Multiple Traveling Salesmen and Related Problems: A Maximum-Entropy Principle based Approach

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Abstract— **This paper presents a new heuristic approach for multiple traveling salesmen problem (mTSP) and other variants of the TSP. In this approach, the TSP and its variants are seen as constrained resource allocation problems, where an ordered set of resources is associated to the cities, and the allocation is done through an iterative algorithm in such a way that eventually each city gets associated with a resource. The approach allows adding constraints on resources which translate to objectives such as minimum tour length (or multiple tour lengths as in mTSP) and other constraints that define the variants on the TSP problem. The algorithm for the associated resource allocation problem is based on maximum entropy principle (MEP) and the deterministic annealing algorithm. Besides mTSP, this article demonstrates this approach for close enough traveling salesman problem (CETSP), which is known to be computationally challenging since there is a continuum of possible edges between a pair of cities. The examples presented in this paper illustrate the effectiveness of this new framework for use in TSP and many variants thereof. Simulations demonstrate that the proposed MEP algorithm achieves significantly better solutions than the ones provided by the most commonly used simulated annealing algorithm with only marginal increase in run-time.**

I. INTRODUCTION

The Traveling Salesman Problem (TSP) [1] is one of the most extensively studied optimization problems. A TSP considers the following optimization problem: *Given a set of cities and the associated cost of travel between each pair of cities, find the route that minimizes the total cost of travel such that each city is visited exactly once and the route ends at the origin city*. Each route through all the cities is referred to as a tour and the *optimal* tour is the one that minimizes the total travel cost to the salesman. There are several applications of the TSP to real world problems. Common applications of the TSP are vehicle delivery route planning and toolhead path planning for VLSI circuit boards. Junger *et al.* [1] as well as Bektas [2] have explored many more applications of the TSP to more specialized problems, demonstrating the real world value and importance of developing effective solutions to the TSP.

The TSP belongs to the class of NP-hard problems [2]. Generally, finding the optimal solution requires a calculation time given by $O(n!)$, where n is the number of cities in the problem. For TSPs with relatively few cities, the optimal solution can be determined by solving associated linear programs within a short period of time; but for larger data sets the computations can become extremely time intensive. Only with the development of more powerful computers the optimal solutions have been discovered for certain TSPs, as computation times in the hundreds of CPU-years had made those solutions infeasible in the past [3]. Many heuristics have been developed for the TSP [1], [2] which offer significant computational savings at the cost of some deviation from the optimal solution.

Despite the success of heuristics for the basic TSP, there are quite a few variants of the TSP that these methods cannot efficiently address. Variants to the basic TSP are necessary to appropriately model realistic situations. In this paper, we present a new framework for solving two such variants of the TSP - a) the *multi-Traveling Salesmen Problem* (mTSP) which allows more than one 'salesman' to operate between the cities, such that the solution to the mTSP is comprised of several routes, one for each salesman, and the optimal tour would be the set of routes such that the total distance traveled is minimized. We also consider variants of this mTSP problem, where additional constraints such as requiring each salesman to start at the same point (representing a warehouse or depot) are included. In [4], few transformations have been suggested, using which a certain mTSP can be viewed as an equivalent "asymmetric" single TSP, which then allows using conventional heuristics for the single TSP; however these transformations are restricted to only one type of mTSP formulation presented in [4] and do not extend to a broader class of variants of the basic TSP and mTSP. b) the *Close Enough Traveling Salesman Problem* (CETSP) is a variant where it suffices for a salesman to reach within a certain radius of each city on the tour. This adds great complexity to the problem; since there is a continuum of possible edges between a pair of cities. Because of the significant increase in the number of edges, many conventional heuristics are unable to address this variant. Special formulations have been developed to address this problem [5], [6]; however, the formulation is not very general and requires uniform radii for all the cities.

The central concept in the proposed framework is viewing the TSP and its variants as resource allocation problems. In this viewpoint, an ordered set of resources that are equal to the number of cites are introduced, and constraints are imposed on the resources that reflect objectives such as minimum tour length that are specific to the TSP variant of interest. Then a resource allocation problem is solved that minimizes the sum of the distances of each resource to its nearest city. This results in each resource being allocated to a distinct city (and its location coincides with that of the city), and consequently the *order* of the resource set specifies the tour. This viewpoint allows efficient resource allocation algorithms such as deterministic annealing (DA)

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to be modified appropriately to address TSP and its variants. DA is well-suited to combinatorial clustering/resource allocation problems that require obtaining an optimal partition of an underlying domain, and optimally assigning resources to each cell of the partition. DA-based methods have been reported in a vast number of applications such as minimum distortion problems in data compression [7], routing problems in multiagent networks [8], locational optimization problems [9], and coverage control problems [10]. While the original DA algorithm was developed in the context of clustering, it was later adapted to the basic TSP as a case of constrained clustering [7], [11], which serves as the foundation for this extension to the mTSP. We recently demonstrated the usefulness of DA in the context of capacitated vehicle routing problems (CVRPs) [12].

