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HAMILTONICITY AND THE 3-OPT PROCEDURE FOR THE TRAVELING SALESMAN PROBLEM

Abstract. The 3-Opt procedure deals with interchanging three edges of a tour with three edges not on that tour. For $n \geq 6$, the 3-Interchange Graph is a graph on $\frac{1}{2}(n-1)!$ vertices, corresponding to the hamiltonian tours in K_n; two vertices are adjacent iff the corresponding hamiltonian tours differ in an interchange of 3 edges; i.e. the tours differ in a single 3-Opt step. It is shown that the 3-Interchange Graph is a hamiltonian subgraph of the Symmetric Traveling Salesman Polytope. Upper bounds are derived for the diameters of the 3-Interchange Graph and the union of the 2- and the 3-Interchange Graphs. Finally, some new adjacency properties for the Asymmetric Traveling Salesman Polytope and the Assignment Polytope are given.

1. Introduction. The 3-Opt procedure is used to decrease the length of a given tour by interchanging three edges of the given tour with three new edges. The use of interchanging two edges and the corresponding 2-Interchange Graph have been studied in [9]. We concentrate in this paper on the 3-Interchange Graph. $K_n = (V, E)$ denotes the complete graph on n vertices. Denote by S_n the set of all tours (hamiltonian cycles) in K_n. Define the *characteristic vector* of $t \in S_n$, $x^t \in \mathbb{R}^E$, by $x^t_e = 1$ if $e \in t$ and $x^t_e = 0$ if $e \notin t$. The polytope $Q^n_T := \mathrm{conv}\{x^T \in \mathbb{R}^E \mid T \in S_n\}$ is called the *Symmetric Traveling Salesman Polytope*; see e.g. [2]. Its skeleton is denoted by $\mathrm{Skel}(Q^n_T)$. Note that the vertex set of $\mathrm{Skel}(Q^n_T)$ is S_n, and that

(1.1) $t_1, t_2 \in S_n$ are adjacent on $\mathrm{Skel}(Q^n_T)$ iff for every λ with $0 \leq \lambda \leq 1$, the point $\lambda t_1 + (1-\lambda)t_2$ cannot be expressed as a convex combination of elements of $S_n \setminus \{t_1, t_2\}$.

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Let $E(t) := \{e \in E \mid x_e^t = 1\}$ be the edge set of the tour t. Then (see e.g. [3], Lemma 1.2.23) the following holds:

(1.2) $t_1, t_2 \in S_n$ are adjacent in $\mathrm{Skel}(Q_T^n)$ if there does not exist a tour $t \neq t_1, t_2$ such that $E(t_1) \cap E(t_2) \subset E(t) \subset E(t_1) \cup E(t_2)$.

The *k-Interchange Graph* of Q_T^n, denoted by $\mathrm{Int}_k(Q_T^n)$, is the graph with the same vertex set as Q_T^n and with $t_1, t_2 \in S_n$ adjacent on $\mathrm{Int}_k(Q_T^n)$ iff t_1 and t_2 differ in an interchange of k edges; $2 \leq k \leq n$. In this paper we concentrate on the case $k = 3$. The case $k = 2$ is discussed in [9], and the case $k \geq 4$ in [10].

2. Adjacency on $\mathrm{Skel}(Q_T^n)$**.** In [9] it is shown that $\mathrm{Int}_2(Q_T^n)$ is a spanning subgraph of $\mathrm{Skel}(Q_T^n)$. The following theorem asserts that the same holds for $\mathrm{Int}_3(Q_T^n)$. In [10] it is shown that $\mathrm{Int}_k(Q_T^n)$ is in general not a subgraph of $\mathrm{Skel}(Q_T^n)$ for $n \geq 4$.

THEOREM 1. *For* $n \geq 3$, $\mathrm{Int}_3(Q_T^n)$ *is a spanning subgraph of* $\mathrm{Skel}(Q_T^n)$.

