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THE TRAVELING SALESMAN PROBLEM: THE SPECTRAL RADIUS AND THE LENGTH OF AN OPTIMAL TOUR

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Dedicated to Professor Bogoljub Stanković (1924–2018)

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A b s t r a c t. *We consider the symmetric traveling salesman problem* (*TSP*) *with instances represented by complete graphs with distances between cities as edge weights. Computational experiments with randomly generated instances on* 50 *and* 100 *vertices with the uniform distribution of integer edge weights in interval* $[1, 100]$ *show that there exists a correlation between the sequences of the spectral radii of the distance matrices and the lengths of optimal tours obtained by the well known TSP solver Concorde. In this paper we give a partial theoretical explanation of this correlation.*

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1. *Introduction*

The traveling salesman problem (TSP) is one of the best-known NP-hard combinatorial optimization problems. There is an extensive literature on both theoretical and practical aspects of the TSP (see e.g. Lawler et al. [12], Gutin and Punnen [10], Applegate et al. [1]). The symmetric traveling salesman problem, which will be considered in this paper, consists of finding a Hamiltonian cycle of the minimal length in a weighted complete undirected graph without loops.

Computational experiments with instances on 50 and 100 vertices with the uniform distribution of integer edge weights in interval $[1, 100]$ show that there exists a correlation between the sequences of spectral radii of distance matrices and lengths of optimal tours obtained by the well known TSP solver Concorde. In this paper we give a partial theoretical explanation of this correlation.

Let $\lambda_1, \ldots, \lambda_n$ be eigenvalues of the distance matrix D. The k-th spectral moment M_k of D is defined by the expression $M_k = \lambda_1^k + \cdots + \lambda_n^k$.

In paper [4] we have extended our previous work on estimating the length of an optimal solution of the TSP using spectral moments of the weight matrix [5]. Namely, in some numerical experiments with TSP instances with up to 14 vertices which were carried out in 1987, it has been noted that there exists a strong correlation between spectral moments M_3, M_4, M_5 and M_6 of the distance matrix and the length of an optimal solution of the TSP with values of correlation coefficients between 0.8 and 0.9 [2]. A partial theoretical explanation of these empirical results has been given in [5]. New numerical experiments which will be reported in this paper are related to TSP problems with 50 and 100 vertices.

For numerical experiments we use the software package Concorde TSP Solver, a program for solving the symmetric traveling salesman problem. It was written by David Applegate, Robert E. Bixby, Vašek Chvátal, and William J. Cook, in ANSI C, and is freely available for academic use [1]. Concorde is widely regarded as the fastest TSP solver currently in existence.

In this paper we use the same TSP instances as in [3] and [4]. For dimension $n = 50$ we have generated randomly two sets $S(1)$ and $S(2)$, each consisting of hundred TSP instances with integer weights uniformly distributed in interval $[1, 100]$. The second set is used in our experiments as a control set. We considered also sets $S(3)$ and $S(4)$ each with hundred instances of dimension $n = 100$.

The Frobenius norm of a square matrix is the square root of the sum of squares of all entries of the matrix. When dividing a matrix by its Frobenius norm, the sum of squares of all entries becomes equal to 1. We shall say that the matrix transformed in this way is normalized and we shall assume that the matrices of the considered TSP instances are normalized. In normalized matrices we have $M_0 = n$ (as in all matrices of order n), $M_1 = 0$ (as in all matrices with zero trace) and $M_2 = 1$ and this fact was the reason to use normalization.

A matrix is called *non-negative (positive)* if all its entries are non-negative (positive). The distance matrix D is a symmetric non-negative matrix. The Perron-

Frobenius theory of non-negative matrices can be applied to matrix D similarly as it is applied to the theory of graph spectra [9].

Eigenvalues $\lambda_1, ..., \lambda_n$ of D are reals. The largest eigenvalue λ_1 is called the *spectral radius* or the *index* of D. The whole spectrum lies in the interval $(-\lambda_1, \lambda_1]$. (In the theory of graph spectra eigenvalue $-\lambda_1$ appears only in the case when a component with the largest eigenvalue of the underlying graph of the considered matrix is bipartite, [9], p. 87).