II. PROBLEM FORMULATION

In this section, we describe some variants of the TSP. The set of locations of cities is denoted by $\{x_i : x_i \in \mathbb{R}^2, 1 \leq i \leq n\}$, where n is the number of cities. In some variants of the basic TSP, the starting location (same as the end-point location) is often specified. This starting location is commonly referred to as *depot* and often show up in the context of vehicle routing problems with route of each vehicle starting and finishing at the depot. We use $\alpha \in \mathbb{R}^2$ to denote the location of depot. The distance between any two cities i and j is denoted by $d_{i,j}$. For example, for squared-euclidean distance, we have $d_{i,j} = \|x_i - x_j\|_2^2$. Any routing sequence that visits each city (and depot) exactly once is referred to as *tour*. Based on the requirements of the underlying problem, a tour may or may not conclude at the starting location. A *tour* is defined by the sequence $(\sigma_1, \ldots, \sigma_{n+1})$ (or $(\sigma_1, \ldots, \sigma_n)$ depending upon whether or not the starting and end locations coincide), where $\sigma_i \in \{1, \ldots, n\}$ denotes the index of the ith city in the tour; note that $\sigma_i \neq \sigma_j$ when $i \neq j$ and $1 \leq i, j \leq n$ and that $\sigma_{n+1} = \sigma_1$. Therefore each tour is completely specified by an index vector (ordered set) $\sigma = (\sigma_1, \ldots, \sigma_n)$.

A. Non-Returning Multi-Traveling Salesmen Problem

In this problem, we are given a set of n cities $\{x_i\}$ and m salesmen to traverse these cities. The objective is to minimize the total tour-length such that each city is visited just once by only one salesman. The starting and ending city locations of each salesman can not coincide. This formulation is applicable to problems pertaining to non-recurring events, such as the scheduling of orders at a steel rolling company [13]. The non-returning mTSP can be viewed as an equivalent single TSP in which $m-1$ edges are removed to give rise to m disjoint tours. The optimization problem is mathematically described as

$$\min_{\substack{\sigma \\ \{\alpha_{k_j}\}}} \left\{ \sum_{i=1}^{n-1} d_{\sigma_i,\sigma_{i+1}} - \sum_{j=1}^{m-1} \alpha_{k_j} d_{\sigma_{k_j},\sigma_{k_j+1}} \right\}$$
$$\text{s.t.} \quad \forall j, \sum_{k_j} \alpha_{k_j} = 1, \quad \alpha_{k_j} \in \{0,1\}, \quad 1 \leq k_j \leq n-1.$$

Note that the first term in the above cost function corresponds to minimizing the total distance between the neighboring cities (as in the basic TSP), while the second term corresponds to removing $m-1$ edges, thereby giving rise to m disjoint tours. The quantity $\alpha_{k_j} = 1$ if the edge corresponding to the cities $(\sigma_{k_j}, \sigma_{k_j+1})$ is removed. This optimization is explained in Fig. 1a.

B. Returning Multi-Traveling Salesmen Problem

In this problem, we are given a set of n cities $\{x_i\}$ and m salesmen, and the objective is to minimize the total tour length such that each city is visited by only one salesman, and the start and end positions of each salesman must be coincident. Many recurring events, such as job scheduling [14] fall under this category. The returning mTSP can be mathematically described as

$$\min_{\substack{\sigma \\ \{\alpha_{k_j}\}}} \left\{ \sum_{i=1}^{n} d_{\sigma_i,\sigma_{i+1}} + \sum_{j=1}^{m} \alpha_{k_j} \left[-d_{\sigma_{k_j},\sigma_{k_j+1}} + d_{\sigma_{k_j},\sigma_{k_{(j-1)}+1}} \right] \right\}$$
$$\text{s.t.} \quad \forall j, \sum_{k_j} \alpha_{k_j} = 1, \quad \alpha_{k_j} \in \{0,1\}, \quad 1 \leq k_j \leq n; k_0 = k_m.$$

As before, the first term in the above cost function corresponds to minimizing the total distance between the neighboring cities (as in the basic TSP). Removal of edge $\sigma_{k_j}, \sigma_{k_j+1}$ accounts for separating the route between two salesmen j and $j+1$, while addition of edge $\sigma_{k_j}, \sigma_{k_{(j-1)}+1}$ ensures that a salesman j returns back to its starting city. Fig. 1b shows a schematic of a returning mTSP. Note that the dashed blue lines indicate the removal of edges $(-d_{\sigma_{k_j},\sigma_{k_j+1}})$, while solid blue lines indicate the addition of links $(d_{\sigma_{k_j},\sigma_{k_{(j-1)}+1}})$.

C. Single-Depot Returning Multi-Traveling Salesmen Problem

In this problem, we are given a set of n cities $\{x_i\}$, a depot (α) and m salesmen, and the objective is to determine the optimal tour such that each city is visited once by only one salesman. Each salesman must start and end at the depot. The total distance traveled by all salesmen is minimized. Real-world problems such as vehicle routing problem (VRP) with single-depot [12] fall under this category. The single-depot mTSP is mathematically described as

$$\min_{\substack{\sigma \\ \{\alpha_{k_j}\}}} \Bigg\{ \sum_{i=1}^{n-1} d_{\sigma_i,\sigma_{i+1}} + d_{\sigma_1,\alpha} + d_{\sigma_n,\alpha}$$
$$+ \sum_{j=1}^{m-1} \alpha_{k_j} \left[-d_{\sigma_{k_j},\sigma_{k_j+1}} + d_{\sigma_{k_j},\alpha} + d_{\sigma_{k_j+1},\alpha} \right] \Bigg\}$$
$$\text{s.t.} \quad \forall j, \sum_{k_j} \alpha_{k_j} = 1, \quad \alpha_{k_j} \in \{0,1\}, \quad 1 \leq k_j \leq n-1.$$

where, $d_{\sigma_l,\alpha}$ denotes the distance between the city located at x_{σ_l} and depot α. The first part of the cost function corresponds to solving a single TSP with depot included in the list of cities. Removal of edge $\sigma_{k_j}, \sigma_{k_j+1}$ accounts for separating the route between two salesmen j and $j+1$, while addition of edges σ_{k_j}, α and σ_{k_j+1}, α ensure that the route for salesman j finishes at the depot and the route for salesman $j+1$ starts at the depot. Fig. 1c shows a schematic of a single-depot returning mTSP.

