PERGAMON

Applied Mathematics Letters 16 (2003) 401–407

Applied Mathematics Letters

www.elsevier.com/locate/aml

Weakly Symmetric Graphs, Elementary Landscapes, and the TSP

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(Received October 2001; accepted March 2002)

Abstract—Weakly symmetric graphs are defined and their construction from symmetric graphs is explained. It is shown that the TSP on a weakly symmetric graph joined with each of a number of well-known local search neighbourhoods yields elementary landscapes (in which local minima are better than the average). In conclusion, an $\mathcal{O}(n^2)$ algorithm for identifying weakly symmetric graphs is described.

Keywords—Elementary landscapes, Laplacian, TSP, Weakly symmetric matrices.

1. INTRODUCTION

The traveling salesman problem (TSP) requires that we identify a shortest path which starts at one of n-cities, visits each precisely once and returns to the starting city. Formally, let C be an $n \times n$ matrix with real entry $c_{i,j}$ at position (i, j). The matrix C then defines a weighted digraph, where one may think of the vertices as cities, and $c_{i,j}$ as the cost of travelling from city i to city j. Let π be any n-cycle permutation. Then π defines a Hamiltonian path through the graph whose cost is given by

$$c(\pi) = \sum_{i=1}^{n} c_{i,i\pi}.$$

The object of the TSP is to find an n-cycle π for which $c(\pi)$ is a minimum. In general, this problem is NP-Hard [1], and the motivation of this paper is to find a path π whose cost is low but not necessarily the minimum.

Local search, and its many variants, are techniques for finding low cost solutions to the TSP whereby the set of all $(n-1)!$ solutions are regarded as the vertices of a *multigraph* (a graph in which multiple edges between two vertices are allowed). Under local search, the graph is traversed according to certain rules until it stops at some vertex, none of whose neighbours has a lower cost. Such a vertex is said to be a *local minimum*.

 Typeset by $\mathcal{A}\mathcal{M}\mathcal{S}$-TEX
PII: S0893-9659(02)00212-4

Typically, the multigraph is defined by specifying, for each solution π, a *neighbourhood* $N(\pi)$ which is a multiset (repetitions are allowed) of solutions obtained from π by some operation. Operations such as two-*swap* (swap the position of two cities in the path) and two-*opt* (invert some segment of the path) are known to produce low cost local minima when the cost matrix is symmetric. In this paper, it is shown that we may significantly weaken the symmetry condition on the cost matrix and retain the same objective function, and therefore, the fact that local minima are of low cost.

1.1. Landscapes

We now give a general setting for local search applied to combinatorial optimization problems and some general results on when local minima have low cost. Suppose the solution set X has cardinality m. A multigraph G with vertex set X may be represented by an $m \times m$ *adjacency* matrix A whose (x, y) entry is the number of edges from vertex x to vertex y. We further define the *degree* matrix D to be an $m \times m$ diagonal matrix with $D(x, x)$ the total number of edges originating at x. We are now able to define the normalized *Laplacian* to be the matrix $L = I - D^{-1}A$ where I is the $m \times m$ identity matrix.

The objective function, f, of the combinatorial optimization problem is a real-valued function on X and is regarded as an m-dimensional vector. Together, G and f define a *landscape*. Let μ be the mean value of f over X. Then the vector whose value at x is $f(x) - \mu$ is the *normalized objective function* and denoted $\tilde{f}$. A landscape (G, f) such that $\tilde{f}$ is an eigenvector of L is called *elementary*.

The following result is suggested by the work of Stadler [2], Barnes and Colletti [3], Codenotti and Margara [4], and Grover [5].

PROPOSITION 1. *If a landscape is elementary then local minima are lower than the global average μ, and local maxima are greater than μ.*

Elementary landscapes as defined above comprise various types of landscape depending on the eigenvalue. For each type, we may state results on the 'smoothness' of the landscape and on the number of steps in a local search for a better than average solution.

In the sequel, we cite results stating that if the objective function arises from a TSP in which the cost matrix is symmetric then, with certain neighbourhoods, the landscape is elementary. This paper extends the class of cost matrices which are known to give rise to elementary landscapes.

