



A LETTERS JOURNAL EXPLORING
THE FRONTIERS OF PHYSICS

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EPL, **113** (2016) 30004

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Phase transitions of Traveling Salesperson problems solved with linear programming and cutting planes

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received 2 January 2016; accepted in final form 12 February 2016

published online 25 February 2016

PACS 02.10.0x – Combinatorics; graph theory

PACS 89.70.Eg – Computational complexity

PACS 64.60.-i – General studies of phase transitions

Abstract – The Traveling Salesperson problem asks for the shortest cyclic tour visiting a set of cities given their pairwise distances and belongs to the NP-hard complexity class, which means that with all known algorithms in the worst case instances are not solvable in polynomial time, *i.e.*, the problem is *hard*. However, this does not mean that there are not subsets of the problem which are *easy* to solve. To examine numerically transitions from an *easy* to a *hard* phase, a random ensemble of cities in the Euclidean plane, given a parameter σ , which governs the hardness, is introduced. Here, a linear programming approach together with suitable cutting planes is applied. Such algorithms operate *outside* the space of feasible solutions and are often used in practical applications but rarely studied in physics so far. We observe several transitions. To characterize these transitions, scaling assumptions from continuous phase transitions are applied.

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The *Traveling Salesperson Problem* (TSP) [1] is to find the shortest tour through a given set of cities, with known pairwise distances, and going back to the initial city. TSP belongs to the class of NP-hard optimization problems [2], where so far only algorithms with exponentially growing *worst-case* running time are known. Thus, a good tour optimization can not only save money when used for real-world applications, but it has also a history as a testbed for exact [1,3] as well as heuristic optimization algorithms, *e.g.*, *simulated annealing* [4], *taboo search* [5] or *ant colony algorithms* [6]. Also, for the TSP there exist specific heuristics [6–8]. For the Euclidean case (which is still NP-hard [9]), *i.e.*, the pairwise distances are the Euclidean distances, a polynomial-time approximation scheme [10] is known. For special corner cases [11] even polynomial-time algorithms exist.

Interestingly, NP-complete problems often show phase transitions [12–14] where instances are *typically easy* to solve in one region and *typically hard* in another region. Some of the classical NP-complete problems [15] were examined with respect to phase transitions with methods of statistical mechanics in refs. [16–20]. Note that in the statistical-mechanics literature usually algorithms like branch-and-bound [21–23], stochastic search [24] and message-passing algorithms [25] are studied which operate *inside* the space of feasible configurations. In contrast,

for practical applications, algorithms based on linear programming (LP) dominate because they are very efficient. These LP-based algorithms operate *outside* the space of feasible solutions and they should be given more attention in the physics community. For this reasons we study here LP algorithms with respect to phase transitions for the TSP.

In ref. [26] the Euclidean TSP decision problem on random realizations of cities scattered on the unit square was under scrutiny and shows a “transition” when asking when the tour length exceeds a certain rescaled threshold. But here the two “phases” are not taken with respect to the basic properties of the instances, and there is no parametrized ensemble. Rather, the instances are sorted into two classes after they are solved, basically reflecting the typical growth of the tour length. Instead, here we define a parametrized ensemble of TSP instances. We study the solvability by a polynomial-time standard LP approach together with several types of so-called *cutting planes*. We find *several* “easy-hard” transitions, similar to one previously found for the vertex-cover problem [27,28].

The two-dimensional Euclidean TSP is under scrutiny [26,29]. Each city from the set of cities V has coordinates on a plane determining the pairwise distances c_{ij} as their Euclidean distances, in particular $c_{ij} = c_{ji}$. We generated each instance of N cities by

