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The Random Link Approximation for the Euclidean Traveling Salesman Problem

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Abstract. — The traveling salesman problem (TSP) consists of finding the length of the shortest closed tour visiting N “cities”. We consider the Euclidean TSP where the cities are distributed randomly and independently in a d -dimensional unit hypercube. Working with periodic boundary conditions and inspired by a remarkable universality in the k th nearest neighbor distribution, we find for the average optimum tour length $\langle L_E \rangle = \beta_E(d) N^{1-1/d} [1 + O(1/N)]$ with $\beta_E(2) = 0.7120 \pm 0.0002$ and $\beta_E(3) = 0.6979 \pm 0.0002$. We then derive analytical predictions for these quantities using the random link approximation, where the lengths between cities are taken as independent random variables. From the “cavity” equations developed by Krauth, Mézard and Parisi, we calculate the associated random link values $\beta_{RL}(d)$. For $d = 1, 2, 3$, numerical results show that the random link approximation is a good one, with a discrepancy of less than 2.1% between $\beta_E(d)$ and $\beta_{RL}(d)$. For large d , we argue that the approximation is exact up to $O(1/d^2)$ and give a conjecture for $\beta_E(d)$, in terms of a power series in $1/d$, specifying both leading and subleading coefficients.

Résumé. — Le problème du voyageur de commerce (TSP) consiste à trouver le chemin fermé le plus court qui relie N “villes”. Nous étudions le TSP euclidien où les villes sont distribuées au hasard de manière décorrélée dans l’hypercube de côté 1, en dimension d . En imposant des conditions aux bords périodiques et guidés par une universalité remarquable de la distribution des k ièmes voisins, nous trouvons la longueur moyenne du chemin optimal $\langle L_E \rangle = \beta_E(d) N^{1-1/d} [1 + O(1/N)]$, avec $\beta_E(2) = 0,7120 \pm 0,0002$ et $\beta_E(3) = 0,6979 \pm 0,0002$. Nous établissons ensuite des prédictions analytiques sur ces quantités à l’aide de l’approximation de liens aléatoires, où les longueurs entre les villes sont des variables aléatoires indépendantes. Grâce aux équations “cavité” développées par Krauth, Mézard et Parisi, nous obtenons dans le cas de liens aléatoires les valeurs, $\beta_{RL}(d)$, analogues à $\beta_E(d)$. Pour $d = 1, 2, 3$, les résultats numériques confirment que l’approximation de liens aléatoires est bonne, conduisant à un écart inférieur à 2,1% entre $\beta_E(d)$ et $\beta_{RL}(d)$. Pour d grand, nous donnons des arguments montrant que cette approximation est exacte jusqu’à l’ordre $1/d^2$ et nous proposons une conjecture pour $\beta_E(d)$, exprimée en fonction d’une série en $1/d$, dont on donne les deux premiers ordres.

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1. Introduction

Given N “cities” and the distances between them, the traveling salesman problem (TSP) consists of finding the length of the shortest closed “tour” (path) visiting every city exactly once, where the tour length is the sum of the city-to-city distances along the tour. The TSP is NP-complete, which suggests that there is no general algorithm capable of finding the optimum tour in an amount of time polynomial in N . The problem is thus simple to state, but very difficult to solve. It also happens to be the most well known combinatorial optimization problem, and has attracted interest from a wide range of fields. In operations research, mathematics and computer science, researchers have concentrated on algorithmic aspects. A particular focus has been on heuristic algorithms — algorithms which do not guarantee optimal tours — for cases where exact methods are too slow to be of use. The most effective heuristics are based on local search methods, which start with a non-optimal tour and iteratively improve the tour within a well-defined “neighborhood”; a famous example is the Lin-Kernighan heuristic [1]. More recent efforts have involved combining local search and non-deterministic methods, in order to refine heuristics to the point where they give good enough solutions for practical purposes; a powerful such technique is Chained Local Optimization [2].

Over the last fifteen years, physicists have increasingly been drawn to the TSP as well, and particularly to *stochastic* versions of the problem, where instances are randomly chosen from an ensemble. The motivation has often been to find properties applicable to a large class of disordered systems, either through good approximate methods or through exact analytical approaches. In our work, we consider two such stochastic TSPs. The first, the Euclidean TSP, is the more classic form of the problem: N cities are placed randomly and independently in a d -dimensional hypercube, and the distances between cities are defined by the Euclidean metric. The second, the random link TSP, is a related problem developed within the context of disordered systems: rather than specifying the positions of cities, we specify the lengths l_{ij} separating cities i and j , where the l_{ij} are taken to be independent, identically distributed random variables. The appeal of the random link problem is, on the one hand, that an analytical approach exists for solving it [3, 4], and on the other hand, that when certain correlations are neglected this TSP can be made to resemble the Euclidean TSP. We therefore consider the random link problem as a *random link approximation* to the (random point) Euclidean problem. Researchers outside of physics remain largely unaware of the analytical progress made on the random link TSP; one of our hopes is to demonstrate how these results are of direct interest in problems where the aim is to find the optimum Euclidean TSP tour length.

Our approach in this paper is then to examine both the Euclidean problem and the random link problem — the latter for its own theoretical interest as well as for a better understanding of the Euclidean case. We begin by considering in depth the Euclidean TSP, including a review of previous work. We find that, given periodic boundary conditions (toroidal geometry), the Euclidean optimum tour length L_E averaged over the ensemble of all possible instances has the finite size scaling behavior

$$\langle L_E \rangle = \beta_E(d) N^{1-1/d} \left[1 + O\left(\frac{1}{N}\right) \right]. \quad (1)$$

From simulations, we extract very precise numerical values for $\beta_E(d)$ at $d = 2$ and $d = 3$; methodological and numerical procedures are detailed in the appendices. We also give numerical evidence that the probability distribution of L_E becomes Gaussian in the large N limit. In addition to these TSP results, we find a surprising universality in the scaling of the mean distance between k th nearest neighbors, for points randomly distributed in the d -dimensional hypercube. Finally, we discuss the expected behavior of $\beta_E(d)$ in the large d limit.

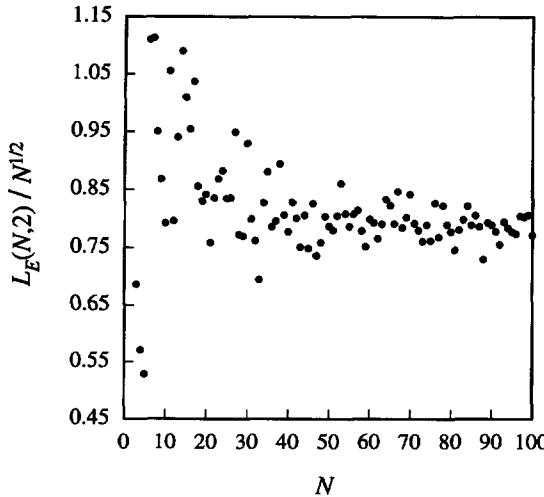


Fig. 1. — Self-averaging of 2-D Euclidean TSP optimum: convergence of $L_E(N, 2)/N^{1/2}$ on a sequence of random instances at increasing N .

In the second part of the paper we discuss the random link problem, considering it as an approximation to the Euclidean problem. Making use of the cavity method, we compare the random link $\beta_{\text{RL}}(d)$ with the Euclidean $\beta_E(d)$ values obtained from our simulations. We find that the random link approximation is correct to within 2% at $d = 2$ and 3. The rest of the section studies the large d limit of the random link model and its implications for the Euclidean TSP. We examine analytically how $\beta_{\text{RL}}(d)$ scales at large d , and we relate the $1/d$ coefficient of the associated power series to an underlying d -independent “renormalized” model. Finally, we present a theoretical analysis based on the Lin-Kernighan heuristic, suggesting strongly that the relative difference between $\beta_{\text{RL}}(d)$ and $\beta_E(d)$ is positive and of $O(1/d^2)$. The random link results then lead to our large d Euclidean conjecture:

$$\beta_E(d) = \sqrt{\frac{d}{2\pi e}} (\pi d)^{1/2d} \left[1 + \frac{2 - \ln 2 - 2\gamma}{d} + O\left(\frac{1}{d^2}\right) \right], \quad (2)$$

where γ is Euler’s constant.

