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On the statistical mechanics of optimization problems of the travelling salesman type

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Résumé. — Nous montrons qu'il existe deux régimes très différents en température pour les problèmes du type voyageur de commerce, et que l'approximation recuite est correcte dans le régime de haute température. Nous introduisons des modèles de liaisons aléatoires et obtenons des bornes inférieure et supérieure pour leur énergie libre, dans le régime basse température. Nous présentons un modèle soluble, qui possède une transition de phase rappelant fortement la transition verre de spin.

Abstract. — We show that two very different temperature regimes exist for problems of the travelling salesman type, and that the annealed approximation is valid for the high-temperature regime. Random-link models are introduced, for which upper and lower bounds on the free energy are obtained in the low-temperature regime. A soluble model is presented, which possesses a phase transition strongly reminiscent of the spin-glass transition.

1. Introduction.

The travelling salesman problem [1, 2] consists in finding the shortest closed path through N given points and is a standard example of hard combinatorial optimization problems : the number of possible tours is finite but it increases very rapidly with the size N , and known algorithms which find the optimal tour in all cases need a time which increases exponentially with N [2]. In similar problems encountered in practical situations, e.g., in computer engineering, N is large and the time necessary to find the best solution becomes prohibitive. One then looks for algorithms which give a near-optimal solution in practically all situations in an acceptable time.

For several years, S. Kirkpatrick has advocated the use of statistical mechanics tools for the study of such problems [3]. A breakthrough in this area came with the adaptation to opti-

mization problems of the probabilistic Metropolis algorithm used in Monte-Carlo methods [4]. This approach introduces a « temperature » and a « partition function » in a way that closely follows the introduction of the canonical ensemble in statistical mechanics. The energy of a configuration corresponds to the length of a tour, the phase space is the space of all possible tours, the ground state corresponds to the optimal tour. The Monte-Carlo moves are given by Lin's two-bond rearrangements [5], and a suitable cooling procedure is followed to reach a tour of near-optimal length. This allows the system to escape trapping in a metastable state which is a local minimum for two-bond transformations (two-opt state).

In order to take full advantage of this method, it is necessary to study the connection between optimization problems and statistical mechanics in greater detail. In particular, it is important to know whether a phase transition occurs when the temperature is lowered, and to elucidate the structure of the phase space. This structure has been recently studied by Kirkpatrick and Toulouse [6], who have emphasized the deep analogy with spin glasses. More generally, some of the powerful methods of modern statistical mechanics may provide new insights and results in an area of considerable practical interest, e.g., in computer wiring and in electronic circuit design [3, 7].

In the present Letter, we study some properties of the partition function for models of the travelling salesman type. There exist two very different regimes in temperature for these models, where the thermodynamic quantities (e.g., the average length of a tour) scale differently with N . Exact results can be obtained in the high-temperature regime, but the most interesting regime is the low-temperature one. There the problem can be formulated in terms of statistical mechanics and is very reminiscent of spin glasses.

We exhibit a particular model which we can solve exactly. We obtain the free energy at all temperatures, hence the exact asymptotic behaviour of the optimal length, and we show that there is a phase transition in the low-temperature regime.

2. Statistical mechanics formulation.

We introduce a generalized travelling salesman problem (T.S.P.) where one is given N points $i = 1, \dots, N$, and a matrix of distances l_{ij} between them. The problem is to find the « tour » P of the shortest length L_P , where P is any permutation of N objects and

$$L_P = \sum_{i=1}^N l_{P(i)P(i+1)} \quad (1)$$

with $P(N+1) = P(1)$.

In the most studied T.S.P. (random-point problem), the positions of the points \mathbf{x}_i are chosen at random independently in some portion of a D -dimensional space, and $l_{ij} = l_{ji} = \sqrt{(\mathbf{x}_i - \mathbf{x}_j)^2}$. In the following we shall also study another version (the random-link problem) where the lengths $l_{ij} = l_{ji}$ are independent random variables, with a distribution $\rho(l)$. This is an equally interesting model, which is technically somewhat simpler since one can neglect the triangular correlations introduced by Euclidean distances. The case where $\rho(l)$ is constant for $0 \leq l \leq 1$ has been studied by Kirkpatrick and Toulouse [6].

