Characterization of the probabilistic traveling salesman problem

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We show that stochastic annealing can be successfully applied to gain new results on the probabilistic traveling salesman problem. The probabilistic "traveling salesman" must decide on an *a priori* order in which to visit *n* cities (randomly distributed over a unit square) *before* learning that some cities can be omitted. We find the optimized average length of the pruned tour follows $E(\overline{L_{\mathrm{pruned}}})=\sqrt{np}(0.872-0.105p)f(np)$, where p is the probability of a city needing to be visited, and $f(np)\to 1$ as $np\to\infty$. The average length of the *a priori* tour (before omitting any cities) is found to follow $E(L_{a\ priori})=\sqrt{n/p}\,\beta(p)$, where $\beta(p)=1/[1.25-0.82\ln(p)]$ is measured for $0.05\leqslant p\leqslant 0.6$. Scaling arguments and indirect measurements suggest that $\beta(p)$ tends towards a constant for $p<0.03$. Our stochastic annealing algorithm is based on limited sampling of the pruned tour lengths, exploiting the sampling error to provide the analog of thermal fluctuations in simulated (thermal) annealing. The method has general application to the optimization of functions whose cost to evaluate rises with the precision required.

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I. INTRODUCTION

Many real systems present problems of stochastic optimization. These include communications networks, protein design [1], and oil field models [2], in all of which uncertainty plays a central role. We will consider the case where the outcome $g(x,\omega)$ depends not only on parameters x to be chosen, but also on unknowns ω. We can only average with respect to these unknowns, aiming to find the "solution" x which optimizes the average outcome. Thus we seek to find $x\in X$ which minimizes

$$\overline{g}(x)=\int g(x,\omega)f(\omega)d\omega, \tag{1}$$

where X is the solution space of the problem and $f(\omega)$ is the probability distribution of the uncertain variables.

Stochastic optimization was born out of an idea by Robbins and Monro [3]. They considered solving the problem of finding

$$G(x)=\alpha, \tag{2}$$

where G is some monotonic function of x and α is a parameter. G is not known directly, but can only be estimated. Their technique to solve this problem is called stochastic approximation, and a number of variants of this scheme have since been developed [4–7].

For function minimization where the function must be estimated and may have multiple minima, the term stochastic optimization is used. This term has sometimes been used for certain heuristic algorithms applied to normal optimization problems, but here it is used exclusively to describe the optimization of a function which must be estimated.

In this paper our focus is on heuristic approaches to the solution of stochastic optimization problems, since these are the appropriate tool for the solution of NP-complete problems, such as the (PTSP) [8]. A number of heuristics already exist to tackle stochastic optimization problems [9–13]. Many of these are developments from simulated annealing [14–17], which has itself been shown [18] to solve stochastic optimization problems with probability 1, provided $\overline{g}(x)$ can be estimated with precision greater than $O(t^{-\gamma})$ for time step t, where $\gamma>1$. A number of authors [15–17,19] have used a modified simulated annealing algorithm in which the acceptance probability is modified to take some account of the precision of the estimates of $\overline{g}(x)$, and in these cases there are a number of convergence results [19,17]. Ceperley and Dewing [20] have developed a penalty method for simulated annealing which permits exact simulation of a thermal system, where the errors of the estimation of $\overline{g}(x)$ are assumed to be Gaussian.

