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The Cavity Method and the Travelling-Salesman Problem.

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Abstract. – For the random link travelling-salesman problem we solve the zero-temperature cavity equations, assuming that there is only one pure state. We get precise predictions for the length of the optimal tour and the probability distribution of links in this tour. These are compared with numerical simulations using the Lin-Kernighan algorithm and the one-tree relaxation of Held and Karp.

Among the several problems of combinatorial optimization which have been studied from the point of view of statistical physics [1, 2], the travelling salesman occupies a choice place: it is considered as an important laboratory for testing ideas on *NP*-complete problems. The problem consists in the following: given N points $i = 1, ..., N$, and the distances l_{ij} between points i and j, one must find the shortest closed line of N links going through all the points. For N large (thermodynamic limit) this can be seen as a problem in statistical physics. One introduces a temperature T, and each tour $\mathcal{J}$ of length $l_{\mathcal{J}}$ is weighted by a Boltzmann factor $\exp[-l_{\mathcal{J}}/T]$. One can then try to predict the asymptotic value (for $N \to \infty$) of the length of the optimal tour, for some sets of samples. One such set which has received much attention is the random link problem in which the l_{ij} are independent random variables, with a probability distribution $\rho(l)$ (here we keep to the symmetric case $l_{ij} = l_{ji}$).

There have been several studies of this problem in the literature before [1-8], mainly numerical ones. On the analytical side, the TSP can be written as a self-avoiding walk interacting through random couplings. It has been studied with the replica method [3] within the replica symmetric approximation. However, the equations satisfied by the order parameters were very complicated. An estimate of the length of the optimal tour was obtained only in one specific case of «flat distances»: a uniform distribution of distances on $[0, 1]$.

On the numerical side, physicists have concentrated on the use of simulated annealing [1, 4, 5] and on the study of finite-temperature properties.

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Our analytic approach does not use replicas, but the cavity method [2]. The cavity equations have been written down in [6], within the hypothesis that there exists only one pure state. Adding a new point $i=0$ to a system of N points $i=1,\ldots,N$, the magnetization of the new point is $m_0=2A_1/((A_1)^2-A_2)$, where $A_k=\sum_{i=1}^{N} T_{0i}^k m_i^k$ and m_i is the magnetization on site i before the addition of the new point. The coupling constant is $T_{0i}=\exp[-\beta N^\delta l_{0i}]$, with β the inverse temperature. For a length distribution $\rho(l)$ scaling as $\rho(l)\sim l^r/r!$ $(l\to 0)$, $\delta=1/(r+1)$ must be chosen to have a good thermodynamic limit [7].

As we are interested in the zero-temperature limit $\beta\to\infty$, it is natural to parametrize $m_i=\exp[\beta\varphi_i]$, and the cavity equation for m_0 simplifies at zero temperature to

$$\varphi_0=N^\delta l_{02}-\varphi_2\,. \tag{1}$$

In eq. (1) we reordered the points $i=1,\ldots,N$ in such a way that $N^\delta l_{01}-\varphi_1\leqslant \leqslant N^\delta l_{02}-\varphi_2\leqslant\ldots\leqslant N^\delta l_{0N}-\varphi_N$.

Denoting by $\overline{(\,)}$ the average over the distribution of links, eq. (1) implies a self-consistent equation for the probability distribution of the φ_i:

$$P(\varphi)=\overline{\delta(\varphi-\varphi_0)}=\overline{\delta(\varphi-\varphi_i)}\,,\quad i=1,\ldots,N\,. \tag{2}$$

To write this self-consistency equation explicitly, we first deduce from eq. (2) the distribution $\Pi(\chi)$ of $\chi=N^\delta l-\varphi$

$$\Pi(\chi)=\frac{1}{N}\int_0^\infty \frac{l^r}{r!}\,\mathrm{d}l\,P(l-\chi)\,. \tag{3}$$

(For N finite the integral has a cut-off, which diverges with N.) In the cavity method the N random variables $\chi_i=N^\delta l_{0i}-\varphi_i$ are independent, so that the distribution of the second smallest of all the χ_i's (see eq. (1)) is easily derived. Using eqs. (2), (3), this leads to

$$P(\varphi)=N(N-1)\Pi(\chi)\left(\int_{-\infty}^{\chi}\Pi(u)\,\mathrm{d}u\right)\left(\int_{\chi}^{\infty}\Pi(u)\,\mathrm{d}u\right)^{N-2}\,, \tag{4}$$

which for large N is equal to $P(\varphi)=(\mathrm{d}G/\mathrm{d}\varphi)\,G(\varphi)\exp[-G(\varphi)]$, with

$$G(\varphi)=\int_0^\infty \mathrm{d}u\,\frac{u^{r+1}}{(r+1)!}P(u-\varphi)\,. \tag{5}$$

From this we can deduce the closed integral equation for G, the order parameter function of the TSP:

$$G(x)=\int_{-x}^{\infty}\frac{(x+y)^r}{r!}\{1+G(y)\}\exp[-G(y)]\,\mathrm{d}y\,, \tag{6}$$

G can be computed precisely by iteration. Its relation with the order parameter function defined in the replica approach is complicated.