2. The Euclidean TSP

2.1. SCALING AT LARGE N . — One of the earliest analytical results for the Euclidean TSP is due to Beardwood, Halton and Hammersley [5] (BHH). The authors considered N cities, distributed randomly and independently in a d -dimensional volume with distances between cities given by the Euclidean metric. They showed that, when the volume is the unit hypercube and the distribution of cities uniform, $L_E/N^{1-1/d}$ is self-averaging. This means that with probability 1,

$$\lim_{N \rightarrow \infty} \frac{L_E}{N^{1-1/d}} = \beta_E(d), \quad (3)$$

where $\beta_E(d)$ is independent of the randomly chosen instances. This property is illustrated in Figure 1. (In fact, the BHH result is more general than this and concerns an arbitrary volume and arbitrary form of the density of cities.) For a physics audience this large N limit

is equivalent, in appropriate units, to an infinite volume limit at constant density. $L_E/N^{1-1/d}$ then corresponds to an energy density that is self-averaging and has a well-defined infinite volume limit. The original proof by BHH is quite complicated; simpler proofs have since been given by Karp and Steele [6, 7].

One of our goals is to determine $\beta_E(d)$. BHH gave rigorous lower and upper bounds as a function of dimension. For any given instance, a trivial lower bound on L_E is the sum over all cities i of the distance between i and its nearest neighbor in space. In fact, since a tour at best links a city with its *two* nearest neighbors, this bound can be improved upon by summing, over all i , the mean of i 's nearest and next-nearest neighbor distances. Taking the ensemble average of this quantity (that is, the average over all instances) leads to the best analytical lower bound to date. For upper bounds, BHH introduced a heuristic algorithm, now known as "strip", in order to generate near-optimal tours (discussed also in a paper by Armour and Wheeler [8]). In two dimensions the method involves dividing the square into adjacent columns or strips, and sequentially visiting the cities on a given strip according to their positions along it. The respective lower and upper bounds give $0.6250 \leq \beta_E(2) \leq 0.9204$.

In addition to bounds, it is possible to obtain numerical *estimates* for $\beta_E(d)$. BHH used two instances, $N = 202$ and $N = 400$, from which they estimated $\beta_E(2) \approx 0.749$ using hand-drawn tours. Surprisingly little has been done to improve upon this value in two dimensions, and essentially nothing in higher dimensions. Stein [9] has found $\beta_E(2) \approx 0.765$, which is frequently cited. Only recently have better values been obtained, but as they come from near-optimal tours found by heuristic algorithms, they should be considered more as upper bounds than as estimates. Using a local search heuristic known as "3-opt" [10], Ong and Huang [11] have found $\beta_E(2) \leq 0.743$; using another heuristic, "tabu" search, Fiechter [12] has found $\beta_E(2) \leq 0.731$; and using a variant of simulated annealing, Lee and Choi [13] have found $\beta_E(2) \leq 0.721$. In what follows we shall show what is needed for a more precise estimate of $\beta_E(d)$ with, furthermore, a way to quantify the associated error.

2.2. EXTRACTING $\beta_E(d)$. — As $N \rightarrow \infty$, $L_E/N^{1-1/d}$ converges with probability 1 to the instance-independent $\beta_E(d)$. Our estimate of $\beta_E(d)$ must rest on some assumptions, though, since only finite values of N are accessible numerically. Note first that at values of N where computation times are reasonable, L_E has substantial instance-to-instance fluctuations. To reduce and at the same time quantify these fluctuations, we average over a large number of instances. We thus consider the numerical mean of L_E over the instances sampled, which itself satisfies the asymptotic relation (3) but with a smoother convergence. To extract $\beta_E(d)$, we must understand precisely what this convergence in N is.

If cities were randomly distributed in the hypercube with open boundary conditions, the cities near the boundaries would have fewer neighbors and therefore lengthen the tour. In standard statistical mechanical systems at constant density, boundary effects lead to corrections of the form surface over volume. For the TSP at constant density, the volume grows as N and the surface as $N^{1-1/d}$. In a d -dimensional unit hypercube, then, the ensemble average of L_E would presumably have the large N behavior

$$N^{1-1/d} \beta_E(d) \left(1 + \frac{A}{N^{1/d}} + \frac{B}{N^{2/d}} + \dots \right). \quad (4)$$

In order to extract $\beta_E(d)$ numerically, it would be necessary to perform a fit which includes these corrections. A reliable numerical fit, however, must have few adjustable parameters, and the slow convergence of this series would prevent us from extracting $\beta_E(d)$ to high accuracy. We therefore have chosen to eliminate these boundary (surface) effects by using *periodic* boundary conditions in all directions. This should not change $\beta_E(d)$, but leaves us with fewer adjustable

parameters and a faster convergence, enabling us to work with smaller values of N where numerical simulations are not too slow.

For the hypercube with periodic boundary conditions, let us introduce the notation

$$\beta_E(N, d) \equiv \frac{\langle L_E(N, d) \rangle}{N^{1-1/d}}, \quad (5)$$

where $\langle L_E \rangle$ is the average of L_E over the ensemble of instances. ($\beta_E(N, d)$ is, in physical units, the zero-temperature energy density.) We then wish to understand how $\beta_E(N, d)$ converges to its large N limit, $\beta_E(d)$. In standard statistical mechanical systems, there is a characteristic correlation length ξ . Away from a critical point, ξ is finite, and finite size corrections decrease as $e^{-W/\xi}$, where W is a measure of the system “width”. At a critical point, ξ is infinite, and finite size corrections decrease as a power of $1/W$. For *disordered* statistical systems, however, this picture must be modified. Even if ξ is finite for each instance in the ensemble, the fluctuating disorder can still give rise to power-law corrections for ensemble averaged quantities. In the case of the TSP, this is particularly clear: the disorder in the positions of the cities induces large finite size effects even on simple geometric quantities.

To see how this might affect the convergence of $\beta_E(N, d)$, consider the following. For a given configuration of N points, call $D_k(N, d)$ the distance between a point and its k th nearest neighbor, where $k = 1, \dots, N - 1$. Take the points to be distributed randomly and uniformly in the unit hypercube. Let us find $\langle D_k(N, d) \rangle$. Under periodic boundary conditions, the probability density $\rho(l)$ of finding a point at distance l from another point is simply equal (for $0 \leq l \leq 1/2$) to the surface area at radius l of the d -dimensional sphere:

$$\rho(l) = \frac{d\pi^{d/2}}{\Gamma(d/2 + 1)} l^{d-1} \quad (6)$$

The probability of finding a point's k th nearest neighbor at distance l (see Fig. 2) is equal to the probability of finding $k - 1$ (out of $N - 1$) points within l , one point at l and the remaining $N - k - 1$ points beyond l :

$$P[D_k(N, d) = l] = \binom{N-1}{k-1} \left[\int_0^l \rho(l') dl' \right]^{k-1} (N-k) \rho(l) \left[1 - \int_0^l \rho(l') dl' \right]^{N-k-1} \quad (7)$$

$$= \binom{N-1}{k-1} (N-k) d \left[\frac{\pi^{d/2}}{\Gamma(d/2 + 1)} \right]^k l^{dk-1} \left[1 - \frac{\pi^{d/2}}{\Gamma(d/2 + 1)} l^d \right]^{N-k-1}, \quad (8)$$

giving the ensemble average

$$\begin{aligned} \langle D_k(N, d) \rangle &= \binom{N-1}{k-1} (N-k) d \left[\frac{\pi^{d/2}}{\Gamma(d/2 + 1)} \right]^k \\ &\times \int_0^{1/2} l^{dk} \left[1 - \frac{\pi^{d/2}}{\Gamma(d/2 + 1)} l^d \right]^{N-k-1} dl + . \end{aligned} \quad (9)$$

where the corrections are due to the $l > 1/2$ case, and are exponentially small in N .