Proof. Let t_1 be any tour in K_n and let (a, b), (c, d) and (e, f) be pairwise different edges of t_1. Using (1.2), we will show that two adjacent vertices on $\mathrm{Int}_3(Q_T^n)$ are also adjacent on $\mathrm{Skel}(Q_T^n)$.

Case 1: No two of the edges (a, b), (c, d) and (e, f) are adjacent. The edge set $E(t_1) \setminus \{(a, b), (c, d), (e, f)\}$ can then be extended in K_n to a tour different from t_1 in four different ways. Let t_2, t_3, t_4, t_5 be these tours, schematically depicted in Fig. 1. Note that the tours t_2, t_3, t_4 have the same structure.

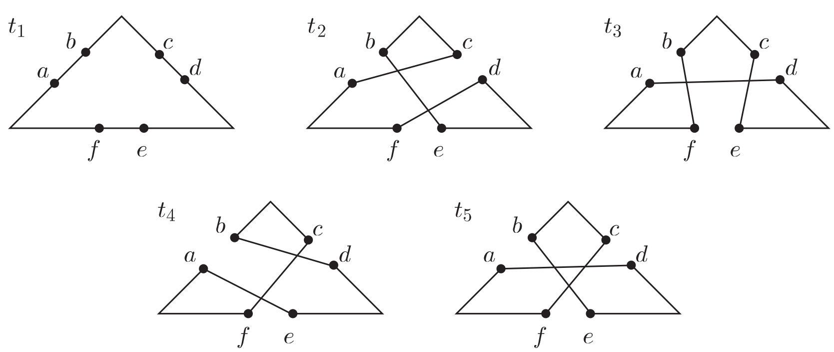

Fig. 1

We will restrict ourselves to the proof that t_1 and t_2 are adjacent and show that there is no tour $t \neq t_1, t_2$ such that $E(t_1) \cap E(t_2) \subset E(t) \subset E(t_1) \cup E(t_2)$. Suppose, to the contrary, that such a tour t exists. If $(a, b) \in E(t)$, then (a, c), $(b, e) \notin E(t)$ and hence $(c, d), (e, f) \in E(t)$, so that $t = t_1$, which is a contradiction. If $(a,c) \in E(t)$, then $(a,b),(c,d) \notin E(t)$ and hence $(b,e),(d,f) \in E(t)$, so that $t = t_2$, which is also a contradiction. Therefore, t_1 and t_2 are adjacent.

Case 2: If two of the edges $(a,b),(c,d),(e,f)$ of t_1 are adjacent, say (a,b) and (e,f) with $a = f$, then there is precisely one way to extend the edge set $E(t_1) \setminus \{(a,b),(c,d),(e,f)\}$ to a tour in K_n different from t_1; see Fig. 2.

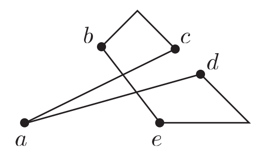

Fig. 2

The proof of Case 2 is left to the reader. The conclusion is that any two tours t_1 and t in K_n with precisely three edges interchanged are adjacent in $\mathrm{Skel}(Q_T^n)$. ■

3. The degree of the vertices of $\mathrm{Int}_3(Q_T^n)$**.** In [9] it is shown that the degree of $\mathrm{Int}_2(Q_T^n)$ is $\binom{n}{2} - \binom{n}{1}$. In the following theorem the degree of the vertices of $\mathrm{Int}_3(Q_T^n)$ is calculated.