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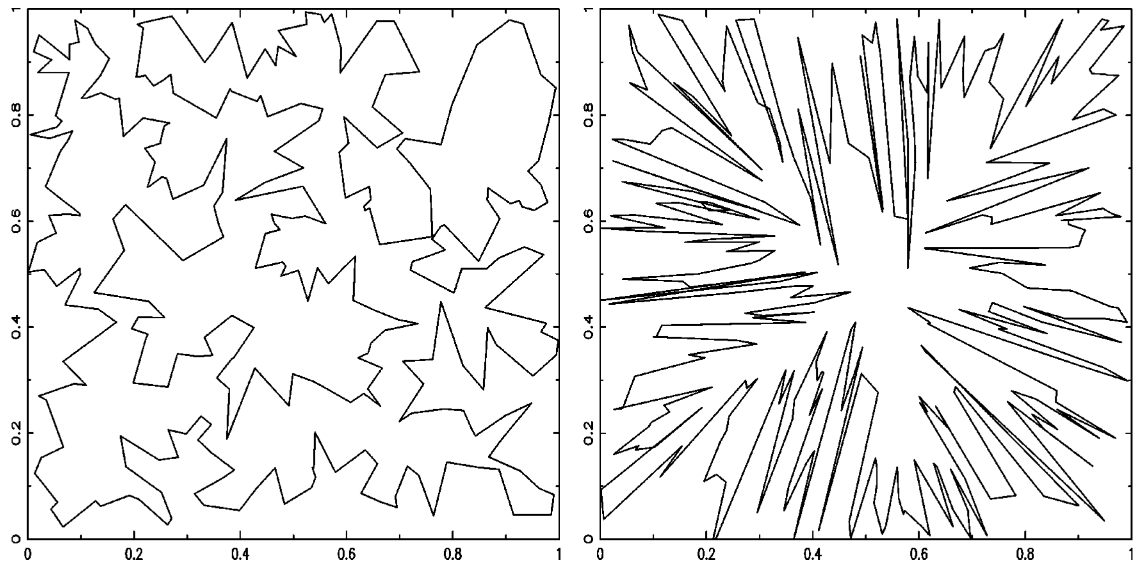

FIG. 1. Typical near optimal *a priori* PTSP tours with $n=300$ for $p=0.5$ (left) and $p=0.1$ (right), respectively.

Stochastic annealing [1] is a more general approach which allows the simulation of thermal equilibrium even if the distribution of errors in the estimation of $\overline{g(x)}$ is not known. In this technique the noise present in the estimates is positively exploited as mimicking thermal noise in a slow cooling, as opposed to being regarded as something whose influence should be minimized from the outset. It is a simplification of this method which we use to approximately solve the PTSP.

We estimate $\overline{g(x)}$ by taking r repeated, statistically independent, measurements of $g(x,\omega)$, each of which we call an instance. All moves for which one estimate (based on r instances) for a new state is more favorable than an equivalent estimate for the old are accepted. This simple procedure does not exactly simulate a thermal system, where the acceptance probabilities should obey

$$\frac{P_{A\to B}}{P_{B\to A}}=e^{-\beta\Delta\mu}, \tag{3}$$

where $\beta=1/k_BT$ and $\Delta\mu$ is the exact difference in $\overline{g(x)}$ between states A and B. However, if we assume that our estimate of $\Delta\mu$ is Gaussian distributed around $\overline{g(x)}$ with standard deviation $\sigma/\sqrt{r}$, where r is the number of instances used for each estimate, then it follows that the acceptance probability is [1]

$$P^G_{A\to B}=\frac{1}{2}\left[1-\mathrm{erf}\left(\frac{\sqrt{r}\Delta\mu}{\sqrt{2}\sigma}\right)\right]. \tag{4}$$

The approximation to a thermal acceptance rule is then quite good since

$$\ln\left(\frac{P_{A\to B}}{P_{B\to A}}\right)=\ln\left(\frac{1-\mathrm{erf}\left(\frac{\sqrt{r}\Delta\mu}{\sqrt{2}\sigma}\right)}{1+\mathrm{erf}\left(\frac{\sqrt{r}\Delta\mu}{\sqrt{2}\sigma}\right)}\right)$$
$$\simeq-\beta_G\Delta\mu-\frac{4-\pi}{48}(\beta_G\Delta\mu)^3-\cdots, \tag{5}$$

where

$$\beta_G=\frac{\sqrt{8r}}{\sqrt{\pi}\sigma} \tag{6}$$

identifies the equivalent effective temperature. The small coefficient ($\simeq 0.02$) of the cubic term in Eq. (5) makes this a rather good approximation to true thermal selection.

