Statistical Physics of the Travelling Salesman Problem

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Abstract

If one places $N$ cities randomly on a continuum in an unit area, extensive numerical results and their analysis (scaling, etc.) suggest that the best optimized travel distance per city becomes $l_E \simeq 0.72/\sqrt{N}$ for the Euclidean metric, and $l_M \simeq 0.92/\sqrt{N}$ for the Manhattan metric. The analytic bounds, we discuss here, give $0.5 < l_E \sqrt{N} < 0.92$ and $0.64 < l_M \sqrt{N} < 1.17$. When the cities are randomly placed on a lattice with concentration $p$, we find (with $N = p$ for unit area of the country) $l_E \sqrt{p}$ and $l_M \sqrt{p}$ vary monotonically with $p$: $l_E \sqrt{p} = l_M \sqrt{p} = 1$ for $p = 1$, and $l_E \sqrt{p} \simeq 0.72$ and $l_M \sqrt{p} \simeq 0.92$ as $p \to 0$. The problem is trivial for $p = 1$ but it reduces to the continuum TSP for $p \to 0$. We did not get any irregular behaviour at any intermediate point, e.g., the percolation point. The crossover from the triviality to the NP-hard problem seems to occur at $p < 1$.

1. Introduction

In everyday life we face several complex problems, classified as combinatorial optimization problems, the solutions of which are of great practical importance. Research in this area tries to find different efficient techniques for finding the extremum (maximum or minimum) values of a function of many different independent variables [1-3].

The travelling salesman problem (TSP) is a simple example of a combinatorial optimization problem and perhaps the most famous one. Given a certain set of cities and the intercity distance metric, a travelling salesman must find the shortest tour in which he visits all the cities and comes back to his starting point. It is a non-deterministic polynomial complete (NP-complete) problem. NP problems are those for which a potential solution can be checked efficiently for correctness, but finding such a solution appears to take time which scales exponentially with the size $N$ in the worst case. The completeness property of NP-complete problems means that if it is possible to find a deterministic algorithm that solves one NP-complete problem in polynomial time, then the other NP-complete problems could also be solved in polynomial time.

In the TSP, the most naive algorithm for finding the optimal tour would have to consider all the $(N - 1)!/2$ possible tours for $N$ number of cities and check for the shortest of them. Working this way, the fastest computer available today would require more time than the current age of the universe to solve a case with about 30 cities. The typical-case behaviour is difficult to characterize for the the TSP though it is believed to require exponential time to solve in the worst case. For this reason the TSP serves as a prototype problem for the study of the combinatorial optimization problems in general.

In the normal TSP, we have $N$ number of cities distributed in some continuum space and we determine the average optimal travel distance per city $\bar{l}_E$ in the Euclidean metric (with $\Delta r_E = \sqrt{\Delta x^2 + \Delta y^2}$), or $\bar{l}_M$ in the Manhattan metric (with $\Delta r_M = |\Delta x| + |\Delta y|$). Since the average distance per city (for fixed area) scales with the number of cities $N$ as $1/\sqrt{N}$, we find that the normalized travel distance per city $\Omega_E = \bar{l}_E\sqrt{N}$ or $\Omega_M = \bar{l}_M\sqrt{N}$ become the optimized constants and their values depend on the method used to optimize the travel
distance. In section 2, we discuss some algorithms used to determine the optimal tour and find the values of the constants $\Omega_E$ and $\Omega_M$ for the optimized travel. In section 3, we present an analytic method to estimate the upper and lower bounds of $\Omega_E$ and $\Omega_M$.

In the lattice version of the TSP, the cities are represented by randomly occupied lattice sites of a two-dimensional square lattice; the fractional number of occupied sites being $p$ (lattice occupation concentration). In this case the average optimal travel distance in the Euclidean metric $\bar{l}_E$, and in the Manhattan metric $\bar{l}_M$, vary with the lattice concentration $p$. Then the normalised travel distance per city are defined as $\Omega_E = \bar{l}_E \sqrt{p}$ and $\Omega_M = \bar{l}_M \sqrt{p}$. In section 4, we study the variation of $\Omega_E$ and $\Omega_M$, and the ratio $\Omega_M/\Omega_E$ with $p$. Finally, we draw conclusions in section 5.