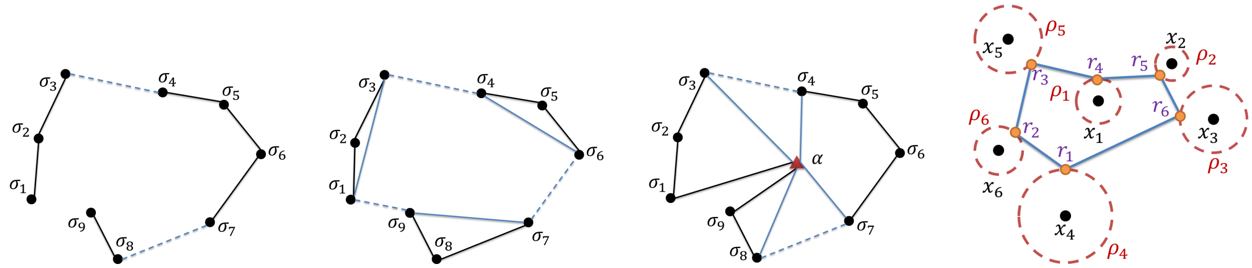


Fig. 1. Schematic of a (a) 9-cities non-returning 3TSP. The dashed blue lines indicate the removal of links, which corresponds to $\alpha_{k_1=3}=1, \alpha_{k_2=7}=1$ (b) 9-cities returning 3TSP. The dashed blue lines indicate the removal of links ($-d_{\sigma_{k_j},\sigma_{k_j+1}}$), while solid blue lines indicate the addition of links ($d_{\sigma_{k_j},\sigma_{k_{(j-1)}+1}}$). (c) 9-cities single-depot returning 3TSP. (d) Single salesman returning CETSP. Each city x_i is provided with a radius parameter ρ_i. The orange dots indicate r_j such that $v_{ij}=1$ for some city i.

D. Close Enough Traveling Salesmen Problem (CETSP)

In this problem, we are given a set of n cities $\{x_i\}$, each with a specified radius $\{\rho_i\}$, and a set of m salesmen. In CETSP, a city located at x_i is considered to be *visited* if a salesman reaches anywhere within ρ_i radius of the city i. CETSPs are used to represent problems such as aerial reconnaissance [6] and establishing a wireless meter reader [5]. The CETSP variant may be applied to any of the TSP class of problems. The most significant difference between point-based TSPs and the CETSP is that due to the radius associated with each city, the CETSP does not define a specific edge between a pair of cities, rather there is a continuum of possible edges between a pair of cities. As a result, there are infinitely many possible solutions to this problem. We use $\{r_j\}$, $j \in \{1,\dots,n\}$ to denote locations where a salesman *visits* all the cities. Consequently, a CETSP *tour* is mathematically described by a sequence of locations $(r_1, r_2, \dots, r_n)$. A single salesman returning CETSP is mathematically described as

$$\min_{\{v_{ij}\},\{r_j\}} \sum_{j=1}^{n} \left\{ \sum_{i=1}^{n} v_{ij} d_{CE}(x_i, r_j) + d(r_j, r_{j+1}) \right\}; r_{n+1} = r_1$$

$$\text{s.t.} \quad v_{ij} \in \{0,1\}, \quad \sum_{i=1}^{n} v_{ij} = 1 \forall j, \quad \sum_{j=1}^{n} v_{ij} = 1, \forall i$$

$$\text{where,} \quad d_{CE}(x_i, r_j) = \begin{cases} 0 & \text{if} \|r_j - x_i\| < \rho_i \\ \infty & \text{else} \end{cases}$$

Note that in this formulation the cost function becomes infinity unless for each city i there is a location on salesman tour within the radius ρ_i of its location x_i. Also, in this case, it is possible that the number of *distinct* locations on salesman tour may be less than n, that is, it is possible that one location on salesman tour can cover multiple cities; for instance in cases when the distances between two cities is less than the sum of the corresponding radii around the respective cities. Fig. 1d shows a schematic of a single salesman returning CETSP. Note that the current framework is flexible in the sense that an mCETSP problem can also be easily formulated by combining the CETSP cost function with the cost functions from previous variants.

III. SOLUTION APPROACH: A MAXIMUM ENTROPY PRINCIPLE FRAMEWORK

A distinct feature of our approach is to view TSP and its variants as combinatorial resource allocation problems. The primary advantages of reformulation in terms of resource allocation are (i) it becomes possible to develop approaches for many variants of TSP, and (ii) one can avail the vast literature of combinatorial resource allocation problems. In the next section, we present how TSP and its variants can be reformulated as resource allocation problems.

In this section, we present a facility location problem (FLP), which is a combinatorial resource allocation problem, and the *deterministic algorithm* (DA) which addresses it. Both the reformulation of the TSP variants considered in this article, and our solution approach are closely related to FLP and DA algorithm, and therefore we give here a brief introduction to both (for more details see [7]). The FLP is described as: For given n city locations, find K facility (resource) locations such that the total *sum of the distance of each city to its nearest facility is minimized*. In other words, if x_i and $y_j \in \Omega \subset \mathbb{R}^2$ denote the locations of i^{th} city and j^{th} facility, respectively, then the FLP addresses the following optimization problem

$$\min_{y_j \in \Omega, 1 \le j \le K} \sum_{i=1}^{n} \left\{ \min_{y_j, 1 \le j \le K} d(x_i, y_j) \right\}, \tag{1}$$

where $d(x_i, y_j) \in \mathbb{R}_+$ denotes the distance between the i^{th} city location x_i and j^{th} facility location y_j, and $\Omega \subset \mathbb{R}^2$ is a compact domain. Most algorithms for FLP (such as Lloyd's) are very sensitive to the initial facility locations. This is primarily due to the distributed aspect of FLPs, where any change in the location of the i^{th} city affects $d(x_i, y_j)$ only with respect to the *nearest* facility j. The DA algorithm suggested by Rose [7], overcomes this sensitivity by allowing each city to be *partially* associated to every facility through an association probability.

