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Finding maximizing Euclidean TSP tours for the Häme-Hyytiä-Hakula conjecture

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Finding maximizing Euclidean TSP tours for the Häme-Hyytiä-Hakula conjecture

Christian L. Müller [1]

1 Introduction

In the open problem session of the 27th European workshop on Computational Geometry (EuroCG 2011), Lauri Häme posed the problem of finding optimal tours of Euclidean TSP instances that maximize a certain objective function. Let $\mathbf{p}_j = (x_j, y_j)^T$ be the coordinates of the j^{th} city in the 2D plane. Let us assume that the optimal TSP tour is given by the permutation $\pi(j) = i$ that defines the ordering of the points along the tour. The coordinates of the ordered N cities are stored in a vector $\mathbf{x} = [\mathbf{p}_1, \mathbf{p}_2, \ldots, \mathbf{p}_i, \ldots, \mathbf{p}_N]^T \in \mathbb{R}^n$ with $n = 2N$. Let α_i be the non-reflex angle spanned by the triplet $\mathbf{p}_{i-1}, \mathbf{p}_i, \mathbf{p}_{i+1}$. For the special case $\mathbf{p}_1$ the preceding city is $\mathbf{p}_N$. A sketch is given in Figure 7.

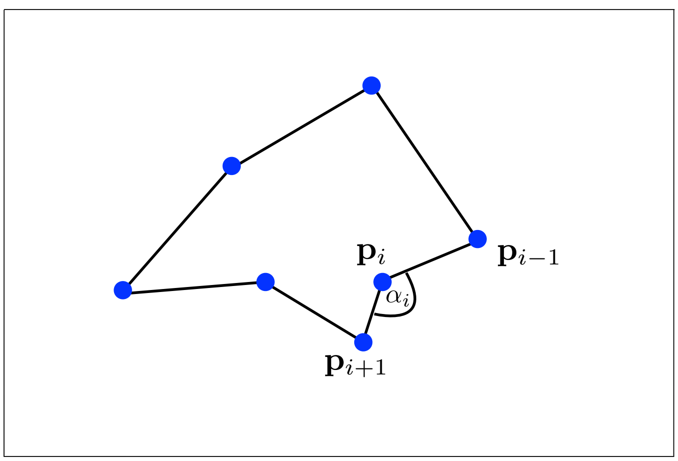

Figure 1: Sketch of an optimal TSP tour for $N = 7$ cities $\mathbf{p}_i$ and the corresponding non-reflex angle α_i.

We now define the following objective function $f_{\text{Häme}}$:

$$f_{\text{Häme}}(\mathbf{x}) = 2/N \sum_{i=1}^{N} \cos(\alpha_i/2) \tag{1}$$

The optimization problem consists now in the task to find the arrangement $\mathbf{x}^*$ of N cities that maximizes $f_{\text{Häme}}(\mathbf{x})$, that is:

$$\mathbf{x}^* = \arg\max_{\mathbf{x} \in \mathbb{R}^n} f_{\text{Häme}}(\mathbf{x}) \,. \tag{2}$$

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In [1] Häme, Hyytiä, and Hakula conjecture that the objective function defined in eq. (1) is bounded by $\sqrt{3}$ for any optimal tour of any instance of the Euclidean TSP. We call this conjecture for short HHH-conjecture. Such a bound would be useful because it would provide an easy way to reject putative optimal solutions of some TSP instance that do not satisfy this criterion. Häme et al. show that the bound is tight for the equilateral triangle for $N = 3$. They furthermore provide a constructive method for optimal TSP tours $\mathbf{x}^*_{\text{HHH}}$ with $\lim_{N\to\infty} f_{\text{Häme}}(\mathbf{x}^*_{\text{HHH}}) = \sqrt{3}$ (see Figure 4 in [1]). However, for small N it is not known (i) whether the conjecture is valid and (ii) whether there exist a regular geometric pattern for maximal tours. In this report we tackle these questions by using a numerical black-box optimization approach. We search for optimal TSP tours $\mathbf{x}^* \in \mathbb{R}^n$ for up to $N = 8$ cities. In Section 2 we describe the formulation of the problem, the used optimizers, and the set-up of the numerical experiments. In Section 3 we present and discuss the obtained results. We conclude this report in Section 4.