Increasing the sample size r means that we are more stringent about not accepting moves that are unfavorable, equivalent to lowering the temperature, which is quantified by Eq. (6) for the Gaussian case. As with standard simulated annealing [21–23], the question of precisely what cooling schedule to use remains something of an art.

II. PROBABILISTIC TRAVELING SALESMAN PROBLEM

We adopt the PTSP as a good test bed amongst stochastic optimization problems, in much the same way as the traveling salesman problem (TSP) has been considered a standard amongst deterministic optimization problems. The PTSP falls into the class of NP-complete problems [8], and the TSP is a subset of the PTSP.

The original traveling salesman problem is to find the shortest tour around n cities, in which each city is visited once. For small numbers of cities this is an easy task, but the problem is NP complete: it is believed for large n that there is no algorithm which can solve the problem in a time poly-

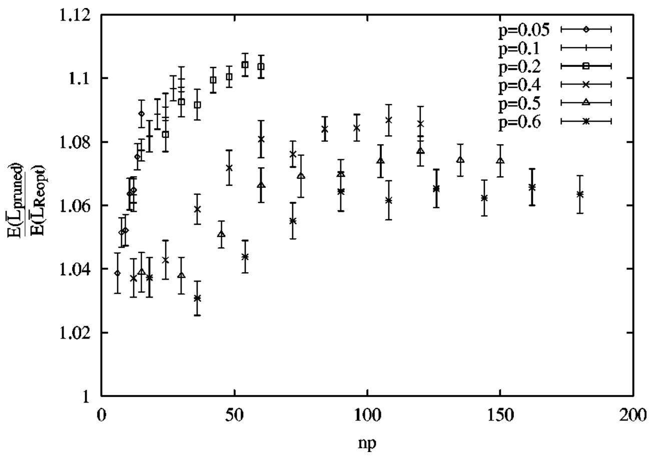

FIG. 2. The expected pruned tour length divided by the expected reoptimized tour length. This indicates the improvement one would expect from reoptimization.

nomial in n. Consideration of the traveling salesman problem began with Beardwood *et al.* [24]. They showed that in the limit of large numbers of cities which are randomly distributed on a unit square, the optimal tour length L_{TSP} follows [25]

$$E(L_{\mathrm{TSP}})=\beta_{\mathrm{TSP}}\sqrt{n}+\alpha_{\mathrm{TSP}}, \tag{7}$$

where β_{TSP} and α_{TSP} are constants. Here and below $E(L)$ denotes the quantity L averaged, after optimization, with respect to different city positions, randomly placed on a unit square. Numerical simulation [26] gives $\beta_{\mathrm{TSP}}=0.7211(3)$ and $\alpha_{\mathrm{TSP}}=0.604(5)$ as estimates when $n\geqslant 50$. Significant divergence from this behavior is found for $n\leqslant 10$, but numerical estimates can be found quickly (see Table I).

The probabilistic traveling salesman problem, introduced by Jaillet [27,28], is an extension of the traveling salesman problem to optimization in the face of unknown data. Whereas all of the cities in the TSP must be visited once, in the PTSP each city only needs to be visited with some probability p. One first decides upon the order in which the cities are to be visited, the "*a priori*" tour. Subsequently, it is revealed which cities need to be visited, and those which do not need to be visited are skipped to leave a "pruned tour." The order in which the cities are to be visited is preserved when pruning superfluous cities. The objective is to choose an *a priori* tour which minimizes the average length of the pruned tour. It is clear from Fig. 1 that near optimal *a priori* tours may appear very different for different values of p.

TABLE I. The average length of the near-optimal TSP tours for a small number of cities.

