Construction of Hamiltonian Cycles with a Given Spectrum of Edge Directions in an n-Dimensional Boolean Cube

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Abstract—The *spectrum of a Hamiltonian cycle* (of a *Gray code*) in an *n*-dimensional Boolean cube is the series $a = (a_1, \ldots, a_n)$, where a_i is the number of edges of the *i*th direction in the cycle. The necessary conditions for the existence of a Gray code with the spectrum *a* are available: the numbers a_i are even and, for $k = 1, \ldots, n$, the sum of *k* arbitrary components of *a* is at least 2^k . We prove that there is some dimension *N* such that if the necessary condition on the spectrum is also sufficient for the existence of a Hamiltonian cycle with the spectrum in an *N*-dimensional Boolean cube then the conditions are sufficient for all dimensions *n*.

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INTRODUCTION

In the chapter of [8] dealing with the Gray codes (Hamiltonian cycles of a Boolean *n*-cube), D. Knuth pointed out the three problems unresolved at the time of publication. The first problem is to estimate the number of distinct Gray codes in a Boolean *n*-cube. The degree of the logarithm of this number is found in [1], and the asymptotic behavior of the logarithm of this number as $n \to \infty$ is determined in [6]. The second problem poses the question that was earlier brought up by G. Kreweras [9]: *Can each perfect matching of a Boolean n-cube be extended to a Hamiltonian cycle*? The affirmative answer to this is given by J. Fink [7]. In the case when the matching contains the edges only of a few directions, the extendability of a perfect matching to a Hamiltonian cycle is proved in [1]. In the third problem, the question is put whether the necessary conditions (formulated in the annotation) on the spectrum of a Hamiltonian cycle are also sufficient for the existence of a Gray code with such a spectrum.

In this article, some asymptotic solution is offered as a solution to the last problem. Namely, if the necessary conditions are sufficient in a Boolean n-cube for a reasonably large n then they are sufficient for all n. This result is announced in [4]. Note that several methods are available for construction of some Gray codes with various properties; in particular, in [5, 10], the Hamiltonian cycles are constructed with a totally balanced spectrum.

1. DEFINITIONS

The *Boolean n-cube* is the set Q_n of the binary words of length n. A graph GQ_n with vertices from Q_n in which two vertices are connected if and only if the corresponding words differ in exactly one position is also called a *Boolean n-cube*. Each edge $\{u, v\}$ of GQ_n has direction $i \in \{1, ..., n\}$ if i is equal to the number of the position in which the words u and v differ. A collection P of edges of a graph G is called a *perfect matching* if each vertex of G is incident to exactly one edge from P. A *Hamiltonian cycle* of G is a cycle including each vertex exactly once. In a bipartite graph and, in particular, in GQ_n , the vertices of each Hamiltonian cycle can be decomposed into some two perfect matching. The *spectrum of a Hamiltonian cycle of the Boolean n-cube* is the series $a = (a_1, a_2, ..., a_n)$, where a_i is the number

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of edges of the *i*th direction in the cycle. The spectrum of a perfect matching of GQ_n is defined in a similar fashion. It is known [2] that an arbitrary series of integers (a_1, \ldots, a_n) that meets the following conditions

1) a_i is a nonnegative even number for i = 1, ..., n;

2) $\sum_{i=1}^{n} a_i = 2^{n-1}$

is a spectrum of some perfect matching of GQ_n . These conditions are not only sufficient, but necessary as well [2]. The necessary conditions for a set of integers (a_1, \ldots, a_n) to be a spectrum of some Hamiltonian cycle of GQ_n are also available [8]:

(*) a_i is a nonnegative even number for i = 1, ..., n;

(**)
$$\sum_{i=1}^{n} a_i = 2^n;$$

(***) $\sum_{i=1}^{k} a_{\pi(i)} \ge 2^k$ for every permutation $\pi \in S_n$ and $k = 1, \ldots, n-1$.