Below we briefly describe the DA algorithm (see [7] for details). Note that a solution to FLP results in a partition of the set Ω into K clusters $\{C_j\}$ such that for any city $x_i \in C_j$, the nearest facility is located at y_j. Also any partition $\{C_j\}$ of Ω can be described in terms of set $\mathcal{V} = \{v_{ij}\} \in \{0,1\}^{n \times K}$ of association values given by

$$v_{ij} = \begin{cases} 1 & \text{if } x_i \in C_j \\ 0 & \text{else} \end{cases}. \tag{2}$$

Now if we define *an instance* $(\mathcal{Y}, \mathcal{V})$ of an FLP by the set of facility locations $\mathcal{Y} = \{y_j\}$, and a partition via the set $\mathcal{V} = \{v_{ij}\}$, and for each *instance* associate a cost $D(\mathcal{Y}, \mathcal{V}) = \sum_{i=1}^{n} \sum_{j=1}^{K} v_{ij} d(x_i, y_j)$, then FLP in (1) can be rewritten as

$$\min_{(\mathcal{Y}, \mathcal{V})} D(\mathcal{Y}, \mathcal{V}). \tag{3}$$

In DA algorithm, a probability distribution $P(\mathcal{Y},\mathcal{V})$ is ascribed on the space of instances (the decision variables), and it solves the following related problem

$$\begin{aligned}&\min_{(\mathcal{Y},\mathcal{V})} \langle D(\mathcal{Y},\mathcal{V})\rangle \\ &\text{subject to } H(P(\mathcal{Y},\mathcal{V})) = H_0,\end{aligned} \tag{4}$$

where $D = \langle D(\mathcal{Y},\mathcal{V})\rangle = \sum_{\mathcal{Y},\mathcal{V}} P(\mathcal{Y},\mathcal{V})D(\mathcal{Y},\mathcal{V})$ is the expected cost and H is the Shannon entropy of the probability distribution $P(\mathcal{Y},\mathcal{V})$ and quantifies the randomness of the distribution. Accordingly a Lagrangian $\langle D\rangle - \frac{1}{\beta}H$ is minimized. In DA the above problem is solved for many values of the annealing parameter β as it is increased from 0 to a large value; where the solution at an iteration of β is used as the initial guess for the next iteration. Note that for each β, the cost function is convex in $P(\mathcal{Y},\mathcal{V})$ (in fact it is equivalent to the optimization problem in MEP), and the optimal distribution can be shown to be a Gibbs distribution given by

$$P(\mathcal{Y},\mathcal{V}) = \frac{e^{-\beta D(\mathcal{Y},\mathcal{V})}}{\sum\limits_{\mathcal{Y}',\mathcal{V}'} e^{-\beta D(\mathcal{Y}',\mathcal{V}')}}. \tag{5}$$

Note that for large values of β, $P(\mathcal{Y},\mathcal{V})$ is either approximately 1 or 0, which reduces the cost function in (4) to (3). DA seeks the most probable set of facility locations, it considers the marginal probability, given by

$$P(\mathcal{Y}) = \frac{e^{-\beta F(\mathcal{Y})}}{\sum\limits_{\mathcal{Y}'} e^{-\beta F(\mathcal{Y}')}}, \tag{6}$$

where $F(\mathcal{Y})$ is the analog of *free energy* in statistical mechanics and is given by,

$$F(\mathcal{Y}) = -\frac{1}{\beta}\log Z(\mathcal{Y}) = -\frac{1}{\beta}\sum_{i=1}^{n}\log\left(\sum_{j=1}^{K} e^{-\beta d(x_i,y_j)}\right). \tag{7}$$

In the DA algorithm, this free energy function is then deterministically optimized at successively increased β values over repeated iterations. The set $\mathcal{Y}$ of facility locations that optimizes the free energy at each β satisfies

$$\frac{\partial}{\partial y_j}F = 0 \quad \forall j \quad \Rightarrow \sum_{i=1}^{n} p(j|i)\frac{\partial}{\partial y_j}d(x_i,y_j) = 0 \quad \forall j, \tag{8}$$

where $p(j|i) = \dfrac{e^{-\beta d(x_i,y_j)}}{\sum\limits_{k=1}^{K} e^{-\beta d(x_i,y_k)}}$. The readers are encouraged to refer to [15] for detailed analysis on the complexity of the DA algorithm.

Remark: It should be noted DA algorithm prescribes a probability distribution on the space of decision variables (instances) $(\mathcal{Y},\mathcal{V})$ and then finds the most probable resource locations $\mathcal{Y}$ by maximizing the marginal distribution $P(\mathcal{Y})$. The most probable $\mathcal{Y}$ is shown to be one that minimizes a corresponding Free Energy F. In the next section this process is repeated for the larger decision space related to the TSP problems.

