Travelling Salesman Problem with a Center

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We study a travelling 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 behaviour of $L$ and $C$, in efficiency of SA, and in the shape of minimal paths.

In the travelling 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 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 TSP is known to be NP-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 TSP for quite a large values of $N$, these algorithms are usually dedicated only to this particular task. Consequently, they are not suitable for more general versions of 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 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 formulae $^6$. 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 of the transition point $^7$. A related phase transition was found in a certain version of TSP where distances between points are randomly drawn integer numbers $\{1,2,..,k\}$. In such a case the time needed to find the minimal solution using branch-and-bound algorithm dramatically increases when $r$ 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 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 to a 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, minimal paths in these two phases have 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 with 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 coordinates of $i$-th point as $(x_i, y_i)$, we have

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

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

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 reason. Another application might be a “just-in-time vehicle routing problem”, in which truck drivers might be called to the center depot immediately 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.
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 positions of two points. Such a move is accepted with a probability $\min(1,e^{-\delta E/T})$ where $\delta E$ is the energy difference between a trial and 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 a unit of time is defined as an 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 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. Such moves are known to be more effective than exchanges of two points. Both methods, however, yields essentially the same behaviour of our model with respect to e.g., location of the transition point or $N$-dependence of $L$ and $C$. Unless specified otherwise, described below results 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 the maximum of the variance of $L$ and the abrupt change of $C$. These results suggest that a certain phase transition takes place around $r = 2$.

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 $r \sim 2.0$ 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 $(r = 0)$.

As for the second relation $(C \sim N)$, there is a simple argument that justifies it. Indeed, since in the $L$-phase a minimal path is relatively uniformly distributed in the unit square one can assume that central points of links are almost uniformly distributed. It means that there is a positive (and $N$-independent in the limit $N \to \infty$) average distance of a central point from $(1/2,1/2)$ and then $C \sim N$ easily follows.

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 a typical distance $\bar{c}$ of a 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 a minimum $c_m$ of distances of a center of a link between $(x_1,y_1)$ and any of the remaining $N - 1$ points. It means that we have to find a minimum of $\frac{1}{2}\sqrt{(x_1 + x_i - 1)^2 + (y_1 + y_i - 1)^2}$ where $i = 2,3,\ldots,N$. 

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

\[ \begin{align*}
\text{FIG. 2: Typical shapes of nearly minimal paths for (from left to right) } r = 0.0, 2.0 \text{ and } 2.5. \text{ Calculations were made for } N = 100 \text{ and } c = 10^{-6}.
\end{align*} \]
Let us notice that in a (two-dimensional) unit square \(N - 1\) points set a characteristic distance between points as \(1/\sqrt{N}\). Thus one can expect that in a circle of a 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. 4. We expect that in the minimal path \(\hat{c}\) 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 role 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.

As it might be expected, the scaling of \(L\) and \(C\) at the transition point \(r = 2.0\) is different than 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. 5) 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 a 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 simulations were made for \(N = 200\) and the exponential cooling schedule was used \(T(t) = T_0(1 - c)^t\), whose effectiveness was already demonstrated [10]. Results of these simulations, shown in Fig. 5 confirm the change of efficiency of SA at the transition point of our model.

A main difficulty with finding a minimal path in 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, a 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 new and it would be desirable to have its better understanding. Another type of a transition in TSP appears in the time-dependent version of this problem [17].

In conclusion, we studied a version of the travelling salesman problem where the cost function includes both the length of a path as well as its distance from a 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 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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