2 Computational Experiments

The present problem is a formidable challenge for black-box optimization because the objective of finding an arrangement of cities that maximize eq. (1) is most certainly highly non-convex and discontinuous. Given a collection of points in 2D, we first have to find the optimal TSP tour $\tilde{\mathbf{x}}$, a classic NP-hard combinatorial problem. We then calculate $f_{\text{Häme}}(\tilde{\mathbf{x}})$ and try to perturb the location of the points in such a way that we maximize this objective. Note that analytic gradients are not available for this objective function. It is conceivable that a slight perturbation of a city location results in a completely different optimal tour, thus leading to different angles α_i and objective function values.

We use the following strategy to tackle the problem. For a fixed arrangement of N cities we solve the TSP problem by using a slightly modified naive algorithm of enumerating all possible $N!$ tours and choosing the minimal one. In order to remove the two translation degrees of the freedom of the problem, we fix the location of the first city to the origin $\mathbf{p}_1 = (0, 0)^T$. We furthermore remove N degrees of freedom in the enumeration problem by just considering all possible tour that start and end at the first city.

We consider two different variable-metric randomized search heuristics, the Evolutions Strategy with Covariance Matrix Adaptation (CMA-ES) [2] and Gaussian Adaptation (GaA) [3, 4] for the outer maximization problem. These search heuristics are known to perform well in practice for a wide variety of black-box problems where gradients or higher-order information are not explicitly available or do not exist. Both algorithms are iterative methods that sample a set of candidate solutions from a multivariate normal distribution. In each iteration the mean and covariance matrix of the distribution are adapted based on the information about the sampled positions in the search space and their corresponding objective function values. While CMA-ES intends to increase the likelihood of generating successful search directions, GaA adapts the normal distribution using maximum entropy arguments. An excellent tutorial about CMA-ES can be found in [5]. Further information about GaA are available in [4, 6, 7]. Compared to the standard CMA-ES parameter settings outlined in [5], we use the slightly bigger sample size $s = 5n$ instead of $s = 4 + 3\lfloor \log n \rfloor$ per iteration. The standard settings of GaA (outlined in [6]) are changed for the learning parameter of the covariance matrix N_{C} for the $N = 8$ case. It is set to a more conservative value of $N_{\text{C}} = 1e3$. Preliminary runs showed that the covariance can be become badly-conditioned otherwise (due to the presence of very small and very large scales in the resulting solutions).

The only initial objective function information needed by the algorithm is a feasible

CMA-ES	$N=3$	$N=4$	$N=5$	$N=6$	$N=7$	$N=8$
Run 1	1.73205081	1.70708836	1.70065854	1.75496939	1.74383666	1.76663567
Run 2	1.73205081	1.70706045	1.70065856	1.75504088	1.74383673	1.76662842
Run 3	1.73205081	1.70697116	1.70065861	1.75506263	1.74383673	1.76662587
Run 4	1.73205081	1.70707805	1.70065837	1.75502498	1.74383671	1.76662127
Run 5	1.73205081	1.70702984	1.70065857	1.75506401	1.74383673	1.61106728

Table 1: Maximum values of $f_{\text{Häme}}$ reached by CMA-ES.

GaA	$N=3$	$N=4$	$N=5$	$N=6$	$N=7$	$N=8$
Run 1	1.73205081	1.41421356	1.70065862	1.58842787	1.70680148	1.76664982
Run 2	1.73205081	1.60980706	1.70065785	1.75454531	1.65459858	1.76660479
Run 3	1.73205081	1.70608257	1.70065774	1.75492896	1.65399433	1.76633620
Run 4	1.73205081	1.47066969	1.70065800	1.75383153	1.65344645	1.76662802
Run 5	1.73205081	1.70708590	1.70057451	1.58480209	1.74383672	1.76663370

Table 2: Maximum values of $f_{\text{Häme}}$ reached by GaA.

