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## A THEORY FOR VALIANT'S MATCHCIRCUITS (EXTENDED ABSTRACT)

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ABSTRACT. The computational function of a matchgate is represented by its character matrix. In this article, we show that all nonsingular character matrices are closed under matrix inverse operation, so that for every  $k$ , the nonsingular character matrices of  $k$ -bit matchgates form a group, extending the recent work of Cai and Choudhary [1] of the same result for the case of  $k = 2$ , and that the single and the two-bit matchgates are universal for matchcircuits, answering a question of Valiant [4].

### 1. Introduction

Valiant [4] introduced the notion of matchgate and matchcircuit as a new model of computation to simulate quantum circuits, and successfully realized a significant part of quantum circuits by using this new model. Valiant's new method organizes certain computations based on the graph theoretic notion of perfect matching and the corresponding algebraic object of the Pfaffian. This leaves an interesting open question of characterizing the exact power of the matchcircuits. To solve these problems, a significant first step would be a better understanding the structures of the matchgates and the matchcircuits, to which the present paper is devoted.

In [6], Valiant introduced the notion of *holographic algorithm*, based on matchgates and their properties, but with some additional ingredients of the choice of a set of linear basis vectors, through which the computation is expressed and interpreted.

Matchgates and their character matrices have some nice properties, which have already been extensively studied. In [1], Cai and Choudhary showed that a matrix is the character matrix of a matchgate if and only if it satisfies all the useful Grassmann-Plücker identities, and all nonsingular character matrices of two bits matchgates form a group.

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In the present paper, we show that for every  $k$ , all the nonsingular character matrices of  $k$ -bit matchgates form a group, extending the result of Cai and Choudhary of the same result for the case of  $k = 2$ .

Furthermore, we show that every matchcircuit based on  $k$ -bit matchgates for  $k > 2$  can be realized by a series of compositions of either single bit or two bits matchgates. This result answers a question raised by Valiant in [4]. The result is an analogy of the quantum circuits in the matchcircuits [3].

We organize the paper as follows. In section 2, we outline necessary definitions and background of the topic. In section 3, we state our results, and give some overview of the proofs. In section 4, we establish our first result that for every  $k$ , all nonsingular  $k$ -bit character matrices form a group. In section 5, we prove the second result that level 2 matchgates are universal for matchcircuits.

## 2. Definitions

### 2.1. Graphs and Pfaffian

Let  $G = (V, E, W)$  be a weighted undirected graph, where  $V = \{1, 2, \dots, n\}$  is the set of vertices each represented by a distinct positive integer,  $E$  is the set of edges and  $W$  is the set of weights of the edges. We represent the graph by a skew-symmetric matrix  $M$ , called the *skew-symmetric adjacency matrix* of  $G$ , where  $M(i, j) = w(i, j)$  if  $i < j$ ,  $M(i, j) = -w(i, j)$  if  $i > j$ , and  $M(i, i) = 0$ .

The *Pfaffian* of an  $n \times n$  skew-symmetric matrix  $M$  is defined to be 0 if  $n$  is odd, 1 if  $n$  is 0, and if  $n = 2k$  where  $k > 0$  then it is defined by

$$\text{Pf}(M) = \sum_{\pi} \epsilon_{\pi} w(i_1, i_2) w(i_3, i_4) \dots w(i_{2k-1}, i_{2k}),$$

where

- $\pi = [i_1, i_2, \dots, i_{2k}]$  is a permutation on  $[1, 2, \dots, n]$ ,
- the summation is over all permutations  $\pi$ , where  $i_1 < i_2, i_3 < i_4, \dots, i_{2k-1} < i_{2k}$  and  $i_1 < i_3 < \dots < i_{2k-1}$ ,
- $\epsilon_{\pi}$  is the sign of the permutation  $\pi$ , or equivalently,  $\epsilon_{\pi}$  is the sign or parity of the number of overlapping pairs, where a pair of edges  $(i_{2r-1}, i_{2r}), (i_{2s-1}, i_{2s})$  is *overlapping* iff  $i_{2r-1} < i_{2s-1} < i_{2r} < i_{2s}$  or  $i_{2s-1} < i_{2r-1} < i_{2s} < i_{2r}$ .

A *matching* is a subset of edges such that no two edges share a common vertex. A vertex is said to be *saturated* if there is a matching edge incident to it. A *perfect matching* is a matching which saturates all vertices. There is a one-to-one correspondence between the monomials in the Pfaffian and the perfect matchings in  $G$ .