From $G(x)$, we now compute the length of the optimal tour. Let us define the distribution of the (rescaled) links, $\mathscr{P}(l)$ as

$$\mathscr{P}(l)=\frac{1}{N}\overline{\sum_{1\leqslant i<j\leqslant N}\delta(l-l_{ij}N^\delta n_{ij})}=\frac{1}{2}\overline{\sum_i\delta(l-l_{0i}N^\delta n_{0i})}\,, \tag{7}$$

where n_{ij} is the thermal average of the occupation number of link ij. At zero temperature, the cavity equation for n_{0l}, written down in [6], tells us that $n_{01} = n_{02} = 1$, and $n_{0i} = 0\,(i \geqslant 3)$. (The points are ordered as introduced after eq. (1).) Using this result and eq. (7), we find after some work the following expression for $\mathscr{P}$ at zero temperature:

$$\mathscr{P}(l) = \frac{1}{2}\frac{l^r}{r!}\left(-\frac{\partial}{\partial l}\right)\int \mathrm{d}x\,(1+G(x))\exp[-G(x)](1+G(l-x))\exp[-G(l-x)], \qquad (8)$$

where G is the solution of eq. (6). The length of the optimal tour (as $N \to \infty$) is then $L \sim N^{1-1/(r+1)}\hat{L}_r$ with

$$\hat{L}_r = \int \mathscr{P}(l)\,\mathrm{d}l = \frac{r+1}{2}\int \mathrm{d}x\,G(x)\,\{1+G(x)\}\exp[-G(x)]. \qquad (9)$$

We summarize our theoretical results: for any r we can solve for $G(x)$ in eq. (6) and then get from eqs. (8), (9) the length of the optimal tour and the distribution of lengths of occupied links in this tour.

In the case $r = 0$ (flat distances) we find $L = \hat{L}_{r=0} = 2.0415\ldots$ and for $r = 1$ we have $\hat{L}_{r=1} = 1.8175\ldots$. This random link case with $r = 1$ is an approximation for the Euclidean TSP in 2 dimensions. Following [9], we estimate the length of a TSP for N points uniformely distributed in the unit square as $\hat{L}_{r=1}/\sqrt{2\pi} = 0.7251$ which is close to the known bounds [10]. A commonly accepted numerical result is 0.749.

We now turn to the numerical checks of these results (restricted to the case of flat distances $r = 0$, *i.e.*, $l_{ij} = l_{ji}$ are uniform random numbers on $[0, 1]$). The TSP being *NP*-complete, there are no tractable algorithms for solving large instances of it. The long-standing interest into the TSP has, however, led to the following situation: there do exist (very involved) algorithms using linear programming [11] or branch and bound strategies [12], the best of which are presently capable of solving instances with several hundreds of points.

On the other hand, a number of methods are available which provide good sub-optimal tours and thus upper bounds on the optimal tour length. Furthermore, algorithms are known which solve «relaxed» TSP problems, leading to lower bounds on the length of the shortest tour. It has been known for some time [12, 13] that these bounds might be quite tight, even for the random link TSP.

We used two well-known heuristics to determine upper and lower bounds for the TSP, following [13]. For the lower bound we used the Lagrangian one-tree relaxation of Held and Karp [14] (our implementation follows ref. [12]). This relaxation solves the problem

$$L_{\text{one-tree}} = \max_{\lambda}\left\{\left(\min_{\substack{n_{ij}=0,1 \\ n_{ij}\,\in\,\text{one-tree}}} \sum_{i,j}(l_{ij}+\lambda_i+\lambda_j)\,n_{ij}\right) - 2\sum_j \lambda_j\right\}, \qquad (10)$$

where the min (for fixed λ) is taken on certain spanning graphs containing exactly one cycle (cf. [12]). The upper bound on the optimal TSP-tour was determined with the Lin-Kernighan algorithm, which was implemented using the original ref. [15]. Both methods are quite fast: for an instance of 400 points we can calculate both the upper and the lower bound in less than 1 minute on a Convex C1 computer.

Our numerical results for the bounds are given in fig. 1. In both cases we find good agreement with a dependence linear in $1/N$. As $N \to \infty$ we get $2.039 \pm 3 \cdot 10^{-3} \leqslant$ $\leqslant L \leqslant 2.21 \pm 1.3 \cdot 10^{-2}$. The theoretical value $L = 2.0415\ldots$ is in agreement with the bounds,