IV. METHODOLOGY: MODIFICATIONS OF THE DA ALGORITHM

In this section, we develop a DA based generalized heuristic for variants on the classical TSP. The framework in the DA algorithm is modified to include routing as constrained resource allocation problem. Rose has previously explored the application of DA to the TSP [11]. The heuristic behind the DA based TSP approach is that if we employ same number of facilities as the number of cities, i.e. $K = n$, then the optimal solution for the FLP is given by the case when all the resource locations are coincident with the city locations; therefore as $\beta \to \infty$ for the corresponding DA algorithm, the resource locations $\{y_j\}$ will coincide with the city locations $\{x_i\}$. We can convert a TSP variant into a resource allocation problem by including a constraint on tour length. For instance, if we pose a problem of finding the resource locations $\{y_j\}$ such that total distance of each city x_i to its nearest resource location y_j, that is $\sum_i \min_j d(x_i,y_j)$ is minimized under a given constraint on tour length $\sum_j d(y_j,y_{j+1}) = L$; it approximates the TSP problem. In fact, if L = optimal tour length of the TSP, then the solution will be such that each resource location will be coincident with a city location and the jth city on the optimal tour will correspond to the resource location y_j.

Note that in the DA, adding this extra constraint to the resource allocation problem will introduce a corresponding extra Lagrange multiplier in addition to the first Lagrange multiplier $\frac{1}{\beta}$. Solving repeatedly as in the original DA by changing these Lagrange multipliers ((annealing)) leads to a solution of the TSP (and its variants). We also discuss an effective scheme to vary the Lagrange multipliers and in this section.

We now describe the problem setting. We are given a set of n cities whose locations are given by $\{x_i\} \subset \mathbb{R}^2, \quad 1 \le i \le n$ and a depot with coordinates $\alpha \in \mathbb{R}^2$. These cities have to be traversed by a maximum of m salesmen under several constraints (which essentially constitute the variants on the TSP) on the optimal tours. As before, we use $\mathcal{Y} = \{y_j\}_{j=1}^n$ and $\mathcal{V} = \{v_{ij}\}_{i,j=1}^n$ to denote the set of facility locations and set of associations, respectively. The distance function $d(x_i,y_j)$ between city i and facility j is considered to be squared-euclidean, i.e., $d(x_i,y_j) = \|x_i - y_j\|_2^2$.

Remark: For brevity and ease of exposition, the results are derived for a special case of $m = 2$ salesmen. The results are easily extendable for any general m.

A. Approach for Non-returning mTSP

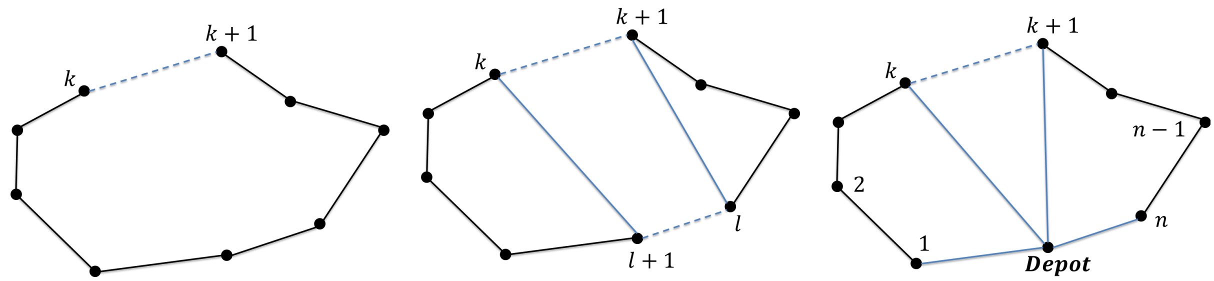
Unlike the basic FLP where an instance is defined by the parameters $(\mathcal{Y},\mathcal{V})$, in this case we modify the definition of an instance to include three parameters, $\mathcal{Y},\mathcal{V}$ and $\mathcal{R}$. Here $\mathcal{Y} = \{y_j\}$ represent the set of facilities located at y_j, $\mathcal{V} = \{v_{ij}\}$ is a set of associations and describes the membership of city x_i to facility y_j (see Eq. 2), and $\mathcal{R}$ is a set of locations of the partition representing the breaks between subsequent salesmen in the chain of consecutive facilities (see Fig. 2a). We consider the case for $m = 2$ salesmen. Therefore in this case $\mathcal{R} \in \{1,\dots,m\}$ such that

$$\mathcal{R} = k; \quad \text{implies there is no link b/w } y_k \text{ and } y_{k+1}.$$

For a given instance of the problem $(\mathcal{Y},\mathcal{V},\mathcal{R})$, the distortion function in original DA formulation is modified as

$$D(\mathcal{Y},\mathcal{V},\mathcal{R}) = D_1(\mathcal{Y},\mathcal{V}) + D_2(\mathcal{Y}) + D_3(\mathcal{Y},\mathcal{R}), \tag{9}$$

where $D_1(\mathcal{Y},\mathcal{V})$ is same as defined in original DA formulation. $D_2(\mathcal{Y})$ captures the tour length in the cost function



(a) (b) (c)

Fig. 2. Schematic of a (a) Non-returning 2TSP, with $\mathcal{R} = k$. (b) Returning 2TSP, with $\mathcal{R} = \{k, l\}$. (c) Returning 2TSP (with Depot), with $\mathcal{R} = k$. The dashed blue lines indicate the removal of links, while solid blue lines indicate the addition of links.

to represent a TSP and is given by

$$D_2(\mathcal{Y}) = \theta \sum_{j=1}^{n-1} d(y_j, y_{j+1}). \tag{10}$$

The final component $D_3(\mathcal{Y}, \mathcal{R})$ represents the partition of facilities for the independent salesmen and subtracts the distance at the partition between the facilities y_k and y_{k+1} from the original distortion function.