THEOREM 2. *For* $n \geq 3$, $\mathrm{Int}_3(Q_T^n)$ *is a* $\left[4\binom{n}{3} - 6\binom{n}{2} + 5\binom{n}{1}\right]$*-regular subgraph of* $\mathrm{Skel}(Q_T^n)$*.*

Proof. The proof is carried out simply by counting the number of tours that can be obtained by replacing three edges in a given tour in K_n. In general, there are $\binom{n}{3}$ ways for choosing three edges from a tour. Taking the adjacency of these three edges into account, there are three possibilities to be considered. First, there are n ways to choose three pairwise adjacent edges. Clearly, it is not possible to construct a new tour by replacing these three edges. Second, there are $n(n-4)$ ways to choose three edges with precisely two adjacent ones. There is only one way to construct a new tour. See Case 2 of Theorem 1. Third, there remain $\binom{n}{3} - n(n-5)$ ways to choose three non-adjacent edges. Then there are four ways to construct a new tour; see also Case 1 of Theorem 1. Adding the number of tours that can be constructed by replacing three edges of a given tour, we obtain the desired formula. ■

Since $\mathrm{Int}_2(Q_T^n)$ and $\mathrm{Int}_3(Q_T^n)$ are edge-disjoint subgraphs of $\mathrm{Skel}(Q_T^n)$, it follows that $\mathrm{Skel}(Q_T^n)$ is a regular graph with degree at least $4\binom{n}{3} - 5\binom{n}{2} + 4\binom{n}{1}$. An interesting open problem is to determine the degree of the vertices of $\mathrm{Skel}(Q_T^n)$. The following table shows some calculations for $n = 4$ to 12. In the second column the number of vertices of $\mathrm{Skel}(Q_T^n)$ is listed. The third, fourth and fifth columns contain the degrees of $\mathrm{Int}_2(Q_T^n)$, $\mathrm{Int}_3(Q_T^n)$

and $\mathrm{Skel}(Q_T^n)$ respectively; the calculations are carried out by brute force computer calculations.

n	$\lvert S_n\rvert$	$\delta(\mathrm{Int}_2(Q_T^n))$	$\delta(\mathrm{Int}_3(Q_T^n))$	$\delta(\mathrm{Skel}(Q_T^n))$
4	3	2		2
5	12	5	5	10
6	60	9	20	41
7	360	14	49	168
8	2520	20	96	730
9	20160	27	165	3555
10	181440	35	260	19391
11	1814400	44	385	115632
12	19958400	54	544	741273

4. Hamiltonicity of $\mathrm{Int}_3(Q_T^n)$**.** The Grötschel–Padberg conjecture (see [2]), stating that the skeleton of the Symmetric Traveling Salesman Polytope is hamiltonian, was settled in [6]. The proof in [9] relies on the hamiltonicity of the 2-Interchange Graph. In this section we will show that $\mathrm{Int}_3(Q_T^n)$ is hamiltonian as well, giving rise to a new and simple proof of the hamiltonicity of the Grötschel–Padberg conjecture. For $k \geq 4$, $\mathrm{Int}_k(Q_T^n)$ is not a subgraph of $\mathrm{Skel}(Q_T^n)$ (see [10]), so we cannot hope for an even more elegant proof by exploring $\mathrm{Int}_k(Q_T^n)$. On the other hand, the hamiltonicity of $\mathrm{Int}_k(Q_T^n)$ itself is open for $4 \leq k \leq n-1$; the case $k = n$ is settled in [10].

Theorem 3. *For* $n \geq 6$, $\mathrm{Int}_k(Q_T^n)$ *is hamiltonian.*

Proof. By a *cycle* we mean a hamiltonian tour on the vertices of the 3-Interchange Graph. The proof is by induction on n. Suppose we have a cycle on the vertices of $\mathrm{Int}_3(Q_T^n)$. We will "expand" every vertex of $\mathrm{Int}_3(Q_T^n)$ to n vertices of $\mathrm{Int}_3(Q_T^{n+1})$, and then expand the cycle in $\mathrm{Int}_3(Q_T^n)$ to a cycle in $\mathrm{Int}_3(Q_T^{n+1})$. The construction is as follows. Let $t = (1\ i_2\ i_3 \ldots\ i_n)$ be a vertex of $\mathrm{Int}_3(Q_T^n)$. Using the "bell-switch" method of Steinhaus (see e.g. [4]) with the new vertex $n+1$, this tour gives rise to n different tours in $\mathrm{Int}_2(Q_T^n)$, namely:

$$\begin{aligned} t_1 &= (1\ n+1\ i_2\ i_3\ \ldots\ i_n),\\ t_2 &= (1\ i_2\ n+1\ i_3\ \ldots\ i_n),\\ &\ \vdots\\ t_n &= (1\ i_2\ i_3 \ldots i_n\ n+1). \end{aligned}$$

