Traveling salesman problem with a center

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We study a traveling salesman problem where the path is optimized with a cost function that includes its length L as well as a certain measure C of its distance from the geometrical center of the graph. Using simulated annealing (SA) we show that such a problem has a transition point that separates two phases differing in the scaling behavior of L and C, in efficiency of SA, and in the shape of minimal paths.

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In the traveling salesman problem (TSP), which is perhaps the most famous combinatorial optimization problem, one has to find the shortest path that joins a given set of N points. In addition to pure academic interest the TSP appears naturally in some transportation applications or production and testing of integrated circuits [1]. This easy to formulate problem is, however, very difficult to solve. Actually the TSP is known to be NP (nondeterministic polynomial)–complete [2] and it is believed that there is no algorithm that can find a solution in time increasing as a finite order polynomial in N. Although advanced algorithms can find exact solutions of the TSP for quite large values of N, these algorithms are usually dedicated only to this particular task. Consequently, they are not suitable for more general versions of the TSP nor for some other numerically difficult optimization problems. It is thus desirable to develop approximate but more versatile methods such as genetic programming [3], simulated annealing (SA) [4], or extremal optimization [5], and for such a purpose the TSP appears to be an excellent testing ground.

Another NP-complete problem that is of considerable interest is the so-called satisfiability problem where one examines conditions needed to satisfy certain Boolean formulas [6]. Recently, it was shown that there is a phase transition in this class of problems that separates two regimes: easy and hard to satisfy. It turns out that such problems are most difficult to examine right at the transition point and computational complexity decreases when one moves away from the transition point [7]. A related phase transition was found in a certain version of the TSP where distances between points are randomly drawn integer numbers $\{1,2,\ldots,k\}$. In such a case the time needed to find the minimal solution using a branch-and-bound algorithm dramatically increases when k exceeds a certain threshold value [8]. Methods used to establish these results very often originate from statistical mechanics providing thus an interesting multidisciplinary bridge [9]. Although some other examples of connections between statistical mechanics and computational complexity were already examined [10], further explorations of this subject would be very desirable.

In the present paper we examine a certain version of the TSP where one requires the minimization of $E=L+rC$, where L is the total length of a path, C is the sum of distances of middle points of links from the geometrical center of the graph, and r is a control parameter of the model (of course, $r=0$ corresponds to the original TSP). Using simulated annealing we show that upon increasing r the model undergoes a phase transition from the L(-dominated) phase (small r) to the C(-dominated) phase (large r). In the L phase we find $L\sim N^{1/2}$ and $C\sim N$, while in the C phase a reverse scaling holds with $L\sim N$ and $C\sim N^{1/2}$. Moreover, the minimal paths in these two phases have a qualitatively different shape. What is also interesting is the change of efficiency of SA. The r-dependent optimization problem that we study does not seem to be easier than the $r=0$ case, and we expect that for any r our problem is also NP-complete. Nevertheless, in the C phase SA has a much better efficiency than in the L phase at least with respect to finding nearly minimal paths. Such an effect might be related to a change of the energy landscape of the problem, but further studies would be needed to verify such a claim.

To define our problem, let us consider N points distributed in a unit square of a Euclidean plane. Denoting the coordinates of the ith point as (x_i,y_i), we have

$$L=\sum_{k=1}^{N}\sqrt{(x_{i_k}-x_{i_{k+1}})^2+(y_{i_k}-y_{i_{k+1}})^2}, \tag{1}$$

$$C=\frac{1}{2}\sum_{i=1}^{N}\sqrt{(x_{i_k}+x_{i_{k+1}}-1)^2+(y_{i_k}+y_{i_{k+1}}-1)^2}, \tag{2}$$

where we assume that in a given path, points appear in the order $i_1,i_2,\ldots,i_N$, i_1 and $i_{N+1}=i_1$. Next, we introduce the cost function $E=L+rC$. We cannot provide an immediate application of such a problem, but one can imagine that in some transportation tasks staying during the tour close to (or far from) the center might be of some importance. Such an additional condition might be particularly relevant in war areas where staying near a military base is important for safety reasons. Another application might be a "just-in-time vehicle routing problem," in which truck drivers might be called to the center depot at intermediate times in order to get further goods that have to be delivered to the customers. It is easy to realize that minimization of L usually does not minimize C and competition of these two terms might lead to some interesting effects.