$$D_3(\mathcal{Y}, \mathcal{R}) = -\theta d(y_k, y_{k+1}) \tag{11}$$

Similar to the original formulation of the DA algorithm, the probability of any instance $(\mathcal{Y}, \mathcal{V}, \mathcal{R})$ is determined by the MEP. Following the steps adopted in Sec. III, the free energy of this system is obtained as

$$\begin{aligned} F \quad = \quad & -\frac{1}{\beta}\sum_{i=1}^{n} \log\left(\sum_{j=1}^{n} e^{-\beta d(x_i, y_j)}\right) + \theta \sum_{j=1}^{n-1} d(y_j, y_{j+1}) \\ & -\frac{1}{\beta} \log\left(\sum_{k=1}^{n-1} e^{\beta\theta d(y_k, y_{k+1})}\right). \end{aligned} \tag{12}$$

Taking the derivative of (12) with respect to each facility allows determination of the set of facilities that maximize entropy in the system.

$$\begin{aligned} \frac{\partial F}{\partial y_j} &= -2\sum_{i=1}^{n} p(j|i)(y_j - x_i) + 2\theta(2y_j - y_{j+1} - y_{j-1}) \\ &+2\theta\,(y_{j+1} - y_j)\,\mathcal{P}(j) + 2\theta\,(y_{j-1} - y_j)\,\mathcal{P}(j-1) = 0 \end{aligned}$$

where $p(j|i)$ is same as before (see Eq. (8)). $\mathcal{P}(j)$ represents the probability that the partition occurs at facility j (i.e. $\mathcal{R} = j$) and is given by

$$\mathcal{P}(j) = \frac{e^{\beta\theta d(y_j, y_{j+1})}}{\sum\limits_{j=1}^{n-1} e^{\beta\theta d(y_j, y_{j+1})}}. \tag{13}$$

Solving for each y_j provides the solution to the system at this pair of β and θ values, so that for every facility

$$y_j = \frac{\sum\limits_{i=1}^{n} p(j|i)x_i + \theta y_{j+1}(1-\mathcal{P}(j)) + \theta y_{j-1}(1-\mathcal{P}(j-1))}{\sum\limits_{i=1}^{n} p(j|i) + \theta\,(2-\mathcal{P}(j)-\mathcal{P}(j-1))} \tag{14}$$

Note that the Eq. (14) is only slightly more complex than the basic TSP proposed in [11]. In fact, setting $\mathcal{P}(j) = 0, \forall j$ transforms the 2TSP into the basic TSP formulation.

B. Approach for Returning mTSP

In case of returning mTSP, the start and end positions of each salesmen must be coincident. In this case, the partition function $D_3(\mathcal{Y}, \mathcal{R})$ not only considers the distance between the facilities where the partition occurs, it must also account for the distance incurred in completing the continuous tour by reconnecting to the other end of the loop (see Fig. 2b). Similar to the non-returning mTSP, we derive the results for $m = 2$ salesmen. The partition parameter $\mathcal{R}$ in this case is described by two parameters.

$$\mathcal{R} = k, l \quad \text{if} \begin{cases} \text{no links b/w } y_k \text{ and } y_{k+1},\ y_l \text{ and } y_{l+1}; \\ \text{links b/w } y_k \text{ and } y_{l+1},\ y_l \text{ and } y_{k+1}; \end{cases}$$

It should be noted that the facilities y_1 and y_n are considered to be adjacent, i.e. $y_0 = y_n$ and $y_{n+1} = y_1$. The tour-length distortion function is given by $D_2(\mathcal{Y}) = \sum\limits_{j=1}^{n} d(y_j, y_{j+1})$. The distortion function $D_3(\mathcal{Y}, \mathcal{R})$ pertaining to the partition parameter is defined as

$$D_3 = \theta\big(-d(y_k, y_{k+1}) - d(y_l, y_{l+1}) + d(y_k, y_{l+1}) + d(y_l, y_{k+1})\big).$$

An important consequence of this framework is that if $k = l$, then the problem reduces to the classical returning TSP. Thus, this framework allows automatic determination of the optimal number of salesmen. With the above modified distortion functions, the update equation for each facility y_j is given by

$$y_j = \frac{\begin{aligned}&\sum\limits_{i=1}^{n} p(j|i)x_i + 2\theta\Big(\sum\limits_{l\neq j-1} \mathcal{P}(j,l)y_{l+1} + \sum\limits_{l\neq j} \mathcal{P}(j-1,l)y_l\Big) \\ &+\theta\left[(1-2\textstyle\sum_l \mathcal{P}(j,l))y_{j+1} + (1-2\textstyle\sum_l \mathcal{P}(j-1,l))y_{j-1}\right]\end{aligned}}{\sum_{i=1}^{n} p(j|i) + 2\theta\big(1 - 2\mathcal{P}(j, j-1)\big)} \tag{15}$$

C. Approach for Single Depot Returning mTSP

Fig. 2c shows the schematic of the proposed framework for the returning version of a single depot multiple salesmen problem. We denote the depot location by $\alpha \in \mathbb{R}^2$. We formulate the framework for $m = 2$ salesmen. The partition parameter $\mathcal{R}$ in this case is defined as

$$\mathcal{R} = k, \quad \begin{cases} \text{no link b/w } y_k \text{ and } y_{k+1}; \\ \text{links b/w } y_k \text{ and } \alpha,\ y_{k+1} \text{ and } \alpha. \end{cases}$$