If  $M$  is an  $n \times n$  matrix and  $A = \{i_1, \dots, i_r\} \subseteq \{1, \dots, n\}$ , then  $M[A]$  denotes the matrix obtained from  $M$  by deleting the rows and columns of indices in  $A$ . The *Pfaffian Sum* of  $M$  is a polynomial over indeterminates  $\lambda_1, \lambda_2, \dots, \lambda_n$  defined by

$$\text{PfS}(M) = \sum_A \left( \prod_{i \in A} \lambda_i \right) \text{Pf}(M[A])$$

where the summation is over the  $2^n$  subsets of  $\{1, \dots, n\}$ . There is a one-one correspondence between the terms of the Pfaffian sum and the matchings in  $G$ . We consider only instances such that each  $\lambda_i$  is fixed to be 0 or 1. In this case, Pfaffian Sum is a summation over all

matchings that match all nodes with  $\lambda_i = 0$ . It is well known that both the Pfaffian and the Pfaffian Sum are computable in polynomial time.

**2.2. Matchgate**

A *matchgate*  $\Gamma$ , is a quadruple  $(G, X, Y, T)$ , where  $G = (V, E, W)$  is a graph,  $X \subseteq V$  is a set of input nodes,  $Y \subseteq V$  is a set of output nodes, and  $T \subseteq V$  is a set of *omittable nodes* such that  $X, Y$  and  $T$  are pairwise disjoint. Usually the numbers of nodes in  $V$  are consecutive from 1 to  $n = |V|$  and  $X, Y$  have minimal and maximal numbers respectively. Whenever we refer to the Pfaffian Sum of a matchgate fragment, we assume that  $\lambda_i = 1$ , if  $i \in T$ , and 0 otherwise. Each node in  $X \cup Y$  is assumed to have exactly one incident *external edge*. For a node in  $X$ , the other end of the external edge is assumed to have index less than the index for any node in  $V$ , and for a node in  $Y$ , the other end node has index greater than that for every node in  $V$ . If  $k = |X| = |Y|$ , then  $\Gamma$  is called *k-bit matchgate*. A matchgate is called a *level k matchgate*, if it is an  $n$ -bit matchgate for some  $n \leq k$ . If a matchgate only contains input nodes, output nodes and one omittable node, then it is called a *standard matchgate*.

We define, for every  $Z \subseteq X \cup Y$ , the *character*  $\chi(\Gamma, Z)$  of  $\Gamma$  with respect to  $Z$  to be the value  $\mu(\Gamma, Z)\text{PfS}(G - Z)$ , where  $G - Z$  is the graph obtained from  $G$  by deleting the vertices in  $Z$  together with their incident edges, and the *modifier*  $\mu(\Gamma, Z) \in \{-1, 1\}$  counts the parity of the number of overlaps between matched edges in  $G - Z$  and matched external edges. We assume that all the nodes in  $Z$  are matched externally. By definition of the modifier, it is easy to verify that  $\mu(\Gamma, Z) = \mu(\Gamma, Z \cap X)\mu(\Gamma, Z \cap Y)$ , and that if  $X = \{1, 2, \dots, k\}$  and  $Z \cap X = \{i_1, i_2, \dots, i_l\}$ , then  $\mu(\Gamma, Z \cap X) = (-1)^{\sum_{j=1}^l (i_j - j)}$ .

The *character matrix*  $\chi(\Gamma)$  is defined to be the  $2^{|X|} \times 2^{|Y|}$  matrix such that entry  $(i_1 i_2 \dots i_k, i_n i_{n-1} \dots i_{n-k+1})$  is  $\chi(\Gamma, X' \cup Y')$ , where  $X' = \{j \in X | i_j = 1\}$ ,  $Y' = \{j \in Y | i_j = 1\}$  and  $i_1 i_2 \dots i_k, i_n i_{n-1} \dots i_{n-k+1}$  are binary expression of numbers between 0 and  $2^k - 1$ . We also use  $(X', Y')$  to denote this entry. We call an entry  $(X', Y')$  *edge entry*, if  $0 < |(X - X') \cup (Y - Y')| \leq 2$ . Throughout the paper, we identify a matchgate and its character matrix. An easy but useful fact is that for every  $k$ , the  $2^k \times 2^k$  unit matrix is a character matrix.

**2.3. Properties of character matrix**

We introduce several properties of character matrices, which will be used in the proof of our results.

**Theorem 2.1** ([4]). *If  $A$  and  $B$  are character matrices of size  $2^k \times 2^k$ , then  $AB$  is a character matrix.*

**Theorem 2.2** ([4]). *Given any matchgate  $\Gamma$  there exists another matchgate  $\Gamma'$  that has the same character as  $\Gamma$  and has an even number of nodes, exactly one of which is omittable.*

**Theorem 2.3** ([1]). *Let  $A$  be a  $2^k \times 2^l$  matrix. Then  $A$  is the character matrix of a  $k$ -input,  $l$ -output matchgate, if and only if  $A$  satisfies all the useful Grassmann-Plücker identities.*

This is a very useful characterization of the character matrices generalizing the characterization for a major part of all 2-input 2-output matchgates in [4]. The proof of this theorem implies the following:

**Corollary 2.4** ([1]). *Let  $A$  be a  $2^k \times 2^l$  matrix whose right-bottom most entry is 1 satisfying all the useful Grassmann-Plücker identities. Then  $A$  is uniquely determined by its edge entries and  $A$  is the character matrix of a standard matchgate  $\Gamma$  containing  $k + l + 1$  nodes ( $k$  input nodes,  $l$  output nodes and 1 omissible node).*

Recently, Cai and Choudhary also showed that:

**Theorem 2.5** ([1]). *Let  $A$  be a  $4 \times 4$  character matrix. If  $A$  is invertible, then  $A^{-1}$  is a character matrix. Consequently, the nonsingular  $4 \times 4$  character matrices form a group.*

**2.4. Matchcircuit**

Given a matchgate  $\Gamma = (G, X, Y, T)$ , we say that it is *even*, if  $\text{PfS}(G - Z)$  is zero whenever  $Z = X \cup Y$  has odd size, and *odd* if  $\text{PfS}(G - Z)$  is zero whenever  $|Z|$  is even.

**Theorem 2.6** ([4],[1]). *Consider a matchcircuit  $\Gamma$  composed of gates as in [4]. Suppose that every gate is:*

- (1) *a gate with diagonal character matrix,*
- (2) *an even gate applied to consecutive bits  $x_i, x_{i+1}, \dots, x_{i+j}$  for some  $j$ ,*
- (3) *an odd gate applied to consecutive bits  $x_i, x_{i+1}, \dots, x_{i+j}$  for some  $j$ , or*
- (4) *an arbitrary gate on bits  $x_1, \dots, x_j$  for some  $j$ .*

*Suppose also that every parallel edge above any odd matchgate, if any, has weight  $-1$  and all other parallel edges have weight 1. Then the character matrix of  $\Gamma$  is the product of the character matrices of the constituent matchgates, each extended to as many inputs as those of  $\Gamma$ .*

From now on, whenever we say a matchcircuit, we mean that it satisfying the requirements in the above theorem. An example circuit is shown in Fig. 1, where the edges in a matchgate are not drawn, and each node has index smaller than that of all nodes located to the right of the node. We call a matchcircuit is of *level  $k$* , if it is composed of matchgates no more than  $k$  bits.

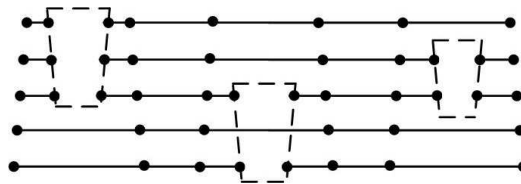


Figure 1: An example of matchcircuit.

The *character matrix of a matchcircuit* is defined by the same way as that of a matchgate except that there is no modifier  $\mu$ .

### 3. The results and overview of the proofs

**Theorem 3.1.** *For every  $k$ , the nonsingular  $2^k \times 2^k$  character matrices form a group under the matrix multiplication.*

We will prove theorem 3.1 by induction on the size of matchgates. The proof proceeds as follows. Based on corollary 2.4, we observe that all  $2^k \times 2^k$  character matrices can be transformed to a special form  $2^k \times 2^k$  character matrices. This suggests the following:

**Definition 3.2.** We say that a  $k$ -bit matchgate is a *reducible matchgate*, if the bottom pair of nodes  $k$  and  $n - k + 1$  are connected by a weight 1 edge, and there is no other edge incident to any of the nodes  $k$  and  $n - k + 1$ .

The character matrix of a reducible matchgate is called a *reducible character matrix*.

By corollary 2.4, a character matrix  $B$  is a reducible character matrix if it satisfies the following:

- (1)  $B_{2^k-1, 2^k-1} = B_{2^k-2, 2^k-2} = 1$ .
- (2) All the edge entries in the last two columns and the last two rows are 0 except for  $B_{2^k-2, 2^k-2}$ .

Firstly we prove that if the  $k$ -bit nonsingular character matrices are closed under matrix inverse operation, then so are the  $(k + 1)$ -bit nonsingular reducible character matrices .

Secondly, we introduce some elementary nonsingular matchgates so that every nonsingular  $2^k \times 2^k$  character matrix can be transformed to a reducible character matrix by multiplying with the character matrices of the elementary matchgates.

This transformation is realized by four phases as follows. Starting from  $A = A^{(0)}$ , we need the following:

**Phase T1** ( $A^{(0)} \Rightarrow A^{(1)}$ ). Turn the right-bottom most entry to 1.

**Phase T2** ( $A^{(1)} \Rightarrow A^{(2)}$ ). Turn the edge entries in the last row and column to 0's, while keeping the right-bottom most entry 1.

**Phase T3** ( $A^{(2)} \Rightarrow A^{(3)}$ ). Turn the entry  $A_{2^k-2, 2^k-2}^{(2)}$  to 1, while keeping the right-bottom most entry 1 and the edge entries in the last row and column 0's.