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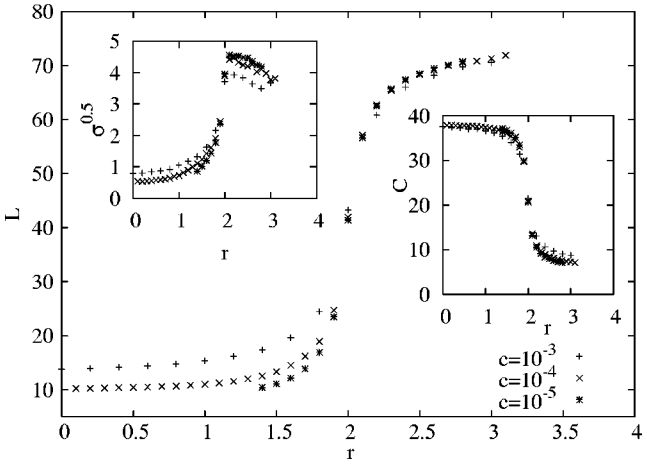

FIG. 1. The length L of the minimal path as a function of r for $N=100$. The left inset shows the square root of its variance $\sqrt{\sigma}$ as a function of r. The right inset shows the total distance from the center C as a function of r.

To find a path that minimizes E we use a standard simulated annealing technique. For a given configuration, we produce a trial configuration by exchanging randomly the positions of two points. Such a move is accepted with a probability $\min(1, e^{-\delta E/T})$ where δE is the energy difference between a trial and the initial configuration, and T is a fictitious temperature. During simulations, the temperature T is reduced to zero linearly in time t according to $T(t)=1-ct$ where c is the cooling rate and the unit of time is defined as the attempt to make N moves. For a small cooling rate c such a method finds a path of a low (and for small N perhaps even the lowest) value of E. To check that the properties of our model are not the consequence of the numerical method, we did additional runs using the so-called LIN-2-OPT moves that cut a configuration in two pieces, turn the direction of one piece around, and reconnect [11]. Such moves are known to be more effective than exchanges of two points [12]. Both methods, however, yield essentially the same behavior of our model with respect to, e.g., the location of the transition point or N dependence of L and C. Unless specified otherwise, the results described below are obtained with the use of the exchange algorithm.

In Fig. 1 we show the length L of a minimal path as a function of r averaged over 1000 distributions of $N=100$ points. One can see that L is a slowly increasing function of r except around $r=2.0$ where the increase is more abrupt. Around the same value of r there is a maximum of the variance of L and an abrupt change of C. These results suggest that a certain phase transition takes place around $r=2$.

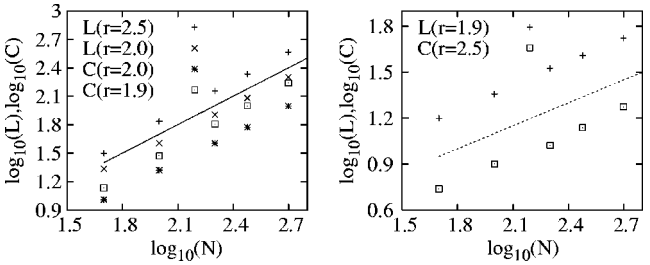

FIG. 3. Size dependence of L and C for $r=1.9$, 2.0, and 2.5. Calculations made for $c=10^{-4}$,10^{-5}, and 10^{-6} were extrapolated to $c=0$ and the average was made over 1000 independent samples. Continuous and dotted lines have slope 1.0 and 0.5, respectively.