2. WEAKLY SYMMETRIC GRAPHS

A weighted digraph may be represented by a matrix where entry (i, j) is the *weight* of the edge from vertex i to vertex j. The definition of weight extends naturally to paths in the graph. By definition, a symmetric matrix represents a *symmetric* graph.

A *weakly symmetric graph* is a graph in which the weight of any cycle is equal to the weight of its reverse. (A matrix is *weakly symmetric* if it represents a weakly symmetric graph.) Obviously, every symmetric graph is weakly symmetric, but the following construction shows that not every weakly symmetric graph is symmetric.

Define a *deformation pair* to be a pair of elements $\mathbf{q}, \mathbf{r} \in \mathbf{R}^n$ such that

$$\sum_{i=1}^{n} q_i + r_i = 0. \tag{1}$$

Deformation pairs exist because for any choice of the $2n - 1$ entries

$$q_1, \dots, q_n, \qquad r_1, \dots, r_{n-1},$$

setting r_n equal to the negative of their sum produces such a pair.

Let $(\mathbf{q}, \mathbf{r})$ be a deformation pair and define

$$Q = \begin{pmatrix} q_1 & q_2 & \cdots & q_n \\ q_1 & q_2 & \cdots & q_n \\ \vdots & \vdots & \vdots & \\ q_1 & q_2 & \cdots & q_n \end{pmatrix} \quad \text{and} \quad R = \begin{pmatrix} r_1 & r_1 & \cdots & r_1 \\ r_2 & r_2 & \cdots & r_2 \\ \vdots & \vdots & \vdots & \\ r_n & r_n & \cdots & r_n \end{pmatrix}. \tag{2}$$

Any matrix $D = R + Q$ is a *deformation matrix.*

PROPOSITION 2. *Graphs representable by deformation matrices are weakly symmetric and are not necessarily symmetric.*

PROOF. To see that a deformation matrix, D, defines a weakly symmetric graph, consider any cycle

$$1 \to 2 \to \cdots \to k \to 1.$$

The weight of this cycle is

$$\begin{aligned} d_{1,2} + d_{2,3} + \cdots + d_{k-1,k} + d_{k,1} &= (r_1 + q_2) + (r_2 + q_3) + \cdots + (r_{k-1} + q_k) + (r_k + q_1) \\ &= (r_2 + q_1) + (r_3 + q_2) + \cdots + (r_k + q_{k-1}) + (r_1, q_k) \\ &= d_{2,1} + d_{3,2} + \cdots + d_{k,k-1} + d_{1,k}. \end{aligned}$$

Thus, the matrix and its associated graph are weakly symmetric.

If D is symmetric, an asymmetric deformation matrix D' may be constructed by defining a new deformation pair $(\mathbf{q}', \mathbf{r}')$ identical to $(\mathbf{q}, \mathbf{r})$ excepting that $q'_2 = q_2 + \epsilon$ and $r'_2 = r_2 - \epsilon$ for some $\epsilon > 0$. Since $r_1 + q_2 = r_2 + q_1$, we have

$$\begin{aligned} d'_{1,2} = r'_1 + q'_2 &= r_1 + q_2 + \epsilon \\ &= r_2 + q_1 + \epsilon \\ &= r'_2 + q'_1 + 2\epsilon \neq d'_{2,1} \end{aligned}$$

and the deformation matrix obtained from $(\mathbf{q}', \mathbf{r}')$ is asymmetric. ∎

As an immediate consequence, we have the following.

PROPOSITION 3. *The sum of a deformation matrix and a symmetric matrix is a weakly symmetric matrix.*

We now wish to prove the converse.