The conditions (*) and (**) are evident, and (* * *) follows from the connectivity of the cycle. Without loss of generality we can assume that the spectrum of a Hamiltonian cycle is ordered so that $a_i \leq a_j$ if $i \leq j$. Then (* * *) can be rewritten as

$$\sum_{i=1}^k a_i \ge 2^k \quad \text{for } k \le n.$$

Define the nonnegative function μ_a of an ordered spectrum as

$$\mu_a(k) = \sum_{i=1}^k a_i - 2^k.$$

If a series of integers satisfies the above necessary conditions (*)-(***) then we call it *admissible*. Denote the set of admissible *n*-dimensional series by \mathbb{D}_n . It is clear that each Hamiltonian cycle of GQ_n contains the edges of all directions, while a perfect matching of GQ_n can contain the edges from 1 to *n* directions inclusively. Let us call a matching of GQ_n that contains the edges from all *n* directions a *matching of full rank*. We call a Hamiltonian cycle that contains a perfect matching of full rank a cycle of full rank.

Proposition 1. If each admissible integer-valued series is a spectrum of a Hamiltonian cycle of GQ_n for some n then the same holds for all m such that $2 \le m \le n$.

Proof. Indeed, let (a_1, \ldots, a_m) be an admissible series. Then the series

$$(a_1, \ldots, a_m, 2^m, \ldots, 2^{n-1})$$

is also admissible. And the projection of a Hamiltonian cycle with spectrum

$$(a_1, \ldots, a_m, 2^m, \ldots, 2^{n-1})$$

onto the first *m* direction produces a Hamiltonian cycle with spectrum (a_1, \ldots, a_m) . The proof is over.

Each (in particular, Hamiltonian) cycle C of a graph GQ_n can be associated with a cyclical *transient* word X in the alphabet $\{1, \ldots, n\}$ in which the *j*th letter x_j is defined as the direction of the *j*th edge in C. Let $S(X) = (s_1, \ldots, s_n)$ denote the *series constituted* by the word X modulo 2; i.e., $s_i = 0$ if the letter $i \in \{1, \ldots, n\}$ occurs evenly many times in S(X) and $s_i = 1$ otherwise.

Proposition 2 [3]. A cyclic word X in the alphabet $\{1, ..., n\}$ defines a simple cycle of a graph GQ_n if and only if $S(X) = \overline{0}$ and $S(Y) \neq \overline{0}$. for each subword $Y \neq X$.

From this we immediately obtain

Corollary 1. A cyclical word X in the alphabet $\{1, ..., n\}$ defines a Hamiltonian cycle in GQ_n if and only if the length of X equals 2^n , S(X) = 0, and $S(Y) \neq \overline{0}$ for each subword $Y \neq X$.

2. CONSTRUCTION OF A HAMILTONIAN CYCLE

The purpose of this article is to prove that each admissible series is a spectrum of some Hamiltonian cycle in Boolean n-cube if this is so for a Boolean N-cube for a sufficiently large N. Let us construct a Hamiltonian cycle by using the representation of a Boolean n-cube as the Cartesian product of the cubes of dimensions k and n - k.

Consider a Hamiltonian cycle of GQ_k that consists of the edges from some disjoint perfect matchings P_1 and P_2 . We embed P_1 into GQ_n in a natural way. Since each vertex of GQ_k in the Cartesian product $GQ_k \times GQ_{n-k}$ corresponds to a Boolean (n-k)-cube; therefore, each edge of P_1 can be associated with a pair of parallel (n-k)-cubes; i.e., one (n-k+1)-cube. Let us replace each edge $v \in P_1$ with a Hamiltonian cycle H_v in the (n-k+1)-cube containing this edge. By removing P_1 from the union of P_2 and the cycles H_v , $v \in P_1$, we obtain a new Hamiltonian cycle of

$$GQ_k \times GQ_{n-k} = GQ_n.$$

We formulate the above construction as

Lemma 1. Let some matchings of GQ_k with spectra (b_1, \ldots, b_k) and (b'_1, \ldots, b'_k) make up a Hamiltonian cycle, and let there be 2^{k-1} Hamiltonian cycles in GQ_{n-k+1} with spectra

$$(a_1^i, \dots, a_{n-k}^i, c^i), \qquad i = 1, \dots, 2^{k-1}.$$

Then there is a Hamiltonian cycle of GQ_n with spectrum (d_1, \ldots, d_n) , where