Note that by applying this construction to every vertex in $\mathrm{Int}_3(Q_T^n)$, all vertices of $\mathrm{Int}_3(Q_T^{n+1})$ are obtained. Let $B_3(t, Q_T^{n+1})$ denote the subgraph of $\mathrm{Int}_3(Q_T^{n+1})$ on the n expanded vertices of the vertex t of $\mathrm{Int}_3(Q_T^n)$.

Claim 1. $B_3(t, Q_T^{n+1})$ *is hamiltonian connected.*

This follows from the fact that $B_3(t, Q_T^{n+1})$ is a complete graph without the edges (t_1, t_2), (t_2, t_3), $\ldots$, (t_{n-1}, t_n), (t_n, t_1). Namely, two vertices t_i and t_{i+1} $(i = 1, \ldots, n)$ with $t_{n+1} = t_1$ differ in an interchange of two edges and all other pairs of vertices differ in an interchange of three edges.

CLAIM 2. *For any two adjacent vertices $t, t' \in \mathrm{Int}_3(Q_T^n)$, the adjacency of vertices in $B_3(t, Q_T^{n+1})$ to vertices in $B_3(t', Q_T^{n+1})$ is at least one-to-one.*

To prove this, let t and t' be two adjacent vertices in $\mathrm{Int}_3(Q_T^n)$, differing in an interchange of three edges, say e_1, e_2, e_3 are in t but not in t' and e_4, e_5 e_6 are in t' but not in t. Recall that a vertex of $B_3(t, Q_T^{n+1})$ is obtained by replacing an edge (v_i, v_j) in t by two edges $(v_i, n+1)$ and $(n+1, v_j)$.

There are now two cases:

Case 1: $(v_i, v_j) \notin \{e_1, e_2, e_3\}$. Then (v_i, v_j) must also be in t'. Clearly, the new tours t and t' differ in an interchange of three edges, and hence they are adjacent in $\mathrm{Int}_3(Q_T^{n+1})$.

Case 2: $(v_i, v_j) \in \{e_1, e_2, e_3\}$, say $(v_i, v_j) = e_1$. Without loss of generality, assume that e_1 and e_4 have v_i in common. The edge e_1 in t is replaced by $(v_i, n+1)$ and $(n+1, v_j)$, and e_4 in t' is replaced by $(v_i, n+1)$ and $(n+1, v_k)$. Therefore, the two new tours differ in an interchange of three edges; namely, e_2, e_3 and $(n+1, v_j)$ in t, versus e_5, e_6 and $(n+1, v_k)$ in t', and hence they are adjacent on $\mathrm{Int}_3(Q_T^{n+1})$.

The theorem is true for $n = 6$. Take for instance the cycle in $\mathrm{Int}_3(Q_T^6)$ shown in Fig. 3.