**Phase T4** ( $A^{(3)} \Rightarrow A^{(4)}$ ). Turn the edge entries in the row  $2^k - 2$  and column  $2^k - 2$  to 0's, while keeping the last two diagonal entries 1's and the edge entries in the last row and column 0's.

Each phase consists of several *actions* (or for simplicity, steps). In each step, either the positions of entries are changed, or the values of some entries are changed.

An action is defined to be the multiplication of a character matrix with an elementary character matrix. The role of an action is to change some specific entries to be some fixed value 0 or 1. However, such an action will certainly injure other entries which are undesired.

The crucial observation is that an appreciate sequence of actions will gradually satisfy all the entries requirements. During the course of the transformation, once an entry requirement is satisfied by some action, it will never be injured again by the future actions. That is to say, an action may injure only the entries which have not been satisfied. This ensures that all the entries requirements will be eventually satisfied.

This describes the idea of the proof of theorem 3.1. The proof will also build an essential ingredient for our second result, the theorem below.

**Theorem 3.3.** *For every  $k > 2$ , if  $\Gamma$  is a matchcircuit composed of level  $k$  matchgates, then:*

- (1)  $\Gamma$  can be simulated by a level 2 matchcircuit  $\Delta$ .
- (2) A  $k$ -bit matchgate can be simulated by  $O(k^4)$  many single and two-bit matchgates. And every matchcircuit  $\Gamma$  can be simulated by a level 2 matchcircuit in polynomial time.

Our proof of theorem 3.3 is a composition of the proof of theorem 3.1 and some more elementary matchgates. On the other hand, one could firstly prove theorem 3.3, then prove 3.1 by combining theorem 3.3 and theorem 2.5. However there are subtle difference between character matrices of matchgate and matchcircuit. Therefore, this approach needs additional technique.

### 4. Group property of the $k$ -bit character matrices

In this section, we prove theorem 3.1. To proceed an inductive argument, we exploit the structure of the reducible character matrices which pave the way to the reductions.

#### 4.1. Reducible matchgates

**Lemma 4.1.** *Let  $\Delta_1$  be a  $(k+1)$ -bit reducible matchgate, that is, the bottom edge  $(k+1, k+3)$  having weight 1 and there is no any other edge incident to any of the nodes  $k+1$  and  $k+3$ . Let  $\Gamma_1$  be the  $k$ -bit matchgate obtained from  $\Delta_1$  by deleting the edge  $(k+1, k+3)$ . Then:*

- (i) *If  $\Delta_1$  is invertible, so is  $\Gamma_1$ .*
- (ii) *If  $\chi(\Gamma_1)^{-1}$  is a character matrix, so is  $\chi(\Delta_1)^{-1}$ .*

*Proof.* (Sketch) For (i). This holds because  $\chi(\Delta_1)$  is a block diagonal matrix after rearranging the order of rows and columns, and  $\chi(\Gamma_1)$  is equal to one block.

For (ii). We prove this by constructing the inverted matchgate  $\Delta_2(F_2, W_2, Z_2, T_2)$  of  $\Delta_1(F_1, W_1, Z_1, T_1)$  from the inverted gate  $\Gamma_2(G_2, X_2, Y_2, T_2)$  of  $\Gamma_1(G_1, X_1, Y_1, T_1)$ .

It suffices to prove that the composition of  $\Delta_1$  and  $\Delta_2$  has the unit matrix as its character matrix. See Fig. 2 for the intuition of the proof, while detailed verification will be given in the full version of the paper.

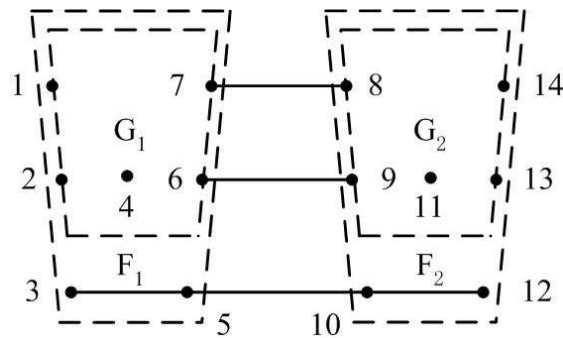


Figure 2: Example of  $k = 2$ .  $X_1 = \{1, 2\}$ ,  $Y_1 = \{6, 7\}$ ,  $T_1 = \{4\}$   $X_2 = \{8, 9\}$ ,  $Y_2 = \{13, 14\}$ ,  $T_2 = \{11\}$ ,  $W_1 = \{1, 2, 3\}$ ,  $Z_1 = \{5, 6, 7\}$ ,  $W_2 = \{7, 8, 9\}$ ,  $Z_2 = \{12, 13, 14\}$ .