Let us briefly recall how the T.S.P. can be formulated as a statistical mechanics problem :

- a configuration is a permutation P of the N points. (Actually there are $(N-1)!/2$ configurations since the starting point and the direction of a tour are irrelevant.)
- the energy of configuration P is its length L_P
- the partition function Z is naturally defined as

$$Z = \sum_P e^{-\beta L_P}, \quad (2)$$

where $\beta = 1/T$ is the inverse temperature

— for a given matrix $\{l_{ij}\}$, we are interested in the behaviour of the average tour length L as a function of temperature :

$$L(T) = - \frac{\partial \ln Z}{\partial \beta}, \quad (3)$$

and in the length L_{\min} of the optimal tour, which is the zero temperature limit of the free energy :

$$L_{\min} \equiv \text{Min}_P L_P = \lim_{T \rightarrow 0} L(T) = \lim_{T \rightarrow 0} - T \ln Z \quad (4)$$

— the entropy S is defined, as usual, from the derivative of the free energy $F = - T \ln Z$:

$$S(T) \equiv - \frac{\partial F}{\partial T} = \ln Z + \beta L(T). \quad (5)$$

An important question which we shall discuss in the following is the way $L(T)$ scales with N , when $N \rightarrow \infty$. In the random-point model, one usually chooses the N points in a cube of fixed volume $V = a^D$ of a D -dimensional space. One expects *a priori* two regimes of temperature :

— at high temperature (regime \mathcal{K}), one can forget about the Boltzmann weights in (2), any permutation is equally probable, hence $L \sim Na$.

— at low temperature (regime \mathcal{L}), the average length L of the tours should be of the order of N times the average distance between two neighbouring cities :

$$L \sim N \left(\frac{V}{N} \right)^{1/D} \sim N^{1-1/D} a. \quad (6)$$

(Rigorous bounds for L_{\min} with a $N^{1-1/D}$ behaviour have been given by Beardwood *et al.* [1].)

A similar scaling can be recovered in the independent-link model, provided the short-distance behaviour of the distribution $\rho(l)$ is $\rho(l) \sim l^{D-1}$. For this reason, we shall consider the family of independent-link T.S.P. with distributions

$$\rho_r(l) = \frac{l^r e^{-l}}{r!}, \quad (7)$$

with results which map on the D -dimensional random-point model (as far as the scaling in N is concerned) through the identification $r \rightarrow D - 1$.

In the following we shall make clear what is meant by high and low temperature in this discussion, and why the behaviour of $L(T)$ is so different in the regimes \mathcal{K} and \mathcal{L} .

3. The annealed approximation.

It is well known in the statistical mechanics of disordered systems that extensive thermodynamic quantities (free energy, internal energy, ...) are « self-averaging », which means that they have a fixed (sample independent) limiting behaviour in the thermodynamic limit ⁽¹⁾. This behaviour can then be obtained by taking the so-called « quenched » average of the free energy F over the

⁽¹⁾ The self-averageness of for instance the average length $L(T)$ in T.S.P.'s is not obvious, but there are strong indications that this property holds at least in the \mathcal{L} regime of the random-point models :

— the self averageness of L_{\min} is proven in [1];

$L(T)$ is extensive since the \mathcal{L} regime can be studied by working at a fixed density of points $\rho = N/V$, while taking $N \rightarrow \infty$.

disorder (here the values of the matrix elements l_{ij}), which we denote by $\langle F \rangle$. The minimal length (whose self-averageness was proven in [1]) is thus obtained as

$$L_{\min} = \lim_{T \rightarrow 0} - T \langle \ln Z \rangle. \quad (8)$$

As Z itself is in general not self-averaging, the quenched average $\langle \ln Z \rangle$ is different from the « annealed » one $\ln \langle Z \rangle$, and much harder to compute [8]. The annealed average is sometimes used as an approximation which is often rather crude. It has been recently observed by Bonomi and Lutton [9] and by Kirkpatrick [10] that the two averages give very similar numerical results for the random-point T.S.P. in two dimensions, except at very low temperatures. This interesting fact was one of the motivations of the present work : it will be explained in the following in the independent-link model, showing the usefulness of the annealed approximation.