Recognizing the integral, up to a simple change of variable, as a Beta function ($B(a, b) \equiv \int_0^1 t^{a-1}(1-t)^{b-1} dt = \Gamma(a)\Gamma(b)/\Gamma(a+b)$) plus a further remainder term exponentially small in

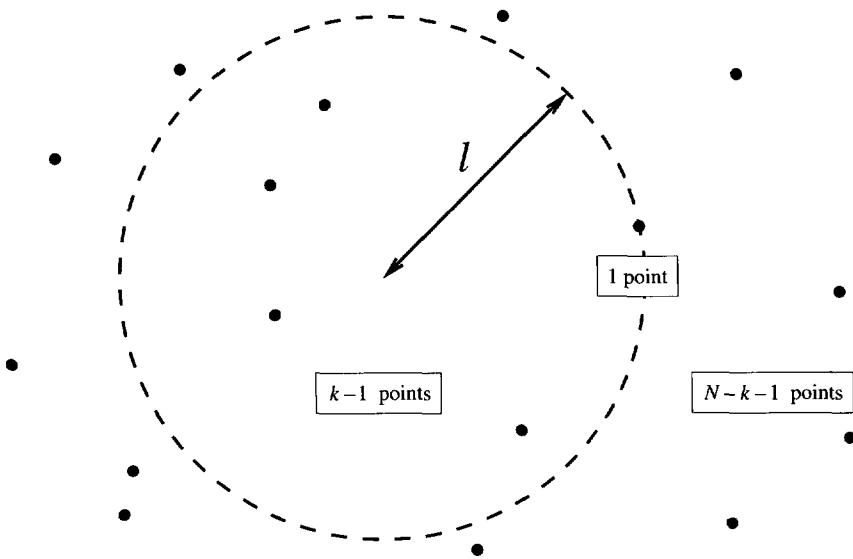


Fig. 2. — A point's $N - 1$ neighbors: $k - 1$ nearest neighbors are within distance l , k th nearest neighbor is at l , and remaining $N - k - 1$ points are beyond l .

N , we see that

$$\langle D_k(N, d) \rangle = \frac{\Gamma(d/2 + 1)^{1/d}}{\sqrt{\pi}} \frac{\Gamma(k + 1/d)}{\Gamma(k)} \frac{\Gamma(N)}{\Gamma(N + 1/d)} + \dots \quad (10)$$

$$= \frac{\Gamma(d/2 + 1)^{1/d}}{\sqrt{\pi}} \frac{\Gamma(k + 1/d)}{\Gamma(k)} N^{-1/d} \left[1 + \frac{1/d - 1/d^2}{2N} + O\left(\frac{1}{N^2}\right) \right]. \quad (11)$$

We are confronted here with a remarkable, and hitherto unexplored, universality: the *exact* same $1/N$ series gives the N -dependence regardless of k . The same finite size scaling behavior therefore applies to all k th nearest neighbor distances.

It might be hoped then that the typical link length in optimum tours would have this N -dependence, and that $\beta_E(N, d)$ would therefore have the same $1/N$ expansion. This is not quite the case. The link between cities i and j figures in the average $\langle D_k(N, d) \rangle$ whenever j is the k th neighbor of i ; it figures in $\beta_E(N, d)$, however, only when it belongs to the optimal tour. Two different kinds of averages are being taken, and so finite size corrections need not be identical. Nevertheless, it remains plausible that $\beta_E(N, d)$ has a $1/N$ series expansion, albeit a different one from (11). While we cannot prove this property, it is confirmed by an analysis of our numerical data.

Our approach to finding $\beta_E(d)$ is thus as follows: (i) we consider the ensemble average $\langle L_E \rangle$, rather than L_E for a given instance, in order to have a quantity with a well-defined dependence on N ; (ii) we use periodic boundary conditions to eliminate surface effects; (iii) we sample the ensemble using numerical simulations, and measure $\beta_E(N, d)$ within well controlled errors; (iv) we extract $\beta_E(d)$ by fitting these values to a $1/N$ series.

2.3. FINITE SIZE SCALING RESULTS. — Let us consider the $d = 2$ case in detail. We found the most effective numerical optimization methods for our purposes to be the local search heuristics Lin-Kernighan (LK) [1] and Chained Local Optimization (CLO) [2] mentioned in

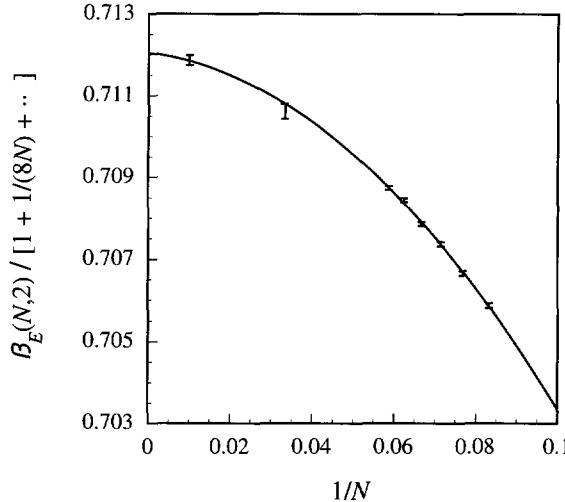


Fig. 3. — Finite size dependence of the rescaled 2-D Euclidean TSP optimum. Best fit ($\chi^2 = 5.56$) gives: $\beta_E(N, 2)/[1 + 1/(8N) + \dots] = 0.7120(1 - 0.0171/N - 1.048/N^2)$. Error bars represent statistical errors.

the introduction. Both heuristics, by definition, give tour lengths that are not always optimal. However, it is not necessary that the optimum be found 100% of the time: there is already a significant statistical error arising from instance-to-instance fluctuations, and so a further systematic error due to non-optimal tours is acceptable as long as this error is kept negligible compared to the statistical error. Our methods, along with relevant numerical details, are discussed in the appendices. For the present purposes, let us simply mention the general nature of the two heuristics used. LK works by performing a “variable-depth” local search, as discussed further in Section 3.6. CLO works by an iterative process combining LK optimizations with random perturbations to the tour, in order to explore many different local neighborhoods. We used LK for “small” N values ($N \leq 17$), averaging over 250,000 instances at each value of N , and we used CLO for “large” N values ($N = 30$ and $N = 100$), averaging over 10,000 and 6,000 instances respectively.

We fitted our resulting $\beta_E(N, d)$ estimates to a truncated $1/N$ series: the fits are good, and are stable with respect to the use of sub-samples of the data. For a fit of the form $\beta_E(N, d) = \beta_E(d)(1 + A/N + B/N^2)$, we find $\beta_E(2) = 0.7120 \pm 0.0002$, with $\chi^2 = 5.57$ for 8 data points and 3 fit parameters (5 degrees of freedom). Our error estimate for $\beta_E(2)$ is obtained by the standard method of performing fits using a range of fixed values for this parameter: the error bar ± 0.0002 is determined by the values of $\beta_E(2)$ which make χ^2 exceed its original result by exactly 1, *i.e.*, making $\chi^2 = 6.57$ in this case.

It is possible to extract another $\beta_E(N, d)$ estimate by making direct use of the universality discussed previously: the universal $1/N$ series in (11) suggests that there will be a faster convergence if we use the rescaled data $\beta_E(N, 2)/[1 + 1/(8N) + \dots]$. This also has the appealing property of leading to a function monotonic in N , as shown in Figure 3. We find

$$\frac{\beta_E(N, 2)}{1 + 1/(8N) + \dots} \approx 0.7120 \left(1 - \frac{0.0171}{N} - \frac{1.048}{N^2} \right) \quad (12)$$

with the leading term having the same error bar of ± 0.0002 as before. Note that the $1/N$ term in the fit is small — 2 orders of magnitude smaller than the leading order coefficient — and so to first order the $1 + 1/8N + \dots$ series is itself a good approximation.

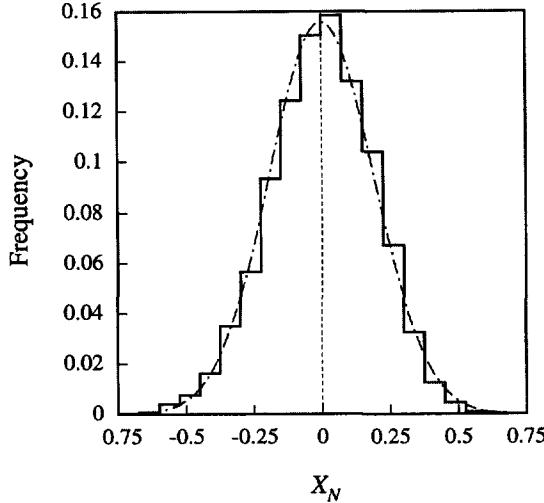


Fig. 4. — Distribution of 2-D Euclidean TSP scaling variable $X_N = (L_E - \langle L_E \rangle)/N^{1/2-1/d}$. Shaded region is for $N = 12$ (100,000 instances used) and solid line is for $N = 30$ (10,000 instances used). Superimposed curve shows (extrapolated) limiting Gaussian.

