Using Entropy-Based Methods to Study General Constrained Parameter Optimization Problems

M. Argollo de Menezes\textsuperscript{1} and A. R. Lima\textsuperscript{2} \textsuperscript{*}

\textsuperscript{1} Instituto de Física, Universidade Federal Fluminense
Av. Litorânea 24210-340, Niterói, RJ, Brazil, marcio@if.uff.br
\textsuperscript{2} Laboratoire de Physique et Mécanique des Milieux Hétérogènes, ESPCI Paris
10 rue Vauquelin, 75231 Paris Cedex 05, France

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Abstract

In this letter we propose the use of physics techniques for entropy determination on constrained parameter optimization problems. The main feature of such techniques, the construction of an unbiased walk on energy space, suggests their use on the quest for optimal solutions of an optimization problem. Moreover, the entropy, and its associated density of states, give us information concerning the feasibility of solutions.

Statistical physicists are constantly developing new computational and theoretical tools to unravel the complex behavior of systems composed by many simple, interacting units. In the last years, many works \textsuperscript{[1]} have showed us that one could “translate” a variety of problems, ranging from biology to economy, to a physicist’s language. One such example is the work

\textsuperscript{*}Electronic Addresses: marcio@if.uff.br, arlima@pmmh.espci.fr
of Rosé et. al., who extended the concept of “density of states” to complex optimization problems\[2, 3\].

This paper follows the same guidelines: we propose the use of methods which obtain the entropy of physical systems to study constrained parameter optimization problems. These include important tasks, such as production planning, decision problems, structural optimization \[4\] and design of semiconductor quantum devices \[5\]. From the operational point of view these problems are usually analytically untractable and numerically hard to solve, mainly due to the intricate shape of the space of feasible solutions.

A general constrained optimization problem can be formulated as follows:

\[
\begin{align*}
\text{Minimize (or Maximize)} & \quad E(\vec{x}) \\
\text{Subject to} & \quad g_i(\vec{x}) \leq 0, \quad i=1,...,q \\
& \quad h_i(\vec{x}) = 0, \quad i=q+1,...,m
\end{align*}
\]

where $\vec{x} = (x_1, x_2, x_3, ..., x_n)$ is an $n$-component vector, $g_i(\vec{x})$ are $q$ inequality constraints and $h_i(\vec{x})$ are $m - q$ equality constraints. The functions $E(\vec{x})$, $g_i(\vec{x})$ and $h_i(\vec{x})$ can be either linear or nonlinear, continuous or discontinuous. 

**Feasible solutions** can be defined as the set $A(\{\vec{x}\})$ of vectors which satisfy all the constraints, and **optimal solutions** as the subset $B \in A$ of the feasible ones which minimize (maximize) the cost $E$.

Although there are many well-established heuristic algorithms for such problems, like evolutionary algorithms \[5, 6\] and Constrained Simulated Annealing\[7, 8\], none of them give, in a simple way, any information about the structure of the problem.

The “translation” of the abovementioned problem to a physicist’s language proceeds as follows: the variables $x_i$ of the optimization problem \[1\] are identified with the simple interacting units (pointed out in the first paragraph) and the vector $\vec{x}$ with a physical state. $E(\vec{x})$ is the energy (or cost) of the state $\vec{x}$. The density of states is here identified with the ratio between the number of solutions with a given cost $E$ and the total number of solutions. Mathematically it reads

\[
g(E) = \frac{\sum_{\vec{x}} \delta_{E(\vec{x})=E}}{\sum_{\vec{x}} 1} \quad (2)
\]

where the summation runs over all feasible solutions. The entropy $S(E)$, in units of $k_B$, is defined as $S(E) = \ln g(E)$. 