A visual indication of a qualitative change around $r \sim 2.0$ is shown in Fig. 2. For large r (C-dominated phase), paths that minimize E have large length L but many intersections around the center $(1/2,1/2)$ yield a small value of C. For small r (L-dominated phase) typical minimal paths have a much different shape. They have only few intersections and are more or less uniformly distributed in a unit square.

That in our problem there are two phases separated by a transition point around ~ 2.0 is also seen in Fig. 3 which presents the N dependence of L and C. These results show that in the L phase ($r=1.9$) $L \sim N^{1/2}$ and $C \sim N$. Consequently, the cost function E is dominated by the distance C. Let us notice that the scaling $L \sim N^{1/2}$ was already proven for the original TSP ($r=0$) [13]. As for the second relation ($C \sim N$), there is a simple argument that justifies it. Indeed, since in the L phase the minimal path is relatively uniformly distributed in the unit square one can assume that central points of links are also almost uniformly distributed. It means that there is a positive (and N independent in the limit $N \to \infty$) average distance of the central point from $(1/2,1/2)$ and then $C \sim N$ easily follows [14].

In the C phase we find $L \sim N$ and $C \sim N^{1/2}$. Such relations can be deduced from the structure of a typical minimal path as seen in Fig. 2. In the C phase points that are approximately opposite with respect to $(1/2,1/2)$ are pairwise linked. It means that there is a finite (N-independent) length of such a link and thus $L \sim N$ follows. The relation $C \sim \sqrt{N}$ is more subtle and we can justify it only approximately. In the following we argue that for a minimal path the typical distance $\bar{c}$ of the center of a link to $(1/2,1/2)$ scales as $1/\sqrt{N}$ from which the relation $C \sim \sqrt{N}$ easily follows. To show that $\bar{c} \sim 1/\sqrt{N}$ let us consider, e.g., a point (x_1,y_1) and ask what is the minimum c_m of distances of the center of a link between (x_1,y_1) and any of the remaining $N-1$ points. It means that we have to find the minimum of

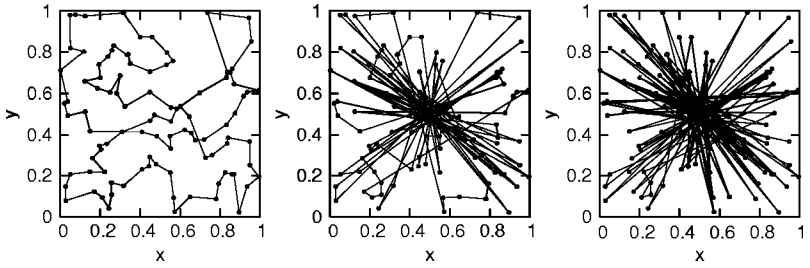

FIG. 2. Typical shapes of nearly minimal paths for (from left to right) $r=0.0$, 2.0, and 2.5. Calculations were made for $N=100$ and $c=10^{-6}$.

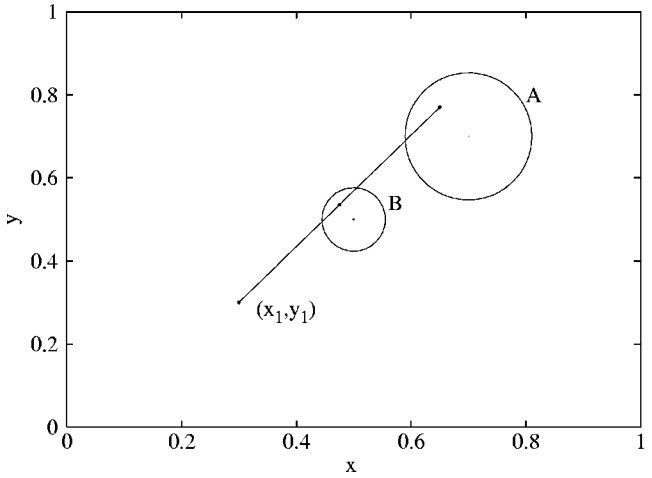

FIG. 4. A link with a point inside circle A has its center inside circle B with a twice smaller radius.