The same methodology was applied to the $d = 3$ case. The χ^2 's again confirmed the functional form of the fit, and we find from our data $\beta_E(3) = 0.6979 \pm 0.0002$. Also, since our initial work [14], Johnson *et al.* have performed simulations at $d = 2, 3, 4$, obtaining results [15] consistent with ours: $\beta_E(2) \approx 0.7124$, $\beta_E(3) \approx 0.6980$ and $\beta_E(4) \approx 0.7234$.

2.4. DISTRIBUTION OF OPTIMUM TOUR LENGTHS. — While BHH and others [6, 7] have shown that the variance of $L_E/N^{1-1/d}$ goes to zero as $N \rightarrow \infty$ (see also Fig. 1), they have not determined how fast this variance decreases. More generally, one might ask how the distribution of $L_E/N^{1-1/d}$ behaves as $N \rightarrow \infty$. We are aware of only one result, by Rhee and Talagrand [16], showing that the probability of finding L_E with $|L_E - \langle L_E \rangle| > t$ is smaller than $K \exp(-t^2/K)$ for some K . Unfortunately this is not strong enough to give bounds on the variance.

Let us characterize the distribution at $d = 2$ by numerical simulation. For motivation, consider the analogy between $L_E/N^{1-1/d}$ and E/V , the energy density in a disordered statistical system. If the system's correlation length ξ is finite (the system is not critical), E/V has a distribution which becomes Gaussian when $V \rightarrow \infty$. This is because as the subvolumes increase, the energy densities in each subvolume become uncorrelated; the central limit theorem then applies. A consequence is that σ^2 , the variance of E/V , decreases as V^{-1} . If ξ is infinite (the system is critical), then in general the distribution of E/V is not Gaussian. In both cases though, the self-averaging of E/V suggests that the scaling variable $X = (E - \langle E \rangle)/\sigma V$ has a limiting distribution when $V \rightarrow \infty$.

In the case of the TSP, it can be argued using a theoretical analysis of the LK heuristic that at $d \geq 2$ the system is not critical. By analogy with E/V , if we take subvolumes to contain a fixed number of cities, the central limit theorem then suggests that $L_E/N^{1-1/d}$ has a Gaussian distribution with σ^2 decreasing as N^{-1} . The scaling variable $X_N = (L_E - \langle L_E \rangle)/N^{1/2-1/d}$ should consequently have a Gaussian distribution with a finite width for $N \rightarrow \infty$ (and at $d \geq 2$). Numerical results at $d = 2$ (see Fig. 4) give good support for this.

2.5. CONJECTURES ON THE LARGE d LIMIT. — In most statistical mechanics problems, the large dimensional limit introduces simplifications because fluctuations become negligible. For the TSP, can one expect $\beta_E(d)$ to have a simple limit as $d \rightarrow \infty$? Again, consider the property of the k th nearest neighbor distance D_k . In the large N limit, (11) gives

$$N\langle D_k(N, d) \rangle \sim N^{1-1/d} \frac{\Gamma(d/2 + 1)^{1/d}}{\sqrt{\pi}} \frac{\Gamma(k + 1/d)}{\Gamma(k)}, \text{ or at large } d, \quad (13)$$

$$\sim N^{1-1/d} \sqrt{\frac{d}{2\pi e}} (\pi d)^{1/2d} \left[1 + \frac{A_k}{d} + \dots \right], \quad (14)$$

where $A_k \equiv -\gamma + \frac{1}{k-1} + \frac{1}{k-2} + \dots$ (γ is Euler's constant). Notice that $A_k \sim \ln k$ at large k . This suggests strongly that unless the “typical” k used in the optimum tour grows exponentially in d , we may write for $d \rightarrow \infty$:

$$\beta_E(d) = \lim_{N \rightarrow \infty} \frac{\langle L_E(N, d) \rangle}{N^{1-1/d}} \sim \sqrt{\frac{d}{2\pi e}} (\pi d)^{1/2d} \left[1 + O\left(\frac{1}{d}\right) \right]. \quad (15)$$

Up to $O(1/d)$, this expression is identical to the BHH lower bound on $\beta_E(d)$ discussed in Section 2.1, given by the large N limit of $N^{1/d} \langle D_1(N, d) + D_2(N, d) \rangle / 2$.

A weaker conjecture than (15) has been proposed by Bertsimas and van Ryzin [17]:

$$\beta_E(d) \sim \sqrt{d/2\pi e} \text{ as } d \rightarrow \infty. \quad (16)$$

This limiting behavior was motivated by an analogous result for a related combinatorial optimization problem, the minimum spanning tree. Unfortunately, there is no proof of either (15) or (16); in particular, the upper bound on $\beta_E(d)$ given by strip, discussed in Section 2.1, behaves as $\sqrt{d/6}$ at large d . Thus if the conjectures are true, the strip construction leads asymptotically to tours which are on average 1.69 times too long. Can we derive stronger upper bounds? A number of heuristic construction methods should do better than strip, but there are no reliable calculations to this effect. The only improvements over the BHH results are due to Smith [18], who generalized the strip algorithm by optimizing the shape of the strips, leading to an upper bound which is $\sqrt{2}$ times greater than the predictions of (15) and (16) at large d .

In spite of our inability to derive an upper bound which, together with the BHH lower bound, would confirm the two conjectures for $d \rightarrow \infty$, we are confident that (15) and (16) are true because of non-rigorous yet convincing arguments. One is a proof that (16) is satisfied for the TSP if it is satisfied for another related combinatorial optimization problem (see Appendix D for details). A more powerful argument, presented in Section 3.6, relies on a theoretical analysis of the LK heuristic. It suggests that up to $O(1/d^2)$, $\beta_E(d)$ is given by a random link approximation, leading to a conjecture even stronger than (15).

3. The Random Link TSP

3.1. CORRESPONDENCE WITH THE EUCLIDEAN TSP. — Let us now consider a problem at first sight dramatically different from the Euclidean TSP. Instead of taking the positions of the N cities to be independent random variables, take the lengths $l_{ij} = l_{ji}$ between cities i and j ($1 \leq i, j \leq N$) to be independent random variables, identically distributed according to some $\rho(l)$. We speak of lengths rather than distances, as there is no distance metric here. This problem, introduced by physicists in the 1980s [19, 20] in search of an analytically tractable form of the traveling salesman problem, is called the *random link TSP*.

The connection between this TSP and the Euclidean TSP is not obvious, as we now have random links rather than random points. Nevertheless, one can relate the two problems. To see this, consider the probability distribution for the distance l between a fixed pair of cities (i,j) in the Euclidean TSP. This distribution, in the unit hypercube with periodic boundary conditions, is given for $0 \leq l \leq 1/2$ by the expression in (6):

$$\rho(l) = \frac{d \pi^{d/2}}{\Gamma(d/2 + 1)} l^{d-1} \quad (17)$$

Of course, in the Euclidean TSP the link lengths are by no means *independent* random variables: correlations such as the triangle inequality are present. However, as noted by Mézard and Parisi [3], correlations appear exclusively when considering three or more distances, since any two Euclidean distances are necessarily independent. Let us adopt (17) as the l_{ij} distribution in the limit of small l for the random link TSP, where d in this case no longer represents physical dimension but is simply a parameter of the model. The Euclidean and random link problems then have the same small l one- and two-link distributions. In the large N limit the random link TSP may therefore be considered, rather than as a separate problem, as a *random link approximation* to the Euclidean TSP. Only joint distributions of three or more links differ between these two TSPs. If indeed the correlations involved are not too important, then the random link $\beta_{\text{RL}}(d)$ can be taken as a good estimate of $\beta_E(d)$. We shall see that this is true, particularly for large d .