starting configuration $\mathbf{x}_0$ and a step size parameter σ_0 that determines the standard deviation of the initial spherical multivariate normal distribution. Note that by fixing the location of the first city, our problem dimension is reduced by two, i.e. for N cities we have $n = 2N - 2$. The initial arrangement of cities $\mathbf{x}_0 \in \mathbb{R}^n$ is drawn uniformly at random from the $[0, 10]^n$ hypercube. The initial step size $\sigma_0 = 1$. We restrict the feasible region to the $[-1000, 1000]^n$ hypercube in order to disallow an unbounded growth of the city locations. This is necessary because the objective function only depends on angles α_i which are independent of the scale of the underlying tour. We consider TSP problems with $N = 3, \ldots, 8$ cities. We bound the number of allowed function evaluations (FES) of the objective by MAX_FES= $2 \cdot 10^4 n$. However, we do not exhaust this budget if other convergence criteria are reached, i.e., we do not perform restarts. For each N we perform five repetitions of the described numerical optimization experiments.

3 Results: Putative maximal tours for $N \leq 8$ cities

We first summarize the general results of the optimization runs. Plots and coordinates of the maximizing configurations are discussed in the subsequent subsections. We observe that CMA-ES shows slightly better average performance than GaA in terms of maximum objective function value reached. However, both methods agree on the maximal solutions (at least up to the third digit for each instance). Table 1 and Table 2 summarize the reached objective function values of CMA-ES and GaA, respectively, for all instances and repetitions.

These results suggest that the HHH-conjecture is valid for $N = 3, 4, 5$, but not for $N = 6, 7, 8$. However, this needs further independent geometric checking by Häme and co-workers. Especially the double-precision number model we use might affect the determination of the optimal tour. It is noteworthy that all solutions that violate the HHH conjecture are unstable in the sense that slight perturbations to the configurations can result in different optimal tours that satisfy the conjecture. This also suggests that an "intuitive" rational design of these tours is potentially very hard and the used black-box optimization approach is a useful tool.

We now provide figures for all maximal tours found by CMA-ES (which are geometrically almost equivalent to GaA's). For convenience, we scale down all configurations to the [-1,1] box. Occasionally, we also provide detailed views of small-scale structures of the maximal tours. The coordinates of the tours are listed as $2 \times N$

matrices.

3.1 Maximizing tours for $N = 3$

We use the $N = 3$ case as a simple double-check whether the implementation of our objective function as well as the chosen black-box optimization approach makes sense at all. We know *a priori* that the optimal solution is the equilateral triangle. Indeed, both GaA and CMA-ES rapidly find this solution and approximate the optimal objective function value $\sqrt{3}$ up to the ninth digit.

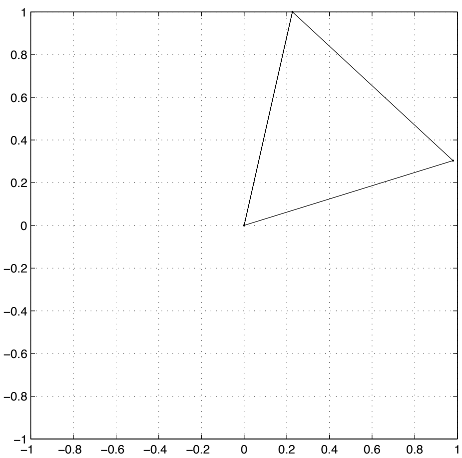

Figure 2: Maximal TSP tour for $N = 3$ cities with $f_{\text{Häme}}(\mathbf{x}) = \sqrt{3}$.

3.2 Maximizing tours for $N = 4$

The maximal tour for $N = 4$ already reveals an interesting pattern. It is very similar to the configuration provided by Häme (see Figure 8). It consists of two distant cities which are separated by two cities that are very close to each other and the line connecting the two distant cities. The limiting configuration would lead to two angles α_3, α_4 approaching 0, and two angles α_1, α_2 approaching 90° thus resulting in $f_{\text{Häme}} = 2/4 \cdot 2(\cos(0) + \cos(\pi/4)) = 1 + 1/\sqrt{2}$. Based on our numerical optimization results we thus suggest that the latter expression is the *supremum* of $f_{\text{Häme}}$ for $N = 4$. The coordinates of the depicted cities are:

0.000000000000000	0.000313790523645	0.762830610905362	-1.000000000000000
0.000000000000000	0.000344627762314	-0.666435000801989	0.948694904709909

The optimal order is $[1, 2, 3, 4]$.