Number of cities n	Number of instances I	Average tour length	$\sigma/\sqrt{I-1}$
2	100000	1.043	0.002
3	100000	1.564	0.002
4	5000	1.889	0.006
5	5000	2.123	0.006
6	5000	2.311	0.005
7	5000	2.472	0.005
8	5000	2.616	0.005
9	5000	2.740	0.005
10	5000	2.862	0.005

In our terminology, the average pruned tour length is averaged over all possible instances of which cities require to be visited. This was given by Jaillet as [27,29]

$$\overline{L}_{\mathrm{pruned}}=\sum_{q=0}^{n-2} p^2(1-p)^q L^{(q)}, \tag{8}$$

where

$$L^{(q)}=\sum_{j=1}^{n} d(j,1+(j+q)_{\mathrm{mod}\ n}) \tag{9}$$

is the sum of the distances between each city and its $(q+1)$th following city on the *a priori* tour, and the factors $p^2(1-p)^q$ in the preceding equation simply give the probability that any particular span skipping q cities occurs in the pruned tour. Jaillet's closed form expression for the average pruned tour length renders the PTSP to some extent accessible as a standard (but still NP complete) optimization problem, and provides some check on the PTSP results by stochastic optimization methods.

It has been conjectured [8] that, in the limit of large n, the PTSP strategy is as good as constructing a TSP tour on the cities requiring a visit, the reoptimization strategy. This would mean that

$$\lim_{n\to\infty}\left(\frac{E(\overline{L}_{\mathrm{pruned}})}{\sqrt{np}}\right)=\beta_{\mathrm{TSP}}, \tag{10}$$

where $E(\overline{L}_{\mathrm{pruned}})$ is the average pruned tour length further averaged over city positions after optimization, which we will refer to as the expected pruned tour length. Figure 2 shows the expected pruned tour length divided by the expected reoptimized tour length. Since this quantity is tending towards a value significantly greater than 1 for $p<1$ it demonstrates that the PTSP strategy can be worse than the reoptimization strategy. Jaillet [27] and Bertsimas and Howell [29] have also shown that there is a limit to how much worse it can be, with

$$\lim_{n\to\infty}\left(\frac{E(\overline{L}_{\mathrm{pruned}})}{\sqrt{np}}\right)=\beta_{\mathrm{pruned}}(p), \tag{11}$$

where

$$\beta_{\mathrm{TSP}}\leqslant\beta_{\mathrm{pruned}}(p)\leqslant\mathrm{Min}\left(0.9212,\frac{\beta_{\mathrm{TSP}}}{\sqrt{p}}\right). \tag{12}$$

One attempt to solve the PTSP using an exact method was taken by Laporte *et al.* [30] who introduced the use of integer linear stochastic programming. This study was severely limited in the size of problem attempted and the stochastic programming algorithm failed to solve the PTSP on certain occasions. Thus the accuracy of any statistics generated using this method are dubious.

Three studies have used heuristics to solve the PTSP [31–33]. None of these studies used global search heuristics, and all were very restricted in the problem size attempted due to computational cost. The evaluation of a move for the PTSP using Eq. (8) involves the computation of $O(n^2)$ terms compared to $O(1)$ computations to evaluate a move in the TSP. Thus, to solve a 100-city problem for the PTSP would take $O(10\,000)$ times longer than it would to solve a 100-city problem for the TSP. It should be noted, however, that it is only possible to make this comparison due to the relative simplicity of the PTSP. For many more stochastic optimization problems, standard optimization techniques are simply not applicable.

III. FORM OF THE OPTIMAL TOUR AND SCALING ARGUMENTS

Optimal *a priori* PTSP tours for small p, as exemplified in Fig. 1 for $p=0.1$, resemble an "angular sorting"—where cities are visited in an order given by their angle with respect to the center of the square. Bertsimas [31] proposed that an angular sorting is optimal as $p\to 0$, but we can show this to be false by comparison to a space-filling curve algorithm which is generally superior as $n\to\infty$. Such an algorithm was introduced by Bartholdi and Blatzman [34] using a technique based on a Sierpinski curve.