$\frac{1}{2}\sqrt{(x_1+x_i-1)^2+(y_1+y_i-1)^2}$ where $i=2,3,\ldots,N$. Let us notice that in a (two-dimensional) unit square $N-1$ points set the characteristic distance between points as $1/\sqrt{N}$. Thus one can expect that in a circle of radius $1/\sqrt{N}$ that is opposite [with respect to $(1/2,1/2)$] to the point (x_1,y_1) there is approximately one of these $N-1$ points (see Fig. 4). A link with such a point has a center that is inside a circle around $(1/2,1/2)$ and has a twice smaller radius (but still it is of the order of $1/\sqrt{N}$). Consequently, the smallest distance c_m of a center of link to the point $(1/2,1/2)$ should scale as $1/\sqrt{N}$ and this argument is supported by simple numerical calculations that we present in Fig. 5. We expect that in the minimal path $\overline{c}$ also scales as c_m i.e., as $1/\sqrt{N}$, and thus the relation $C\sim\sqrt{N}$ follows. Let us notice that scaling of L and C in the C phase is analogous to the scaling in the L phase but with the roles of L and C interchanged. We do not know whether this relation is accidental or indicates a deeper relation (e.g., certain duality) between these two phases.

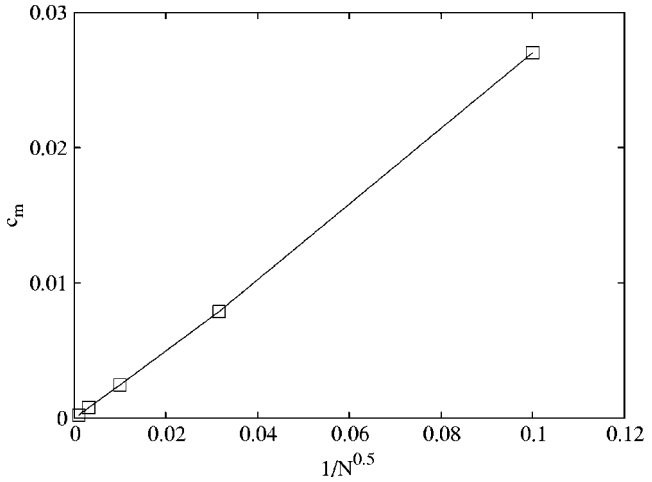

FIG. 5. The minimal distance c_m from the center of a link to $(1/2,1/2)$ as a function of $1/\sqrt{N}$. Links are made between a randomly chosen point (x_1,y_1) and $N-1$ other randomly chosen points. Presented results are averages over 100 choices of (x_1,y_1).

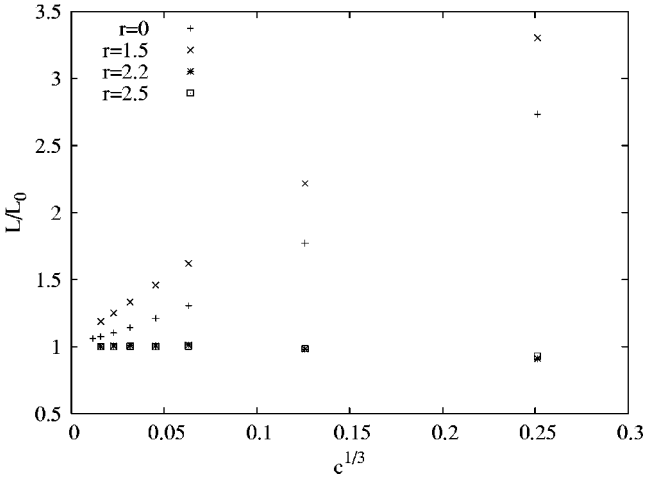

FIG. 6. The average normalized length L/L_0 as a function of cooling rate c, where L_0 is the extrapolated value of L at the zero cooling rate ($N=100$).