2. Some heuristic algorithms

The most naive method to obtain an approximate solution of travelling salesman problem is the “greedy” heuristic algorithm [1, 2]. Suppose we have a random arrangement of $N$ cities in a square (country) of fixed area (taken to be unity). Let us think of any tour to start-with and then make a local exchange of a pair of cities in the tour. We compute the new tour length and if it is lower than the previous one, then the greedy algorithm accepts the new tour as the starting point for further such modifications. The “Lin- Kernighan” algorithm [4, 5] considers local exchange between three or more cities.

The essential drawback of such local search algorithms is the obvious one of getting stuck at a local minimum, where any local rearrangement in the tour does not improve the optimized tour length. The “simulated annealing method” [2, 6] is an ingenious method in analogy with the thermodynamic way of avoiding such local minima in free energy (glass formations) and achieving the global minimum of a many-body system by slow cooling or annealing. The rapid quenching of the system leads to the trapping of the system in a local minimum (or glass) state. The system cannot get out of it, since the Boltzmann probability to get out of the minimum drops to zero, as the temperature becomes zero due to quenching. This is similar to the greedy or other local search algorithms. In the annealing, the system
is slowly cooled so that as the system falls in a local trap, the finite Boltzmann probability
\( \sim \exp(E' - E)/kT \), for trap energy \( E \) and barrier height \( E' \) allows the system to get out
of the trap, maintaining a general flow to lower energy states as temperature decreases.
Eventually the system anneals to the ground state at the lowest temperature.

In the TSP case, one takes the total tour length \( L = NL \) as the energy \( E \) and one
introduces a fictitious temperature \( T \). Initially one takes \( T \) very high such that the average
total tour length \( \bar{L} \) is much higher than the global minimum. The tours are then modified
locally and the modified tours are accepted with probability \( \sim \exp(\Delta L/kT) \) where \( \Delta L \) is
the change in the tour length. In greedy algorithm the probability is unity for negative \( \Delta L \)
and it is zero for positive \( \Delta L \) cases. Here, probability is non-vanishing even for \( \Delta L \) positive
as long as the temperature is nonzero!

Simulated annealing and numerous heuristic generalizations of the local search algorithm
optimize very effectively on small scales involving a small number of variables, but fail for the
larger scales that require the modification of many variables simultaneously. To deal with
the large scales, “genetic algorithms” [7] use a “crossing” procedure which takes two good
configurations — “parents”, from a population and finds sub-paths that are common to the
parents. It generates a “child” by reconnecting those sub-paths, either randomly or by using
large parts of its parents. A population of configurations is evolved from one generation to
the next using these crossings followed by a selection of the best children. However, this
approach supposedly does not work well in practice since it is extremely difficult to produce
two parents and cross them to make a child as good as them. This is a major drawback of
the genetic algorithms and is responsible for their limited use.

So far, careful analysis of the numerical results obtained indicates that \( \Omega_E \approx 0.72 \) [8] for
TSP on continuum.

3. Some analytical results for the bounds for \( \Omega \)

Although the TSP problem is a multivariable optimization problem (real number of variables
\( \sim N! \) in an \( N \) city problem), we now look for an approximate analytical solution (upper
bound) by expressing the travel distance as a function of a single variable and optimizing the distance with respect to that variable [9]. As is obvious, the problem is trivial in one dimensional case where any directed tour will solve it. In two dimensions, one can again reduce it (approximately) to an one dimensional problem, where the square (country) is divided into strips of width $W$ and within each strip, the salesman visits the cities in a directed way. The total travel distance is then optimized with respect to $W$.

Let the strip width be $W$ and the probability density of cities be $p$ (= $N$ for unit area). We have a city at $(0, y_1)$ [See Fig. 1]. The probability that the next city is between distances $x$ and $x + \Delta x$, is $pW\Delta x$. The probability that there is no city in the distance $x = n\Delta x$, is $(1 - pW\Delta x)^n \sim e^{-(pWx)}$. The probability that there is a city between $y$ and $y + \Delta y$, is $\Delta y/W$. Hence the probability that there is no other city within distance $y$ is $(1 - y/W)$.