For the angular sort with $np\gg 1$ only cities that are separated by a small angle will contribute significantly to Eq. (8). For two cities which are separated by a large angle the probability that they are adjacent on the pruned tour (i.e., no cities between them require a visit) is vanishingly small. Thus for an n-city tour chosen by angular sorting we may approximate Eq. (9) by

$$L_{\rm ang}^{(q)}\simeq L_o n, \tag{13}$$

where L_o is some fraction of the side of a unit square, since cities which are sorted with respect to angle will be unsorted with respect to radial distance. This leads to

$$E(\overline{L}_{\rm ang})\simeq L_o n p^2 \sum_{q=0}^{n-2} (1-p)^q. \tag{14}$$

For $np\gg 1$, we find that the angular sorting yields

$$E(\overline{L}_{\rm ang})\to L_o np. \tag{15}$$

By contrast it has been shown [29] that

$$\frac{E(\overline{L}_{\tau_{\rm sf}})}{E(\overline{L}_{\rm Reopt})}=C, \tag{16}$$

with probability 1, where $E(\overline{L}_{\tau_{\rm sf}})$ is the expected length of a tour generated by a heuristic based on a space-filling curve approach of Bartholdi and Blatzman [34] and $E(\overline{L}_{\rm Reopt})$ is the expected length for the reoptimization strategy. Using previous computational results [29,26], we estimate $C\simeq 1.33$, which is worse than we achieve using stochastic annealing. Hence, $E(\overline{L}_{\tau_{\rm sf}})$ is given by

$$E(\overline{L}_{\tau_{\rm sf}})=O(\sqrt{np}), \tag{17}$$

which leads to

$$\frac{E(\overline{L}_{\tau_{\rm sf}})}{E(\overline{L}_{\rm ang})}=O\left(\frac{1}{\sqrt{np}}\right). \tag{18}$$

So for large enough np the angular sorting is not optimal.

From inspection of near-optimal PTSP tours such as Fig. 1, we propose that the tour behaves differently on different length scales; the tour being TSP-like at larger length scales, but resembling a locally directed sorting at smaller length scales. A locally directed sorting sorts cities according to their distance in a particular direction. We may construct such a tour and use scaling arguments to analyze both the pruned and *a priori* lengths of the optimal tour. Consider dividing a unit square into a series of "blobs," each blob containing $1/p$ cities so that on average one city within each blob requires a visit. The number of such blobs is given by

$$N\simeq np, \tag{19}$$

and for these to approximately cover the unit square their typical linear dimension ξ must obey

$$N\xi^2\sim 1. \tag{20}$$

Since a pruned tour will visit each blob once on average, we can estimate the expected pruned tour length to be

$$E(\overline{L}_{\rm pruned})\sim N\xi\sim\sqrt{np}, \tag{21}$$

which we will see below is verified numerically. We can similarly estimate the *a priori* tour length to be n times the distance between two cities in the same blob. Thus, the expected *a priori* tour length is

$$E(L_{a\ priori})\sim n\xi\sim\sqrt{\frac{n}{p}}, \tag{22}$$

which is more difficult to confirm numerically.

IV. COMPUTATIONAL RESULTS FOR THE PTSP

We have investigated near optimal PTSP tours for a range of different numbers of cities, and various values of p. We used stochastic annealing with effective temperatures in the range $1/\beta_G=0.07-0.01$, corresponding to sample sizes in the range $r=2-500$. Between 10 and 80 different random city configurations were optimized (80 configurations of 30 cities, 40 configurations of 60 cities, 20 configurations of 90 cities, and 10 configurations for $n\geq 120$ cities).

Figure 3 shows a master curve for the expected pruned tour length divided by $\beta_{\rm pruned}(p)\sqrt{np}$ as a function of np. The shift factors $\beta_{\rm pruned}(p)$ have been chosen to give the best