The distortion function $D_3(\mathcal{Y}, \mathcal{R})$ and the corresponding probability distribution $\mathcal{P}(\mathcal{R} = k)$ pertaining to the partition parameter are given by

$$\begin{aligned} D_3(\mathcal{Y}, \mathcal{R}) \quad &= \quad \theta\,(-d(y_k, y_{k+1}) + d(y_k, \alpha) + d(y_{k+1}, \alpha)) \\ \mathcal{P}(\mathcal{R}) \quad &= \quad \frac{e^{-\beta\theta\{-d(y_k, y_{k+1}) + d(y_k, \alpha) + d(y_{k+1}, \alpha)\}}}{\sum_{k=1}^{n-1} e^{-\beta\theta\{-d(y_k, y_{k+1}) + d(y_k, \alpha) + d(y_{k+1}, \alpha)\}}}. \end{aligned}$$

The distortion function corresponding to the tour-length constraint is modified to include the links between y_1 and α, and between y_n and α, i.e., $D_2(\mathcal{Y}) = \theta\left\{\sum_{j=1}^{n-1} d(y_j, y_{j+1}) + d(y_1, \alpha) + d(y_n, \alpha)\right\}$. If we define $\mathcal{P}(0) = \mathcal{P}(n) = 1$, then the corresponding update equation for each facility y_j is given by

$$y_j = \frac{\begin{array}{c}\sum_{i=1}^{n} p(j|i)x_i + \theta\left\{\mathcal{P}(j) + \mathcal{P}(j-1)\right\}\alpha \\ + \theta\left\{1 - \mathcal{P}(j)\right\} y_{j+1} + +\theta\left\{1 - \mathcal{P}(j-1)\right\} y_{j-1}\end{array}}{2\theta + \sum_{i=1}^{n} p(j|i)}.$$

D. Approach for Close Enough TSP

In the close enough traveling salesman problem (CETSP), an additional radius parameter (ρ_i) corresponding to each city x_i is included in the optimization framework. For ease of exposition, we consider a single salesman CETSP in this work, however, the framework can be modified to additionally incorporate any of the aforementioned variants. Note that there are no partition parameters for a single salesman returning TSP. To simplify the calculations, distance between the city and the facility pairs is modified as

$$d_{CE}(x_i, y_j, \rho_i) = \left(\|y_j - x_i\| - \rho_i\right)^2. \tag{16}$$

Note that in case CETSP, the facility locations $\{y_j\}$ automatically define the points of visit $\{r_j\}$ described in Sec. II-D. The distortion functions corresponding to the city-facility distances and the tour-length constraints are respectively given by

$$\begin{aligned} D_1(\mathcal{Y}, \mathcal{V}) &= \sum_{i=1}^{n}\sum_{j=1}^{n} v_{ij} d_{CE}(x_i, y_j, \rho_i) \\ D_2(\mathcal{Y}) &= \theta\sum_{j=1}^{n} d(y_j, y_{j+1}) \end{aligned} \tag{17}$$

The free energy of this system is obtained as

$$F = -\frac{1}{\beta}\sum_{i=1}^{n}\log\left(\sum_{j=1}^{n} e^{-\beta d_{CE}(x_i, y_j, \rho_i)}\right) + \theta\sum_{j=1}^{n} d(y_j, y_{j+1}).$$

Taking derivative of the free-energy term and setting it to 0, we obtain the update equation for each facility given by

$$y_j = \frac{\sum_{i=1}^{n} p(j|i)(x_i + \rho_i \operatorname{sgn}(y_j - x_i)) + \theta(y_{j+1} + y_{j-1})}{2\theta + \sum_{i=1}^{n} p(j|i)},$$

where, the association probability distribution is now given by $p(j|i) = \left(\frac{e^{-\beta d_{CE}(x_i, y_j, \rho_i)}}{\sum_{k=1}^{n} e^{-\beta d_{CE}(x_i, y_k, \rho_i)}}\right)$ and $\operatorname{sgn}(\cdot)$ is a vector-valued *signum* function.

E. Controlling Lagrange Multipliers

It is desirable to have a consistent and repeatable method for varying the Lagrange multipliers β and θ which govern the distortion function and the tour length. In this study, the β multiplier is considered as the main driver, and the θ multiplier is secondary. As such, the θ parameter is decreased according to an exponential function until a stable tour length is reached, at which point β is increased according to an exponential function. This process is repeated until a sufficiently high β value and sufficiently low θ value are both reached, leaving the final solution. This is addressed by Rose [11] in the context of classical TSP, which is generalized to mTSP case in this work; not presented here due to lack of space.

V. RESULTS AND DISCUSSIONS

This section provides an overview of the results of the MATLAB implementations of the proposed heuristic. As yet, the MATLAB code used for this implementation has not been optimized for minimum computation time, so valid comparisons on the basis on run time are not currently available, however the heuristic is shown to achieve high quality results based on tour lengths in fairly reasonable amount of time. The heuristics are evaluated on synthetic data. We also compare the proposed MEP based approach against the optimized simulated annealing implementation ([16]) on synthetic dataset of 30 different instances, each comprising of total number of cities ranging from 100 to 200, uniformly spanned in an area of $[-30, 30] \times [-30, 30] \in \mathbb{R}^2$.

