The Landscape of the Traveling Salesman Problem

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Abstract

The landscapes of Traveling Salesman Problems are investigated by random walk techniques. The autocorrelation functions for different metrics on the space of tours are calculated. The landscape turns out to be AR(1) for symmetric TSPs. For asymmetric problems there can be a random contribution superimposed on an AR(1) behaviour.

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1. Introduction

The *traveling salesman problem* (TSP) [1] is the most prominent classical example of an $\mathcal{NP}$-complete [2] combinatorial optimization problem. Given a distribution of cities the task is to find the shortest tour visiting each city once and returning to the starting point with prescribed costs η_{ij} for traveling from i to j.

The symmetric problem $\eta_{ij} = \eta_{ji}$ has applications in X-ray crystallography [3], electronics [4] and the study of protein conformations [5]. For these problems the Lin-Kernighan [6] heuristic has proven to be highly successful. The asymmetric case [7] is much more problematic for heuristic algorithms. Asymmetric costs arise in scheduling chemical processes or from pattern allocation problems in glas industry.

Let $\mathcal{T}$ be the set of all possible tours t. We impose a topology on this set by defining the nearest neighbours for each tour. A transition from one tour, t_1, to another one, t_2, is allowed if t_1 and t_2 are nearest neighbours of each other. On the other hand, one may also define a set of moves—operations which modify a given tour in a certain way. Then the set of moves defines the neighbourhoods. If nearest neighbours are connected by edges the set $\mathcal{T}$ becomes a graph. By $\ell(t)$ we denote the length of a tour t. The map

$$\ell : \quad \mathcal{T} \to \mathbb{R}, \quad t \mapsto \ell(t) \tag{1}$$

is known as the value landscape of the TSP.

The term "landscape" originated in theoretical biology and refers in general to a map from some combinatorial object (graph) into the real numbers [8].

Although few mathematical problems have attracted as much attention as the traveling salesman problem, very little is known on the structure and statistical properties of its landscape. Recently Weinberger [9,10] has shown that unbiased random walks are an appropriate method for investigating landscape structures. The autocorrelation function of the "time series" obtained by sampling the values $\ell(t_i)$ along the walk $\{t_i\}$ turns out to be the crucial quantity:

$$\rho(s) = \frac{1}{\mathrm{var}(\ell)} \cdot \lim_{N\to\infty} \frac{1}{N} \sum_{i=1}^{N} (\ell(t_i) - \langle\ell\rangle)(\ell(t_{i+s}) - \langle\ell\rangle) \tag{2}$$

In the most simple case $\rho(s)$ is just a decaying exponential; such a landscape is called an AR(1) landscape, since the values along the random walk form an Ornstein-Uhlenbeck process, or AR(1)-process, in the limit of large landscapes:

$$\ell(t_k) = \langle\ell\rangle + \rho \cdot (\ell(t_{k-1}) - \langle\ell\rangle) + \Delta \tag{3}$$

where Δ denotes white noise with some variance σ^2.

Two different types of averages occur in the analysis of random TSPs: for each instance of the problem one averages over configurations (tours) and there is the ensemble average over different instances. Fortunately the autocorrelation function a self-averaging quantity, thus for large systems one can use the configuration average as an estimate for the ensemble average which is, of course, the desired quantity. For the TSP, some 10 cities is large enough for the two averges to coincide within statistical errors.

We remark that there is a close connection between the notion of fractal landscapes and the autocorrelation function [11] of a landscape: Sorkin [12,13] used unbiased walks on value landscapes to define *fractalness* by

$$\langle(\ell(t_i) - \ell(t_j))^2\rangle \propto d^{2H}(t_i, t_j) \tag{4}$$

where $d(t_i, t_j)$ denotes the distance between the tours t_i and t_j. $H > 0$ is related to the fractal dimension; in his examples he always finds $H = 1/2$. On the other hand for t_i, t_j fulfilling $d(t_i, t_j) = d$ one has [14]

$$\langle(\ell(t_i) - \ell(t_j))^2\rangle = \mathrm{var}(\ell)(1 - \rho(d)) \tag{5}$$

2. Configuration Space

The natural support of an n-city TSP is the group S_n of all permutations of the n cities. By symmetry we may choose the start of the tour always in 1 thus restricting the problem to the permutations of the remaining $n-1$ cities.