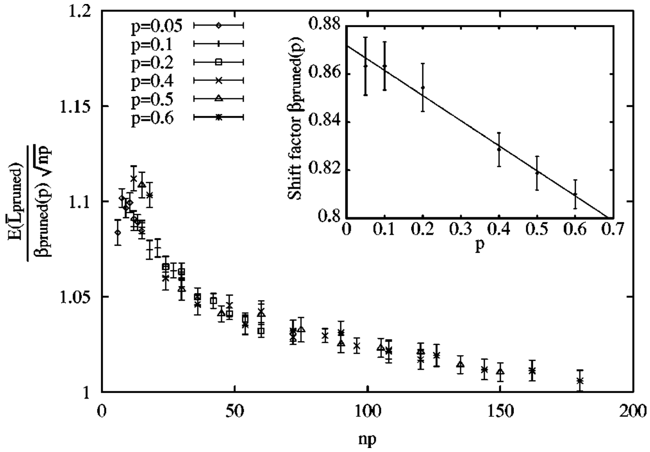

FIG. 3. The master curve for the pruned tour length divided by $\beta_{\text{pruned}}(p)\sqrt{np}$. The data follows a smooth curve for $n>30$, and the shift factors follow a linear relationship, suggesting that $E(\overline{L}_{\text{pruned}})/\sqrt{np}(0.872-0.105p)=f(np)$. Three points with $n=30$ lie significantly above the other data points (here and also in Fig. 4), showing breakdown of the master curve at small n.

fit of the data to a single curve. The shift factors vary only slightly with changing p and appear to have a linear fit. This means the expected pruned tour length is given by

$$\frac{E(\overline{L}_{\text{pruned}})}{\sqrt{np}(a-bp)}=f(np), \tag{23}$$

for $n\gg 1$, where $a=0.872\pm0.002$, $b=0.105\pm0.005$, and $f(np)\rightarrow 1$ for large np. This indicates that the PTSP strategy can be no more than $0.872/0.767-1=14\%(\pm 1\%)$ worse than the reoptimization strategy.

The master curve for the *a priori* tour length is shown in Fig. 4. Our scaling arguments predict that the shift factors $\beta_{a\ priori}(p)$ should tend towards a constant for $p\rightarrow 0$. However, data are fit very well by the relation

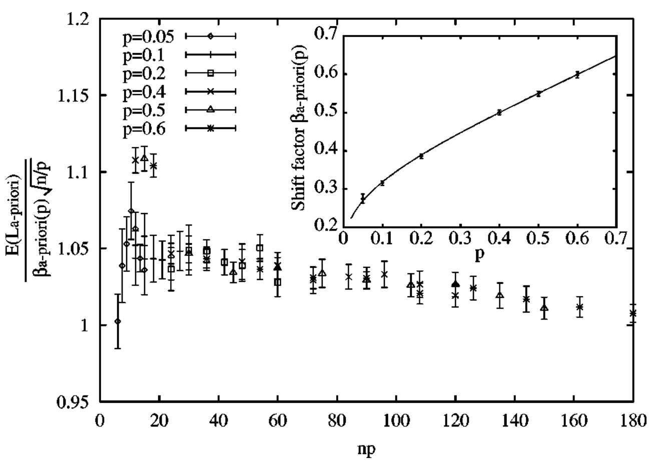

FIG. 4. The master curve for the *a priori* tour length divided by $\sqrt{(n/p)}\beta_{a\ priori}(p)$. The shift factors, inset, are expected to tend towards a constant for $p\rightarrow 0$. The slight, but significant, deviation from linear suggests that this might not be the case.