THEOREM 1. *Every weakly symmetric matrix is the sum of a symmetric matrix and a deformation matrix.*

Let S be a symmetric matrix and D be a deformation matrix. Define $C = S + D$. For any $i \neq j \in \{1, \ldots, n\}$, we have $c_{i,j} = s_{i,j} + d_{i,j} = s_{i,j} + r_i + q_j$ which implies $s_{i,j} = c_{i,j} - r_i - q_j$. Interchanging i and j (since S is symmetric) produces $s_{i,j} = c_{j,i} - r_j - q_i$. Equating these two expressions for $s_{i,j}$ yields

$$r_i - r_j + q_j - q_i = c_{i,j} - c_{j,i}, \qquad \text{for each } i < j. \tag{3}$$

Concatenating equation (1) with the set of $(n^2-n)/2$ equations in (3) produces an $(n^2-n)/2+1$ by $2n$ linear system,

$$A\mathbf{x} = \mathbf{y} \tag{4}$$

where

$$A = \begin{pmatrix} 1 & 1 & 1 & \cdots & 1 & 1 & 1 & 1 & \cdots & 1 \\ 1 & -1 & 0 & \cdots & 0 & -1 & 1 & 0 & \cdots & 0 \\ & & \ddots & & & & & \ddots & & \\ 0 & \cdots & 0 & 1 & -1 & 0 & \cdots & 0 & -1 & 1 \end{pmatrix}.$$

A's first row is denoted e and corresponds to equation (1). The remaining $(n^2-n)/2$ rows correspond to pairs (i,j) with $i<j$ and appear in the order $(1,2),(1,3),\dots(1,n);(2,3),(2,4),\dots(2,n);\dots;(n-1,n)$. We denote the row corresponding to (i,j) by $h(i,j)$. The first n columns are associated with $\mathbf{r}$ and the remaining n columns are associated with $\mathbf{q}$. The row $h(i,j)$ contains 1 in positions i and $n+j$, -1 in positions j and $n+i$, and zero elsewhere. Consistent with A,

$$\mathbf{x} = \begin{pmatrix} r_1 \\ \vdots \\ r_n \\ q_1 \\ \vdots \\ q_n \end{pmatrix} \quad \text{and} \quad \mathbf{y} = \begin{pmatrix} 0 \\ c_{1,2} - c_{2,1} \\ \vdots \\ c_{n-1,n} - c_{n,n-1} \end{pmatrix}.$$

The proceeding discussion leads to the following.

LEMMA 1. *A matrix C is the sum of a symmetric matrix and a deformation matrix if and only if there is some solution $\mathbf{x}$ to equation (4).*

PROOF. If $C = S + (R+Q)$, then the above discussion ensures that

$$\mathbf{x} = \begin{pmatrix} r_1 \\ \vdots \\ r_n \\ q_1 \\ \vdots \\ q_n \end{pmatrix}$$

is a solution to equation (4).

Conversely, suppose $\mathbf{x}$ is a solution to equation (4). By setting $\mathbf{r} = (x_1,\dots,x_n)$, $\mathbf{q} = (x_{n+1},\dots,x_{2n})$, and $s_{i,j} = c_{i,j} - r_i - q_j$, it is easy to verify that $C = S + (Q+R)$ is the sum of a symmetric matrix and a deformation matrix (as required). ∎

Reflecting on the lemma above, we see that Theorem 1 will be proved if we can show the following.

LEMMA 2. *There exists a solution $\mathbf{x}$ to equation (4) if and only if C is weakly symmetric.*

From linear algebra, we know that there is a solution to $A\mathbf{x} = \mathbf{y}$ if and only if the rank of A equals the rank of the augmented matrix $(A \mid \mathbf{y})$. The following two lemmas suffice to prove both Lemma 2 *and* Theorem 1.

LEMMA 3. Rank$(A) = n$.

PROOF. We proceed by selecting a set $\mathcal{F}$ of n rows of A and showing that they form a basis of the row space of A. For each $i<n$, let $f_i = h(i,i+1)$. Let e be the row all of whose entries are 1, i.e., the top row of A. The reader may easily verify that $\mathcal{F} = \{e\} \cup \{f_i \mid i<n\}$ is a basis for the row space of A, i.e., for any $i<j$, the row $h(i,j)$ is equal to $f_i + \cdots + f_{j-1}$, and $\mathcal{F}$ spans the row space of A.