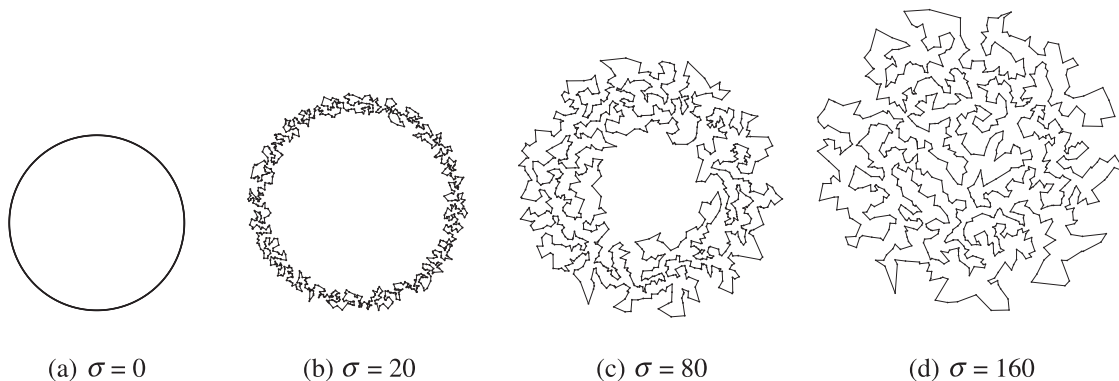


Fig. 1: Evolution of a $N = 1024$ and $R = \frac{N}{2\pi} \approx 160$ system with increasing disorder σ . These sample realizations were solved with *Concorde* [3]. Obviously the leftmost configuration is *easy* to solve, but the other three are probably not.

random displacement of cities from a well-defined start configuration, chosen as N cities lying on a circle with a circumference of $2\pi N$, *i.e.*, the distance between two neighboring cities is approximately 1. Note that for the circle even the simplest greedy heuristics, *e.g.*, *nearest neighbor*, finds the optimal tour. Further the circle fulfills the *necklace condition* [30] which enables a polynomial-time solution algorithm and all points are part of the convex hull which also solves the tour [31]. For each city the displacement is determined by two independent random variables from a uniform distribution. $\phi \in [0, 2\pi)$ is treated as a displacement angle and $r \in [0, \sigma]$ as a radius, such that the new position of a city lies inside of a disk with radius σ around its initial position. Four sample instances together with their optimal tours for $N = 1024$ cities are shown in fig. 1.

Next, we present our numerical approach. LPs can be solved in polynomial time using the *ellipsoid* algorithm [21]. In this study the *simplex* algorithm [21] implemented by the commercial optimization library CPLEX is used instead, for its good runtime behavior in the typical case. If there are constraints which enforce the variables to be integer, it is called *integer program* (IP), which also belongs to the class of NP-hard problems. One can formulate the TSP as an integer program with the objective, eq. (1), and the constraints, eqs. (2) to (4), [32]:

$$\text{minimize } \sum_i \sum_{j < i} c_{ij} x_{ij} \quad (1)$$

$$\text{subject to } x_{ij} \in \{0, 1\}, \quad (2)$$

$$\sum_j x_{ij} = 2, \quad \forall i \in V, \quad (3)$$

$$\sum_{i \in S, j \notin S} x_{ij} \geq 2, \quad \forall S \subsetneq V, S \neq \emptyset, \quad (4)$$

where the variables x_{ij} are 1 if i and j are consecutive in the tour, and 0 otherwise. The *objective*, eq. (1), minimizes the tour length. The *integer constraints*, eq. (2), restrict x_{ij} to the integers 0 and 1, the *degree constraints*, eq. (3), ensure that every city has exactly two neighbors,

one for the salesperson to enter, one to leave. And the *subtour elimination constraints* (SEC), eq. (4), prevent closed subtours, *i.e.*, loops which visit just a subset of all cities, by forcing at least two edges to cross the boundaries of all sets $S \subsetneq V, S \neq \emptyset$, which ensures that the salesperson can enter and leave the set. Hence a closed subtour would violate the constraint for the set S which contains all cities of the subtour. Note that there are exponentially many SECs, because there are exponentially many different subsets $S \subset V$. To solve this integer program, it is first relaxed to a LP, *i.e.*, eq. (2) is replaced by $x_{ij} \in [0, 1]$. The solution of this LP relaxation will always have a better or equal tour length than the solution of the TSP, but may not always be a valid tour, *i.e.*, may have fractional x_{ij} . Though, if the solution of a LP relaxation is integer, it is guaranteed to be the optimal tour.

Because there are exponentially many SECs, they will not be enforced in the beginning, instead SECs will be added if violated by the current LP solution, and the resulting LP is solved again. The violated SECs can be found by a *global minimum cut*, *e.g.*, with the Stör-Wagner algorithm in polynomial time [33]. This is iterated until no violated SEC exists anymore.

A measure of hardness of an instance for a given LP algorithm is as follows: if the LP relaxation results in all variables being integer, *i.e.*, if the instance can be solved in polynomial time [34–36], it is therefore *easy*. Also we will look at the *degree LP relaxation* where the SECs are removed and only the degree constraints, eq. (3), and the bounds are enforced. Here, we also find instances which are solved by this simpler algorithm. Thus, they can be considered even *easier*.