Let $S_1, S_2, \ldots, S_n$ be row sums of matrix D. These row sums play the role of vertex degrees in the corresponding weighted graph. Let S, S_{min}, S_{max} be the average, the minimal and the maximal of these row sums, respectively. By the Perron-Frobenius theory we have (cf. [9], p. 85)

$$S_{min} \leq S \leq \lambda_1 \leq S_{max}. \tag{1}$$

We have used standard tools from mathematical statistics which are appropriate when studying hidden complex connections between apparently non-related quantities. In particular, we use the following correlation coefficients.

The coefficient of linear correlation between two sequences of length s is defined by

$$C_{BC} = \frac{1}{\sqrt{\nu_B \nu_C}} \sum_{i=1}^{s} (b_i - m_B)(c_i - m_C),$$

where $b_i, c_i, m_B, m_C, \nu_B, \nu_C$ are values, mean values and variances of the corresponding sequences B and C, respectively.

The Spearman correlation coefficient S_{BC} is defined as the linear correlation coefficient between the ranked variables. For each b_i, c_i their ranks rgb_i, rgc_i are determined and we have

$$S_{BC} = \frac{1}{\sqrt{\nu_{rg_B} \nu_{rg_C}}} \sum_{i=1}^{s} (rgb_i - m_{rg_B})(rgc_i - m_{rg_C}),$$

where $rg_B = (rgb_i)$ and $rg_C = (rgc_i)$.

The rest of the paper is organized as follows. Section 2 presents numerical results of computer experiments. In Section 3 we show that instead of spectral moments it is sufficient to consider just the spectral radius. In Section 4 we present several facts showing that spectral graph theory is relevant in considering the TSP. Using previously presented results we show in Section 5 that the average length of Hamiltonian cycles is also relevant. Section 6 contains concluding remarks.

2. *Summary of numerical results*

The original strong correlation between spectral moments and the length of an optimal tour (noted in [2] and [5]) looked very promising for estimation of the later. This was a motivation to undertake numerical experiments [4] with instances of higher dimension.

We have computed the linear correlation coefficient between spectral moments M_k and the length of an optimal tour d for the sets of instances $S(1)$ and $S(2)$ for k = 3, 4, 5, 10, 30, 35, 40, 45, 50 and for sets $S(3)$ and $S(4)$ for k = 3, 4, 5, 10, 30, 35, 40, 45, 50, 60, 70, 80, 90, 100. The values of the linear correlation coefficient vary between 0.4154 and 0.5201 and are given in a table in [4].

The values are almost constant for all considered values of k within a set of instances and vary to some extent between the sets.

Correlation coefficients have gone down to a value of about 0.5 when compared to old results in [2] and [5] for instances with up to 14 vertices.

With this moderate correlation it is not reasonable to estimate the length of an optimal tour by spectral moments since standard techniques provide good results (solving relaxation tasks for lower bounds and applying heuristics for upper bounds). Nevertheless, it is challenging to explain the obtained computational results.

We shall explain these data first by analyzing the value domains of several relevant quantities of considered TSP instances:

The Frobenius norm of the non-normalized distance matrix varies
for set $S(1)$ in interval $[2800.4775, 2950.9178]$,
for set $S(2)$ in interval $[2773.2238, 2955.8643]$,
for set $S(3)$ in interval $[5685.1920, 5863.9294]$,
for set $S(4)$ in interval $[5699.4554, 5886.6838]$.

Other data are related to normalized matrices.

The length d of an optimal tour varies
for set $S(1)$ in interval $[0.0583, 0.0957]$,
for set $S(2)$ in interval $[0.0600, 0.1031]$,
for set $S(3)$ in interval $[0.0377, 0.0531]$,
for set $S(4)$ in interval $[0.0352, 0.0540]$.

The largest eigenvalue λ_1 varies
for set $S(1)$ in interval $[0.8506, 0.8745]$,
for set $S(2)$ in interval $[0.8567, 0.8722]$,
for set $S(3)$ in interval $[0.8610, 0.8714]$,
for set $S(4)$ in interval $[0.8618, 0.8716]$.

Let μ be the maximal modulus of other eigenvalues. We have $\mu < \lambda_1$ and the quantity μ varies

for set $S(1)$ in interval $[0.1334, 0.1673]$,
for set $S(2)$ in interval $[0.1339, 0.1608]$,
for set $S(3)$ in interval $[0.0986, 0.1104]$,
for set $S(4)$ in interval $[0.0969, 0.1129]$.