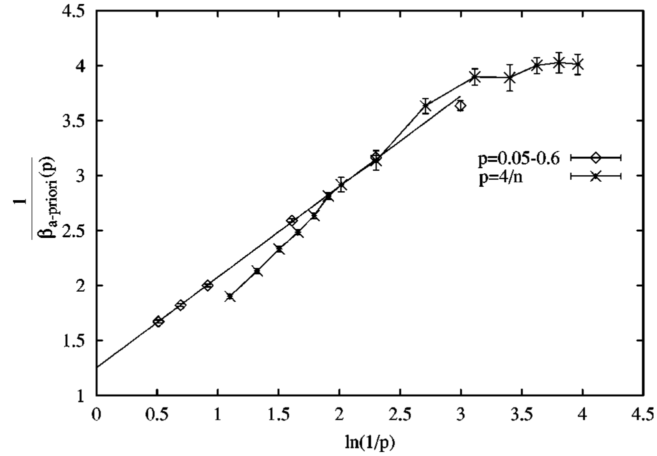

FIG. 5. Reciprocal shift factors for *a priori* tours (diamonds) compared to estimates from 4-city tours (crosses), $1/\beta_{a\ priori}(p)\simeq n/2E(L^{4\ \text{city}}_{a\ priori})$. The 4-city tour data are optimized when each of the instances have 4 cities on the pruned tour. The direct measurements do not appear to saturate within the accessible range of p. The crosses show matching behavior, with saturation at larger n corresponding to inaccessible p, suggesting that $E(L_{a\ priori})=\beta_0\sqrt{(n/p)}$ for small p.

$$\beta_{a\ priori}(p)=\frac{1}{1.25-0.82\ln(p)}, \tag{24}$$

which would tend to zero as $p\rightarrow 0$ in conflict with our scaling arguments. To resolve this dilemma we need to probe very small p.

V. THE LIMITING CASE $p\rightarrow 0$

We are interested in finding whether $\beta_{a\ priori}(p)$ tends towards a constant as $p\rightarrow 0$. To do this using the above approach is difficult, since we need a large number of cities to produce reliable data for this regime. Extraction of this behavior may be achieved by comparing simulations for different values of n, but fixed np. We accomplish this by insisting that each instance has four cities on the pruned tour. 4 city tours are chosen since they are the smallest for which it matters in which order the cities are visited. This can be viewed as an efficient way to simulate (approximately) the PTSP strategy with $p=4/n$.

Since we are considering the PTSP at fixed np, if $\beta_{a\ priori}(p)$ tends towards a (nonzero) constant as $p\rightarrow 0$ then we expect $E(L^{4\ \text{city}}_{a\ priori})/n$ to tend towards a constant as $n\rightarrow\infty$. Simulations in this regime were performed for $n=12-210$, with 100 different random city configurations used for $n<30$, 20 configurations for $n\leqslant 90$, and 10 configurations for $n\geqslant 120$. Figure 5 shows a linear-log plot of $n/2E(L^{4\ \text{city}}_{a\ priori})$ against $\ln(n/4)\cong\ln(1/p)$. For small n these results reasonably match the direct measurements of $\beta_{a\ priori}(p)$, shown for comparison. However, for large $n\sim 100$ which is beyond the range of our $\beta_{a\ priori}(p)$ data, our earlier proposal of scaling behavior is vindicated by $E(L^{4\ \text{city}}_{a\ priori})/n$ approaching a constant value. In summary we have

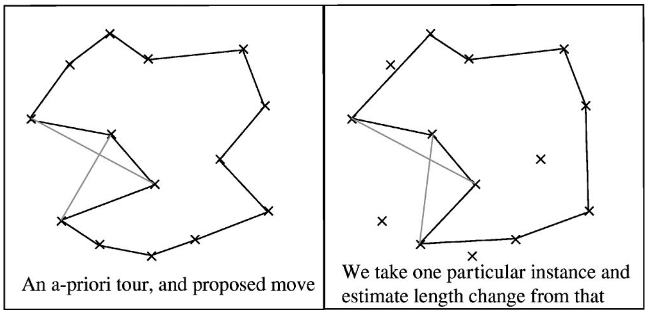

FIG. 6. When estimating the expected length change due to a move, we randomly generate instances. Only the cities that are nearest to the move are needed to calculate the change in the pruned tour length.

$$\lim_{n\to\infty} E(L_{a\ priori}) = \sqrt{\frac{n}{p}}\beta_{a\ priori}(p), \tag{25}$$

where

$$\beta_{a\ priori}(p)\begin{cases} = \dfrac{1}{1.25-0.82\ln(p)} & \text{for } p>0.03 \\ = \beta_0 & \text{for } p<0.03. \end{cases} \tag{26}$$

VI. NOTES ON ALGORITHM IMPLEMENTATION

We applied stochastic annealing to the PTSP using a combination of the 2-opt and 1-shift move sets [35] established for the TSP. Both move sets are applied to the *a priori* tour in the same way as they are applied for the TSP. The expected pruned tour length change for the move is estimated by averaging the change in the tour length for a number of instances. For a given instance it is not necessary to decide whether every city is present, but only the set of cities closest to the move which determine the change in the pruned tour length (see Fig. 6). For the PTSP, the location of the nearest cities on the pruned tour to the move is determined from a Poisson distribution.