Note that this algorithm can easily be extended to find always the optimal solution, by a branch-and-cut search [3] at the cost of a worst-case exponential running time. Nevertheless, here we are mostly interested in the algorithm-dependent hardness of an instance, not necessarily in always finding a solution. The focus on the solvability by LP methods allows reasonable big instances of up to $N = 1448$ cities at 80 different $\sigma \in [0, 60]$ and 5000

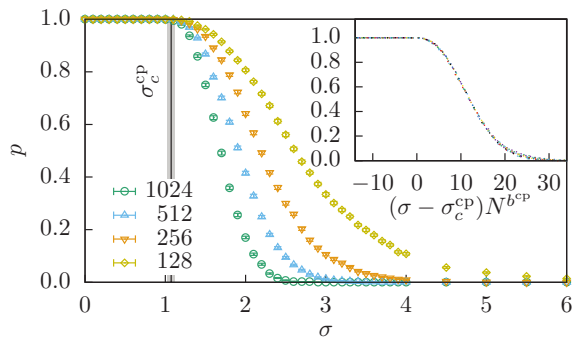


Fig. 2: (Color online) Probability p that the LP relaxation is integer, *i.e.*, the solution can be obtained by LP, as a function of the displacement parameter σ . The inset shows the same p for $N \geq 256$ plotted with a rescaled σ -axis with $\sigma_c^{\text{cp}} = 1.07(5)$ and $b^{\text{cp}} = 0.43(3)$ obtained by fig. 3. Different symbols and error bars are omitted for clarity.

samples each. All error bars are obtained via bootstrap resampling [37–39] if not noted otherwise.

The probability p to find the true integer solution using the LP relaxation is plotted in fig. 2. For small disorder, p is constant at $p = 1$ and falls with increasing σ to $p = 0$. With increasing system size N the curves become steeper. This pattern is typical for a phase transition. Therefore, the results indicate a phase transition from an *easy* phase, where the instances are typically solvable by polynomial-time linear programming techniques, to a *hard* phase. Next, we determined the transition point σ_c^{cp} in the limit $N \rightarrow \infty$ and the exponent b^{cp} , governing the finite-size scaling behavior [40] near the transition point, corresponding to the correlation-length exponent for physical systems. For this purpose we fitted parabolas to the variance of p in the vicinity of the maximum, see fig. 3. For second-order phase transitions the peak positions are expected to follow $\sigma = \sigma_c^{\text{cp}} + aN^{-b^{\text{cp}}}$, which holds well for our data as depicted in the inset of fig. 3.

According to finite-size scaling, rescaling the σ -axis according to $(\sigma - \sigma_c^{\text{cp}})N^{b^{\text{cp}}}$ should yield a collapse of the data onto one curve [41] for big values of N in the vicinity of the critical point. This is true for our data as visible in the inset of fig. 2, confirming the values of σ_c^{cp} and b^{cp} .

To identify a region of even *easier* instances, we studied also the LP by applying only the degree constraints, eq. (3), see fig. 4. We found a second easy-hard transition with $\sigma_c^{\text{lp}} = 0.51(4)$ and $b^{\text{lp}} = 0.29(6)$.

A further class of cutting-plane inequalities for the TSP are blossom inequalities [42] which originate from the two-matching LP [43]. A subset, which is easy to separate using heuristics, consists of *fast blossoms* [3], available in *Concorde* [3]. Doing the same analysis as above revealed a third transition (not shown) at $\sigma_c^{\text{fb}} = 1.47(8)$ with $b^{\text{fb}} = 0.40(3)$.

Next, we want to find out whether the easy-hard transitions are accompanied by changes of suitably defined structural order parameters. For up to $N = 180$ the

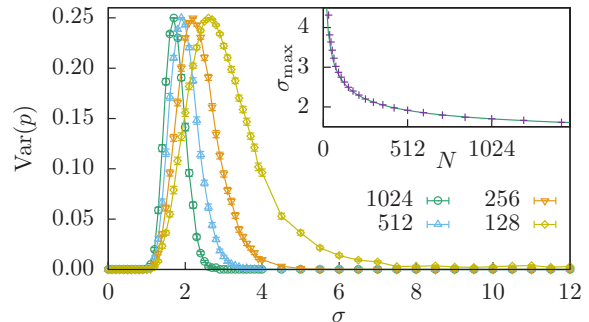


Fig. 3: (Color online) Variance of the solution probability $\text{Var}(p)$ as a function of the disorder σ . The inset shows the position of maximal variance of the solution probability p over the number of cities N . The positions are obtained by second-order polynomials fitted to the 5 data points next to the peak. The power law $\sigma = aN^{-b^{\text{cp}}} + \sigma_c^{\text{cp}}$ is fitted to the peak positions for $N \geq 256$ to minimize the effects of corrections to scaling, yielding $\sigma_c^{\text{cp}} = 1.07(5)$ and $b^{\text{cp}} = 0.43(3)$.