The sum T of the weights of an instance (the sum of entries in the, say, upper triangle in the normalized weight matrix) varies

for set $S(1)$ in interval $[21.1575, 21.7300]$,
for set $S(2)$ in interval $[21.2742, 21.6681]$,
for set $S(3)$ in interval $[42.9270, 43.4221]$,
for set $S(4)$ in interval $[42.9459, 43.4452]$.

We see that Frobenius norms are very big. Because of normalization of all distance matrices, optimal tour lengths, eigenvalues and quantities T are very small.

3. *From moments to spectral radius*

Having in view the intervals of variation of eigenvalue λ_1 and of the quantity μ from Section 2, the term λ_1^k is dominant in the expression for spectral moments $M_k = \lambda_1^k + \cdots + \lambda_n^k$ in all considered TSP instances. Actually, this means that we can assume $M_k \approx \lambda_1^k$ already for very small values of k (say $k \geq 3$).

There are several results in the literature (see, for example, [8], section 3.7. Spectra of Random Graphs, [13], Appendix B: Eigenvalues of Random Graphs) that in random symmetric matrices with identical probability distribution for entries in the upper triangle the second largest eigenvalue should be small, which explains why in our matrices λ_1 is much greater than μ.

The fact that the correlation coefficient between M_k and the length of an optimal tour is independent of k is explained by a very small interval to which λ_1 belongs.

We see that really important parameter is the largest eigenvalue λ_1. It is well-known that the largest eigenvalue (also known as the spectral radius) plays an important role in the theory of graph spectra [9],[14]. It was the purpose of the paper [4] to establish that the spectral radius is also relevant in the theory of the traveling salesman problem.

Therefore in [4] we have computed linear correlation coefficients KK and Spearman correlation coefficients SKK between λ_1 and optimal tour lengths:

for set $S(1)$: KK$= 0.5197$, SKK$= 0.5504$,
for set $S(2)$: KK$= 0.4157$, SKK$= 0.3689$,
for set $S(3)$: KK$= 0.4190$, SKK$= 0.3907$,

for set $S(4)$: KK$= 0.4902$, SKK$= 0.4563$.

The values are again around 0.5 just as for spectral moments.

4. *Using the theory of graph spectra*

The theory of graph spectra [9] was appearing sporadically in treating the traveling salesman problem (see, for example, [6], [7]). Very interesting observations are described in an unpublished doctoral dissertation [11] by O. Halskau.

In this section we shall show, using several facts from the theory of graph spectra, that the spectral radius λ_1 of the distance matrix is approximately equal to the average length of Hamiltonian cycles for the considered TSP instance.

Consider an undirected regular graph of degree r with n vertices. The number N_k of walks of length k in this graph is $N_k = nr^k$. For a complete graph K_n we have $N_k = n(n-1)^k$. Since the spectrum of K_n consists of a simple eigenvalue $n-1$ and of the eigenvalue -1 of the multiplicity $n-1$, for the spectral moment we get $M_k = (n-1)^k + (n-1)(-1)^k$.

In an undirected weighted graph the weight of a walk by definition is equal to the product of weights of edges of which the walk consists. Let $D = ||d_{ij}||_1^n$ any square symmetric matrix and let $D^k = ||d_{ij}^{(k)}||_1^n$. By a well-known result (see, for example, [9], p. 44) the quantity $d_{ij}^{(k)}$ is equal to the sum of weights of all walks of length k starting at vertex i and terminating in vertex j. It follows that the spectral moment M_k, being equal to the trace of D^k, is equal to the sum of weights of all closed walks of length k.

Let now $D = ||d_{ij}||_1^n$ be the normalized weight matrix representing a TSP instance with largest eigenvalue λ_1. Consider an auxiliary weighted graph with the weight matrix $D^* = ||\lambda_1/(n-1)||_1^n$ with zeros on the diagonal and off diagonal entries $\lambda_1/(n-1)$. Since the weight of any edge is equal to $\lambda_1/(n-1)$, the weight of any walk of length k is equal to $(\lambda_1/(n-1))^k$.

As already established we have $M_k \approx \lambda_1^k$ for matrix D.

The k-th spectral moment for matrix D^* can be calculated and for sufficiently large n estimated as

$$\begin{aligned} M_k &= ((n-1)^k + (n-1)(-1)^k)(\lambda_1/(n-1))^k \\ &= \lambda_1^k + (-1)^k(\lambda_1/(n-1))^k(n-1) \\ &\approx \lambda_1^k. \end{aligned}$$

On the basis of this estimation we could consider, for the moment, the weighted graph with the weight matrix D^* instead of the original weighted graph. Since matrices D and D^* assimptotically have equal spectral moments, we can expect that other quantities for these matrices behave similarly.