The average distance between any two consecutive cities is therefore

$$\bar{I}_E = 2 \int_{x=0}^{\infty} \int_{y=0}^{W} \sqrt{x^2 + y^2} \ pW dx \ e^{-pWx} \frac{dy}{W^2} (1 - \frac{y}{W}) .$$

(1)

The factor 2 arises to take care of the fact that $y$ can be both positive and negative. We make the substitutions: $u = pWx$ and $v = y/W$, so that

$$\bar{I}_E = 2 \int_{u=0}^{\infty} \int_{v=0}^{1} \frac{1}{pW} \sqrt{u^2 + p^2W^4v^2} \ e^{-u} (1 - v) du dv .$$

We introduce two dimensionless quantities $\Omega_E = \sqrt{p} \ \bar{I}_E$ and $\bar{W} = \sqrt{p} \ W$, so that

$$\Omega_E = \frac{2}{\bar{W}} \int_{u=0}^{\infty} \int_{v=0}^{1} \sqrt{u^2 + \bar{W}^4v^2} \ e^{-u} (1 - v) du dv .$$

(2)

Using the method of Monte Carlo integration to evaluate the above integral, we get the minimum $\Omega_E \sim 0.92$ at normalized strip width $\bar{W} \sim 1.73$ [See Fig. 2].

In the Manhattan metric the average distance between any two consecutive cities is

$$\bar{I}_M = 2 \int_{x=0}^{\infty} \int_{y=0}^{W} \ (x + y) pW dxe^{-pWx} \frac{dy}{W^2} (1 - \frac{y}{W}) .$$

(3)

As before we introduce $u = pWx$ and $v = y/W$, so that

$$\bar{I}_M = 2 \int_{u=0}^{\infty} \int_{v=0}^{1} \frac{1}{pW} (u + pW^2v)e^{-u} (1 - v) du dv .$$

4
and then introduce the dimensionless quantities $\Omega_M = \sqrt{p} \bar{M}$ and $\bar{W} = \sqrt{p} W$, so that

$$\Omega_M = \frac{2}{\bar{W}} \int_{u=0}^{\infty} \int_{v=0}^{1} (u + \bar{W}^2 v)e^{-u(1-v)}dudv .$$

Using the method of Monte Carlo integration, we get the minimum $\Omega_M \sim 1.15$ at the normalized strip width $\bar{W} \sim 1.73$ [See Fig. 3].

Note that the relation

$$\Omega_M \simeq \frac{4}{\pi} \Omega_E$$

can be explained as follows. Let

$$x = l_E \sin \theta \quad \text{and} \quad y = l_E \cos \theta .$$

Then,

$$l_M = x + y = l_E (\cos \theta + \sin \theta) .$$

Since $\langle x \rangle = \langle y \rangle$, we have

$$\bar{l}_M = 2\bar{l}_E \langle \cos \theta \rangle .$$

We have now

$$\langle \cos \theta \rangle = \frac{2}{\pi} \int_{0}^{\pi/2} \cos \theta d\theta = \frac{2}{\pi} [\sin \theta]_{0}^{\pi/2} = \frac{2}{\pi} .$$

Hence

$$\bar{l}_M = \frac{4}{\pi} \bar{l}_E , \quad \text{or} \quad \Omega_M = \frac{4}{\pi} \Omega_E .$$

Let us now estimate the lower bound of the minimum travel distance per city. Let the distance between any two cities be denoted by $l$. Then the probability that there is a city between $l$ and $l+dl \sim (p-1)2\pi l dl \sim 2p\pi l dl$. Now, the probability that there is no other city in the distance $l \sim (1 - \pi l^2)^{p-2} \sim e^{-\pi l^2} \sim e^{-\pi l^2}$. Therefore, $P(l)dl = (2p\pi l)e^{-\pi l^2} dl$. Note that $\int P(l)dl = 1$. Hence the average distance is

$$\bar{l}_E = \int_{0}^{\infty} lP(l)dl = 2p\pi \int_{0}^{\infty} l^2 e^{-\pi l^2} dl = \frac{1}{2} \frac{1}{\sqrt{p}} .$$

Therefore, the lower bound for $\Omega_E = 1/2$ . The lower bound for $\Omega_M$ can then easily be estimated to be $2/\pi$ in a similar manner.
4. The TSP on randomly diluted lattices

The lattice version of the TSP was first studied by Chakrabarti [10]. In the lattice version
of the TSP, the cities are represented by randomly occupied lattice sites of a two-
dimensional square lattice \((L \times L)\), the fractional number of sites occupied being \(p\) (lattice concentration)
[11-13]. In this case, the average optimal travel distance in the Euclidean metric \(\bar{l}_E\), and in
the Manhattan metric \(\bar{l}_M\), vary with the lattice concentration \(p\). We intend to study in this
case the variation of the normalised travel distance per city, \(\Omega_E = \bar{l}_E \sqrt{p}\) and \(\Omega_M = \bar{l}_M \sqrt{p}\),
with the lattice occupation (city) concentration \(p\).