3.3 Maximizing tours for $N = 5$

The maximal configurations for $N = 5$ agree with the HHH-conjecture. It is formed by a triangle with a kink at one side. This configuration is again similar to the one proposed by Häme (see Figure 9), however, with different side lengths. The coordinates of the depicted cities are:

0.000000000000000	-0.122143427990517	0.865897232779853	0.149052140172011	0.381867065017353
0.000000000000000	0.239188992322131	1.000000000000000	0.094475971836293	-0.815692128401913

The optimal order is $[1, 4, 2, 3, 5]$.

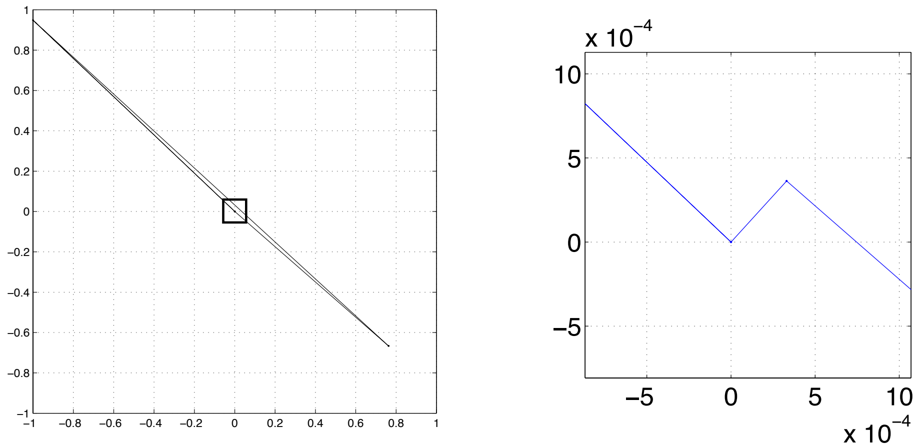

Figure 3: Maximal TSP tour for $N = 4$ cities with $f_{\text{Häme}}(\mathbf{x}) = 1.707088363719576 \approx 1 + \sqrt{2}/2$. The right panel shows a detailed view of the kink region.

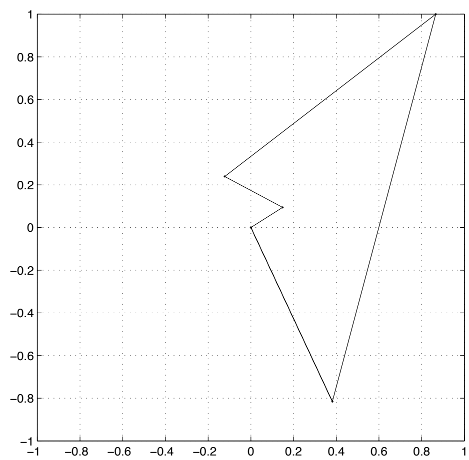

Figure 4: Maximal TSP tour for $N = 5$ cities with $f_{\text{Häme}}(\mathbf{x}) = 1.700658561053293$

3.4 Maximizing tours for $N = 6$

The maximal tour for $N = 6$ is the first instance that seems to violate the HHH-conjecture $f_{\text{Häme}}(\mathbf{x}) = 1.755064005205272$. Its structure is surprisingly similar to the $N = 4$ case. However, this time two distant cities are separated by 4 cities that form a "W" pattern.

The coordinates of the depicted cities are:

0.000000000000000 1.000000000000000 0.009112614136206 -0.003925991818460 0.007025267155736
0.000000000000000 0.470703929148958 -0.006481507533350 0.013830651187737 0.004508984673990

-0.659092389894056
-0.557536857720572

The optimal order is $[1, 3, 6, 2, 4, 5]$.