3.2. SCALING AT LARGE N . — As in the Euclidean case, we are interested in understanding the $N \rightarrow \infty$ scaling law in the random link TSP. It is relatively simple to see, following an argument similar to the one in Section 2.2, that the nearest neighbor distances D_k have a probability distribution with a scaling factor $N^{-1/d}$ at large N . Vannimenus and Mézard [20] have suggested that the random link optimum tour length with N links will then scale as $N^{1-1/d}$, and the tour will be self-averaging, i.e.,

$$\lim_{N \rightarrow \infty} \frac{L_{\text{RL}}}{N^{1-1/d}} = \beta_{\text{RL}}(d), \quad (18)$$

parallel to the BHH theorem (3) for the Euclidean case. This involves the implicit assumption that optimum tours sample a representative part of the D_k distribution, so no further N scaling effects are introduced. The assumption seems reasonable based on the analogy with the Euclidean TSP, and for our purposes we shall accept here that $\beta_{\text{RL}}(d)$ exists. However, there is to our knowledge no mathematical proof of self-averaging in the random link TSP.

Following the discussion of Section 2.1, let us consider some bounds on the ensemble average $\langle L_{\text{RL}} \rangle$ as derived in [20]. As before, we get a lower bound on $\beta_{\text{RL}}(d)$ using nearest and next nearest neighbor distances. For an upper bound, the “strip” algorithm used in the Euclidean case (Sect. 2.1) cannot be applied to the random link case. On the other hand, Vannimenus and Mézard make use of an algorithm called “greedy” [21]: this constructs a non-optimal tour by starting at an arbitrary city, and then successively picking the link to the nearest available city until all cities are used once and a closed tour is formed. At $d > 1$, greedy gives rise to tour lengths that are self-averaging, and leads to the upper bound [20]

$$\beta_{\text{RL}}(d) \leq \frac{1}{\sqrt{\pi}} \frac{\Gamma(d/2 + 1)^{1/d} \Gamma(1/d)}{d - 1} \quad (19)$$

At $d = 1$, the presumed scaling (18) suggests that $\langle L_{\text{RL}} \rangle$ is independent of N , whereas greedy generates tour lengths which grow as $\ln N$. There is numerical evidence [4, 22], however, that the $d = 1$ model does indeed satisfy (18), and that $\beta_{\text{RL}}(1) \approx 1.0208$.

3.3. SOLUTION via THE CAVITY EQUATIONS. — Since the work of Vannimenus and Mézard, several groups [23–25] have tried to “solve” the statistical mechanical problem of the random link TSP at finite temperature using the replica method, a technique developed for analyzing disordered systems such as spin glasses [26]. To date, it has only been possible to obtain part of the high temperature series of this system [23]. In view of the intractability of these replica approaches, Mézard and Parisi have derived an analytical solution using another technique from spin glass theory, the “cavity method”. The details of this approach are beyond the scope of this paper, and are discussed in several technical articles [3, 26, 27]. For readers acquainted with the language of disordered systems, however, the broad outline is as follows: one begins with a representation of the TSP in terms of a Heisenberg (multi-dimensional spin) model in the limit where the spin dimension goes to zero. Under the assumption that this system has only one equilibrium state (no replica symmetry breaking), Mézard and Parisi have then written a recursion equation for the system when a new $(N + 1)$ th spin is added. The cavity method then supposes that this new spin’s effect on the N other spins is negligible in the large N limit, and that its magnetization may be expressed in terms of the magnetizations of the other spins.

Using this method, Krauth and Mézard have derived a self-consistent equation for the random link TSP, at $N \rightarrow \infty$ [4]. They have determined the probability distribution of link lengths in the optimum tour in terms of $\mathcal{G}_d(x)$, where $\mathcal{G}_d(x)$ is the solution to the integral equation

$$\mathcal{G}_d(x) = \int_{-x}^{+\infty} \frac{(x+y)^{d-1}}{\Gamma(d)} [1 + \mathcal{G}_d(y)] e^{-\mathcal{G}_d(y)} dy. \quad (20)$$

Their probability distribution leads to the prediction

$$\beta_{RL}(d) = \frac{d}{2\sqrt{\pi}} \left[\frac{\Gamma(d/2 + 1)}{\Gamma(d + 1)} \right]^{1/d} \int_{-\infty}^{+\infty} \mathcal{G}_d(x) [1 + \mathcal{G}_d(x)] e^{-\mathcal{G}_d(x)} dx. \quad (21)$$

These equations can be solved numerically, as well as analytically in terms of a $1/d$ power series (see next section). At $d = 1$, Krauth and Mézard compared their prediction with the results of a direct simulation of the random link model; their numerical study [4, 22] strongly suggests that the cavity prediction is exact in this case. It has been argued, furthermore, that the cavity method is exact at $N \rightarrow \infty$ for *any* distribution of the independent random links [26]. Good numerical evidence has been found for this, notably in the case of the matching problem, a related combinatorial optimization problem [28]. The validity of the cavity assumptions therefore does not appear to be sensitive to the dimension d , and we shall assume that (21) holds for the random link TSP at all d .

Krauth and Mézard computed the $d = 1$ and $d = 2$ cases to give $\beta_{RL}(1) = 1.0208$ and $\beta_{RL}(2) = 0.7251$. Since $\beta_{RL}(d)$ is taken to approximate $\beta_E(d)$, let us compare these values with their Euclidean counterparts. At $d = 1$, the Euclidean TSP with periodic boundary conditions is trivial ($\beta_E(1) = 1$); the random link TSP thus has a 2.1% relative excess. At $d = 2$, comparing with $\beta_E(2) = 0.7120$ found in Section 2.3, the random link TSP has a 1.8% excess. In low dimensions, the random link results are then a good approximation of the Euclidean results. The approximation is better than Krauth and Mézard believed, since they made the comparison at $d = 2$ using the considerably overestimated Euclidean value of $\beta_E(2) \approx 0.749$ from [5].

Extending the numerical solutions to higher dimensions, at $d = 3$ we find $\beta_{RL}(3) = 0.7100$, which compared with $\beta_E(3) = 0.6979$, has an excess of 1.7%. Some further random link values are $\beta_{RL}(4) = 0.7322$ and $\beta_{RL}(5) = 0.7639$. The value at $d = 4$ may be compared with the Euclidean estimate of Johnson *et al.* [15], $\beta_E(4) \approx 0.7234$, giving an excess of 1.2%. The $\beta_E(d)$ data at $d = 1, 2, 3, 4$ therefore suggest that the random link approximation improves with increasing dimension. This leads us to study the limit when d becomes large.

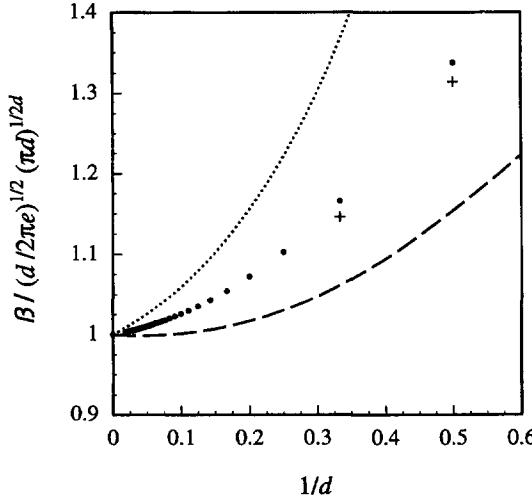


Fig. 5. — Dimensional dependence of rescaled random link TSP optimum, shown by small points, between converging “greedy” upper bound (dotted line) and nearest-neighbors lower bound (dashed line). Plus signs at $d = 2$ and $d = 3$ show Euclidean results for comparison.

3.4. DIMENSIONAL DEPENDENCE. — The large d limit was considered by Vannimenus and Mézard [20]. For $\beta_{RL}(d)$, the lower bound obtained from $(D_1(N, d) + D_2(N, d))/2$ by way of (11) and the upper bound given in (19) differ at large d only by $O(1/d)$, giving:

$$\beta_{RL}(d) = \sqrt{\frac{d}{2\pi e}} (\pi d)^{1/2d} \left[1 + O\left(\frac{1}{d}\right) \right]. \quad (22)$$

Note that this *exact* result is the random link analogue of the Euclidean conjecture (15).