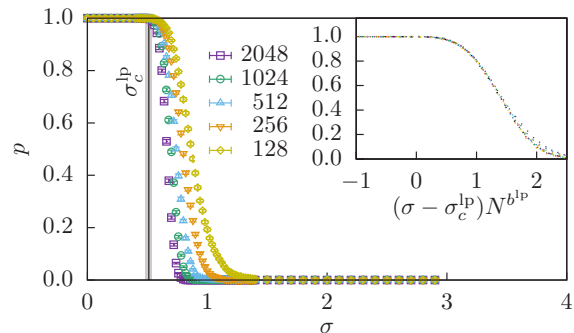


Fig. 4: (Color online) Probability p that the degree LP relaxation is integer. The inset shows the collapse for $N \geq 256$, with $\sigma_c^{\text{lp}} = 0.51(4)$ and $b^{\text{lp}} = 0.29(6)$ obtained from the same type of analysis as in fig. 3 for $N \geq 512$.

optimal tours for all studied samples were obtained by a branch-and-cut procedure, available in *CPLEX*, to examine structural properties of the solutions. With increasing values of σ , optimized tours appear to be more “meandering” as shown in fig. 1. As a measure of this “meandering”, we used the *tortuosity* τ , as defined in ref. [44], where it was used to evaluate images of blood vessels in the retina to detect vascular diseases. To calculate τ , the tour is segmented into n segments, such that each segment has the same curvature sign and is of maximal length. Let the *arc length* L_i be the length of the segment i along the tour and let the *chord length* S_i be the direct distance between the first and last city of the segment i and L the total length of the tour. Then the tortuosity is defined as

$$\tau = \frac{n-1}{L} \sum_{i=1}^n \left(\frac{L_i}{S_i} - 1 \right). \quad (5)$$

When plotting τ as a function of σ in fig. 5, it shows peaks near σ_c^{cp} . As a very rough estimate of the position of

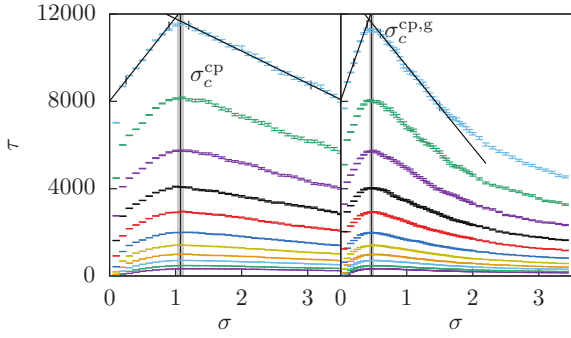


Fig. 5: (Color online) The tortuosity τ of optimal tours as a function of the displacement parameter σ for different system sizes $N \leq 180$ peaks at σ_c^τ , which coincides with σ_c^{cp} determined by the fit in fig. 3 (gray bar = mean + error). On the right side the same is done with data from a slightly modified model, explained later in the text.

this peak, straight lines are fitted to τ at $N = 180$, left and right of the peak, and their intersection is interpreted as an estimate of the peak positions, with errors obtained by error propagation. This is shown for $N = 180$ in fig. 5 and done for all sizes $N \geq 64$. Via a power-law fit to $\sigma^\tau = \sigma_c^\tau + aN^{-c}$, we estimated an asymptotic $\sigma_c^\tau = 1.06(23)$, which is consistent with the estimate σ_c^{cp} from fig. 3. Unfortunately the fit is not good enough to give a meaningful estimate of the more susceptible corresponding exponent b^τ .