3.5 Maximizing tours for $N = 7$

The maximal tour for $N = 7$ is the second instance that seems to violate the HHH-conjecture with $f_{\text{Häme}}(\mathbf{x}) = 1.74383672809659$. Its structure is similar to the $N = 5$ case. However, this time the simple kink is replaced by a "W" pattern as well.

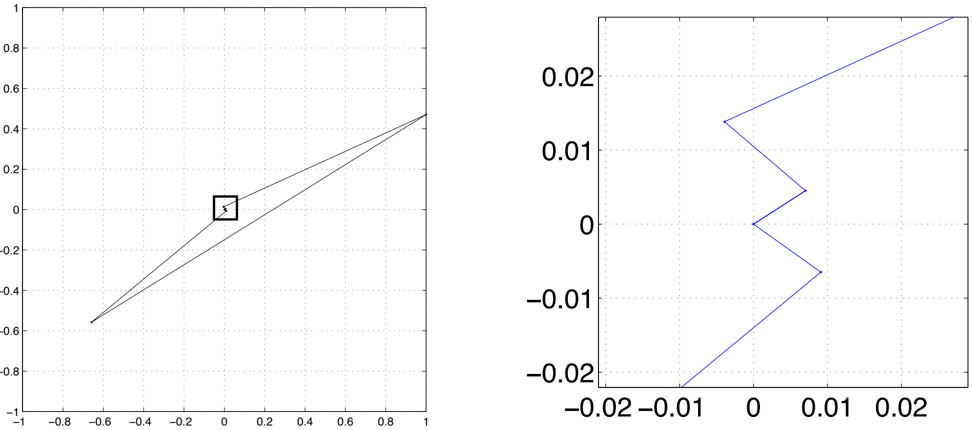

Figure 5: Maximal TSP tour for $N = 6$ cities with $f_{\text{Häme}}(\mathbf{x}) = 1.755064005205272$. The right panel shows a detailed view of the kink region.

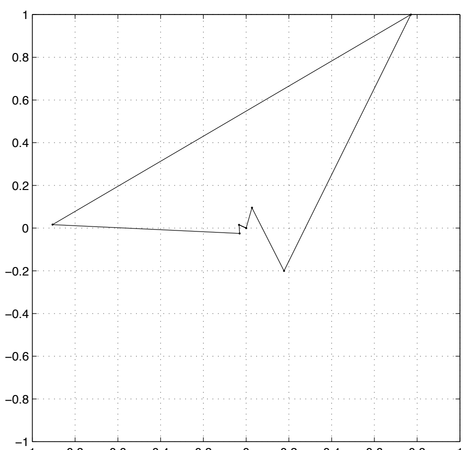

Figure 6: Maximal TSP tour for $N = 7$ cities with $f_{\text{Häme}}(\mathbf{x}) = 1.74383672809659$.

The coordinates of the depicted cities are:

0.000000000000000	-0.032698237006735	0.027255246575148	0.770475677669605	-0.030369722545232
0.000000000000000	0.015171686772064	0.095523150763347	1.000000000000000	-0.025041512723650
-0.905436360341430	0.177356450901677			
0.016561774715430	-0.200421987435255			

The optimal order is $[1, 3, 7, 4, 6, 5, 2]$.

3.6 Maximizing tours for $N = 8$

The maximal tour for $N = 8$ is the third instance that seems to violate the HHH-conjecture with $f_{\text{Häme}}(\mathbf{x}) = 1.766621273793079$. Its structure is different from the previous configurations with even number of cities. It is a kite-like structure with a "W" pattern between the wings. It might be that this structure is sub-optimal and an even better configuration exist similar to the patterns observed in the $N = 4, 6$ case. Further optimization runs might show this.