For values of $d \leq 50$, we have calculated $\beta_{RL}(d)$ numerically using the cavity equations (20,21). The results are shown in Figure 5, along with the converging upper and lower bounds, and our low d Euclidean results.

For large d , we may see whether the cavity equations are compatible with (22) by solving them analytically in terms of a $1/d$ power series. Define $\tilde{\mathcal{G}}_d(x) \equiv \mathcal{G}_d(\Gamma(d+1)^{1/d} [1/2 + x/d])$. (20) may then be written:

$$\tilde{\mathcal{G}}_d(x) = \int_{-x-d}^{+\infty} \left(1 + \frac{x+y}{d}\right)^{d-1} \left[1 + \tilde{\mathcal{G}}_d(y)\right] e^{-\tilde{\mathcal{G}}_d(y)} dy \quad (23)$$

$$= \int_{-x-d}^{+\infty} e^{x+y} \left[1 - \frac{1}{d} \left(x+y + \frac{(x+y)^2}{2}\right) + O\left(\frac{1}{d^2}\right)\right] \left[1 + \tilde{\mathcal{G}}_d(y)\right] e^{-\tilde{\mathcal{G}}_d(y)} dy. \quad (24)$$

Strictly speaking, the expansion of $(1 + [x+y]/d)^{d-1}$ is only valid in the interval $-x - d < y < -x + d$; however, for large y it can be shown that $\tilde{\mathcal{G}}_d(y) \sim y^d$, so the $e^{-\tilde{\mathcal{G}}_d(y)}$ term in the integrand makes the $y > -x + d$ contribution exponentially small in d .

Furthermore, extending the integral's lower limit to include the region $y < -x - d$ also contributes a remainder term exponentially small in d . If we write the integral with its lower

limit at $y = -\infty$, the equation may be solved:

$$\begin{aligned}\tilde{\mathcal{G}}_d(x) &= \sqrt{2}e^x \left[1 - \frac{1}{d} \left(\frac{x^2}{2} + x \frac{3 - \ln 2 - 2\gamma}{2} - \frac{(\ln 2 + 2\gamma)^2 + 6\ln 2 + 12\gamma - 9}{8} \right) \right. \\ &\quad \left. + O\left(\frac{1}{d^2}\right) \right],\end{aligned}\tag{25}$$

where γ , we recall, represents Euler's constant. Using (21), we then find

$$\beta_{\text{RL}}(d) = \sqrt{\frac{d}{2\pi e}} (\pi d)^{1/2d} \left[1 + \frac{2 - \ln 2 - 2\gamma}{d} + O\left(\frac{1}{d^2}\right) \right],\tag{26}$$

which is perfectly compatible with (22). This provides further evidence that the cavity method is exact for the random link TSP.

3.5. RENORMALIZED RANDOM LINK MODEL AT LARGE d . — We can motivate the large d scaling found in the previous section by examining a different sort of random link TSP. Consider a new “renormalized” model where link “lengths” x_{ij} are obtained from the original l_{ij} by the linear transformation $x_{ij} \equiv d[l_{ij} - \langle D_1(N, d) \rangle]/\langle D_1(N, d) \rangle$. Note that the x_{ij} may take on negative values, and that the nearest neighbor length in this new model has mean zero. Since the transformation is linear, there is a direct equivalence between the renormalized x_{ij} and original l_{ij} TSPs, and the two have the same optimum tours. The renormalized optimum tour length L_x may then be given in terms of the original tour length L_l by

$$L_x = d \frac{L_l - N\langle D_1(N, d) \rangle}{\langle D_1(N, d) \rangle}\tag{27}$$

Now take $N \rightarrow \infty$ and $d \rightarrow \infty$. It may be seen from the l_{ij} distribution (17) and the $\langle D_1(N, d) \rangle$ expansion (14) that the random variables x_{ij} have the d -independent probability distribution $\rho(x) \sim N^{-1} \exp(x - \gamma)$. Also, in the large N limit, since L_l scales as $N^{1-1/d}$ and $\langle D_1 \rangle$ scales as $N^{-1/d}$, we expect $\langle L_x \rangle \sim N\mu$ for some μ which must be, like $\rho(x)$, independent of d . Then, from (27), the TSP in the original l_{ij} variables satisfies

$$\langle L_l \rangle \sim N\langle D_1(N, d) \rangle \left[1 + \frac{\mu}{d} + O\left(\frac{1}{d^2}\right) \right],\tag{28}$$

or, using the expansion (14),

$$\beta_{\text{RL}}(d) = \sqrt{\frac{d}{2\pi e}} (\pi d)^{1/2d} \left[1 + \frac{\mu - \gamma}{d} + O\left(\frac{1}{d^2}\right) \right].\tag{29}$$

This result may be compared with our cavity solution of (26), where the $1/d$ coefficient is equal to $2 - \ln 2 - 2\gamma$. If the cavity method is correct at $O(1/d)$, which we strongly believe is the case, then a direct solution of the renormalized model should give $\mu = 2 - \ln 2 - \gamma$. Work is currently in progress to test this claim by numerical methods.

3.6. LARGE d ACCURACY OF THE RANDOM LINK APPROXIMATION. — Since the random link model is considered to be an approximation to the Euclidean case, it is natural to ask whether the approximation becomes exact as $d \rightarrow \infty$. In this section we argue that: (i) in stochastic TSPs, good tours can be obtained using almost exclusively low order neighbors; (ii) the geometry inherent in the Euclidean TSP leads to $\beta_E(d) \leq \beta_{\text{RL}}(d)$ in all dimensions d ;

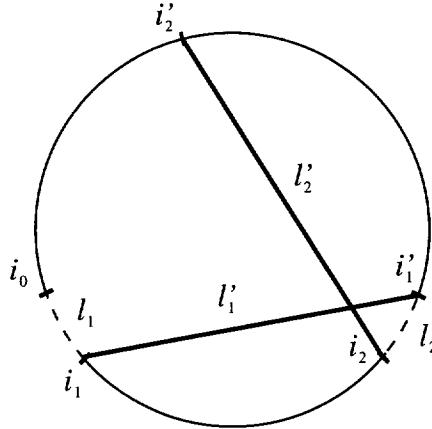


Fig. 6. — Recursive construction of removed links (dashed lines) and added links (bold lines) in an LK search.

(iii) the relative error of the random link approximation decreases as $1/d^2$ at large d . All three claims are based on a theoretical analysis of the Lin-Kernighan (LK) heuristic algorithm for constructing near-optimal tours.

The LK algorithm works as follows [1,29]. An *LK search* starts with an arbitrary tour. The principle of the search is to substitute links in the tour recursively, as illustrated schematically in Figure 6. The first step consists of choosing an arbitrary starting city i_0 . Call i_1 the next city on the tour, and l_1 the link between the two. Now remove this link. Let i'_1 be the nearest neighbor to i_1 that was not connected to i_1 on the original tour, and let l'_1 be a new link connecting i_1 to i'_1 . We now have not a tour but a “tadpole graph”, containing a loop with a tail attached to it at i'_1 . At this point, call i_2 one of the cities next to i'_1 on the original tour, and remove the link l_2 between the two. There are two possibilities for i_2 (and thus l_2): LK chooses the one which, if we were to put in a new link between i_2 and i_0 , would give a single closed tour. Now as before, let i'_2 be the nearest neighbor of i_2 that was not connected to i_2 on the original tour, and let l'_2 be a new link between the two. This gives a new tadpole. The process continues recursively in this manner, with the vertex hopping around while the end point stays fixed, until no new tadpoles are found. At each step, LK chooses the new i_m so as to allow the path to be closed up between i_m and i_0 , forming a single tour; the result of the LK search is then the best of all such closed up tours. The *LK algorithm* consists of repeating these LK searches on different starting points i_0 , each time using the current best tour as a starting tour, until no further tour improvements are possible.