Comparing the solution tour x_{ij} to the circularly shaped optimal tour at $\sigma = 0$, it is expected that they are similar at very small disorder σ . A way to measure this similarity is to look at the number of edges occurring in one tour but not in the other, *i.e.*, the Hamming distance [45]. The tour difference d shown in fig. 6 is the Hamming distance normalized by $2N$, such that two tours with no common edges would result in $d = 1$ while two tours visiting the cities in the same sequence would result in $d = 0$. This observable seems to be roughly independent of N . Figure 6 suggests that the easy-hard transition observed when using the degree LP relaxation alone corresponds to the structural change observed by studying the Hamming distance d .

Unfortunately, we were not able to identify so far an observable which corresponds to the phase transition occurring when using the fast blossoms.

We performed the same analysis for a different random ensemble, where the cities are displaced by Δx and Δy from a Gaussian distribution $G(0, \sigma)$ for each direction. As expected for continuous phase transitions, we obtained (not shown) the same critical exponent $b^{\text{cp},g} = 0.45(5)$ within error bars, which hints that this model exhibits universality with respect to the type of disorder. The resulting values are shown in table 1. Also for the case of cities displaced spherically by ϕ , θ and r from uniform distributions in three dimensions, it shows the same critical exponent $b^{\text{cp},3} = 0.40(4)$. Note that, unlike many other models (*e.g.* Ising ferromagnet or

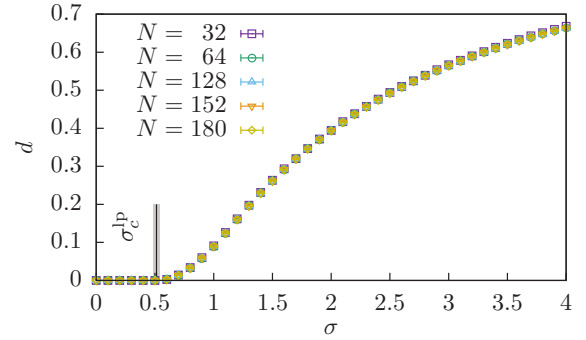


Fig. 6: (Color online) Difference of the optimal tour to the initial circle as a function of σ .

Table 1: Values of critical points and exponents grouped by different types of transitions.

	σ_c	b
With SEC	$\sigma_c^{\text{cp}} = 1.07(5)$	$b^{\text{cp}} = 0.43(3)$
	$\sigma_c^\tau = 1.06(23)$	–
	$\sigma_c^{\text{cp},g} = 0.47(3)$	$b^{\text{cp},g} = 0.45(5)$
	$\sigma_c^{\tau,g} = 0.44(8)$	–
	$\sigma_c^{\text{cp},3} = 1.18(8)$	$b^{\text{cp},3} = 0.40(4)$
Only degree	$\sigma_c^{\text{lp}} = 0.51(4)$	$b^{\text{lp}} = 0.29(6)$
Fast blossoms	$\sigma_c^{\text{fb}} = 1.47(8)$	$b^{\text{fb}} = 0.40(3)$

percolation), the different dimension does not lead to a different exponent.

We have shown that for this random ensemble governed by the parameter σ there exist various easy-hard phase transitions. This indicates a rich behavior of the ensemble with respect to the typical computational hardness. Furthermore, at least for two cases we found that the transitions can be correlated with measurable changes of the solution structure, namely the Hamming distance to the circle solution and tortuosity, respectively. The transitions can be characterized by critical exponents b . Within the statistical accuracy of our data, the critical exponents for the different easy-hard transitions are compatible within two sigmas.

An interesting question for further study would be finding an answer to why the tortuosity τ peaks at σ_c , where the TSP becomes not solvable using LP and SEC. Unfortunately, τ is quite complex to measure. Therefore, the search for a simpler observable showing the transition would be of equal interest.

Besides the blossom inequalities, there are more complicated inequalities valid for the TSP establishing facets on the polytope, which can be implemented as cutting planes and partly already be separated in polynomial time [46]. It would be interesting if those established a further phase transition at higher σ and if the critical exponent b stayed the same.

In general, LP-based algorithms are used a lot in practice and it would be of great interest to study suitable ensembles of other NP-hard optimization problems with respect to easy-hard transitions. Furthermore, a statistical-mechanics analysis of the performance of LP-based algorithms, as done in the past for branch-and-bound algorithms [22,23], would yield more insight into the sources of computational hardness.

The simulations were performed at the HPC Cluster HERO, located at the University of Oldenburg (Germany) and funded by the DFG through its Major Research Instrumentation Programme (INST 184/108-1 FUGG) and the Ministry of Science and Culture (MWK) of the Lower Saxony State.

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