When using stochastic optimization, the only variable over which we have control is the sample size (the number of instances) r, whereas the effective temperature $\sigma/\sqrt{r}$ also entails the standard deviation σ of the pruned length change over instances. As shown in Fig. 7, annealing by controlling r alone exhibits a relatively sharp transition in the expected pruned tour length. The rapid transition appears to ‘‘freeze in’’ limitations in the tours found (analogous to defects in a physical low temperature phase). By comparison we obtain a much smoother change when $\sigma/\sqrt{r}$ is controlled.

The sharpness of the transition under control by r is caused by the fact that σ may vary from move to move, and is on average lower when the expected pruned tour length is less. The jump in the pruned tour length is accompanied by a jump in σ and hence the temperature. We suggest that quite generally controlling $\sigma/\sqrt{r}$ gives a better cooling schedule than focusing on r alone.

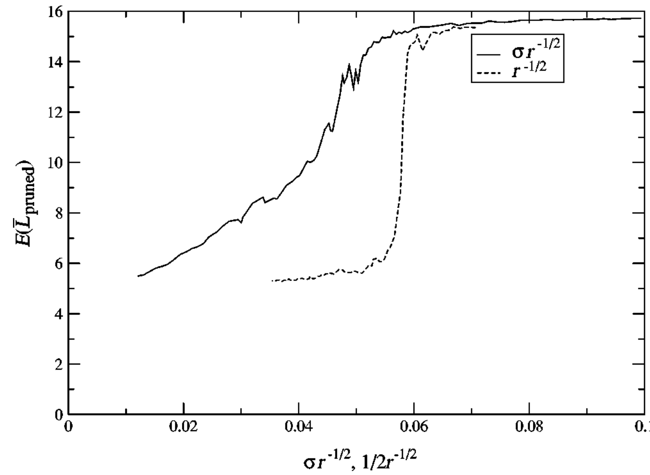

FIG. 7. The expected pruned tour length for annealings when r and $1/T=\sqrt{r}/\sigma$ are increased monotonically. The sharp drop in the pruned tour length is seen when only r is controlled, demonstrating that this ‘‘freezes in’’ imperfections in the tour. The system was annealed at each value of the temperature and value of r for 50 000 Monte Carlo steps with $n=300$ and $p=0.1$.

VII. CONCLUSION

We have shown that earlier incompatible ideas about the form of PTSP, tours especially at small p [31,8,34], are resolved by a new crossover scaling interpretation. At larger length scales the tour appears TSP-like, but resembles a locally directed sorting at smaller scales. The crossover between these two regimes corresponds to a group of cities for which on average one city in this group requires a visit. Our computational results for the pruned tour length are summarized by Eq. (23) and clearly support the crossover scaling.

Computationally the *a priori* tour length is more subtle than the pruned tour length, although it does ultimately conform to expectations from crossover scaling. We introduced 4-city tours to probe the behavior of *a priori* tour length down to very small p. As summarized by Eq. (25), we find a wide preasymptotic regime until recovering the expected crossover scaling only for $p<0.03$. Understanding these anomalies in the *a priori* tour length, and confirming them analytically, is left as a future challenge.

We have shown stochastic annealing to be a robust and effective stochastic optimization technique, taking the PTSP as a representative difficult stochastic optimization problem. In this case it enabled us to obtain representative results out to unprecedented problem sizes, which in turn supported a whole new view of how the tours behave. Of relevance to wider applications of stochastic optimization, we have seen that smoother annealing can be obtained by directly controlling the effective temperature $\sigma/\sqrt{r}$ [1] rather than simply the bare depth of sampling r alone.

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