■

**4.2. The transformation lemma**

In this part, we construct the matchgates to realize the phases T1 – T4 prescribed in section 3, and show that every  $k$ -bit nonsingular character matrix can be transformed to a  $k$ -bit reducible character matrix by using the transformation.

The key point to the proof of the theorem is the following:

**Lemma 4.2.** *Let  $A$  be a  $2^k \times 2^k$  nonsingular character matrix. Then there exist nonsingular character matrices  $L_s, \dots, L_2, L_1, R_1, R_2, \dots, R_t$  for some  $s$  and  $t$  such that  $L_s \cdots L_2 L_1 A R_1 R_2 \cdots R_t$  is a reducible character matrix.*

*Proof.* Given a nonsingular character matrix  $A$ , we denote  $A$  by  $A^{(0)}$ . We construct the matchgates to realize the four phases T1 – T4. We use  $A^{(i)}$  to denote the character matrix obtained from  $A^{(i-1)}$  by using phase Ti, where  $i = 1, 2, 3, 4$ . We start with  $A^{(0)}$ , and define the transformation to be a series of actions, defined in section 3. In the discussion below, we will use  $A$  to denote the character matrix obtained so far in the construction from  $A^{(0)}$  (or shortly, the current matrix).

The four phases proceed as follows.

**Phase T1:** Suppose that  $\Gamma_l$  is the  $k$ -bit matchgate such that the  $l$ -th pair of input-output nodes are connected by a path of length 2 on which each edge has weight 1, and each of the other pairs is connected by an edge of weight 1, and  $k+1$  is the only unomittable node other than the input and output nodes. (See Fig. 3 (a)). Let  $C_l$  denote the character matrix of  $\Gamma_l$ .

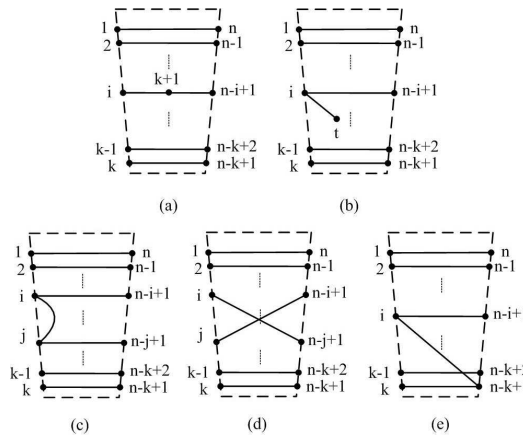


Figure 3:

Suppose without loss of the generality that  $A_{I=i_1 i_2 \dots i_k, J=j_1 j_2 \dots j_k} \neq 0$ . Define

$$L_1 = \prod_{1 \leq l \leq k, i_l=0} C_l, \quad R_1 = \prod_{1 \leq l \leq k, j_l=0} C_l.$$

It is easy to see that the right-bottom most entry,  $a$  say, of  $L_1 A R_1$  is either  $A_{I,J}$  or  $-A_{I,J}$  by computing the  $\text{Pfs}(G - X \cup Y)$  of the composed matchgate corresponding to  $L_1 A R_1$ . Let  $L_2 = \frac{1}{a} E$ , and  $A^{(1)} = L_2 L_1 A R_1$ . Clearly  $L_2$  is a character matrix, so is  $A^{(1)}$ , by theorem 2.1.



**Phase T2:** Phase T2 will change the edge entries in the last column and the last row to 0's. We first describe the actions for the column as follows.

**Phase T2 for the last column:**

We turn the edge entries in the last column to 0's one by one from bottom to top. To turn an edge entry  $(X', 2^k - 1)$  to zero, we need a row transformation applied to the current matrix  $A$ , which adds the multiplication of  $-b$  and the last row to row  $X'$ , where  $b$  is the value of entry  $(X', 2^k - 1)$  of the current matrix.

Therefore phase T2 for the last column consists of the following actions. In decreasing order of  $X'$ , for every edge entry  $(X', 2^k - 1)$ , we have:

**Action**  $(X', 2^k - 1)$ : Multiplying an elementary character matrix,  $L$  say, to the current character matrix  $A$  from the left side, where  $L$  is a character matrix satisfying that the diagonal entries are all 1's, and that  $L_{I=X', 2^k - 1} = -b$ .

This makes some row transformations to the current matrix according to the nonzero entries other than the diagonal entries. The row transformation corresponding to  $L_{I=X', 2^k - 1} = -b$  is exactly the one that realizes the goal of this action.

Now we formally construct the matchgate to realize the character matrix  $L$  as required in the action  $(X', 2^k - 1)$  above. The construction is divided into two cases depending on the size of  $X'$  as follows.

**Case 1.**  $X' = X - \{i\}$  for some  $i$ .

We use the matchgate with the following properties: (1) each input-output pair of the gate is connected by an edge of weight 1, and (2) it contains one more edge  $(i, t)$  to realize  $L$ , where  $t$  is the unique omissible node, and the weight of  $(i, t)$  is either  $b$  or  $-b$  ensuring  $L_{I, 2^k - 1} = -b$ . For intuition of the matchgate, a reader is referred to Fig. 3 (b).