$$
\begin{array}{ccccccccc}
123645 & \rightarrow & 123456 & \rightarrow & 126345 & \rightarrow & 123465 & \rightarrow & 162345 \\
 & & & & & & & & \downarrow \\
124563 & \leftarrow & 126453 & \leftarrow & 124536 & \leftarrow & 124653 & \leftarrow & 162453 \\
\downarrow & & & & & & & & \\
125643 & \rightarrow & 162534 & \rightarrow & 125364 & \rightarrow & 126534 & \rightarrow & 125346 \\
 & & & & & & & & \downarrow \\
132654 & \leftarrow & 163254 & \leftarrow & 132564 & \leftarrow & 136254 & \leftarrow & 132436 \\
\downarrow & & & & & & & & \\
134265 & \rightarrow & 136425 & \rightarrow & 134256 & \rightarrow & 134625 & \rightarrow & 163425 \\
 & & & & & & & & \downarrow \\
164235 & \leftarrow & 142634 & \leftarrow & 142356 & \leftarrow & 146235 & \leftarrow & 142365 \\
\downarrow & & & & & & & & \\
162354 & \rightarrow & 123654 & \rightarrow & 123546 & \rightarrow & 126354 & \rightarrow & 123564 \\
 & & & & & & & & \downarrow \\
162335 & \leftarrow & 124365 & \leftarrow & 126435 & \leftarrow & 124356 & \leftarrow & 124635 \\
\downarrow & & & & & & & & \\
162543 & \rightarrow & 125643 & \rightarrow & 125436 & \rightarrow & 126543 & \rightarrow & 125463 \\
 & & & & & & & & \downarrow \\
163245 & \leftarrow & 132465 & \leftarrow & 136245 & \leftarrow & 132456 & \leftarrow & 132645 \\
\downarrow & & & & & & & & \\
163524 & \rightarrow & 135264 & \rightarrow & 136524 & \rightarrow & 135246 & \rightarrow & 135624 \\
 & & & & & & & & \downarrow \\
164325 & \leftarrow & 143625 & \leftarrow & 143625 & \leftarrow & 146325 & \leftarrow & 143265
\end{array}
$$

Fig. 3

For $n \geq 7$, the induction hypothesis is now an immediate consequence of Claims 1 and 2. ∎

5. The diameter of $\mathrm{Int}_3(Q_T^n)$**.** Diameters of many $(0,1)$-polytopes have been calculated, and a remarkable number have diameter equal to 2; see e.g. [8] and [11]. In [8] it is shown that the diameter of the Asymmetric Traveling Salesman Polytope equals 2. For the symmetric case, it is only conjectured that this diameter is 2; see e.g. [2]. For the 3-Interchange Graph we have the following results.

THEOREM 4. *For* $n \geq 6$,

(a) $\mathrm{Diam}(\mathrm{Int}_3(Q_T^n)) \leq n-1$, *and*
(b) $\mathrm{Diam}(\mathrm{Int}_2(Q_T^n) \cup \mathrm{Int}_3(Q_T^n)) \leq n - \lfloor\sqrt{n-2}\rfloor - 2$.

Proof. Let $t_1 = (1\, i_2 \,\ldots\, i_{p-1}\, i_p\, i_{p+1} \ldots i_q\, i_{q+1} \,\ldots\, i_n)$, with $p < q$, be a hamiltonian tour in K_n. Placing i_p between i_q and i_{q+1} leads to the tour $t' = (1\, i_2 \,\ldots\, i_{p-1}\, i_{p+1} \,\ldots\, i_q\, i_p\, i_{q+1} \,\ldots\, i_n)$. This swop is either a 2-interchange (namely, if $p+1 = q$), or a 3-interchange (if $p+1 < q$). The tours $t = (1\,2 \ldots n)$ and t_1 differ in at most $n-1$ edges. In [10], one can find a theorem that asserts that in any sequence of p^2+1 elements, there is a monotone subsequence of at least $p+1$ elements. Taking $p = n-1$, it follows that at least $\lfloor\sqrt{n-2}\rfloor + 1$ of the elements $i_2, \ldots, i_n$ form an increasing sequence. The remaining $n - \lfloor\sqrt{n-2}\rfloor - 2$ elements can be moved to the natural position (i.e. corresponding to the ordering $1, \ldots, n$) by a sequence of 2- and 3-interchanges. This proves part (b) of the theorem.