Let us first sketch why the LK algorithm leads to tours which use only links between “near” neighbors, where “near” means that the neighborhood order k is small and does not grow with d . Consider any tour where a significant fraction of the links connect distant neighbors (large k). The links l'_m which the LK search substitutes for the l_m are, by definition, between very near neighbors ($k \leq 3$). As long as many long links exist, the probability at each step of substituting a near neighbor in place of a far neighbor is significant. Towards the beginning of an LK search this probability is relatively constant, so the *expected* tadpole length will decrease linearly with the number of steps. Even taking into account the fact that closing up the path between i_m and i_0 might require inserting a link with $k > 3$, there is a high probability as $N \rightarrow \infty$ that the improvement in tadpole length far outweighs this cost of closing the tour. Thus for stochastic TSPs, regardless of d , the LK algorithm can at large N replace all but a

tiny fraction of the long links with short links. It follows that in accordance with our Euclidean TSP assumption of Section 2.5, the “typical” k used in the optimum tour remains small at large d . This provides very powerful support for the $\beta_E(d)$ conjectures (15) and (16). A consequence, making use of the exact asymptotic $\beta_{RL}(d)$ result (22), is that the relative difference between $\beta_E(d)$ and $\beta_{RL}(d)$ is at most of $O(1/d)$.

Our second argument concerns why $\beta_{RL}(d)$ must be greater than $\beta_E(d)$ at all d . For the random link TSP there is no triangle inequality, which means that given two edges of a triangle, the third edge is on average longer than it would be for the Euclidean TSP. Applying this to our LK search, we can expect the link between ι_m and ι_0 closing up the tour to be longer in the random link case than in the Euclidean case. Thus on average, the LK algorithm will find longer random link tours than Euclidean tours. In fact, this property holds as well for any LK-like algorithm where the method of choosing the l_m and l'_m links is generalized. If the algorithm were to allow *all* possibilities for l_m and l'_m , we would be sure of obtaining the exact optimum tour, given a long enough search. In that case, the inequality on the tour lengths found by our algorithm leads directly to $\beta_{RL}(d) > \beta_E(d)$. Not surprisingly, the numerical data confirm this inequality at d up to 4 (although one should be cautious when applying the argument at $d = 1$). Note also that the inequality in itself implies conjectures (15) and (16) for the Euclidean model, since it supplies precisely the upper bound we need on $\beta_E(d)$.

Finally let us explain why the relative difference between $\beta_{RL}(d)$ and $\beta_E(d)$ should be of $O(1/d^2)$. This involves quantifying the tour length improvement discussed above. It is clear that any non-optimal tour can be improved to the point where links are mostly between neighbors of low order. If LK, or a generalized LK-like algorithm, is able to improve the tour further, the relative difference in length will be of $O(1/d)$; we see this from (14), noting that the neighborhood order k is small both before and after the LK search. Now we need to quantify the *probability* that LK indeed succeeds in improving the tour. We may consider the vertex of the LK tadpole graph as executing a random walk, in which case the probability of closing up a tour by a sufficiently short link is equivalent to the probability of the random walk’s end-to-end distance being sufficiently small. In that case it may be shown that, over the course of an LK search, the probability of successfully closing a random link tour minus the probability of successfully closing a Euclidean tour scales at large d as $2/(d - 2)$. From this, we conclude that improvements in the Euclidean model are $O(1/d)$ more probable than in the random link model. Now, the relative tour length improvement for the Euclidean TSP compared to the random link TSP is simply the relative tour length improvement *when a better tour is found*, times the probability of finding a better tour — hence $O(1/d^2)$. If we consider a generalized LK search as described in the previous paragraph, where the algorithm necessarily finds the true optimum, then this result applies to the exact β ’s: the relative difference between $\beta_{RL}(d)$ and $\beta_E(d)$ will scale at large d as $1/d^2$.

Three comments are in order concerning this surprisingly good accuracy of the random link approximation. First, the factor $2/(d - 2)$ is only appropriate for large d . It is not small even for $d = 4$. (Its divergence at $d = 2$ is associated with the fact that a two-dimensional random walk returns to its origin with probability 1.) We therefore expect the $1/d^2$ scaling to become apparent only for $d \geq 5$, beyond the range of our numerical data. Second, we have seen that the coefficient of the $1/d$ term in $\beta_{RL}(d)$ may be obtained by the cavity method. Assuming that this method is correct and that $\beta_{RL}(d)$ and $\beta_E(d)$ do indeed converge as $1/d^2$, this leads to a particularly strong conjecture for the Euclidean TSP:

$$\beta_E(d) = \sqrt{\frac{d}{2\pi e}} (\pi d)^{1/2d} \left[1 + \frac{2 - \ln 2 - 2\gamma}{d} + O\left(\frac{1}{d^2}\right) \right]. \quad (30)$$

Third, this type of LK analysis can in fact be extended to many other combinatorial optimization problems, such as the assignment, matching and bipartite matching problems. In these cases, we expect the random link approximation to give rise to a $O(1/d^2)$ relative error just as in the TSP.

4. Summary and Conclusions

The first goal in our work has been to investigate the finite size scaling of L_E , the optimum Euclidean traveling salesman tour length, and to obtain precise estimates for its large N behavior. Motivated by a remarkable universality in the k th nearest neighbor distribution, we have found that under periodic boundary conditions, the convergence of $\langle L_E \rangle / N^{1-1/d}$ to its limit $\beta_E(d)$ is described by a series in $1/N$. This has enabled us to extract $\beta_E(2)$ and $\beta_E(3)$ using numerical simulations at small values of N , where errors are easy to control. Furthermore, thanks to a bias-free variance reduction method (see Appendix B), these estimates are extremely precise.

Our second goal has been to examine the random link TSP, where there are no correlations between link lengths. We have considered it as an approximation to the Euclidean TSP, in order to understand better the dimensional scaling of $\beta_E(d)$. For small d , we have used the cavity method to obtain numerical values of the random link $\beta_{RL}(d)$. Comparing these with our numerical values for $\beta_E(d)$ shows that the random link approximation is remarkably good, accurate to within 2% at low dimension. For large d , we have solved the cavity equations analytically to give $\beta_{RL}(d)$ in terms of a $1/d$ series. We have then argued, using a theoretical analysis of iterative tour improvement algorithms, that the relative difference between $\beta_{RL}(d)$ and $\beta_E(d)$ decreases as $1/d^2$. This leads to our conjecture (30) on the large d behavior of $\beta_E(d)$, specifying both its asymptotic form and its leading order correction.

Let us conclude with some remaining open questions. First of all, while the cavity method most likely gives the exact result for the random link TSP, we would be interested in seeing this argued on a more fundamental physical level. Readers with a background in disordered systems will recognize that the underlying assumption of a unique equilibrium state is false in many NP-complete problems, and in particular in the spin-glass problem that has inspired the cavity method. What makes the TSP different? Second of all, our renormalized random link model provides an alternate approach to finding the $1/d$ coefficient of the power series in $\beta_{RL}(d)$, and could prove a useful test of the cavity method's validity. A solution to the renormalized model using heuristic methods appears within reach. Third of all, the $O(1/d^2)$ convergence of the random link approximation merits further study, from both numerical and analytical perspectives. Numerically, Euclidean simulations at $d \geq 5$ could provide powerful support for the form of the convergence, and thus for our conjecture (30). Analytically, the qualitative arguments presented in Section 3.6, based on the LK algorithm, could perhaps be refined by a more quantitative approach. Lastly, it is worth noting that the $O(1/d^2)$ convergence should apply equally well to the *distribution* of link lengths in the optimum tour. The random link prediction for this distribution can be obtained from the cavity method [4]; an interesting test would then be to compare it with simulation results for the true Euclidean distribution.

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Appendix A

Overview of the Numerical Methodology

In the following, we discuss the procedures used to obtain the raw data from which $\beta_E(d)$ and the finite size scaling coefficients are extracted. Two major problems must be solved in order to get good estimates of $\beta_E(N, d)$. First, $\beta_E(N, d)$ is defined as an ensemble average $\langle L_E(N, d) \rangle / N^{1-1/d}$, but is measured by a numerical average over a finite sample of instances. The instance-to-instance fluctuations in L_E give rise to a statistical error, which decreases only as the inverse square root of the sample size. Keeping the statistical error down to acceptable levels could require inordinate amounts of computing time. We therefore find it useful to introduce a variance reduction trick: instead of measuring L_E , we measure $L_E - \lambda L^*$, where λ is a free parameter and L^* can be any quantity which is strongly correlated with L_E . Details are given in Appendix B.

