1, c_2] \subset (0, \infty)$ there exists a penalizing pair $(\overline{\mathcal{S}}, \overline{f}_c)$ such that for $c_1 \leq c \leq c_2$:

$$(i) \quad \forall i \in \mathcal{S}: \quad 0 < \overline{q}_i(c) < \varepsilon \tag{5.29}$$

$$(ii) \quad 0 < \overline{S}_c < \varepsilon \tag{5.30}$$

$$(iii) \quad \langle \overline{f}_c \rangle_c - f_{opt} < -R. \tag{5.31}$$

Proof Without loss of generality we may represent $\mathcal{S}$ by $\mathcal{S} = \{1, 2, \ldots, k\}$ for some positive integer k.
Now define

$$\overline{\mathcal{S}} = \mathcal{S} \cup \{k+1\} \tag{5.32}$$

$$\overline{f}_c(k+1) = f_{opt} - \alpha + \frac{1}{c}, \tag{5.33}$$

where α is a positive parameter to be chosen shortly.
To facilitate the discussion let us fix $\rho > 1$ such that

$$(i) \quad (1+\rho)\exp(-\rho) < \frac{\varepsilon}{|\mathcal{S}|} \tag{5.34}$$

$$(ii) \quad \rho > R + \varepsilon(1 + L) \tag{5.35}$$

with

$$L = \sum_{i \in \mathcal{S} \setminus \mathcal{S}_{opt}} (f(i) - f_{opt}). \tag{5.36}$$

From now on let $c_1 \leq c \leq c_2$.
In terms of ρ we choose α as follows:

$$\alpha > \max(g(c_1), g(c_2)) \tag{5.37}$$

with

$$g(c) = \frac{1}{c} + \rho \max(1, c). \tag{5.38}$$

With $N_0(c)$ as in (2.6) we have for $i \in \mathcal{S}$

$$\begin{aligned} \overline{q}_i(c) &= \frac{\exp\left(\frac{-f(i)}{c}\right)}{N_0(c) + \exp\left(\frac{\alpha - f_{opt}}{c} - \frac{1}{c^2}\right)} \\ &< \exp\left(\frac{-\alpha}{c} + \frac{1}{c^2}\right) \\ &\leq \exp\left(\frac{-\alpha + g(c)}{c} - \rho\right) \\ &< \exp(-\rho) \;<\; \varepsilon, \end{aligned} \tag{5.39}$$

which proves (5.30).
To demonstrate (5.31) note that

$$\begin{aligned} \frac{1}{\overline{q}_{k+1}(c)} &= 1 + N_0(c) \exp\left(\frac{f_{opt} - \alpha}{c} + \frac{1}{c^2}\right) \\ &\leq 1 + |\mathcal{S}| \exp\left(\frac{-\alpha}{c} + \frac{1}{c^2}\right) \\ &< 1 + |\mathcal{S}| \exp(-\rho). \end{aligned} \tag{5.40}$$

Hence

$$\begin{aligned} 0 < \overline{S}_c &< -\sum_{i \in \mathcal{S}} \exp(-\rho) \ln \exp(-\rho) + \ln\left(\frac{1}{\overline{q}_{k+1}(c)}\right) \\ &< |\mathcal{S}|(1+\rho)\exp(-\rho) < \varepsilon. \end{aligned} \tag{5.41}$$

Finally, we have for $\langle \overline{f}_c \rangle_c$

$$\langle \overline{f}_c \rangle_c - f_{opt} < \sum_{i \in \mathcal{S} \setminus \mathcal{S}_{opt}} (f(i) - f_{opt}) \exp(-\rho) + \left(-\alpha + \frac{1}{c}\right) \overline{q}_{k+1}(c), \tag{5.42}$$

which, when combined with the fact that

$$-\alpha + \frac{1}{c} < -\rho \max(1, c) \leq -\rho, \tag{5.43}$$

gives us

$$\begin{aligned} \langle \overline{f}_c \rangle_c - f_{opt} &< L \exp(-\rho) - \rho(1 - |\mathcal{S}| \exp(-\rho)) \\ &< -R + |\mathcal{S}|\rho \exp(-\rho) - \varepsilon + L(\exp(-\rho) - \varepsilon) \\ &< -R. \end{aligned} \tag{5.44}$$

Herewith the proof of lemma 5.2 is completed. □

Figure 5.1 shows the entropy as well as the expected cost as a function of the cooling parameter for a penalization chosen in accordance with (5.33).