We generate the randomly diluted lattice configuration following the standard Monte
Carlo procedure for 64(= \(N\)) randomly positioned (on the lattice) cities. We vary the lattice
size from \((8 \times 8)\) to \((48 \times 48)\) so that the lattice concentration \(p\) varies from 1.000 to 0.028.
For each such lattice configuration, the exact optimum tour [See Fig. 4] is obtained with the
help of the GNU tsp.solve [14]. We then calculate \(l_E\) and \(l_M\). At each lattice concentration
\(p\), we take different lattice configurations and then obtain the averages, \(\bar{l}_E\) and \(\bar{l}_M\). We then
determine \(\Omega_E = \bar{l}_E \sqrt{p}\) and \(\Omega_M = \bar{l}_M \sqrt{p}\) and study the variation of \(\Omega_E\) and \(\Omega_M\), and of
the ratio \(\Omega_M/\Omega_E\) with \(p\). We find that \(\Omega_E\) has monotonic variation from 1 (for \(p = 1\)) to
a constant \(\sim 0.79\) (for \(p \to 0\)) and \(\Omega_M\) has monotonic variation from 1 (for \(p = 1\)) to the
constant 1.01 (for \(p \to 0\)) respectively. We believe, with bigger \(N\) the value of \(\Omega_E\) eventually
reduces to about 0.72 as in continuum TSP. Results for higher values of \(N\) (\(\approx 100\)) [15] indeed
suggest the same. The ratio \(\Omega_M/\Omega_E\) changes from 1 to 1.26 \((\approx 4/\pi)\), as \(p\) varies from 1 to 0
[See Fig. 5]. We note that the TSP on randomly diluted lattice is certainly a trivial problem
when \(p = 1\) (lattice limit) as it reduces to the one-dimensional TSP (the connections in
the optimal tour are between the nearest neighbours along the lattice; Hamiltonian walks).
However, it is certainly hard at the \(p \to 0\) (continuum) limit. It is clear that the problem
crosses from triviality (for \(p = 1\)) to the NP-hard problem (for \(p \to 0\)) at a certain value of
\(p\). It seems the transition occurs at \(p < 1\). This requires further investigation.
5. Conclusions

If one places $N$ cities randomly on a continuum in an unit area, the best numerical results and their analysis (scaling, etc.) suggest that the best optimized travel distance per city becomes $l_E \simeq 0.72/\sqrt{N}$ for the Euclidean metric and $l_M \simeq 0.92/\sqrt{N}$ for the Manhattan metric. The analytic bounds we discussed in section 3, gives $\Omega_E(=l_E\sqrt{N}) < 0.92$ and $\Omega_M(=l_M\sqrt{N}) < 1.17$. When the cities are randomly placed on a lattice with concentration $p$, as discussed in section 4, we find (with $N = p$ for unit area of the country) that $\Omega_E(p)$ and $\Omega_M(p)$ are monotonically varying with $p$. The problem is trivial for $p = 1$ where $\Omega_E(p) = \Omega_M(p) = 1$ and it certainly reduces to the continuum TSP discussed before for $p \to 0$ ($\Omega_E \simeq 0.72$ and $\Omega_M \simeq 0.92$; although we observed higher values, viz., $\Omega_E \simeq 0.79$ and $\Omega_M \simeq 1.01$, since $N$ is not sufficiently large). The variations of $\Omega$ with $p$ are found to be monotonic without any irregular behaviour at any intermediate point like the percolation point, etc. The crossover from the triviality to the NP-hard problem seems to occur at $p < 1$. However, this requires further investigation.

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References

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Figure captions

**Fig. 1**: Calculating the average distance between two nearest neighbours along a strip of width $W$.

**Fig. 2**: Plot of $l_E \sqrt{p}$ against $W \sqrt{p}$ from eqn. (2).

**Fig. 3**: Plot of $l_M \sqrt{p}$ against $W \sqrt{p}$ from eqn. (4).

**Fig. 4**: A typical optimized tour for TSP on dilute lattice in the Euclidean metric for $N = 64$ cities.

**Fig. 5**: Plot of $\Omega_E$, $\Omega_M$ and $\Omega_M/\Omega_E$ against $p$ for TSP on dilute lattice, obtained using the optimization programs (exact) for $N = 64$ cities (fixed). The error bars are due to configuration to configuration variations.
Fig. 5