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As pointed by H. Rosé [2], independently of the complexity of the space of solutions, the density of states is a direct measure which reflects how sparsely states with a given quality $E$ are distributed. Thus, from the density of states (or, equivalently, the entropy $S(E)$) we can estimate whether solutions with a given cost $E$ represent global optimal values or if further optimization could lead to better results with reasonable computational effort[2]. Unfortunately, it is not a simple task to obtain the entropy or to estimate it from traditional simulations (Metropolis importance sampling, microcanonical simulations, etc...) [9, 10]. Over the past few years, many efficient algorithms have been developed aiming at an efficient calculation of this quantity. Those include multicanonical methods [11], the “Broad Histogram Method” [12, 13] and, more recently, the “Multiple Range Random Walk” algorithm (MRRW) [14]. Since the latter seems to be the most simple to implement and easiest to generalize [14, 15], we adopted it as a calculational tool to study optimization problems on this letter, and before applying it to our problem, let us briefly review its most important points.

The main idea of the MRRW algorithm is to obtain the density of states (DOS) recursively. For a good resolution on the DOS, one must visit the energy axis on a non-biased way, what can be done by performing a random walk in energy space with the probability of visiting a state $\vec{x}$ being proportional to the reciprocal of the density of states, $1/g(E)$. Since $g(E)$ is not known a priori, it is set to $g(E) = 1$ for all $E$ at the beginning of the random walk, and then configurations are randomly chosen. If a given choice changes the energy of the system from $E_1$ to $E_2$, the new configuration is accepted according to

$$p(E_1 \rightarrow E_2) = \min \left( \frac{g(E_1)}{g(E_2)}, 1 \right).$$

(3)

Then, after the energy level $E$ is visited, $g(E)$ is updated on a multiplicative fashion, $g(E) \rightarrow g(E) \times f$, and the histogram of visits $H(E)$ on an additive way, $H(E) \rightarrow H(E) + 1$. When fluctuations on $H(E)$ are sufficiently small (the magnitude of $f$ is related to the “flatness” of the histogram), the multiplicative factor $f$ is decreased to $f' = \sqrt{f}$. This sequence is repeated until a predefined value of $f$ is achieved (for more details, we refer to the original paper [14].

In principle, this prescription for a “flat histogram” assures that all energy
levels are visited equally and, in practice, one expects that the extreme values of the accessible energies will be visited with the same probability as any other energy level. Since on optimization problems one is interested in extremal values of a cost function (or energy) which characterizes the best solution of a given problem, it is natural to think that “flat histogram” algorithms are good candidates for solving optimization tasks, as we will show on the rest of the paper.

A great advantage of these methods over traditional techniques is that there are no restrictions on how one should make changes to the state \( \vec{x} \), as long as the new state sampled is accepted according to the transitional probability (3). So, this choice can always be made such that it handles the constraints of the problem \([16]\).

Let us take as a simple test case a parabola \( E(x) = x^2 \) on the interval \( 0 \leq x \leq 1 \), with \( x \) being a random variable. From the analysis of functions of random variables \([17]\), one can obtain the probability distribution function \( P(E) dE \), from which the entropy \( S(E) \) can be determined. In this simple case it reads \( S(E) = -\ln E/2 \). To recover this entropy with the MRRW algorithm we simply need to initialize our “system” with an initial “state” \( x = 0 \), then choose randomly another “state” \( x' \). The latter is accepted according to the transitional probability (3), and then histograms are updated. After accomplishing all steps of the method, \([18]\), we compare our numerical estimate with the analytical result (fig. 1) and find a root mean square deviation of order \( 10^{-2} \).

Once we verified the correctness of the method, let us focus on harder problems:

1) Find the maximum of

\[
E_1(\vec{x}) = \left| \frac{\sum_{i=1}^{n} \cos^4(x_i) - 2 \prod_{i=1}^{n} \cos^2(x_i)}{\sqrt{\sum_{i=1}^{n} ix_i^2}} \right|
\]

subject to \( \prod_{i=1}^{n} x_i \geq 0.75 \), \( \sum_{i=1}^{n} x_i \leq 7.5n \) and \( 0 \leq x_i \leq 10 \).
2) Find the maximum of

\[ E_2(\vec{x}) = \left( \sqrt{n} \right)^n \prod_{i=1}^{n} x_i \]  \hspace{1cm} (5)

subject to \( \sum_{i=1}^{n} x_i^2 = 1.0 \).

