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The Centred Traveling Salesman at High Temperature

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A recently formulated statistical mechanics method is used to study the phase transition occurring in a generalisation of the Traveling Salesman Problem (TSP) known as the centred TSP. The method shows that the problem has clear signs of a crossover, but is only able to access (unscaled) finite temperatures above the transition point. The solution of the problem using this method displays a curious duality.

I. INTRODUCTION

In a recent paper, Lipowski and Lipowska [1] considered a generalisation of the geometric TSP by adding a new term to the cost function:

$$H = (1-\alpha)H_L + \alpha H_C \tag{1}$$

$$H_L = \sum_i V_L(\mathbf{r}_{i+1}, \mathbf{r}_i) = \sum_i |\mathbf{r}_{i+1} - \mathbf{r}_i| \tag{2}$$

$$H_C = \sum_i V_C(\mathbf{r}_{i+1}, \mathbf{r}_i) = \sum_i |\mathbf{r}_{i+1} + \mathbf{r}_i| \tag{3}$$

The familiar term H_L of the traditional TSP is the total path length of a cyclic tour defined by some permutation of the N city indices. The new term H_C is a measure of the distance of the tour from the centre of the geometry. Here we shall only consider the two-dimensional problem in a square domain, and shall take this centre, the origin of the city coordinates, $\mathbf{r}_i$, to be the centre of the square. The parameter α, $0 \leq \alpha \leq 1$, specifies the relative strength of each term.

The authors of [1] gave example motivations for the centred model, but the fact that they found a transition as α is varied and were able to identify it as a complexity transition provides sufficient interest. Specifically, they used simulated annealing techniques to numerically study zero temperature optimum configurations for instances with cities placed randomly according to a flat probability distribution. While these configurations appear similar to standard TSP tours for small α, the picture is rather different at large α. For $\alpha = 1$, rather than connecting near neighbour cities ($\mathbf{r}_{i+1} \sim \mathbf{r}_i$), the tour connects cities lying on points that are almost inverted with respect to the origin ($\mathbf{r}_{i+1} \sim -\mathbf{r}_i$). Sharp changes in quantities such as $\langle H_L \rangle$ (where the average is over the random instances), as α is varied suggest a phase transition. Moreover, this transition was identified as a complexity transition [2], since the simulated annealing schedule required to reach optima in the (large α) C-phase is much less stringent than that required in the (small α) L-phase, indicating a difference in characteristic difficulty of the problem as the transition is crossed. Complexity transitions have recently been of strong interest to computer scientists, combinatorial optimists and physicists, and although a transition has already been identified [3] in other versions of the TSP, the geometric basis and simplicity of this centred model are very appealing.

Many questions about the nature of the transition remain, and the aim of this paper is to investigate the model using analytic techniques recently developed to study the statistical mechanics of stochastic TSP-like models [4]. The stochastic TSP has cities randomly placed according to some probability distribution, usually taken to be flat. These techniques allow a full solution of the stochastic theory in the region of high city density and finite temperature. In particular, expectation values for the path length $\langle H_L \rangle$ and its fluctuations can be computed and these provide evidence for a smoothed transition at finite temperature. The technique is not able to access the optima at low temperature and we cannot use it to compute critical indices for example. Nonetheless, our methods produce other insights such as a duality; $\alpha \leftrightarrow (1-\alpha)$ between thermodynamic quantities that may have a role beyond the region of applicability of the technique.