To see that the rows of $\mathcal{F}$ are independent is an elementary exercise in linear algebra and is omitted. ∎

LEMMA 4. Rank$(A \mid \mathbf{y}) = n$ *if and only if C is weakly symmetric.*

PROOF. If Rank$(A \mid \mathbf{y}) = n$, there is a solution to equation (4). Therefore, by Lemma 1, $C = S + D$ for some symmetric matrix S and deformation matrix D and by Proposition 3, C is weakly symmetric.

To complete the proof, we suppose that C is weakly symmetric and show that each row of the augmented matrix can be expressed as a linear combination of the rows $\gamma_i = (f_i \mid c_{i,i+1} - c_{i+1,i})$, $i < n$ and $\epsilon = (e \mid 0)$.

Let $\rho_{i,j} = (h(i,j) \mid c_{i,j} - c_{j,i})$ be an arbitrary row of the augmented matrix. We must show that $\rho_{i,j} = \gamma_i + \cdots + \gamma_{j-1}$. It was shown in the previous lemma that $h(i,j) = f_i + \cdots + f_{j-1}$, so it only remains to show that

$$\sum_{k=i}^{j-1} c_{i,i+1} - c_{i+1,i} = c_{i,j} - c_{j,i}. \tag{5}$$

Denote the cycle $i \to i+1 \to \cdots \to j \to i$ by ω and its reverse by ω^r. Denote their weights under C by $c(\omega)$ and $c(\omega^r)$, respectively.

Consider the left-hand side of equation (5). Adding all the left summands $(c_{i,i+1})$ is easily seen to give $c(\omega) - c_{j,i}$ while the sum of the right summands $c_{i+1,i}$ is $c(\omega^r) - c_{i,j}$. But since C is weakly symmetric, $c(\omega) = c(\omega^r)$ so that we are left with $c_{i,j} - c_{j,i}$ (as required). ∎

3. THE TSP AND ELEMENTARY LANDSCAPES

In this section, we build on Theorem 1 to identify large new classes of graphs which give rise to elementary landscapes for a local search approach to the TSP.

PROPOSITION 4. *Every Hamiltonian tour on a graph defined by a deformation matrix has weight zero.*

PROOF. Let $D = R+Q$ be a deformation matrix and let π be an n-cycle permutation representing a Hamiltonian tour. Then the weight of π is

$$\begin{aligned} d(\pi) &= \sum_{i=1}^{n} d_{i,i\pi} = \sum_{i=1}^{n} r_i + q_{i\pi} = \sum_{i=1}^{n} r_i + q_i, && \text{by commutativity of addition,} \\ &= 0, && \text{by equation (1).} \end{aligned}$$

∎

The result of this proposition is that adding a deformation matrix to a cost matrix does not change the objective function. Therefore, if a matrix S yields an elementary landscape under a particular neighbourhood definition, then, for any deformation matrix D, $S + D$ also yields an elementary landscape. Therefore, we are able to deduce the following corollaries to earlier results concerning the TSP.

According to Colletti and Barnes [3] TSP on a symmetric graph gives rise to an elementary landscape under a complete conjugative neighbourhood (for example, a complete swap neighbourhood).

COROLLARY 1. *The TSP on a weakly symmetric graph gives an elementary landscape under any complete conjugative neighbourhood.*

The TSP on a symmetric graph gives an elementary landscape under two-opt neighbourhoods [2]. Therefore, we can conclude the following.

COROLLARY 2. *The TSP on a weakly symmetric graph gives an elementary landscape under a two-opt neighbourhood.*

Antisymmetric graphs also give rise to elementary landscapes under swap and two-opt neighbourhoods [2]. Hence, we have the following corollary.

COROLLARY 3. *The sum of an antisymmetric matrix and a deformation matrix represents a graph which yields an elementary landscape under both swap and two-opt neighbourhoods.*

4. EFFICIENT IDENTIFICATION OF WEAKLY SYMMETRIC GRAPHS

When a TSP joined with a stipulated search neighbourhood yields an elementary landscape, local search approaches to the TSP are particularly effective [5]. Therefore, it is of interest to be able to efficiently identify weakly symmetric graphs so that a neighbourhood which will yield an elementary landscape is selected.