Let  $(I', J')$  be an arbitrary nonzero entry of  $L$  other than the diagonal entries. By the construction of the gate, we have that the  $i$ -th bit of  $I'$  and  $J'$  are 0 and 1 respectively, and that  $I'$ , and  $J'$  are identical on the  $j$ -th bit for every  $j \neq i$ . Hence  $I' < J'$  and  $I' \leq I$  (recall that  $I = X'$ ). The action at entry  $(X', 2^k - 1)$  in this case actually makes the following row transformation: For each such pair  $(I', J')$ , row  $I'$  is added by the multiplication of  $L_{I', J'}$  and row  $J'$ . Since  $I' \leq I$ , all the edge entries  $(I_1, 2^k - 1)$  with  $I_1 > I$  have never been injured by the action in this case.

**Case 2**  $X' = X - \{i, j\}$  for some  $i, j$ .

The character matrix  $L$  in this case is constructed by a similar way to that in case 1 above, using the matchgate in Fig. 3 (c).

The cost of the action in this case is similarly analyzed to that for case 1.

Recall that after phase T1, the right-bottom most entry is 1. The actions in both case 1 and case 2 of phase T2 above will never injure the last row of the matrix, so that the satisfaction of T1 is still preserved by the current state of the construction.

**Phase T2 for the last row:** The construction, and analysis for the actions is the same as that for the column case with the roles of rows and columns exchanged.

Therefore, the goal of T2 prescribed in section 3 has been realized.

**Phase T3:** The goal of this phase is similar to that of phase T1, but different actions are needed. T3 consists of 2 actions. The first action moves a nonzero edge entry to position  $(2^k - 1, 2^k - 1)$ , and the second one changes edge entry  $(2^k - 1, 2^k - 1)$  to 1. The actions proceed as follows.

**Action 1:** First, we choose a nonzero edge entry. Since  $A^{(2)}$  is nonsingular, there must be a nonzero edge entry  $A_{X'=X-\{i\},Y'=Y-\{j\}}^{(2)}$  for some  $i$  and  $j$ . (Otherwise, all edge entries are zero's so that  $A^{(2)}$  is a zero matrix, contradicting the non-singularity of  $A^{(0)}$ .)

We use a gate of type  $\Gamma_d$ , defined as follows: (i) connect each input-output pair other than the  $i$ -th or the  $j$ -th pair by an edge, (ii) the  $i$ -th input is connected to the  $j$ -th output, and (iii) the  $j$ -th input is connected to the  $i$ -th output. All edges are of weight 1. (See Fig. 3 (d)) Let  $C_{i,j}$  denote the character matrix of the matchgate described above.

This action just turns  $A^{(2)}$  to  $C_{i,k}A^{(2)}C_{j,k}$  by connecting the matchgate of  $C_{i,k}$  with the gate of  $A^{(2)}$ , and the gate of  $C_{i,k}$  in the order of left to right.

Firstly, we verify that action 1 realizes its goal. Generally, multiplying  $C_{a,b}$  from left (resp. right) side is equivalent to exchanging pairs of rows (resp. columns)  $i_1i_2 \dots i_a \dots i_b \dots i_k$  and  $i_1i_2 \dots i_b \dots i_a \dots i_k$ , modular a factor of 1 or  $-1$ . Hence, the edge entry  $(2^k - 2, 2^k - 2)$  of  $C_{i,k}A^{(2)}C_{j,k}$  is either  $A_{X',Y'}^{(2)}$  or  $-A_{X',Y'}^{(2)}$ .

Secondly, we analyze the cost of the action. Notice that the row exchanges are determined by a bit exchange on the labels of rows, so that the number of zeros in (the string of) the row label is kept unchanged. By definition, an edge entry can be exchanged only with another edge entry. Therefore all edge entries in the last row and column are kept zeros. In addition, it is easy to see that the left-bottom most entry is kept 1.

**Action 2:** We construct a matchgate with all of the input-output pairs connected by an edge of weight 1, except that the last pair is connected by an edge of weight  $w = \frac{1}{A_{2^k-2, 2^k-2}}$ .

All entries of the character matrix of this matchgate are zeros, except for the diagonal entries. A diagonal entry  $(I, I)$  is  $w$ , if the last bit of  $I$  is 0, and 1, otherwise.

We multiply this character matrix with the current matrix, then a straightforward calculation shows that entry  $(2^k - 1, 2^k - 1)$  is turned to 1, while all the satisfied entries achieved previously are still preserved.

The goal of T3 is realized.

**Phase T4:** This phase is similar to phase T2, except that we need consider the consequence on the last column and row. We start from changing the edge entries in column  $2^k - 2$ .