In the independent-link model, the annealed partition function is :

$$\langle Z \rangle = \int \prod_{i < j} \rho(l_{ij}) dl_{ij} \sum_P \exp\left(-\beta \sum_i l_{P(i)P(i+1)}\right). \quad (9)$$

The integral over l_{ij} gives the same result for any permutation P , so :

$$\begin{aligned} \langle Z \rangle &= N! \left(\int_0^\infty \rho(l) e^{-\beta l} dl \right)^N \\ &= N! (g(\beta))^N, \end{aligned} \quad (10)$$

where $g(\beta)$ is the characteristic function of $\rho(l)$. This yields the annealed free energy

$$F_{\text{ann}} = - TN \ln(N/e) - TN \ln g(\beta) + \mathcal{O}(\ln N), \quad (11)$$

and the annealed average length

$$L_{\text{ann}} = - N \frac{d \ln g(\beta)}{d\beta}. \quad (12)$$

Already from equation (11), one can obtain a number of indications which will be shown to hold for the real, quenched quantities in the next two sections :

— any finite temperature (T fixed when $N \rightarrow \infty$) lies in the « \mathcal{H} regime » defined before, where $L(T)$ scales like N . In this whole regime the free energy is completely dominated by the entropic term $- TN \ln \frac{N}{e}$, it is not extensive.

— there is a regime of very low temperatures where entropy and energy have the same scaling in N , in this annealed approximation : one must have $g(\beta) \sim N^{-1}$. Taking for definiteness the links l_{ij} distributed according to $\rho_r(l)$ defined in (7), we get $g_r(\beta) = (1 + \beta)^{-(r+1)}$. The low temperature regime is $\beta = \hat{\beta} N^{1/(r+1)}$ ($\hat{\beta}$ fixed independently of N). It does correspond to the \mathcal{L} regime defined before, where the average length and the entropy both scale as $N^{1-1/(r+1)}$.

4. Fluctuations of the partition function.

The annealed average is usually a good approximation at high temperatures where Z does not fluctuate much. In order to see whether this is the case here, we compute $\langle Z^2 \rangle$ in the independent-link model :

$$\langle Z^2 \rangle = \int \prod_{i < j} \rho(l_{ij}) dl_{ij} \sum_{P, P'} \exp\left(-\beta \sum_{i=1}^N [l_{P(i)P(i+1)} + l_{P'(i)P'(i+1)}]\right). \quad (13)$$

One can always renumber the N cities so that the permutation P reduces to the identity I . The integral depends on P' only through the overlap Q between P' and I , defined as the number of links common to I and P' . This gives :

$$\langle Z^2 \rangle = N! \sum_{Q=0}^N (N! \mathfrak{F}_N(Q)) (g(2\beta))^Q (g(\beta))^{2(N-Q)}, \tag{14}$$

where $\mathfrak{F}_N(Q)$ is the probability that the overlap between two permutations of N objects be Q . Equation (14) can be written as

$$\langle Z^2 \rangle = \langle Z \rangle^2 \left(\sum_{Q=0}^N \mathfrak{F}_N(Q) \left(\frac{g(2\beta)}{g(\beta)^2} \right)^Q \right). \tag{15}$$

To calculate $\mathfrak{F}_N(Q)$, first note that the probability that a tour goes through a given link is $2/(N - 1)$. For Q finite and $N \rightarrow \infty$, it is reasonable to expect that the Q links common to the two permutations are independent, in which case one has :

$$\mathfrak{F}_N(Q) \sim C_{N^2/2}^Q \left(\frac{2}{N} \right)^{2Q} \left(1 - \frac{2}{N} \right)^{N-Q}, \tag{16}$$

$$\xrightarrow{N \rightarrow \infty} \frac{2^Q}{Q! e^2} \equiv \mathfrak{F}_\infty(Q). \tag{17}$$

This Poisson distribution can be derived rigorously by a detailed study of the moments $Q^r \mathfrak{F}_N(Q) dQ$ [11].