$$d_{k+j} = \sum_{i=1}^{2^{k-1}} a_j^i, \qquad j = 1, \dots, n-k,$$

$$d_j = b_j + \sum_{p=s_j+1}^{s_{j+1}} (c^p - 1), \qquad j = 1, \dots, k,$$

$$s_j = \sum_{p=1}^{j-1} b'_p.$$

Proof. Let

$$X = x_1 y_1 x_2 \dots x_{2^{k-1}} y_{2^{k-1}}$$

be a transient word of a Hamiltonian cycle of GQ_k , where the matchings that correspond to the words $x_1x_2 \ldots x_{2^{k-1}}$ and $y_1y_2 \ldots y_{2^{k-1}}$ have the spectra (b_1, \ldots, b_k) and (b'_1, \ldots, b'_k) correspondingly. Let y_iZ^i denote a transient word in a Hamiltonian cycle of GQ_{n-k+1} in the alphabet $\{k + 1, \ldots, n, y_i\}$ with the spectrum

$$(a_1^i, \dots, a_{n-k}^i, c^i), \qquad i = 1, \dots, 2^{k-1}$$

where y_i occurs $c^i - 1$ times in Z^i .

Consider the word Z obtained from X by replacing the letters y_i with the words Z^i ; i.e.,

$$Z = x_1 Z^1 x_2 Z^2 \dots x_{2^{k-1}} Z^{2^{k-1}}$$

Let us show that Z is a transient word of some Hamiltonian cycle of GQ_n . Consider an arbitrary subword

$$W = U_i x_{i+1} Z^{i+1} \dots Z^{j-1} x_j V_j$$

of Z, where U_i is a suffix of the word Z^i and V_j is a prefix of Z^j (the prefix and/or suffix can be empty). If i = j then $S(W) \neq \overline{0}$ since W is a subword of the transient word $y_i Z^i$. Let i < j and, without loss of generality, $y_i = 1$ and $y_j \in \{1, 2\}$. Consider the case when $y_j = 1$. Let

$$0 = S(W)_t = S(x_{i+1}y_{i+1}\dots x_j)_t = S(y_i x_{i+1}y_{i+1}\dots x_j)_t, \qquad t = 2,\dots,k.$$

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Since either $S(x_{i+1}y_{i+1}...x_j)_1 = 0$ or $S(y_ix_{i+1}y_{i+1}...x_j)_1 = 0$; therefore, we have a contradiction to the fact that X is a transient word of a Hamiltonian cycle. The case when $y_i = 2$ can be considered in a similar way. It is easy that

$$S(Z) = S(X) = \overline{0}.$$

Therefore, the word Z satisfies the conditions of Corollary 1, and Z is a transient word of a Hamiltonian cycle of GQ_n . By construction, the Hamiltonian cycle that corresponds to Z has the required spectrum.

The proof of Lemma 1 is complete.

Remark 1. If a matching with spectrum (b'_1, \ldots, b'_k) and at least one of the cycles of GQ_{n-k+1} used in the construction have full rank then we can obtain a Hamiltonian cycle of full rank as a result of the construction (Lemma 1).

3. THE MAIN RESULT

We now prove two lemmas about spectra of Hamiltonian cycles that can be produced using the above construction.

Lemma 2. If every admissible series of integers of length n - k + 1 is the spectrum of some Hamiltonian cycle of GQ_{n-k+1} and there is a Hamiltonian cycle of GQ_k with the spectrum (b_1,\ldots,b_k) then each admissible series of integers $(b_1,\ldots,b_k,a_{k+1},\ldots,a_n)$ is the spectrum of a Hamiltonian cycle of GQ_n .

Proof. Consider the lexicographical order on the set of ordered admissible integer-valued series

$$A = \{ a \in \mathbb{D}_n \mid a_i = b_i, \ 1 \le i \le k \}.$$

The minimal series $(b_1, \ldots, b_k, 2^k, \ldots, 2^{n-1})$ in this order is the spectrum of a Hamiltonian cycle of GQ_n . Indeed, it is enough to choose $(2, 4..., 2^{n-k}, 2)$ as the spectrum of $(a_1^i, \ldots, a_{n-k}^i, c^i)$ for all $i = 1, \ldots, 2^{k-1}$ in the above construction.

Suppose that some admissible series in A are not spectra of Hamiltonian cycles constructed by Lemma 1. Choose a lexicographically minimal $d \in A$ among these series. Consider the preceding series $d' \in A$ within the lexicographical order. It is clear that d and d' differ in the two positions $i, j \in \{k + 1, ..., n\}, i < j$, where

$$d'_i = d_i - 2,$$
 $d'_j = d_j + 2,$ $d'_j \ge d'_i + 4.$

Then, for the spectrum f of one of the Hamiltonian cycles of GQ_{n-k+1} used to construct a cycle with the spectrum d', $f_j - f_i \ge 4$ holds (or $f_j - f_i = 2$ in the spectra of the two cycles). Obviously, if we change f_i with $f_i + 2$ in the integer-valued series f and f_j with $f_j - 2$ then, by hypothesis, the new series f' will also be a spectrum of a Hamiltonian cycle of GQ_{n-k+1} .