**Phase T4 for column  $2^k - 2$ :** Suppose we are going to change edge entry  $(X - \{i\}, Y - \{n - k + 1\})$  to zero by the order from bottom to top. Denote the action realizing this goal by *action at  $(X - \{i\}, Y - \{n - k + 1\})$* .

We construct the elementary matchgate used in the action at  $(X - \{i\}, Y - \{n - k + 1\})$ . Each pair of input-output nodes of this matchgate is connected by an edge of weight 1, furthermore, the  $i$ -th input node is connected to the last output node by an edge of weight  $w$ , where  $w$  is either  $A_{X-\{i\},Y-\{n-k+1\}}$  or  $-A_{X-\{i\},Y-\{n-k+1\}}$  such that entry  $(X - \{i\}, Y - \{n - k + 1\})$  of the character matrix of the matchgate is  $-A_{X-\{i\},Y-\{n-k+1\}}$ . (See Fig. 3 (e).)

We examine the nonzero entries in the character matrix  $L$  of the constructed matchgate. We first note that all diagonal entries are 1's. Let  $(I', J')$  denote an arbitrary nonzero entry other than the diagonal entries of the matrix  $L$ . By construction of the matchgate,  $I'$  and  $J'$  differ at only the  $i$ -th and the  $k$ -th bits, and  $I'|_i = J'|_k = 0$ ,  $I'|_k = J'|_i = 1$ ,  $I' < J'$ ,  $I' < X - \{i\}$  and  $I', J'$  contain the same number of 0's, which is at least 1, where  $I'|_i$  denotes the  $i$ -th bit of  $I'$ . The action at  $(X - \{i\}, Y - \{n - k + 1\})$  multiplies  $L$  with  $A$  from the left side. It makes some row transformations: for every such entry  $(I', J')$  chosen as above, add row  $I'$  by the multiplication of row  $J'$  by  $L_{I',J'}$ . So the goal of this action is realized.

Now we analyze the cost of the action. We first prove that it does not injure the edge entries in column  $2^k - 2$  which have already been satisfied. The reason is similar to that in phase T2. Because  $I' \leq X - \{i\}$ , the action only injures the rows with indices less than  $X - \{i\}$ .

The cost of the action is different from that in phase T2 in that it may affect the edge entries in the last column which have already been satisfied in phases T1 and T2. Because  $I'$  and  $J'$  contain the same number of 0's, which is at least 1, all the row changes made by the action always add a zero edge entry of the last column to another zero edge entry in the same column. Hence, it does not injure the satisfied entries in the last column. Additionally, it is obvious that the last two rows are preserved during the current action, so the left-bottom most entry, the edge entries in the last row and entry  $(2^k - 2, 2^k - 2)$  are all preserved.

**Phase T4 for row  $2^k - 2$ :** Similar actions to that in phase T4 for the column above can be applied to the row  $2^k - 2$  to change its edge entries to 0's.

Therefore, T4 realizes its goal, at the same time, it preserves the satisfied entries in phases T1 – T3.

We have realized the phases T1 – T4 prescribed in section 3, by corollary 2.4,  $B$  is a reducible character matrix. The lemma follows. ■

### 4.3. Proof of theorem 3.1

*Proof.* We prove by induction on  $k$  that for every  $k$ , and every  $2^k \times 2^k$  character matrix  $A$ , if  $A$  is invertible, then  $A^{-1}$  is a character matrix.

The case for  $k = 1$  is easy, the first proof was given by Valiant in [4].

Suppose by induction that the theorem holds for  $k - 1$ . By lemma 4.2, there exist nonsingular character matrices  $L_i$  and  $R_j$  such that  $B = L_s \cdots L_2 L_1 A R_1 R_2 \cdots R_t$  is the character matrix of a reducible matchgate  $\Delta$ . Let  $B'$  be the  $2^{k-1} \times 2^{k-1}$  character matrix of  $\Gamma$  constructed from  $\Delta$  by deleting the bottom edge.

Since  $A$  is invertible, so is  $B$ , and so is  $B'$  by lemma 4.1. By the inductive hypothesis,  $B'^{-1}$  is a character matrix, so is  $B^{-1}$  by lemma 4.1.

By the choice of  $L_i$  and  $R_j$ , for all  $1 \leq i \leq s$  and  $1 \leq j \leq t$ , we have that

$$A^{-1} = R_1 R_2 \cdots R_t B^{-1} L_s \cdots L_2 L_1.$$

By theorem 2.1,  $A^{-1}$  is also a character matrix.

This completes the proof of theorem 3.1. ■

We notice that the inductive argument in the proof of theorem 3.1 also gives a different proof for the result in the case of  $k = 2$ . Our method is a constructive, and uniform one. It may have some more applications.