The length of any Hamiltonian cycle for D^* is $n\lambda_1/(n-1)$ and this is at the same time the average length of all Hamiltonian cycles w.r.t. matrix D^*.

Since for sufficiently large n we have $n\lambda_1/(n-1) \approx \lambda_1$, we arrive at the conclusion that one should expect a correlation between the average length of Hamiltonian cycles and the length of an optimal tour w.r.t. original matrix D.

This will be confirmed in another way and computationally verified in the next section.

O. Halskau has used in [11] the spectral decomposition of the weight matrix to derive several bounds for relevant quantities. For example, it is proved that the sum $E = |\lambda_1| + |\lambda_2| + \cdots + |\lambda_n|$ is an upper bound for the length of any Hamiltonian cycle ([11], p.90). (Recall that the first term reflects the average length of Hamiltonian cycles.) Quantity E is known as the *energy* of a graph (or matrix) (see, for example, [9], p. 237, where it is considered in the context of the adjacency matrix of a graph and in this case is relevant in Chemistry).

5. *Average length of hamiltonian cycles*

The average length of Hamiltonian cycles in a TSP instance will be computed exactly in another way in this section.

Let $D = ||d_{ij}||_1^n$ be a normalized weight matrix representing a TSP instance. For any i, j $(i < j)$ the edge with the weight d_{ij} belongs to $(n-2)!$ Hamiltonian cycles. The number of Hamiltonian cycles is equal to $\frac{1}{2}(n-1)!$. Let d_h be the length of the Hamiltonian cycle h. Then the average length $\overline{d}_h$ of Hamiltonian cycles is equal to

$$\overline{d}_h = \frac{2}{(n-1)!}\sum_h d_h = \frac{2}{(n-1)!}\sum_{i<j} d_{ij}(n-2)! = \frac{2}{n-1}\sum_{i<j} d_{ij} = \frac{2}{n-1}T.$$

For the average value S of row sums of matrix D we obviously have

$$S = \frac{2T}{n}.$$

Example 5.1. Considering the first instance in the set $S(1)$ we find in computed data $\lambda_1 = 0.862$, $d = 0.0788$, $T = 21.4029$. Now we obtain $S = 0.856$ and $\overline{d}_h = 0.8735$. It is interesting that $n\lambda_1/n - 1 = \frac{50}{49} \times 0.862 = 0.8796$, thus quite close to $\overline{d}_h$.

By formula (1) we see that λ_1 is close to S and because S is proportional to T we have computed linear correlation coefficients KK and Spearman correlation coefficients SKK between T and optimal tour lengths:

$S(1)$: KK$= 0.5362$, SKK$= 0.5382$;
$S(2)$: KK$= 0.4113$, SKK$= 0.3576$;
$S(3)$: KK$= 0.4051$, SKK$= 0.3862$;
$S(4)$: KK$= 0.4632$, SKK$= 0.4390$.

Hence we see that there exists a notable correlation between the average length of Hamiltonian cycles and the length of an optimal tour.

6. *Conclusions*

It started with an intriguing observation from 1987 that the correlation coefficient between the length of an optimal tour and spectral moments for TSP instances up to 14 vertices lays between 0.8 and 0.9. Recent experiments with instances on 50 and 100 vertices have reduced this value to about 0.5. Hence, there exists a moderate, but for our purpose significant correlation between sequences of spectral moments and sequences of the optimal tour lengths. More precisely, in spite of obtaining a moderate correlation, the discovery that such apparently quite disconnected quantities are in some connection, is significant.

Since in distance matrices, generated randomly in the described way, the largest eigenvalue is much greater than the moduli of other eigenvalues, it turns out that it is sufficient to consider just the largest eigenvalue instead of the spectral moment. Hence, the spectral radius and the length of an optimal tour are in correlation also with a correlation coefficient of about 0.5.

Using several facts from the theory of graph spectra, we found a close relation between the largest eigenvalue and the average length of all Hamiltonian cycles in a TSP instance. In this way we established a notable correlation between the average length of Hamiltonian cycles and the length of an optimal tour. At the moment we do not see a direct (without using spectral graph theory) explanation of this fact.

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