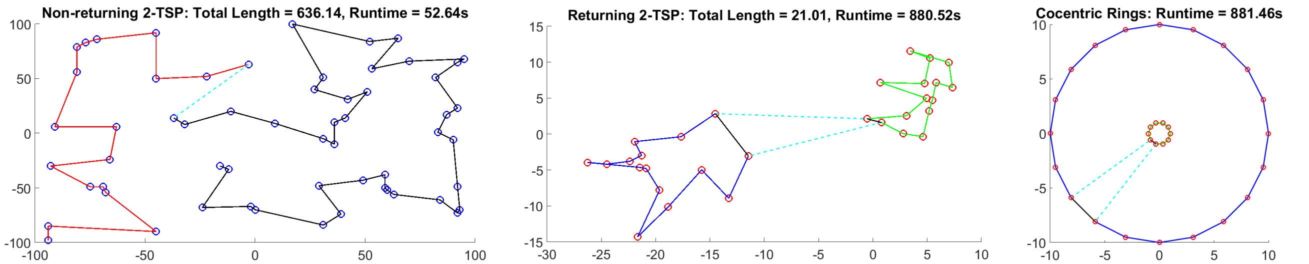
Non-returning 2TSP: Fig. 3a shows the non-returning 2TSP result for a synthetic 59 cities data. The tours of the two salesmen are shown in *red* and *black* respectively, with *cyan* dashed line indicating the partition.

Returning 2TSP: Fig. 3b shows the returning 2TSP result for a randomly generated 30 cities data. The heuristic is able to find the two largest links to be removed from the sequence of facilities. Fig. 3c shows the returning 2TSP result for a 30 cities in concentric rings arrangement. The DA based heuristic finds the two most optimal routes for this configuration. Note that this dataset is particularly challenging for heuristics such as *cluster-first route-second*, where clustering the data first will either result in two symmetric subsets or the only cluster identified will be at the origin and when the two salesmen are allocated to the cities, there is no way to effectively partition the set into two distinct subsets based on the information provided by the clustering solution.

Single depot returning 2TSP: Fig. 4a shows the implementation results for the 59 cities (and a depot) data. The two tours are shown in *cyan* and *black* colors respectively.

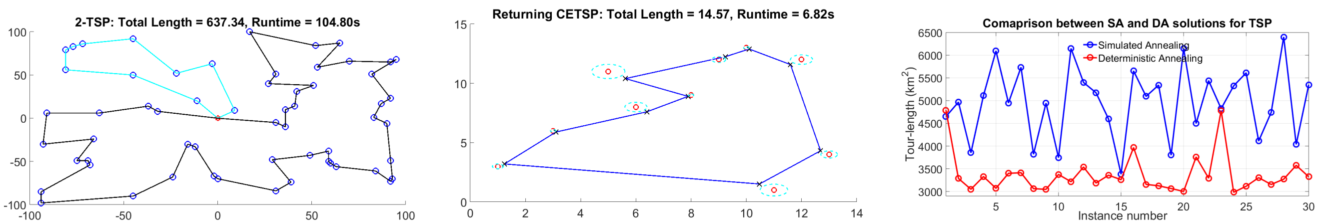
Returning CETSP: Fig. 4b shows the implementation results for the CETSP on a randomly generated 10 cities data with the additional radius parameter. It is difficult to determine whether the algorithm arrives at an optimal solution because this is much more difficult to check manually and unlike the standard TSP, there is no database of optimal tours for the CETSP. We have compared the heuristic against one of the 100 cities sets (kroD100 from TSPLIB [17]) tested by Mennell for equal radii of 11.697 [6]. Mennell achieves a tour length of 58.54 units with a 0.3 overlap ratio on the data. However, there are no details on the calculation time. Our MEP based heuristic finds an optimal tour length of 64.99 units in 949 seconds. Note that in the current formulation, there is a penalty for a facility existing either inside or outside of the circle. However, according to the problem formulation, there should be no penalty when the facility exists within the radius of the city. This can be addressed by setting the derivative of the distance function $d_{CE}(x_i, y_j, \rho_i)$ with respect to y_j to zero whenever y_j exists within ρ_i distance from the city x_i. This negates the penalty incurred for placing a facility within the radius of a city and should help this heuristic identify more accurate solutions.

Comparison with SA: Fig. 4c shows the comparison of the proposed MEP based approach against the simulated



(a) (b) (c)

Fig. 3. (a) Result for non-returning 2TSP for 59 cities data. The dashed line indicates the removal of the link. (b) Result for returning 2TSP for 59 cities data. The dashed lines indicate the removal of links, while the black solid lines indicate the addition of links. (c) Returning 2TSP version for concentric rings.



(a) (b) (c)

Fig. 4. (a) Single-depot returning 2TSP solution to a 59 cities data. The depot location is denoted by *red* marker. (b) CETSP result for single salesman 10 cities returning TSP. The *red* markers denote the city locations, while the *black* '$\times$' denote the facility locations. The *cyan* circles correspond to the radii ρ_i. (c) Comparison between MEP based deterministic annealing (DA) approach and simulated annealing (SA) approach for the non-returning 2TSP (NR2TSP).

annealing (SA) based approach for 30 randomly generated instances for the non-returning 2TSP (NR2TSP). It should be remarked that both the algorithms require similar average computational time for each of the scenarios. We plot the total tour-lengths for each of the instances for the two approaches. Clearly the proposed MEP algorithm outperforms the most widely used simulated annealing algorithm with marginal increase in run-time. Similar comparisons exist for the other scenarios too.

VI. Conclusions and Future Works

In this paper we explore the Maximum-Entropy-Principle as a heuristic for the TSP, as well as many variants. Because the algorithm is independent of the edges between cities, it has more flexibility to address variants such as the CETSP and the mTSP. The algorithm produces high-quality solutions for some challenging scenarios, such as, concentric rings. The next steps for this heuristic framework should be developing the formulation for further variants on the basic TSP. There remain significant opportunities to optimize the code implementation of the MEP framework to achieve more favorable computation times, at which point this algorithm can be run on benchmark mTSP cases and compared against many of the conventional heuristics.

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