The summation in (15) may be performed using $\mathfrak{F}_\infty(Q)$ and yields

$$\langle Z^2 \rangle = \langle Z \rangle^2 \exp \left(2 \frac{g(2\beta)}{g(\beta)^2} - 1 \right), \tag{18}$$

provided the dominant terms in the sum are found for Q finite. The maximum term is for $Q^* \sim 2 g(2\beta)/g(\beta)^2$, which is finite if β is finite. So equation (18) holds for any given finite temperature (\mathcal{H} regime). If on the contrary the temperature is scaled with N in such a way that $g(\beta)$ is of the order of N^{-1} (\mathcal{L} regime), then Q^* is of the order of N and formula (18) is no longer valid.

Equation (18) implies that the fluctuations of Z from sample to sample are extremely small in the \mathcal{H} regime. To make this statement clear, let us assume that $\ln Z$ has a Gaussian distribution (a very reasonable assumption in view of its self-averageness and its extensivity). From (18) we obtain the relative fluctuations of $\ln Z$

$$\frac{(\langle (\ln Z - \langle \ln Z \rangle)^2 \rangle)^{1/2}}{\langle \ln Z \rangle} \sim \frac{1}{N}. \tag{19}$$

Equation (19) implies that the annealed approximation gives in fact the exact result for the free energy and for the average tour length in the whole \mathcal{H} regime. This result justifies the numerical findings of Kirkpatrick [10], Bonomi and Lutton [9], at least for the independent-link model.

The calculation of $\langle Z^2 \rangle$ in the \mathcal{L} regime is more difficult. Nonetheless we show in the next section, using different methods, that the annealed approximation is still useful in this region.

5. Low-temperature regime : bounds on the optimal length.

We will obtain in the \mathcal{L} regime both lower and upper bounds on the free energy and the optimal length in the random-link problem. The lower bounds are derived from the annealed free energy,

following a method already used for spin glasses [8]. The upper bounds follow from the study of a restricted class of paths.

The entropy $S(T)$ defined in (5) must be positive for all T , since the inequality $\ln Z \geq -\beta L_{\min}$ implies

$$S(T) \geq \beta(L(T) - L_{\min}) \geq 0. \quad (20)$$

The average free energy is therefore a decreasing function of T . In addition, one has the convexity inequality $\langle \ln Z \rangle \leq \ln \langle Z \rangle$, hence

$$\langle F(T) \rangle \geq \begin{cases} F_{\text{ann}}(T) & , \quad T \geq T^* \\ F_{\text{ann}}(T^*) & , \quad T < T^* \end{cases} \quad (21)$$

where T^* is the temperature where F_{ann} has a maximum (see Fig. 1), i.e., where the annealed entropy S_{ann} vanishes.

Combining these results with (4) one finds

$$\langle L_{\min} \rangle = F(0) \geq F_{\text{ann}}(T^*) \equiv L^*. \quad (22)$$

The above derivation applies to any problem of the travelling salesman type. For the family of random-link problems introduced above, there is indeed a temperature T^* where S_{ann} vanishes, and it lies in the \mathcal{L} regime :

$$T^* = (N e^r)^{-1/(r+1)}. \quad (23)$$

This gives

$$\langle L_{\min} \rangle \geq L^* \sim N^{1-1/(r+1)}(r+1) e^{-r/(r+1)}. \quad (24)$$

A simple upper bound for L_{\min} can be obtained using an adaptation of the « greedy » algorithm [12] to the random-link problem. Select an arbitrary origin i , choose as first link the smallest l_{ij} among the $(N-1)$ possibilities, as second link the smallest l_{jk} , and so on. The length L_{gr} of the tour so constructed is an upper bound :

$$\langle L_{\min} \rangle \leq \langle L_{\text{gr}} \rangle = \sum_{p=N-1}^1 \langle \text{Min } a_i \rangle, \quad (25)$$

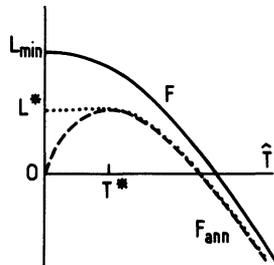


Fig. 1. — The free energy F as a function of the temperature \hat{T} in the \mathcal{L} regime. The dashed curve is the annealed free energy F_{ann} , the dotted curve is the lower bound on F obtained from F_{ann} .