A second and more basic problem is that it is computationally costly to determine the optimal tour lengths for a large number of instances, precisely because the TSP is an NP-complete problem. The most sophisticated “branch and cut” algorithms can take minutes on a workstation to solve a single instance of size $N \leq 100$ to optimality. However, we do not need to guarantee optimality: the statistical error in $\beta_E(N, d)$ already limits the quality of our estimate, and so an additional (systematic) error in L_E is admissible as long as it is negligible compared to the statistical error. We may thus use fast heuristics to measure L_E , rather than exact but slower algorithms. This is discussed further in Appendix C.

Appendix B

Statistical Errors and a Variance Reduction Trick

Consider estimating $\langle L_E(N, d) \rangle$ at a given N by sampling over many instances. If we have M independent instances, the simplest estimator for $\langle L_E(N, d) \rangle$ is $\overline{L_E(N, d)}$, the numerical average over the M instances of the minimum tour lengths. This estimator has an expected statistical error $\sigma(M) = \sigma_{L_E} / \sqrt{M}$, where σ_{L_E} is the instance-to-instance standard deviation of L_E .

Now let us define L_k to be the sum, over all cities, of k th nearest neighbor distances. $\langle L_k \rangle$ is its ensemble average; in terms of the notation used earlier in the text, $\langle L_k \rangle = N \langle D_k \rangle$. It has been noted by Sourlas [30] that L_E is strongly correlated with L_1 , L_2 and L_3 . He therefore suggested reducing the statistical error in $\langle L_E \rangle$ using the estimator

$$E_S = \langle L_{123} \rangle \overline{L_E / L_{123}}, \quad (\text{B.1})$$

where L_{123} is the arithmetic mean of L_1 , L_2 and L_3 . The ensemble average $\langle L_{123} \rangle$ can be calculated analytically from (11), and so the variance of E_S comes from fluctuations in the ratio L_E / L_{123} . If L_E were a constant factor times L_{123} , this estimator would of course be perfect, *i.e.*, it would have zero variance. This is not the case, however, and furthermore the use of a ratio biases the Sourlas estimator: its true mathematical expectation value differs from $\langle L_E(N, d) \rangle$ by $O(1/N)$. To improve upon this, we have introduced our own bias-free estimator [31]:

$$E_{M-P} = \lambda \langle L_{12} \rangle + \overline{L_E - \lambda L_{12}}, \quad (\text{B.2})$$

where L_{12} is the arithmetic mean of L_1 and L_2 , and λ is a free parameter. Our estimator has a reduced variance because L_E and L_{12} are correlated. It is easy to show that the variance

of E_{M-P} is minimized at a unique value of λ , $\lambda^* = C(L_E, L_{12})\sigma_{L_E}/\sigma_{L_{12}}$, where $C(A, B) \equiv \langle (A - \langle A \rangle)(B - \langle B \rangle) \rangle / \sigma_A \sigma_B$ is the correlation coefficient of A and B . The variance then becomes $\sigma_{L_{M-P}}^2 = \sigma_{L_E}^2 [1 - C^2(L_E, L_{12})]/M$. Empirically, we have found this variance reduction procedure to be quite effective, since $\sqrt{1 - C^2} \approx 0.38$ at $d = 2$ and $\sqrt{1 - C^2} \approx 0.31$ at $d = 3$. The statistical error is thus reduced by about a factor of 3; this means that for a given error, computing time is reduced by about a factor of 10.

Appendix C

Control of Systematic Errors

Our procedure for estimating L_E at a given instance involves running a good heuristic m times from random starts on that instance, and taking the best tour length found in those m trials. The expected systematic error can be found from the frequencies with which each local optimum appears in a large number of test trials. (This large number must be much greater than m , the actual number of trials used in production runs.) The measurement is performed on a sufficiently large sample of instances, from which we extract the *average* size of the systematic error in $\langle L_E(N, d) \rangle$ as a function of m . We have found that in practice, this error is dominated by those infrequent instances where a sub-optimal tour is obtained with the highest frequency.

As N increases, the probability of not finding the true optimum increases rather fast; for a given heuristic, it is thus necessary to increase m with N in such a way that the systematic error remains much smaller than the statistical error. If the heuristic is not powerful enough, m will be too large for the computational resources. For our purposes, we have found that the Lin-Kernighan heuristic [1] is powerful enough for the smaller values of N ($N \leq 17$). For $20 \leq N \leq 100$, it was more efficient to switch to Chained Local Optimization (CLO) [2, 32], a more powerful heuristic which can be thought of as a generalization of simulated annealing. (When the temperature parameter is set to zero so that no up-hill moves are accepted, as was the case for our runs, CLO with embedded Lin-Kernighan is called "Iterated Lin-Kernighan" [33, 34].) With these choices, using in two dimensions $m = 10$ for $N \leq 17$ (LK), $m = 5$ for $N = 30$ and $m = 20$ for $N = 100$ (CLO), we have kept systematic errors to under 10% of the statistical errors.

Appendix D

Bounding $\beta_E(d)$ using the Bipartite Matching Problem

Given two sets of N points P_1, \dots, P_N and Q_1, \dots, Q_N in d -dimensional Euclidean space, the bipartite matching (BM) problem asks for the minimum matching cost L_{BM} between the P_i 's and the Q_i 's, with the constraint that only links of the form $P - Q$ are allowed. The cost of a matching is equal to the sum of the distances between matched pairs of points. When points P_i and Q_j are chosen at random in a d -dimensional unit hypercube, it is natural to expect $L_{BM}/N^{1-1/d}$ to be self-averaging as $N \rightarrow \infty$. To date, a proof of this property has not been given, even though the self-averaging of the analogous quantity in the more general matching problem (where links $P - P$ and $Q - Q$ are allowed as well) can be shown at all d in essentially the same way as for the TSP, following arguments developed by Steele [7]. For $d = 1$, it is in fact known that self-averaging *fails* in the BM. For large d , however, let us assume that $L_{BM}/N^{1-1/d}$ does converge to some $\beta_{BM}(d)$ in the large N limit.

We shall now derive a bound for the Euclidean TSP constant $\beta_E(d)$ in terms of $\beta_{BM}(d)$. Consider K disjoint sets S_1, \dots, S_K , together forming a large set $S \equiv S_1 \cup \dots \cup S_K$, and let each S_i contain N random points in the d -dimensional unit hypercube. Construct the K minimum matchings $S_1 - S_2, S_2 - S_3, \dots, S_{K-1} - S_K$ and $S_K - S_1$. Starting at any point in S_1 , generate a loop (a closed path) in S by following the matchings $S_1 - S_2, S_2 - S_3, \dots$ until the path returns to its starting point. The set of all such distinct loops $\Omega_1, \dots, \Omega_M$ ($M \leq N$) is then equivalent to the set S , and furthermore the sum of the loop lengths is equal to the sum of all minimum matchings costs $(L_{BM})_{S_i-S_{i+1}}$. (Note that $(L_{BM})_{S_K-S_1}$ is defined as $(L_{BM})_{S_K-S_1}$.)

Now, consider the optimum TSP tour through all the points of S_1 . Construct a giant closed path visiting every point in S at least once, by substituting into this TSP tour the loops $\Omega_1, \dots, \Omega_M$ in place of their starting points in S_1 . Using standard techniques [6], we can construct from this path of length $(K+1)N$ a shorter closed path of length KN which visits every point in S exactly once. For the Euclidean TSP tour length L_E , we then obtain the inequality

$$(L_E)_S \leq (L_E)_{S_1} + \sum_{i=1}^K (L_{BM})_{S_i-S_{i+1}}. \quad (\text{D.1})$$

If S consists of random points chosen independently and uniformly in the unit hypercube, then averaging over all configurations, dividing by $N^{1-1/d}$ and taking the limit $N \rightarrow \infty$, we find

$$K^{1-1/d} \beta_E(d) \leq \beta_E(d) + K \beta_{BM}(d). \quad (\text{D.2})$$

Letting $K = d$, this gives in the large d limit $\beta_E(d) \leq \beta_{BM}(d)$. Based on analogies with other combinatorial optimization problems [17], $\beta_{BM}(d)$ is expected to scale as $\sqrt{d/2\pi e}$ when $d \rightarrow \infty$. In that case, $\beta_E(d)$ too must satisfy the Bertsimas-van Ryzin conjecture (16).

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