As might be expected, the scaling of L and C at the transition point $r=2.0$ is different from that in each of the phases. Figure 3 shows that in this case both quantities increase linearly with N.

Finally, we compare the efficiency of the simulated annealing in each phase. Our data (Fig. 6) show that in the C phase SA is much more efficient and already with a relatively fast cooling a (nearly) minimal path is found. In the L phase corrections due to the nonzero cooling rate are much more important (our simulations show that these corrections in the L phase decay approximately as $c^{1/3}$). For $r=0$ our data extrapolated to the limit of zero cooling rate give for $N=100$ the average length of a minimal path as $L_0=7.8$, which is in good agreement with other results quoted in the literature [15]. For comparison, we show also the results obtained using the LIN-2-OPT algorithm [11]. This time simula-

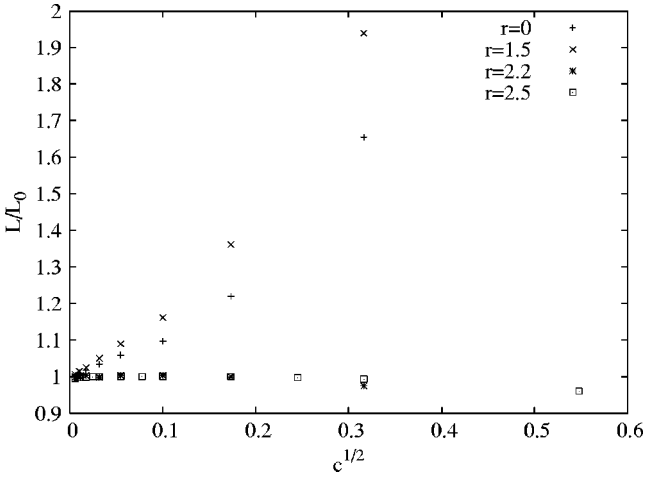

FIG. 7. The average normalized length L/L_0 as a function of exponential cooling rate c, where L_0 is the extrapolated value of L at the zero cooling rate ($N=200$). Simulations were made using LIN-2-OPT moves. Let us notice that L converges to L_0 linearly in $c^{1/2}$. For the algorithm with exchange moves (Fig. 6) convergence is slower and linear in $c^{1/3}$.

tion was made for $N=200$ and an exponential cooling schedule was used $T(t)=T_0(1-c)^t$, whose effectiveness was already demonstrated [16]. Results of these simulations, shown in Fig. 7, confirm the change of efficiency of SA at the transition point of our model.

The main difficulty with finding a minimal path in the TSP is due to the complexity of the cost function and more specifically due to its many local minima. Some of these minima, being quite far from the global minimum, might be at the same time quite deep and the searching algorithm might get stuck in one of them. The landscape of the cost function in our problem is also very complex and has many minima. However, the substantial increase in efficiency of SA in the *C* phase indicates a certain change in this landscape. One possibility is that in the *C* phase local minima are located mainly in the vicinity of the global minimum. As a result, a solution found using SA, which is almost always only a nearly optimal path, is a good approximation of the optimal solution. In our opinion, such a transition for a model that most likely is NP-complete for any r is unusual and it would be desirable to understand it better. Another type of transition in the TSP appears in the time-dependent version of this problem [17].

In conclusion, we studied a version of the traveling salesman problem where the cost function includes both the length of the path as well as its distance from the center. This problem, depending on the control parameter, turns out to have two phases with different kinds of solutions. As indicated by a drastic change in the efficiency of the simulated annealing method, a phase transition in this problem should be accompanied by important changes in the complex landscape of the cost function. Further studies would be needed to clarify more detailed properties of this problem.

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