The two most common sets of generators are T, the set of transpositions and J, the set of inversions which are the moves most frequently used in heuristic optimization algorithms. J corresponds to the set of *2-opt* moves [6]. Transposition means exchange of two cities. Inversions are more involved: the inversion $[r,s]$ exchange not only the cities r and s but also reverts the path from r to s. The sets of k-*opt* moves ($k < n-2$) are obviously also sets of generators of the symmetric group S_n.

For T it is well known that the maximal distance of two points in configuration space is $\max d_{S_n;T}(x,y) = n-1$ [12]. For inversions a corresponding result does not seem to be known. We have, however, $\max d_{S_n;J}(x,y) \leq n-1$. This may be seen as follows: Let x be an arbitrary permutation. Let a_1 be the image of 1. Then the inversion $[1,a_1]$ yields a permutation of the form $(1,x')$, where x' now denotes a permutation of the numbers 2 through n. Iterating this procedure yields $(1,2,\ldots k,x^{(k)})$ after (at most) k steps (with $x^{(k)}$ denoting a permutation of the numbers $k+1$ through n). Thus one obtains the identity after at most $n-1$ steps since $x^{(n-1)} = (n)$. The isometry $d(xy,y) = d(x,e)$ shows that $n-1$ steps are sufficient to transform any two tours into each other. $n/2$ seems to be a lower bound.

3. AR(1)-Landscapes

A time series which is *isotropic*, *Gaussian* and *Markovian* inevitably [15] leads to an autocorrelation function of the form

$$\rho(s) = \rho(1)^s = \exp(-s/\lambda). \tag{6}$$

with λ being the correlation length. A time series may be obtained from a landscape by means of unbiased random walks. A landscape fulfilling equ.(6) with s being the distance between two points is thus called AR(1)-*landscape* [9]. Examples are the Nk-model [16] and the Sherrington-Kirkpatrick spin-glass [17]. For both, the configuration space is the Boolean hypercube $\mathbf{B}^n$ with n denoting the number of sites on the macromolecule and the number of spins, respectively.

Many statistical properties of AR(1) landscapes are then uniquely defined by the mean μ and the variance σ^2 of the distribution of values, by the correlation length λ and the support (configuration space). Specific results for the Nk-model and spin glasses have been obtained by Weinberger [9,10,18].

Number of Local Optima. The distribution of values of the neighbours of a given point x_0 with value E_0 is also Gaussian but with mean $\mu_N = \mu + \rho(E_0 - \mu)$ and variance $\sigma_N^2 = (1-\rho^2)\sigma^2$. Thus Prob$\{E \leq E_0\}$ under the assumption of random sampling is given by the integral of a Gaussian with mean μ_N and variance σ_N^2 from $-\infty$ to E_0 [19]. With the abbreviations

$$\begin{aligned} x &= \frac{\xi - [\mu + \rho(E_0 - \mu)]}{\sqrt{2(1-\rho^2)} \cdot \sigma} \\ c_0 &= \frac{1}{\sqrt{2} \cdot \sigma} \cdot \sqrt{\frac{1-\rho}{1+\rho}} \end{aligned} \tag{7}$$

this Gaussian integral becomes

$$\text{Prob}\{E \leq E_0\} = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{c_0(E_0-\mu)} e^{-x^2} dx \quad =: \quad \Phi\big(c_0(E_0 - \mu)\big) \tag{8}$$