A naive approach starting with the definition of a weakly symmetric graph would suggest checking the weight of each cycle, an operation requiring $\mathcal{O}(n!)$ additions. Using Theorem 1 and Lemma 1 would involve solving a system of n linear equations in $2n$ unknowns requiring $\mathcal{O}(n^3)$ operations [1]. However, Theorem 2 allows identification of a weakly symmetric matrix in $\mathcal{O}(n^2)$ additions.

THEOREM 2. *A graph is weakly symmetric if and only if every three-cycle based at some vertex has the same weight as its reverse.*

The forward implication is trivial. To see the converse, we first show that checking the condition at any selected vertex is equivalent to checking the condition at all vertices.

LEMMA 5. *If every three-cycle at any selected vertex has the same weight as its reverse, then every three-cycle has the same weight as its reverse.*

PROOF. Under the assumption that every three-cycle based at vertex $*$ has the same weight as its reverse, we must show that any three cycle $i \to j \to k \to i$ has the same weight as its reverse. If we add the following three equations:

$$\begin{aligned} c_{*,i} + c_{i,j} + c_{j,*} &= c_{*,j} + c_{j,i} + c_{i,*}, \\ c_{*,k} + c_{k,i} + c_{i,*} &= c_{*,i} + c_{i,k} + c_{k,*}, \\ c_{*,j} + c_{j,k} + c_{k,*} &= c_{*,k} + c_{k,j} + c_{j,*}, \end{aligned}$$

we obtain $c_{i,j} + c_{j,k} + c_{k,i} = c_{i,k} + c_{k,j} + c_{j,i}$. ∎

We complete the proof of the theorem by induction. Assume that all cycles of length less than k have the same weight as their reverses. Under an appropriate renumbering, consider the k-cycle, $1 \to 2 \to \cdots \to k \to 1$. The weight of this cycle is

$$\begin{aligned} c_{1,2} + c_{2,3} + \cdots + c_{k-1,k} + c_{k,1} &= c_{1,2} + c_{2,3} + (c_{3,1} - c_{3,1}) + c_{3,4} \cdots + c_{k-1,k} + c_{k,1} \\ &= (c_{2,1} + c_{3,2} + c_{1,3}) - c_{3,1} + c_{3,4} \cdots + c_{k-1,k} + c_{k,1} \\ &= c_{2,1} + c_{3,2} - c_{3,1} + (c_{1,3} + c_{3,4} \cdots + c_{k-1,k} + c_{k,1}) \\ &= c_{2,1} + c_{3,2} - c_{3,1} + c_{3,1} + c_{4,3} \cdots + c_{k,k-1} + c_{1,k} \\ &= c_{2,1} + c_{3,2} + c_{4,3} \cdots + c_{k,k-1} + c_{1,k}, \end{aligned}$$

(as required). ∎

4.1. A Scholium on the Proof of Theorem 2

For completeness, we note that under the usual matrix operations the distance matrices $\{c_{ij}\}$ defining weakly symmetric graphs form a vector space. Furthermore, the number of defining conditions on the space of these matrices is $\binom{n-1}{2}$ because this is the number of distinct three-cycles $(*, i, j)$ which index the necessary and sufficient conditions for weak symmetry described in Theorem 2. The $\binom{n-1}{2}$ three-cycle conditions are linearly independent because there is an $\binom{n-1}{2} \times \binom{n-1}{2}$ minor which is the identity matrix on the indices $(c_{23}, c_{24}, \dots, c_{2n}, c_{34}, \dots, c_{3n}, \dots, c_{n-1,n})$ in the three-cycle equalities ordered according to $(*,2,3), (*,2,4), \dots, (*,2,n), (*,3,4), \dots,$

$(*, 3, n), \ldots, (*,\ n-1, n)$. Therefore, the dimension of the space of weakly symmetric matrices is the number of c_{ij}s which are free to be chosen

$$n^2 - n - \binom{n-1}{2} = \frac{1}{2}n^2 + \frac{1}{2}n - 1,$$

that is, the difference between the dimension of all TSP matrices (which is $n^2 - n$) and the number of defining three-cycle conditions. As expected the dimension of weakly symmetric matrices, is greater than the dimension, $(1/2)n^2 - (1/2)n$, of symmetric matrices.

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