These are well-known test functions for optimization algorithms \[19\], whereas the optimal solution for the first problem is not known exactly, while for the second one the maximum is at \( E = 1 \).

Following the observation that very often the global solution of many constrained numerical optimization problems lies on the boundary of the feasible region \[8\], we fix the search to the “edge of feasibility”. For instance, in the first example we fix the condition \( \prod x_i = 0.75 \) and perform simultaneous changes to two variables \( x_i \) and \( x_j \) at each change (that is, modify \( x_i \) by a random variable \( 0 < q < 2 \) and divide \( x_j \) by the same \( q \)). Doing so, we obtain the entropy of the former problem, which is depicted in figure (2) for the case \( n = 20 \).
| Problem | n  | MRRW   | EA [4]  | CSA [7, 8] |
|---------|----|--------|---------|------------|
| $E_1$   | 20 | 0.803587 | 0.803553 | 0.803619   |
| $E_1$   | 50 | 0.835131 | 0.833194 | -          |
| $E_1$   | 100| 0.845388 | -       | -          |
| $E_2$   | 20 | 0.999881 | 0.999866 | 1.0        |

Table 1: Comparison between numerical results obtained with multiple range random walks (MRRW), evolutionary algorithms (EA) and constrained simulated annealing (CSA).

On table 1 we compare our results with those obtained with evolutionary algorithms (EA) [4] and constrained simulated annealing (CSA) [7, 8]. We spent approximately $10^6$ MC steps to obtain the entropies for both problems with a nice resolution (which corresponds to 222 seconds for problem 1 with $n = 20$ and 77 seconds for problem 2, both running on a pentium II 400 MHz), while the optimal solutions are obtained in approximately 10 times less MC steps. These results were obtained from only one simulation, and could, in principle, be improved by increasing the number of MC steps or by employing a steepest descent method about the minimum found [20]. Our numerical estimates are always better than those obtained with genetic algorithms, and can get as good as constrained simulated annealing ones with this additional (local) search [20].

As a final test, we apply the MRRW algorithm to the traveling salesman problem (TSP), an archetypal problem on computer science and one of the six basic NP-complete problems [21]. It can be formulated as the quest for the shortest path which connects $N$ cities displaced on a plane map. We try to find optimal tours for two particular instances of the problem, known as ATT48 and kroA100, for which there are known solutions, mathematically proven to be optimal [22]. In order to visit the space of states (the space of feasible solutions) efficiently, we use the Lin Kerninghan algorithm [23] to sample between valid tours. We were able to find optimal tours with approximately $10^6$ MC steps in both instances. On figure (3) we show the entropy of the kroA100 instance with the optimal tour on the inset. From the entropy, one can directly assess how difficult it is to find tours with a specified “quality”, or perimeter $P$ [24].
Figure 2: Entropy as a function of the energy $E = E_1$ when $\prod_{i=1}^n x_i = 0.75$, $n = 20$.

The aim of this paper was to propose the use of a simple and efficient algorithm for entropy determination of physical systems on constrained parameter optimization problems. By performing a biased walk on configuration space, one is able to obtain an unbiased random walk on energy space and then to reconstruct with good precision the density of states. This is the property which makes this “flat histogram” algorithm a good tool for optimization tasks, since the extreme energies of the system are visited at the same frequency as other energies during the visitation scheme of the algorithm. As a result, we were able to obtain, with reduced computational efforts, satisfactory results for classical optimization problems. As an additional feature, we gain insight into the complexity of the problem by means of its associated entropy.

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Figure 3: Entropy of the kroA100 instance. With the MRRW algorithm we were able to find the tour with shortest perimeter $P$, which is exposed on the inset.
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