where the a_i are independent random variables with a common distribution $\rho(a)$. The average value of the minimum of p variables is given by

$$\langle \text{Min} (a_1, \dots, a_p) \rangle = \int_0^\infty (1 - G(x))^p dx, \tag{26}$$

where $G(x) = \int_0^x \rho(a) da$ is the integrated density, and one finds

$$\langle L_{\min} \rangle \leq \int_0^\infty (1 - G - (1 - G)^N) G^{-1} dx. \tag{27}$$

For the densities $\rho_r(x)$, we obtain for $N \rightarrow \infty$ the bound

$$\lim_{N \rightarrow \infty} \frac{\langle L_{\min} \rangle}{(r + 1) N^{1-1/(r+1)}} \leq \frac{((r + 1)!)^{1/(r+1)}}{r(r + 1)} \Gamma\left(\frac{1}{r + 1}\right) = a_r, \tag{28}$$

for $r > 0$. For $r = 0$ (i.e., a constant density for small distances) the bound on $\langle L_{\min} \rangle$ is of the order of $\ln N$.

In order to obtain an upper bound F_B for the free energy, we consider a special family of paths defined as follows : for each partition of the N points into N/n blobs of n points, we take the path corresponding to the greedy algorithm inside each blob, and the shortest interblob connections. All these paths have a length bounded asymptotically by

$$L_B = \frac{N}{n} \langle L_{gr}(n) \rangle \sim \frac{N}{n} n^{1-1/(r+1)}(r + 1) a_r, \tag{29}$$

for N/n finite. The entropy associated with the number of ways of choosing the blobs is

$$S_B \sim \ln(N!) - \frac{N}{n} \ln(n!). \tag{30}$$

Choosing $N/n = e^{\lambda r}$, we find for each $\lambda \geq 0$ a bound

$$F_B(\lambda) = N^{1-1/(r+1)} \{ (r + 1) a_r e^{\lambda r/(r+1)} - \hat{T} r \lambda \}, \tag{31}$$

with $\hat{T} = TN^{1/(r+1)}$. Our final upper bound is the envelope of this family of curves for integer values of $p = N/n$. Combining this with (21) gives a bracket for the quenched free energy in the \mathcal{L} regime :

$$\left. \begin{matrix} c_r & \hat{T} \leq c_r \\ \hat{T} \ln \frac{c_r e}{\hat{T}} & \hat{T} > c_r \end{matrix} \right\} \leq \frac{F(T)}{(r + 1) N^{1-1/(r+1)}} \leq \begin{cases} a_r & \hat{T} \leq \hat{T}_1 \\ a_r p^{1/(r+1)} - \hat{T} \frac{\ln p}{(r + 1)} & \hat{T}_p < \hat{T} \leq \hat{T}_{p+1} \end{cases} \tag{32}$$

where

$$\hat{T}_p = (r + 1) a_r \frac{(p + 1)^{1/(r+1)} - p^{1/(r+1)}}{\ln(p + 1) - \ln p} \underset{p \rightarrow \infty}{\sim} a_r e^{\lambda r/(r+1)},$$

a_r is defined in (28) and $c_r = e^{-r/(r+1)}$. For large p , the upper bound is asymptotically equal to $\hat{T} \ln(e a_r / \hat{T})$.

Formula (32) proves that $F(T)$ in the ℓ regime, and hence L_{\min} , is of the order of $N^{1-1/(r+1)}$ for the random-link problem, a scaling form which agrees with the well known $N^{1-1/D}$ form of the random-point problem [1], via the $r = D - 1$ correspondence. For $r = 0$, no conclusion can be reached because the upper bound is of the order of $\ln N$, the lower one of the order of 1. Of course, other classes of tours may be considered to obtain upper bounds on $F(T)$, but the present choice has the advantage of showing that the dominant term of the quenched free energy is $(-\hat{T} \ln \hat{T})$ in the high- \hat{T} range (upper part of the ℓ regime) and is correctly given by the annealed approximation. This indicates that we have identified the dominant tours in that range.

Let us note that, as far as L_{\min} is concerned, another lower bound can be obtained by considering the average of the smallest link originating from a point :

$$\langle L_{\min} \rangle \geq N \int_0^\infty (1 - G(x))^{N-1} dx. \quad (33)$$

This gives

$$\lim_{N \rightarrow \infty} \frac{\langle L_{\min} \rangle}{(r+1) N^{1-1/(r+1)}} \geq \frac{r}{r+1} a_r, \quad (34)$$

which happens to be in this case slightly better than the annealed bound (24).