Replacing the cycle with spectrum f in Lemma 1 with a cycle with spectrum f', we see that the series d is the spectrum of a Hamiltonian cycle; a contradiction. In the case when $f_i - f_i = 2$ in two spectra, we interchange the amounts of edges of directions i and j and apply the same construction.

The proof of Lemma 2 is complete.

Lemma 3. Let $4 \le s < k < n-1$; let all admissible integer-valued series of length n - s + 1 be spectra of Hamiltonian cycles; let, for some admissible ordered series $b \in \mathbb{D}_n$,

(i) there be an admissible series $b' \in \mathbb{D}_s$ that is the spectrum of a Hamiltonian cycle of full rank such that $b'_i \leq b_i$ for $i = 1, \ldots, s$;

and let the equations

(iii) $\sum_{i=s+1}^{k} b_i \ge 2^k - 2^s$ (ii) $b_s \le 2^{n-s-1}$,

hold for k such that $2^{k-s-1} \leq b_s$.

Then the series b is the spectrum of a Hamiltonian cycle.

Proof. Let $d_i = b_i - b'_i$ for $i = 1, \ldots, s$ and $d = \sum_{i=1}^s d_i$.

From the proof of Lemma 2 it follows that the integer-valued series $(b'_1, \ldots, b'_s, 2^s, \ldots, 2^{n-1})$ is the spectrum of a Hamiltonian cycle of GQ_n constructed by the above construction with s = k. Let m be the least integer such that $2^{m-s-1} > b_s$. Since $d_i \le b_s < 2^{m-s-1}$, the series

$$(2, \ldots, 2^{m-s-1}, 2^{m-s} - d_i, 2^{m-s+1}, \ldots, 2^{n-s}, 2 + d_i)$$

is admissible for all $i = 1, \ldots, s$.

Let us now interchange s Hamiltonian cycles (one for each direction) with spectrum

 $(2, 4, \ldots, 2^{n-s}, 2)$

in this construction with a Hamiltonian cycle with spectrum

$$(2,\ldots,2^{m-s}-d_i,2^{m-s+1},\ldots,2^{n-s},2+d_i)$$

so that as a result we have a cycle with spectrum

$$(b_1,\ldots,b_s,2^s,\ldots,2^m-d,2^{m+1},\ldots,2^{n-1}).$$

Consider the set of ordered admissible integer-valued series

 $A = \{a \in \mathbb{D}_n \mid a_i = b_i, 1 \le i \le s, \text{ the spectrum } a \text{ satisfies condition (iii)}\}.$

It is proven above that the lexicographically least spectrum from A belongs to a Hamiltonian cycle obtained with by our construction (Lemma 1). Suppose that some of the series $a \in A$ are not spectra of so-obtained Hamiltonian cycles. Then there is the lexicographically least spectrum among them. By analogy with the proof of Lemma 2 we have a contradiction.

The proof of Lemma 3 is complete.

Proposition 3. Let $2 \le s \le k \le n$, $a \in \mathbb{D}_n$, and let k be such that

$$\sum_{i=s+1}^{k} a_i < 2^k - 2^s, \qquad 2^{k-s-1} \le a_s.$$
 (A)

Then $\mu_a(s) - \mu_a(k) \ge 2$ and $k \le 2s + \log \mu_a(s)$.

Proof. Since

$$2^{k-s-1} \le a_s \le 2^{s-1} + \mu_a(s) \le 2^{s-1} \mu_a(s),$$

we have $k \leq 2s + \log \mu_a(s)$. From the first inequality in (A) it follows that

$$\sum_{i=s+1}^{k} a_i \le 2^k - 2^s - 2.$$

Therefore,

$$\mu_a(k) = \sum_{i=1}^k a_i - 2^k = \sum_{i=1}^s a_i - 2^s + \sum_{i=s+1}^k a_i - 2^k + 2^s \le \mu_a(s) - 2.$$

The proof is complete.