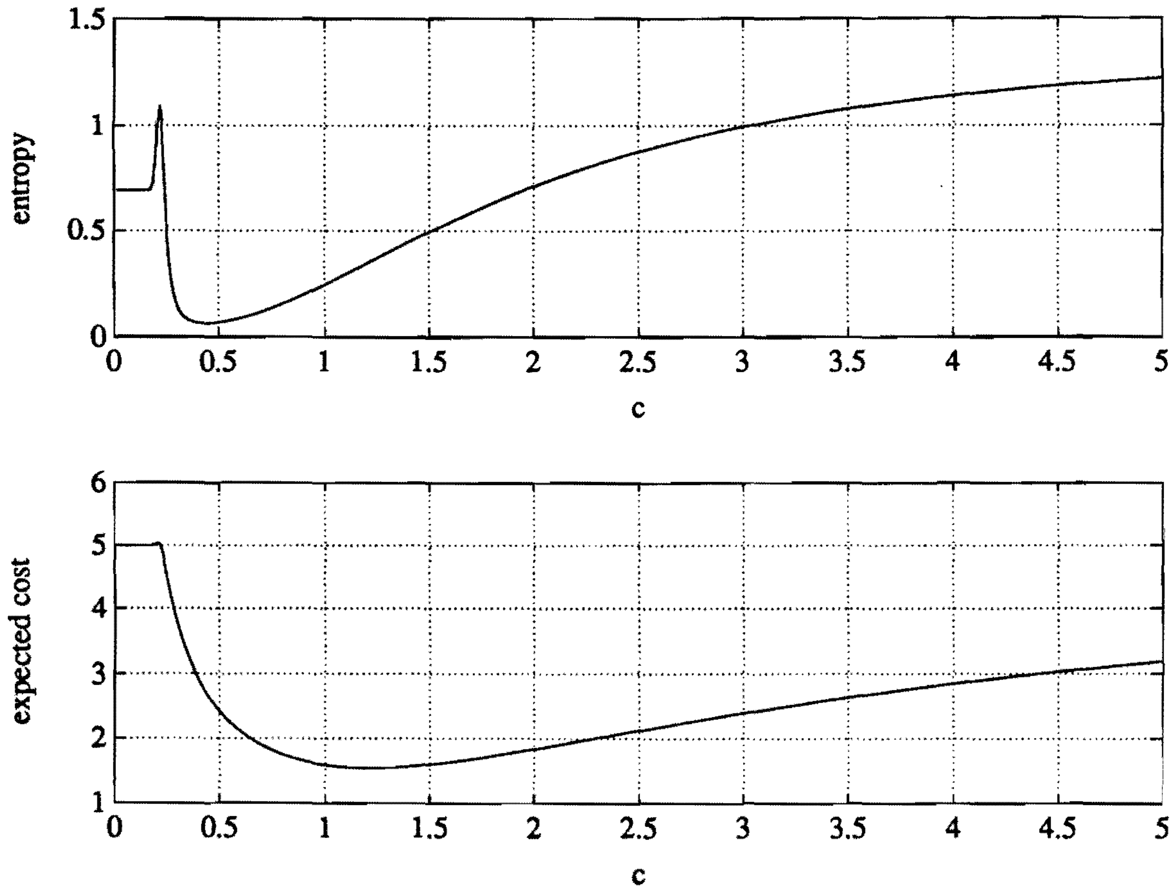

Figure 5.1: *The entropy and the expected cost in the penalized case as a function of c for the problem instance* $\mathcal{S} = \{1,2,3\}$, $f(1) = f(2) = 5$, $f(3) = 9$ *with the penalization* $\overline{\mathcal{S}} = \mathcal{S} \cup \{4\}$, $\overline{f}_c(4) = 0.4 + 1/c$.

Note that the structure of $\overline{f}_c$ as given by (5.33) is the same as that of the penalization (4.6) used in the macro placement problem. Therefore the phenomena described in the preceding lemma and illustrated by the above figure are by no means artificial pathologies but may really influence the outcome of a practical annealing experiment.

6 Concluding remarks

Let us note that, since the unpenalized case is evidently included in the penalized case, this paper implicitly contains detailed asymptotic estimates for the unpenalized case that have not been reported previously in the literature.