In the above described procedure we may have applied a number of 2-interchanges. Each element can be put in its natural position by 3-interchanges, except possibly for the case where the $\lfloor\sqrt{n-2}\rfloor + 1$ $(= m)$ elements, denoted by J, have precisely one neighbor not in J in the wrong position. For instance, in the subsequence $\ldots, 4, 9, 8, 6, 2, 3, \ldots$ with $8 \in J$, the 6 can be put in its natural position by a 3-interchange, so that only the neighbor 9 of 8 is in the wrong position. It needs two 3-interchanges to bring 9 in the natural position (namely, for instance, a three-jump to the right, plus a two-jump to the left). In the most extreme case, all elements of J have a neighbor in the wrong position. Hence, it takes $(n-m-1)-m = n-2m-1$ plus $2m$ 3-interchanges to bring all $n-m-1$ elements in the natural position. Adding these numbers yields a total of $(n-2m-1)+2m = n-1$ 3-interchanges. This proves part (a) of the theorem. ∎

It is an open question whether the upper bounds in Theorem 4 are sharp, so that equalities hold. Note that the upper bound in Theorem 4(b) is an upper bound for $\mathrm{Diam}(\mathrm{Skel}\, Q_T^n)$ as well.

6. The asymmetric TSP and the Assignment Polytope. Let $D_n = (V, A)$ be the complete digraph on n vertices. Denote by $\mathcal{T}_n$ the set of all directed tours in D_n. Then the polytope $P_T^n := \operatorname{conv}\{x^T \in \mathbb{R}^A \mid T \in \mathcal{T}_n\}$ is called the *Asymmetric Traveling Salesman Polytope*. Let Q_A^n and P_A^n denote the Assignment Polytopes on K_n and D_n, respectively; i.e. $Q_A^n := \operatorname{conv}\{x^a \in \mathbb{R}^E \mid a$ is a perfect 2-matching on $K_n\}$, and $P_A^n := \operatorname{conv}\{x^a \in \mathbb{R}^E \mid a$ is an assignment on $D_n\}$.

THEOREM 5. $\mathrm{Int}_3(P_T^n)$ *is an* $\left[\binom{n}{3} - \binom{n}{1}\right]$*-regular spanning subgraph of* $\mathrm{Skel}(P_T^n)$.

Proof. The proof that $\mathrm{Int}_3(P_T^n)$ is a spanning subgraph of $\mathrm{Skel}(P_T^n)$ is similar to the proof of Theorem 1. As for the degree of the vertices of $\mathrm{Int}_3(P_T^n)$, the counting procedure is similar to the one in the proof of Theorem 2. Note that, in contrast to the proof of Theorem 2, we now have only one possibility (instead of four) to construct a new tour. ∎

It is well known that $Q_T^n \subset Q_A^n$, and that $P_T^n \subset P_A^n$. However, adjacent tours on Q_T^n are not always adjacent on Q_A^n. The same is true for P_T^n and P_A^n. On the other hand, the following theorem states, in particular, that any two adjacent tours in both the 2- and the 3-Interchange Graphs are adjacent on the Assignment Polytope. We first give an example. The two tours t_1 and t_2, schematically depicted in Fig. 4, are adjacent on $\mathrm{Skel}(Q_T^n)$. However, since there exist two perfect 2-matchings a_1 and a_2 with $\frac{1}{2}t_1 + \frac{1}{2}t_2 = \frac{1}{2}a_1 + \frac{1}{2}a_2$, they are not adjacent on $\mathrm{Skel}(Q_T^n)$.

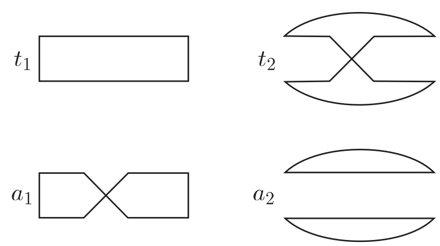

Fig. 4

THEOREM 6. *For* $n \geq 6$, *the following assertions hold*:

(a) $\mathrm{Int}_2(Q_T^n) \cup \mathrm{Int}_3(Q_T^n) \subset \mathrm{Skel}(Q_A^n)$;
(b) $\mathrm{Int}_3(P_T^n) \subset \mathrm{Skel}(P_A^n)$;
(c) $\mathrm{Int}_k(Q_T^n) \not\subset \mathrm{Skel}(Q_A^n)$ *for* $k \geq 4$.

Proof. The proof is left to the reader. ∎

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