We now make the assumption, that equ.(8) holds for all neighbours *independently*. This seems to be a reasonable approximation for not too highly correlated landscapes. The probability for finding a local optimum with value E_0 is then given by

$$\text{Prob}\left\{loc.opt.|E_0\right\} = \text{Prob}\left\{E \leq E_0\right\}^N \tag{9}$$

where $N = N(n)$ denotes the number of neighbours of a given point in configuration space. Note that the crucial parameter is not the size of the system n but the size of the neighbourhood N. From

$$\text{Prob}\left\{loc.opt.\right\} = \int_{-\infty}^{+\infty} \text{Prob}\left\{loc.opt.|E_0\right\} \cdot \text{Prob}\{E_0\} dE_0 \tag{10}$$

we obtain with $\text{Prob}\{E_0\} = \exp\bigl(-\frac{1}{2}(\frac{E_0-\mu}{\sigma})^2\bigr)/\sqrt{2\pi}\sigma$ and a change in variables

$$\text{Prob}\left\{loc.opt.\right\} = \Psi_N(\rho) = \sqrt{\frac{1+\rho}{\pi(1-\rho)}} \int_{-\infty}^{+\infty} e^{-\frac{1+\rho}{1-\rho}y^2} \cdot \Phi^N(y) \cdot dy \tag{11}$$

Note that for $\rho = 0$ this expression reduces to

$$\begin{aligned} \Psi_N(0) &= \int_{-\infty}^{+\infty} \frac{1}{\sqrt{\pi}} e^{-y^2} \cdot \Phi^N(y) dy = \int_{-\infty}^{+\infty} \Phi'(y)\Phi^N(y) dy = \\ &= \frac{1}{N+1} \cdot \Phi^{N+1}(y) \Big|_{-\infty}^{+\infty} = \frac{1}{N+1} \end{aligned} \tag{12}$$

This is a well known result for uncorrelated landscapes [16].

For $\rho \to 1$ the coefficient of $\frac{1+\rho}{1-\rho}$ tends to ∞ and thus the Gaussian function approaches a Dirac δ-distribution. We have thus

$$\lim_{\rho\to 1} \Psi_N(\rho) = \Phi^N(0) = 1/2^N. \tag{13}$$

For a totally correlated landscape we would expect to find a single optimum (i.e. $\Psi_N(0) = 1/n!$), thus equ.(11) is likely to under-estimate the number of local optima in the TSP since for all metrics considered in this contribution we have $N = \mathcal{O}(n^2)$ or even higher powers and $2^{-n^2} n! \to 0$ for large n. We conclude that equ.(11) gives reasonable estimates only for $\rho \ll 1$, i.e. a correlation length much smaller than the diameter of the landscape.

We emphasize that the above estimates depend heavily on the assumption of random sampling. Different distributions of local optima may be obtained from adaptive walks, gradient walks or as suboptimal solutions of heuristic optimization algorithms.

4. Symmetric TSPs

The distribution of the tour lengths is (nearly) Gaussian. This fact is not very surprising. We may consider the length of a tour as the sum of n random variables (the distances between two subsequent cities) drawn from some distribution with mean η and variance s^2. For the distribution of tour lengths we expect, then, a Gaussian with

$$\text{mean} \quad \ell = n \cdot \eta \qquad \text{and variance} \quad \sigma^2 = n \cdot s^2 \tag{14}$$

due to the central limit theorem. This has been checked by numerical investigation of TSPs based on different types of inter-city distance matrices:

(i) Euclidean distance matrices for cities randomly distributed in a d-dimensional hypercube with $d = 2, \ldots, 9$

(ii) Randomly generated symmetric distance matrices.

(iii) The distance matrix of a 442-cities problem by Grötschel [20].

It turned out that the length-distribution of independent tours ($5n$ transpositions separated from each other) is in fact very well modelled by a Gaussian distribution, even for low values, e.g., $n = 20$. The higher moments μ_i converge to the expected values for a Gaussian distribution as n increases:

μ_3/σ^3 lies in $(-0.05, 0.00)$ for $n \geq 100$.

μ_4/σ^4 lies in $(2.98, 3.02)$ for $n \geq 50$.

μ_5/σ^5 is slightly negative (from -0.5 at $n = 50$ to -0.3 at $n = 300$).

μ_6/σ^6 is scattered around the theoretical value (15.0) with a width of approximately 0.3.

Result 1. Symmetric TSPs are AR(1) landscapes for both transposition and inversion metrics.