II. FORMALISM

The analytic techniques we use to solve the model were derived in [4] using a functional formalism and have since been placed on a firm basis via a discrete approach [5]. The continuum equations for a system of unit area and a flat

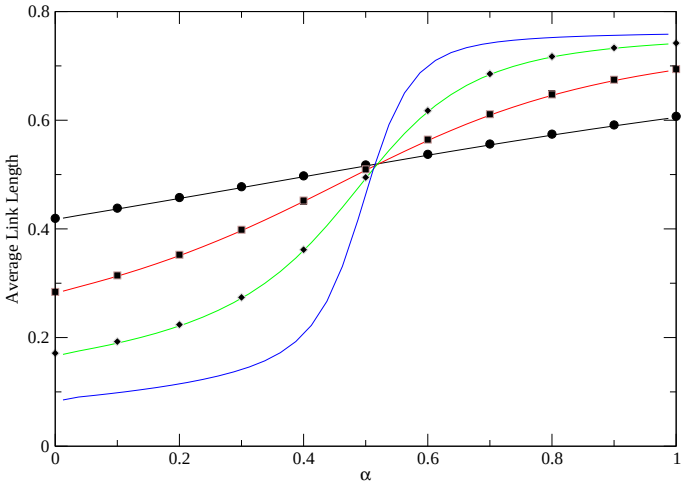

FIG. 1: The average link length $(1/N)\langle H_L\rangle$ for the centred TSP according to the formalism of [4] shown for $\beta = 2.0, 5.0, 10.0, 20.0$ with increasingly sharp step. Points (omitted at $\beta = 20.0$) are from Monte Carlo simulations with $N = 1000$ averaged over 100 random instances.

distribution of cities allow the free energy to be written in terms of a quantity $s(\mathbf{r})$ which is defined by an integral equation,

$$\beta F = -2N \int d^2r \, \log s(\mathbf{r}) - N \log N \tag{4}$$

$$s(\mathbf{r}) = \int d^2r \, \frac{1}{s(\mathbf{r}')} \exp\left(-\beta\left[(1-\alpha)V_L(\mathbf{r},\mathbf{r}') + \alpha V_C(\mathbf{r},\mathbf{r}')\right]\right). \tag{5}$$

Observables can now be obtained by standard thermodynamic relations. For example the expectation values for the total length of the path and its fluctuations are given by,

$$\langle H_L\rangle = N \int d^2r d^2r' \, \frac{V_L(\mathbf{r},\mathbf{r}')}{s(\mathbf{r})s(\mathbf{r}')} \exp\left(-\beta\left[(1-\alpha)V_L(\mathbf{r},\mathbf{r}') + \alpha V_C(\mathbf{r},\mathbf{r}')\right]\right) \tag{6}$$

$$\langle (H_L - \langle H_L\rangle)^2\rangle = \frac{\alpha}{\beta}\frac{\partial\langle H_L\rangle}{\partial\alpha} - \frac{\partial\langle H_L\rangle}{\partial\beta} \tag{7}$$

These expressions are proportional to N in contrast to the expected dependence of the optimum configurations. For example, the optimum path length for the standard ($\alpha = 0$) TSP grows as $\sqrt{N}$, and for $\alpha > 0$ has more complex N dependence reported in [1]. Along with the non-extensive $N \log N$ entropy, this scaling makes it already clear that the region within which the technique is valid is restricted. Similar formulae hold for expectations of H_C, but in all cases we find that the solution of the integral equation (5), obeys a duality relation:

$$s_{1-\alpha}(\mathbf{r}) = s_\alpha(\mathbf{r}) = s_\alpha(-\mathbf{r}) \tag{8}$$

This duality is a consequence of the symmetry that inverts with respect to the centre, $\mathbf{r} \to -\mathbf{r}$, and interchanges $H_L \leftrightarrow H_C$. As a result, $F(1-\alpha) = F(\alpha)$ so expectations of H_C are simply related to those of H_L, for example, $\langle H_C(\alpha)\rangle = \langle H_L(1-\alpha)\rangle$. One immediate result of the duality is that if any transition occurs, it must be at $\alpha_c = 1/2$. We shall return to discuss whether this duality holds outside the range of validity of the equations (5).