Theorem. There is a number N such that if all admissible integer-valued series of length N is the spectrum of some Hamiltonian cycle (of full rank in the case when $\sum_{i=1}^{k} a_i > 2^k$ for all k < N) then, for every integer $n \ge 2$, each admissible integer-valued series of length n is the spectrum of some Hamiltonian cycle of GQ_n .

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Proof. Take $a \in \mathbb{D}_n$. It is easy to prove by simple exhaustive search through the admissible series that $a_2 \ge 4$ and $a_4 \ge 6$, except for the case when $a_1 = a_2 = 2$ and $a_1 = a_2 = a_3 = a_4 = 4$. The Hamiltonian cycle of GQ_4 with the transient series 1213414243212343 has the spectrum (4, 4, 4, 4). The existence of a Hamiltonian cycle with the spectrum $a \in \mathbb{D}_n$ for $n \ge 5$ and $a_1 = a_2 = a_3 = a_4 = 4$ ($a_1 = a_2 = 2$) follows from Lemma 2.

Assume that $a_2 \ge 4$ and $a_4 \ge 6$. It is easy that $a_1 \ge 2$ and $a_3 \ge 4$ in every ordered admissible sequence. There is a Hamiltonian cycle of full rank in GQ_4 with the transient series 4212312141312313 and the spectrum (2, 4, 4, 6). Thus, if s = 4 then the condition (i) of Lemma 3 and the hypothesis of Lemma 2 hold. Consider the conditions (ii) and (iii) of Lemma 3 for s = 4. Let $n \ge 35$, then

$$a_4 \le \frac{2^n}{n-3} \le 2^{n-5}.$$

Suppose that the condition (iii) fails; i.e., for some $k \ge 5$, we have

$$2^{k-5} \le a_4.$$
 $\sum_{i=5}^k a_i < 2^k - 2^4.$

Then

$$(k-4)2^{k-5} \le (k-4)a_4 < 2^k - 2^4,$$

whence it follows that $k \leq 35$ and $a_4 < \frac{2^{35}-2^4}{31}$. Therefore,

$$\mu_a(4) < \mu^* = 4 \cdot \frac{2^{35} - 2^4}{31}$$

Take

$$n \ge N = 2^{2^{\mu^*/2}(4 + \log \mu^*)}$$

and induct. Suppose that, for m < n, all admissible series is a spectrum of a Hamiltonian cycle (I) and if m > 4 and $\sum_{i=1}^{k} a_i > 2^k$ for any k < m then the series $a \in \mathbb{D}_m$ is the spectrum of a Hamiltonian cycle of full rank (II). To perform the inductive step, we check that the hypotheses of Lemma 2 and 3 are met. The condition (i) of Lemma 3 is true by inductive hypothesis. It is easy that

$$a_s \le \frac{2^n}{n-s+1}.$$

Therefore, the inequality (ii) $a_s \leq 2^{n-s-1}$ holds for

$$s \le 2^{\mu^*/2} (4 + \log \mu^*) - 1.$$

If $\mu_a(4) \ge \mu^*$ then, as shown above, the condition (iii) holds. Take $\mu_a(4) < \mu^*$. We define the sequence of numbers s_i recurrently. Let $s_0 = 4$. If s_i is already selected then, for s_{i+1} , we select minimal k such that the condition (iii) of Lemma 3 fails; i.e.,

$$\sum_{i=s_i+1}^{s_{i+1}} a_i < 2^{s_{i+1}} - 2^{s_i}.$$

By Proposition 3, there are at most $M = \mu^*/2$ elements in the sequence $s_1 < s_2 < \cdots < s_M$ such that $\mu_a(s_i) > 0$. Moreover, by Proposition 3,

$$s_M \le 2^M (4 + \log \mu^*) - 1$$

If the next s_j cannot be selected then we use Lemma 3 to construct the desired Hamiltonian cycle; and if $\mu_a(s_j) = 0$ then we use Lemma 2. Thus, the inductive hypothesis (I) is proven. The hypothesis (II) follows from Remark 1.

Proposition 1 completes the proof of the theorem.

To obtain the complete solution for the problem of spectra of the Gray codes we need to provide the base of induction to apply the theorem. The Hamiltonian cycles of GQ_n for $n \leq N$ with arbitrary admissible spectra can be built using the above construction as well as other known constructions such as Bakos's construction [10].

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