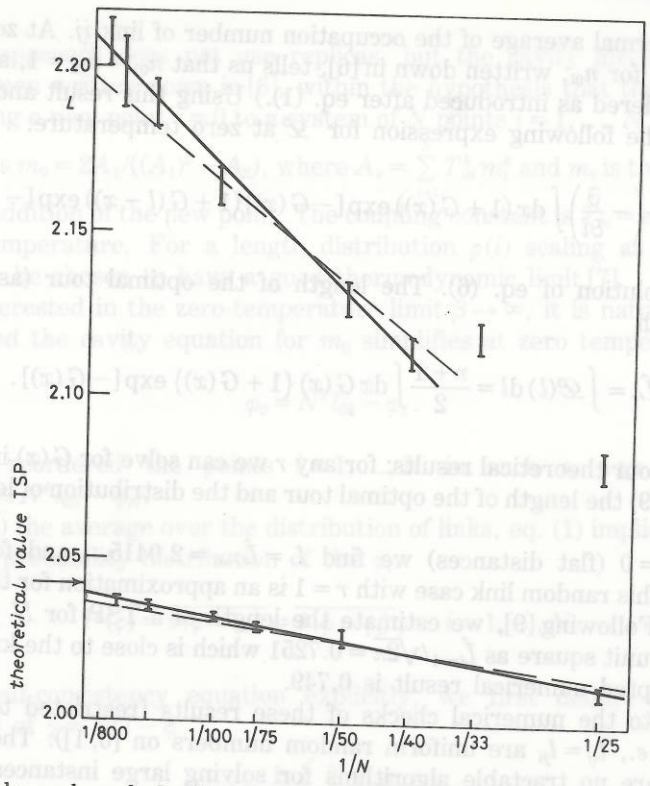

Fig. 1. – Upper and lower bounds for the optimal tour length of the random link TSP (flat distances $l_{ij} \in [0, 1]$). The upper curve was produced using the Lin-Kernighan algorithm, averaged over, *e.g.*, 360 samples for $N = 800$, 5000 samples for $N = 25$. The lower curve results from the Langrangian one-tree relaxation with, *e.g.*, 3000 samples ($N = 400$), 20000 samples ($N = 25$).

in fact it coincides within our 2‰ level of precision with the results of the one-tree relaxation.

We compared also the probability distribution of links both of the Lin-Kernighan solution and of the one-tree relaxation with the theoretical prediction. To eliminate sample-to-sample fluctuations, we rescalded the lengths of occupied links, in each solution, by the average length of the occupied links. The distribution of these rescaled lengths, for $N = 800$, was then averaged over, *e.g.*, 100 Lin-Kernighan tours and compared to the theoretical prediction

$$I(x) = \int_0^{x L_{T=0}} \mathrm{d}l \; \mathscr{P}(l) .$$

The agreement is excellent, see fig. 2. We found equally good agreement with the one-tree relaxation. We do not know why a simple length rescaling makes agree the Lin-Kernighan solution (which we suspect to be 10% above optimal) the one-tree relaxation (which does not produce a tour) and the theoretical result for the optimal solution.

The simulations give the numerical value of the optimal TSP tour length, albeit on a rather crude level. They also illustrate the power of the Lin-Kernighan algorithm, compared to simpler heuristics which up to now have all given bounds on the optimal tour length diverging like $\log N$ for $N \to \infty$ [4]. Finally, the extremely close agreement between the one-

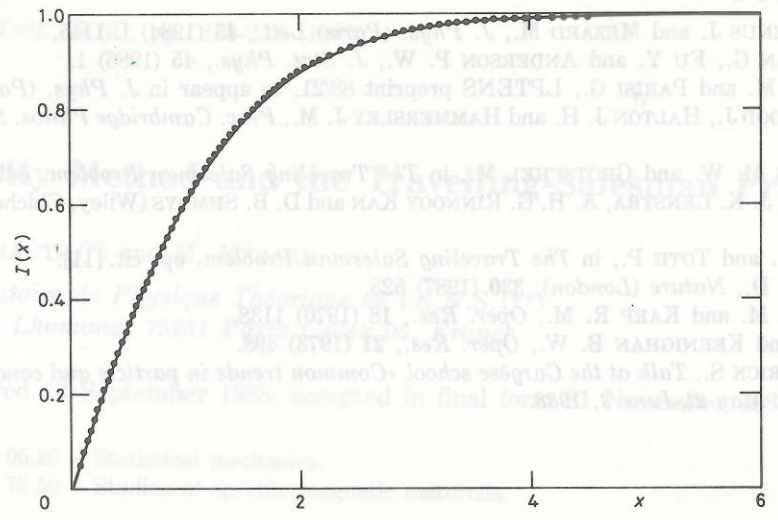

Fig. 2. – Integrated distribution function $I(x)$ for the occupied links in TSP solutions *vs.* reduced length variable x ($x = 1$ corresponds to the mean length of occupied links in each sample). The curve gives the theoretical result, the dotted line the numerical results for Lin-Kernighan solutions (100 samples at $N = 800$).

tree relaxation and the proposed value for the optimal tour suggests to us the exciting conjecture that the two values may indeed be identical. It would be interesting to apply the cavity method directly to the one-tree relaxation.

We found some support for the conjecture in additional simulations using the Lin-Kernighan heuristics repeatedly on each sample and keeping the lowest result. In this way we can lower the upper bound considerably for finite N, but not for $N \to \infty$. (Preliminary results with an exact algorithm, by Kirkpatrick [16], agree with an optimal TSP length around 2.04.)

In conclusion we remark that the recently developed cavity method of statistical physics in combination with rather traditional tools of Operations Research have led to a better understanding of the random link TSP.

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