Because of the random choice of the distance matrix we expect the landscape to be isotropic. The time series obtained by the random walk can be expected to be Markovian since the walk itself is Markovian. From result 1 we conclude that for all three types of problems (i) through (iii) the time series becomes Gaussian, Markovian and isotropic for sufficiently large n and therefore the landscape should be AR(1).

In order to check this prediction numerically autocorrelation functions for symmetric TSPs with 20 to 600 cities, with both random distance matrix and distance matrices taken from Euclidean configurations with various dimensions $2 \leq d \leq 9$ have been investigated for both transposition and inversion metric. In order to improve statistics we calculated random walks with a length of 10^5 steps; the autocorrelation functions obtained for single walks have been averaged over at least 30 different initial positions in the same landscape. The precision of the estimate of $\rho(x)$ is better than 0.003 for $n \leq 100$. Calculations become more expensive for larger landscapes thus we had to be content with a precision of roughly 1 percent for $n = 600$. Within these statistical errors the data are consistent with a single decaying exponential (*cf.* Fig.2a).

Result 2. $\lambda_T/n \approx 1/4$ and $\lambda_J/n \approx 1/2$. The autocorrelation functions are independent of the Euclidean dimension of the space.

These facts may be understood as follows: Let t and t' be two tours with $d(t,t') = 1$ and length ℓ and ℓ' and let b denote the number of edges in which t and t' differ. A short calculation shows [14] that

$$\rho = \rho(1) = 1 - \frac{\langle(\ell - \ell')^2\rangle}{2\sigma^2} = 1 - \xi \tag{15}$$

On the other hand, for ξ sufficiently small we have

$$\lambda = \frac{-1}{\ln\rho} = \frac{-1}{\ln(1-\xi)} = \frac{1}{\xi} + \mathcal{O}(1) = \frac{2\sigma^2}{\langle(\ell-\ell')^2\rangle} + \mathcal{O}(1) \tag{16}$$

Let η_k and η'_k denote the length of edges of two tours t and t'. We expect then that

$$\begin{aligned}\langle(\ell-\ell')^2\rangle &= \langle\Big(\sum_{k=1}^{b}(\eta_k-\eta'_k)\Big)^2\rangle = \\ &= \langle\sum_{k=1}^{b}(\eta_k-\eta'_k)^2\rangle = b\cdot 2s^2\end{aligned} \tag{17}$$

where the sums in equ.(17) run over the edges η_k and η'_k, which are different in the two tours. Inserting this into equ.(16) we find finally

$$\lambda \quad = \quad \frac{n}{b} + \mathcal{O}(1) \tag{18}$$

For inversions exactly 2 edges are different in the symmetric case and thus $b_J = 2$, whereas for transpositions we have 4 different edges except for the exchange of adjacent cities; the expected value is

$$\langle b\rangle_T = \frac{n-3}{n-1}4 + \frac{2}{n-1}2 = 4(1-\frac{1}{n-1}) \to 4.$$

Thus we expect for large n:

$$\lambda_T/n \to 1/4 \qquad \text{and} \qquad \lambda_J/n \to 1/2 \tag{19}$$

Since the Euclidean dimension of the space enters η and s^2 only, we expect the results to be independent of d. We expect that the estimates for λ have to be corrected by terms of size $\mathcal{O}(1)$ for the fact that the n-th edge is not chosen randomly but uniquely determined.

The same arguments will hold of course also for k-*opt* moves [6] since the number of newly introduced edges is $b = k$ by construction of these moves. Thus we expect

$$\lim_{n\to\infty} \lambda_{\text{k-opt}}/n = 1/k. \tag{20}$$

No dependence of the correlation length from d or a difference between Euclidean and random distance matrices could be detected. The correlation lengths obtained by numerical investigation are given in Fig.1. A least square fit to the data presented in Fig.1 yields

$$\begin{aligned} \lambda_T(n) &= -0.583 + 0.246 \cdot n \\ \lambda_J(n) &= -1.661 + 0.494 \cdot n \end{aligned} \tag{21}$$

with correlations coefficients larger that 0.9995. The slopes are consistent with 1/4 and 1/2 respectively.