A lower bound on L_{\min} can be obtained through the computation of $\langle Z \rangle$ in any type of T.S.P. In the case of the random-point problem in a unit hypercube in D dimensions, the bounds so obtained are not as good as those quoted in the literature [1], except for $D \rightarrow \infty$ where we recover the known form $L_{\min} \geq (D/2 \pi e)^{1/2} N^{1-1/D}$.

6. A solvable model of a travelling salesman.

A very interesting model appears when one lets $r \rightarrow \infty$. Then the distribution of lengths $\rho_r(l)$ is peaked around $l \sim r$, which gives a scale of distances. The two bounds we have found for L_{\min} coincide, so that

$$\frac{\langle L_{\min} \rangle}{r N^{1-1/(r+1)}} \sim \frac{1}{e} \quad (r \rightarrow \infty). \quad (35)$$

This limiting case is to our knowledge the first example of a random T.S.P. for which the exact asymptotic behaviour of L_{\min} is known.

Furthermore, the bounds (32) on the free energy in the ℓ regime coincide in this limit, proving that the quenched free energy is :

$$\frac{F(T)}{r N^{1-1/(r+1)}} \sim \begin{cases} \frac{1}{e} & \hat{T} \leq 1/e, \\ -\hat{T} \ln \hat{T} & \hat{T} > 1/e. \end{cases} \quad (36)$$

This is a striking result since it shows that a phase transition occurs in the ℓ regime at a finite \hat{T} . Below the critical temperature $\hat{T}_c = 1/e$, the entropy vanishes and the system is frozen. This behaviour is strongly reminiscent of Derrida's « random energy model » [13] and has a similar origin : the average number of paths of length $L = N^{1-1/(r+1)}(r+1)l$,

$$\langle \mathcal{N}(l) \rangle \sim \exp(N(r+1) \ln(l e^{r/(r+1)})) \quad (37)$$

is exponentially small for $l < l_c = e^{-r/(r+1)}$, hence there are no tours in this region. From our previous result (36), we see that for $r \rightarrow \infty$ and $l > l_c$, the entropy is indeed given by $S \sim \ln \langle \mathcal{N}(l) \rangle$, meaning that the fluctuations in $\mathcal{N}(l)$ can be neglected in that limit.

This similarity gives an analytic basis to the connection between T.S.P. and spin glasses, since the random energy model has been shown to be the simplest model of a spin glass [14]. We hope that the present « infinite dimensional » model of a travelling salesman will play a similar role for optimization problems.

7. Conclusions.

We have clarified the notion that there exist two temperature regimes in the thermodynamic study of the T.S.P., and we have shown that the difference between the high- $T(\mathcal{H})$ regime and low- $T(\mathcal{L})$ regime is not of the same nature as the distinction between two phases separated by a transition point : it corresponds to different behaviours with N of the thermodynamic quantities for large systems. In the \mathcal{H} regime, i.e. finite temperatures in usual units, the free energy is given by the annealed approximation, it is analytic in T and there is no phase transition.

The interesting temperature regime for the T.S.P. is certainly the \mathcal{L} regime, which is also the most appealing one from a purely statistical mechanics point of view for several reasons : it is the regime which corresponds to finite temperatures \hat{T} (in the random-point model) if one takes the limit $N \rightarrow \infty$ keeping the density of points $\rho = N/V$ fixed (rather than the volume V fixed), which is a more physical procedure. The entropy and the energy then balance with the same scaling as functions of N , giving an extensive free energy $F \sim N\rho^{-1/D}$.

The analytic approach to the computation of $\langle \ln Z \rangle$ in this regime is not easy, as can be seen from the fact that a high temperature expansion for $1/\hat{T}$ small but finite is already non trivial. However we have shown that this high- \hat{T} regime is well described by the annealed approximation. Furthermore we have exhibited a solvable model for which there is a phase transition at a finite \hat{T} . Whether a similar transition occurs in other T.S.P. models, and whether this transition is of the same nature as the spin glass transition remain challenging open questions.

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