It has not been possible to analytically solve the integral equation (5), but an iterative procedure on a discretised version converges rapidly and is numerically stable. Monte Carlo simulations with $N = 1000$ and measurements taken over a million Monte Carlo moves following a similar number of moves to equilibriate, independently confirm the results and are shown in the figures below. At the lowest temperatures it becomes hard for the Monte Carlo to reach equilibrium and we omit the $\beta = 20.0$ data. In figure (1) the expectation value of the length per link is shown as a function of α, for a variety of temperatures. Evidently this tends towards a step function and is a smoothed out version of the zero temperature result shown in reference [1].

Fluctuations in the path length also grow as N and figure (2) shows how $(1/N)\langle (H_L - \langle H_L\rangle)^2\rangle$ changes with α. This quantity is numerically more delicate than the simple average, but although it can be computed by solving linear equations for $\partial s/\partial\beta$ and $\partial s/\partial\alpha$, we have simply evaluated the expression in (7) with discrete derivatives. The Monte

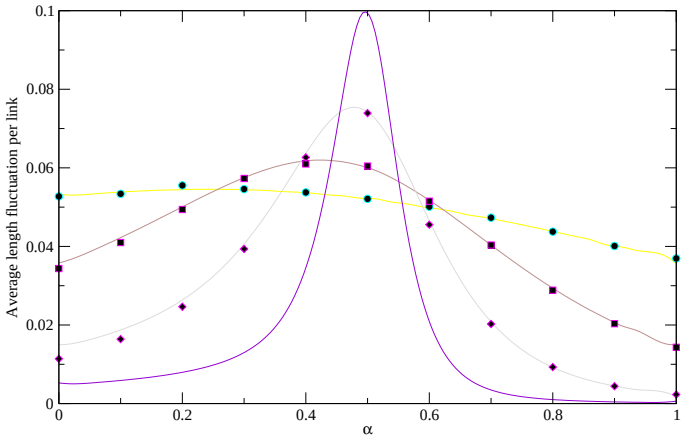

FIG. 2: The average per link length fluctuations $(1/N)\langle(H_L - \langle H_L\rangle)^2\rangle$ for the centred TSP according to the formalism of [4] shown for $\beta = 2.0, 5.0, 10.0, 20.0$ with increasingly pronounced peak. Points (omitted at $\beta = 20.0$) are from Monte Carlo simulations with $N = 1000$ averaged over 100 random instances.

Carlo also suffers from large sample to sample fluctuations at low temperature. As the temperature is reduced, a peak starts to appear at α_c.

Other quantities such as correlations between angles between successive links have also been computed within this formalism and agree with Monte Carlo simulations. The computations are interesting in that they show how to generalise the methods of [4] to compute correlations along the path, however they do not throw any further light on this problem and its transition.

III. LOW TEMPERATURE LIMIT

Although no general analytic solution of the integral equations has been found, the low temperature limit can be understood using a saddle point at large β. Because the formalism does not scale temperature [6] this low temperature limit does not correspond to the TSP optimum.

Writing $s_\alpha(\mathbf{r}) = t_\alpha(\mathbf{r})e^{-\beta w_\alpha(\mathbf{r})}$, the stationarity condition of the exponent at large β is:

$$w_\alpha(\mathbf{r}) = min_{\mathbf{r}'}\left[(1-\alpha)|\mathbf{r}-\mathbf{r}'| + \alpha|\mathbf{r}+\mathbf{r}'| - w_\alpha(\mathbf{r}')\right] \tag{9}$$

A solution exists with $w_\alpha(\mathbf{r})$ linear in $\mathbf{r}$, matching the tendency of the iterative numerical solutions at low temperature. The prefactor $t_\alpha(\mathbf{r})$, can also be determined based on linear rather than the usual quadratic fluctuations [4]. The resulting solution obeys duality:

$$s_\alpha(\mathbf{r}) = \begin{cases} \frac{\sqrt{2\pi}}{\beta(1-\alpha)}\exp\left(-\beta\alpha r\right) & 0 < \alpha \le 1/2 \\ \frac{\sqrt{2\pi}}{\beta\alpha}\exp\left(-\beta(1-\alpha)r\right) & 1/2 < \alpha \le 1 \end{cases} \tag{10}$$