To mention a side effect, in [1], p. 28, a postulate is formulated implying that as c tends to zero the expected cost $\langle f\rangle_c$ in the unpenalized case approaches f_{opt} in a linear way. From lemma 5.1 it is clear that this postulate must be modified somewhat, since the convergence is exponential. In particular $\langle f\rangle_c$ approaches f_{opt} faster than any positive power of c.

It is a remarkable fact that for the derivation of the results in this paper we only needed to include in our definition of penalization the condition (4.3) that as c tends to zero the infeasible values blow up. In many practical cases, such as the macro placement problem (see (4.6)) the structure of the penalization is such that

(PC) The infeasible values of the cost function increase monotonically as $c \downarrow 0$ and tend to a limit as $c \to \infty$.

If this practical condition (PC) holds, then the limits for $c \to \infty$ of $\overline{q}(c)$, $\langle \overline{f}_c\rangle_c$, $\overline{\sigma}_c^2$ and $\overline{S}_c$ all exist. In particular

$$\lim_{c\to\infty} \overline{q}_i(c) = \frac{1}{|\overline{\mathcal{S}}|} \quad \text{for all } i \in \overline{\mathcal{S}} \tag{6.1}$$

$$\lim_{c\to\infty} \overline{S}_c = \ln |\overline{\mathcal{S}}|. \tag{6.2}$$

In this case the entropy at the beginning of the optimization process (i.e. for large c-values) will generally have a higher value ($\approx \ln |\overline{\mathcal{S}}|$) than towards the end of the process ($\approx \ln |\mathcal{S}_{opt}|$). Note that if (PC) holds there is still in general no monotonicity of $\langle \overline{f}_c\rangle_c$ and $\overline{S}_c$ since the penalization (5.33) occurring in the proof of lemma 5.2 already fulfilled condition (PC).
Although not needed for the results in this paper, it is quite natural to impose condition (PC). In fact, if one does not impose such a condition then undesirable things may happen. To illustrate this consider the problem instance

$$\mathcal{S} = \{1,2,3\}, \quad f(1) = f(2) = 0, f(3) = 1 \tag{6.3}$$

with the penalization

$$\overline{\mathcal{S}} = \mathcal{S} \cup \{4\} \quad \overline{f}_c(4) = \frac{1}{c} - c. \tag{6.4}$$

Then

$$\lim_{c\to\infty} \overline{q}_i(c) = \begin{cases} 0 & \text{if } i \in \mathcal{S} \\ 1 & \text{if } i \in \overline{\mathcal{S}} \setminus \mathcal{S} \end{cases} \tag{6.5}$$

$$\lim_{c\to\infty} \langle \overline{f}_c\rangle_c = -\infty \tag{6.6}$$

$$\lim_{c\to\infty} \overline{S}_c = 0 < \lim_{c\downarrow 0} \overline{S}_c = \ln 2. \tag{6.7}$$

Clearly, such a penalization is not suitable for practical implementation since during a major part of the optimization process no feasible solutions will be generated.

To conclude with, let us discuss some implementational consequences of our results.
As we have seen there is a region $0 < c < c_0$ such that all the quantities $\overline{q}(c)$, $\langle \overline{f}_c\rangle_c$, $\overline{\sigma}_c^2$ and $\overline{S}_c$ behave as in the unpenalized case. On the other hand, when the process is outside that region, odd things may happen, such as a dominant appearance of infeasible states, resulting

in extremely low values for the expected cost and entropy (see lemma 5.2). In practice, the implementation of the annealing algorithm is governed by a cooling schedule specifying the initial c-value as well as a decrement rule for c, a stop criterion and the length of the Markov chains. For the unpenalized case there exist some quite elaborated cooling schedules (see [1]). In the penalized case the literature is not very helpful. That the situation is rather difficult can be seen from the results in the present paper. Specifically, let us have a look at the initial value c^* of the cooling parameter. A high value of c^* often means (e.g. in the situation of lemma 5.2 and generally in the macro placement problem) walking around in $\overline{\mathcal{S}} \setminus \mathcal{S}$ for a large part of the optimization process. A low value means (by virtue of (4.14)) staying in $\mathcal{S}$ but at the risk of ending up in a local optimum since the cooling parameter is not large enough to perform any hill climbing in the cost landscape. Therefore, in practice it is advisable to determine c^* experimentally in such a way that for the cooling parameter c^* in a fixed number of trials a large enough percentage of feasible solutions is obtained.

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