Grötschel's Euclidean 442 city problem agrees very well with the predictions from random TSPs. We obtained

$$\begin{aligned} \lambda_T(\text{Grötschel}) &\approx 105 \pm 5, \\ \lambda_J(\text{Grötschel}) &\approx 225 \pm 10, \end{aligned} \tag{22}$$

Concluding the above considerations we find that the autocorrelation functions of symmetric random TSPs are of the form

$$\rho(x) = \exp\left\{ -\left[b/n + \mathcal{O}(1/n^2) \right] \cdot x \right\} \tag{23}$$

This result is reminiscent of the Sherrington-Kirkpatrick spin-glass which is an AR(1) landscape with correlation length [11]

$$\rho_{SP} = 1 - 4/n + \mathcal{O}(1/n^2) \qquad \text{or} \qquad \lambda = n/4 + \mathcal{O}(1) \tag{24}$$

5. Asymmetric TSPs

In an asymmetric TSP the cost functions η_{ij} are no longer symmetric, i.e. it makes a difference whether one goes from i to j or the other way around.

Result 3. For transpositions there is no difference between symmetric and asymmetric problems concerning the correlation structure of the landscapes.

This is what one would expect in the light of the arguments in the previous section. The autocorrelation function depends on n and the number b of edges which are exchanged. Apart from 4 edges the whole tour is preserved in the transposition case in both symmetric and asymmetric problems.

This is no longer true for inversion-type metrics for the asymmetric problems. We have investigated three sets of generators:

- J Inversions $[r, s]$ with $r \neq s$ arbitrary. For simplicity city 1 is always rotated to position 1.
- J_+ Inversions $[r, s]$ with $1 < r < s \leq n$.
- J_- Inversions $[r, s]$ with $1 < s < r \leq n$ taken circularly and afterwards moving city 1 to position 1 again.

The set J is the union of J_+ and J_-; it is the full set of inversions. All three sets lead to essentially identical statistics for the symmetric TSP because all three correspond to the set of all inversions up to the reversal of the tour.

Result 4. For all three sets of inversions the autocorrelation function is found to be

$$\rho(s) = \frac{1}{2}\delta_{0s} + \frac{1}{2}\exp\{-4s/n\} + \mathcal{O}(\frac{1}{n}) \tag{25}$$

The full set of inversions is very close to this expression, even for as few as 20 cities.

The first inversion step on average inverts 50% of the tour. Since the lengths of the edges η_{ij} and η_{ji} may be regarded as independent and uncorrelated random variables we expect $\rho(1) = 1/2 - 2/n$ since half the tour is randomized and two entirely new edges are introduced. This argument also holds for the first few steps, where it is very unlikely to get an edge back by chance which has been changed in a previous step. Thus we expect

$$\rho(s) = \frac{1}{2} - \frac{2}{n} \cdot s \qquad s \ll n \tag{26}$$

On the other hand we expect—apart from the 50% randomization—an AR(1) type behaviour, since the non-randomized part behaves like a symmetric TSP. Interpreting equ.(26) thus as a linearized version and noting that all estimates are of order $\mathcal{O}(1)$ in the numerator, and the denominator scales as $\mathcal{O}(n)$, we arrive at equ.(25). Examples of autocorrelation functions are shown in fig.2. Analogous results are expected for k-*opt* moves with $2 < k \ll n$.

Result 5. For the set of inversions J_- we find that $\rho(n) > \rho(n-1)$ for even n (*cf.* Fig. 2d). The size of the oszillations, formally defined by

$$w(n) = \lim_{s\to\infty} \left| \frac{1}{2}[\rho(s) + \rho(s-2)] - \rho(s-1) \right| \tag{27}$$

scales as $\mathcal{O}(\frac{1}{n})$.