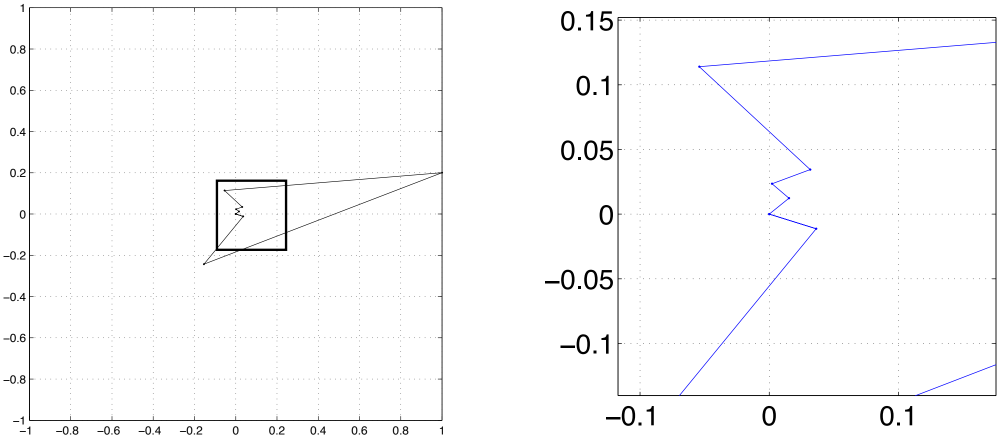

Figure 7: Maximal TSP tour for $N = 8$ cities with $f_{\text{Häme}}(\mathbf{x}) = 1.766621273793079$. The right panel shows a detailed view of the kink region.

0.000000000000000	0.002168676431030	-0.054079526626567	0.015249585316206	-0.153876243875765
0.000000000000000	0.023441257113698	0.114026726096821	0.012317574035279	-0.242980202722913
1.000000000000000	0.031667207745441	0.036360406522439		
0.200504197368216	0.034428868905803	-0.011362848988851		

The optimal order is $[1, 4, 2, 7, 3, 6, 5, 8]$

4 Conclusions

In this technical report we analyzed the validity of the HHH-conjecture for TSP tours up to $N = 8$. Our preliminary results suggest that it is valid for $N = 3, 4, 5$ but not for $N = 6, 7, 8$. For the latter instances we have provided configurations that seem to violate the conjecture. For the $N = 4$ we conjecture the new supremum $1 + 1/\sqrt{2}$ based on the numerically obtained solutions. The reported results need careful double-checking by Häme and co-workers because it might turn out that the double-precision number model might hamper the optimality of the true tours. If so, we might need to consider alternative number representations. In case, the validity of the tours is confirmed, three possible lines of research arise from the current work. First, we may implement an $O(n^2 2^n)$ algorithm for TSP in order to be able to tackle instances $N > 8$. Second, an in-depth analysis of the provided numerical solutions might lead to a constructive way to generate tours for general N that maximize $f_{\text{Häme}}$ and thus lead to the true upper bound. Finally, it might also be possible to prove optimality of the tours using geometric arguments.

5 Acknowledgements

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Appendix

Häme provided a list of putative maximal tours in an email to the author of this report. These tours have been found by pure random search. Their shapes along with the corresponding objective function values are listed below.

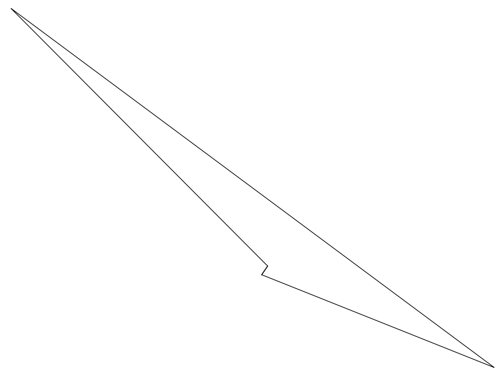

Figure 8: Putative maximal TSP tour for $N = 4$ cities found by Häme with $f_{\text{Häme}}(\mathbf{x}) = 1.7035596210462067$.

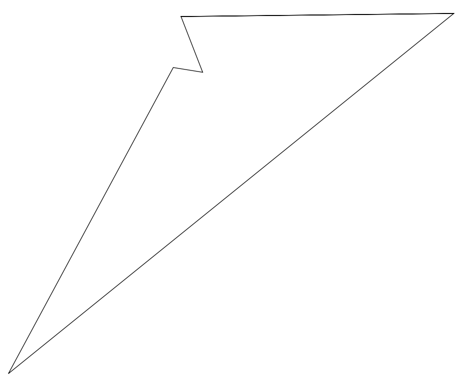

Figure 9: Putative maximal TSP tour for $N = 5$ cities found by Häme with $f_{\text{Häme}}(\mathbf{x}) = 1.67791654156608$.