The resulting expectation values have sharp changes at the transition point. For example,

$$\frac{1}{N}\langle H_L\rangle = \begin{cases} \frac{2}{\beta(1-\alpha)}\exp\left(-\beta\alpha r\right) & 0 < \alpha \le 1/2 \\ 2\int d^2\mathbf{r}\,|\mathbf{r}| = \left(\sqrt{2}+\log(1+\sqrt{2})\right)/3 & 1/2 < \alpha \le 1 \end{cases} \tag{11}$$

The length fluctuations develop a delta function singularity at α_c, with leading coefficient proportional to $1/\beta$,

$$\frac{1}{N}\langle(H_L - \langle H_L\rangle)^2\rangle = \frac{1}{\beta}\left(\frac{\left(\sqrt{2}+\log(1+\sqrt{2})\right)}{6} - \frac{2}{\beta}\right)\delta(\alpha-\alpha_c) + \frac{2}{\beta^2(1-\alpha)^2}\theta(\alpha_c-\alpha) \tag{12}$$

The height of the fluctuation peak as determined by the iterative solution of the integral equation at fixed α_C appears first to grow as β as the temperature is reduced, but eventually this $1/\beta$ behaviour is observed.

IV. CONCLUSIONS

The method of [4] for studying the statistical mechanics of TSP-like problems has been applied to the centred TSP. Both numerical solutions of the equations at finite temperature and the limiting behaviour at large β provide evidence supporting the transition observed though numerical study of optimum configurations in [1]. The method is not able to reach the region where optimal configurations dominate and the character of the evidence is a smoothed signal of the transition indicating that the transition point lies at a temperature below that accessible by this technique.

A noteworthy feature of the solutions is a duality, $F(1-\alpha) = F(\alpha)$, relating observables on either side of the transition. This duality can be understood in terms of the density of states: the number of cyclic tours with H_L between E and $E + dE$ is the same as the number of tours with H_C between E and $E + dE$, where in this regime of high city density and high temperature, E should not be too small. This kind of relationship also exists between a particular pair of one-dimensional Hamiltonians [7] in which the configurations are also specified by permutations of N indices. However, in that case, even at finite N, a map between a configuration with a certain value of one Hamiltonian and another configuration with the same value for the other Hamiltonian was demonstrated. A brief consideration of particular instances of the $N = 4$ case shows that a precise relationship of this kind cannot hold for the centred two-dimensional TSP, so the duality must only be valid in the large N limit. Within the large N limit, even if the duality holds for optima and near optima outside the regime of high temperature, the lack of a definite map prevents one from using the $\alpha = 1$ model on the easy side of the transition to solve the hard TSP at $\alpha = 0$.

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[1] A. Lipowski and D. Lipowska, Phys. Rev.**E** 71, 067701 (2005)
[2] T. Hogg, B.A. Huberman and C. Williams, Artif. Intell. **81**, 1 (1996); O.C. Martin, R. Monasson and R. Zecchina, Theoretical Computer Science **265**, 3 (2001).
[3] W. Zhang and R.E. Korf, Artificial Intelligence **81**, 223 (1996); P. Cheeseman, B. Kanefsky and W.M. Taylor, Proc AAAI-93, Washington, 21 (1993)
[4] D.S. Dean, D. Lancaster and S.N. Majumdar, J. Stat. Mech. L01001 (2005); *ibid.* Phys. Rev. E **72** 026125 (2005).
[5] D.S. Dean and D. Lancaster, in preparation.
[6] J. Vannimenus and M. Mézard, J. Physique Lett. **45** L1145 (1984).
[7] D. Lancaster, J. Phys. A. **37**, 1125 (2004).