J_- is chosen such that the inversions occur predominantly in a particular region of the tour, always including the city 1. Thus a single step randomizes a large part of a tour around the city 1, whereas the next step re-establishes a considerable part of the initial tour which is not compensated by the newly randomized part. Thus we expect the autocorrelation function to be larger at an even than at an odd number of steps (Fig.2c). Since 1 is the only city which is in the inverted part in each step, we expect its effect to decrease as $\frac{1}{n}$ with increasing number n of cities (*cf.* Fig.3).

6. Local Optima

The previous chapters show that the landscapes of the TSPs are highly correlated. We do not expect thus, that the estimate equ.(11) yields reasonable results.

In a fully correlated landscape, i.e. correlation length $\lambda \approx \max d(x,y)$ one expects to find a single minimum. Let $\mathcal{N}(r)$ denote the number of vertices in a neighbourhood with radius r around an arbitrary vertex of the graph with $|G|$ vertices. We expect $\mathcal{O}(1)$ local optima in a patch with radius λ, i.e.

$$\Psi = \mathrm{Prob}\{loc.opt\} \approx \frac{\mathcal{N}(\lambda)}{|G|} \tag{28}$$

In case of the symmetric TSP with transposition metric we may estimate [12]

$$\mathcal{N}(r) \approx \sum_{j=0}^{r} \frac{(n^2/j)^2}{j!} \tag{29}$$

and we find finally

$$\Psi \approx \frac{1}{n!} \sum_{j=0}^{\lfloor (n+2)/4 \rfloor} \frac{(n^2/j)^2}{j!} \tag{30}$$

(the additive constant 2 in the upper limit of the sum has been introduced in order to assure correct rounding the correlation length $n/4$).

Result 6. The probability for finding a local minimum by random sampling in TSP landscapes with a transposition metric agrees quite well with the estimate in equ.(30)

Experimental data and the theoretical estimates Ψ as are shown in fig.4 as a function of the number of cities n. The corners in the estimate come from the fact that the diameter of the neighbourhoods assigned to each minimum increases by 1 each fourth step. Note that for $n = 3$ there is only a single tour, thus for $n = 3$ we have $\Psi = 3$.

Conclusions

The correlation structure of the landscape of the TSP can be understood in terms of simple parameters, namely: mean and variance of the entries in the distance matrix, the number of cities n, the average number b of edges exchanged by an allowed move and the type of the moves. Symmetric TSPs lead to AR(1) landscapes, i.e. to autocorrelation functions which are simple decaying exponentials. For asymmetric TSPs the situation is more involved: depending on the move set one obtains an AR(1) landscape, a superposition of an AR(1) and an uncorrelated landscape or even a landscape with a non-monotonic autocorrelation function.

A very plausible conjecture states that optimization with general algorithms becomes easier when the correlation of the landscape increases. This has originally been observed in computer experiments on evolutionary optimization on fitness landscapes based on the properties of RNA [21,22]. A heuristic explanation for this fact runs as follows: In highly correlated parts a hill climbing process essentially leads to the optimum of this part of the landscape. The smaller such a correlated patch is, the more of them have to be tried on a given support, thus optimization needs more steps if the correlation length is small.

This is supported by well known facts: Simulated Annealing on symmetric TSP works more efficiently using inversions (*2-opt* moves) than using transpositions. A direct comparison with the performance of *3-opt* moves is quite difficult, since the average distance of 2 randomly chosen points is smaller and the neighbourhoods are much larger for *3-opt* moves than for inversions or transpositions. Thus the fact reported in [23], that Simulated Annealing leads to better solutions with *3-opt* moves than with inversions, although the correlation length for the moves is with $\lambda_{\text{3-opt}} = n/3$ smaller than for the inversions $\lambda_J = n/2$, does not contradict the conjecture.

The same behaviour has been observed for the performance of a genetic algorithm based on the concept of quasi-species applied to TSPs [24]. We conclude that heuristic algorithms use predominantly *2-opt* moves for good reasons: It is impossible to make moves exchanging less than 2 edges and thus there is no realization of the configuration space with a correlation length larger than $n/2$. Equ.(25) explains furthermore why such algorithms do much better in symmetric than in asymmetric cases: In the asymmetric case the autocorrelation function is smaller than in a corresponding symmetric case by a factor of 2.

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