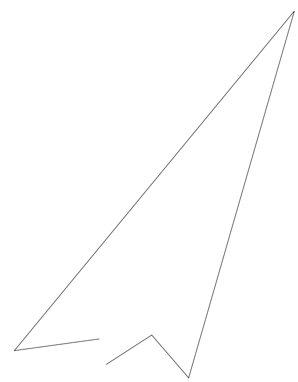

Figure 10: Putative maximal TSP tour for $N = 6$ cities found by Häme with $f_{\text{Häme}}(\mathbf{x}) = 1.6345702280832342$.

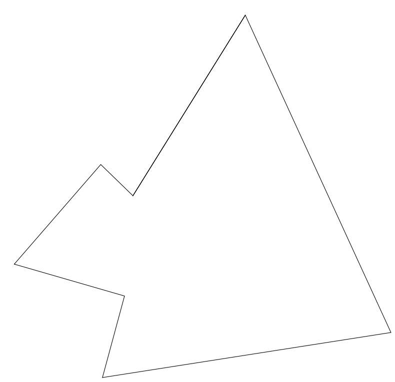

Figure 11: Putative maximal TSP tour for $N = 7$ cities found by Häme with $f_{\text{Häme}}(\mathbf{x}) = 1.5902711443213857$.

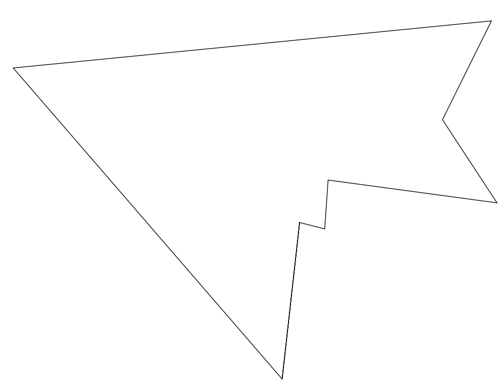

Figure 12: Putative maximal TSP tour for $N = 8$ cities found by Häme with $f_{\text{Häme}}(\mathbf{x}) = 1.5844186365098027$.

References

[1] Lauri Häme, Esa Hyytiä, and Harri Hakula. The Traveling Salesman Problem with Differential Neighborhoods. In *Abstracts from the 27th European Workshop*

on Computational Geometry (EuroCG 2011), pages 51–54, Morschach, March 2011. ETH Zurich.

[2] Nikolaus Hansen and Andreas Ostermeier. Completely Derandomized Self-Adaption in Evolution Strategies. *Evolutionary Computation*, 9(2):159–195, 2001.

[3] Gregor Kjellström and Lars Taxen. Stochastic Optimization in System Design. *IEEE Trans. Circ. and Syst.*, 28(7), July 1981.

[4] Christian L. Müller and Ivo F. Sbalzarini. Gaussian adaptation revisited - an entropic view on covariance matrix adaptation. In C. Di Chio et al., editor, *EvoApplications*, volume I of *Lecture Notes in Computer Science*, pages 432–441. Springer, 2010.

[5] Nikolaus Hansen. The CMA Evolution Strategy: A Tutorial. http://www.lri.fr/ hansen/cmatutorial.pdf, 2008.

[6] Christian L. Müller and Ivo F. Sbalzarini. Gaussian adaptation as a unifying framework for continuous black-box optimization and adaptive monte carlo sampling. In *Evolutionary Computation (CEC), 2010 IEEE Congress on*, pages 1 –8, 2010.

[7] Christian L. Müller. *Black-box Landscapes: Characterization, Optimization, Sampling, and Application to Geometric Configuration Problems.* PhD thesis, Institute of Theoretical Computer Science, Department of Computer Science, ETH Zürich, 2010.