## 5. Level 2 matchgates are universal

We introduce nine types of matchgates as our elementary gates. We use  $\Gamma_a, \dots, \Gamma_i$ , to denote the elementary level 2 matchgates corresponding to that in the following Fig. 4 (a), (b), (c), (d), (e), (f), (g), (h) and (i) respectively.

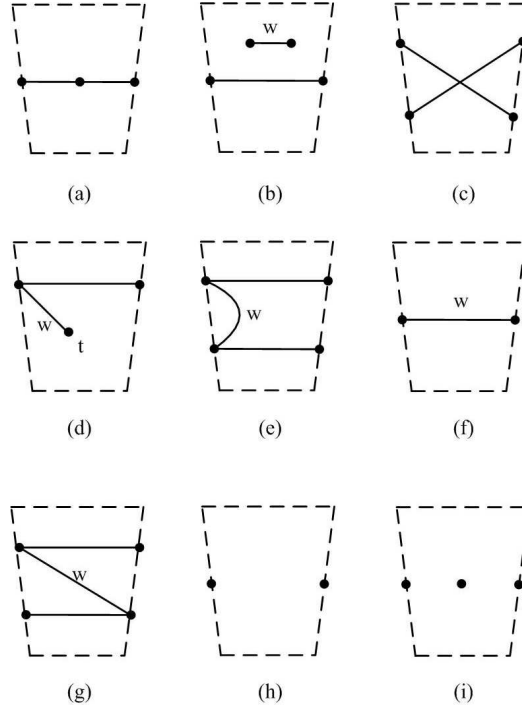


Figure 4:

We describe the elementary gates as follows. All edges in  $\Gamma_a$  have weight 1. All edges connecting an input and an output node except for the edge in  $\Gamma_f$ , and the diagonal edge in  $\Gamma_g$ , are all of weight 1. The remaining edges take weights  $w$ .

$\Gamma_a$  makes a row (or column, when it is multiplied from right side) exchange, which is a special transformation, of the character matrix according to a bit flip on the label, and it is used to move a nonzero entry to the right-bottom most entry by the same way as that in the proof of theorem 2.3 in [1].  $\Gamma_b$  is used to realize  $cE$ , and to turn a nonzero entry to 1. Both  $\Gamma_a$  and  $\Gamma_b$  are only used in the first phase, i.e. T1, of the transformation. Intuitively,  $\Gamma_c$  can exchange two consecutive bits, and it allows us to apply some other elementary gates to nonconsecutive bits.  $\Gamma_d$  and  $\Gamma_e$  are used in phase T2 to eliminate the edge entries in the last column and the last row.  $\Gamma_c$  will be also used in phase T3 to move a nonzero edge entry to position  $(2^k - 2, 2^k - 2)$ , in which case,  $\Gamma_f$  will further turn this entry to 1.  $\Gamma_g$  is used in phase T4 to eliminate the edge entries in the column  $2^k - 2$  and row  $2^k - 2$ . A nonzero singular character matrix will be transformed to a matchcircuit composed of only  $\Gamma_h$ -type gates.  $\Gamma_i$  is used to realize zero matrix. To understand the composition of  $\Gamma_c$  with other elementary gates, we need the following:

**Lemma 5.1.** *Suppose  $A$  is the character matrix of a  $k$ -bit matchcircuit  $\Delta$ , and  $P_1, P_2$  are two arbitrary permutations on  $k$  elements. There exists matchcircuit  $\Lambda$  constructed from  $\Delta$  by adding some gates  $\Gamma_c$ , such that the corresponding character matrices  $B$  satisfying  $B_{2^k-1, 2^k-1} = A_{2^k-1, 2^k-1}$  and  $|B_{i_1 \dots i_k, j_1 \dots j_k}| = |A_{P_1(i_1 \dots i_k), P_2(j_1 \dots j_k)}|$ .*

The following lemma gives the transformation for matchcircuits.

**Lemma 5.2.** *For any  $k > 2$ , and any  $k$ -bit matchcircuit  $\Delta$  consisting of a single nonsingular  $k$ -bit matchgate  $\Gamma$ , there is a new matchcircuit  $\Lambda$  constructed by adding some invertible single and two-bit matchgates to  $\Delta$ , such that the character matrix  $B$  of  $\Lambda$  is reducible. Furthermore,  $B$  is the character matrix of an even reducible matchgate.*

So far we have established the result for the first significant case that a matchgate is applied to the first  $k$  bits.

In the following lemma we consider two more cases:

- a gate applied to consecutive bits but not starting from the first bit,
- a gate applied to nonconsecutive bits.

For the first case, the gate must be an even or an odd gate, we observe that only even and odd gates are used in the transformation for an even or an odd gate. For the second case, we extend its matrix, and replace it by a new even gate which is applied to consecutive bits reducing it to the first case.

**Lemma 5.3.** *For any  $k > 2$ , and any  $m$ -bit matchcircuit  $\Delta$  containing a  $k$ -bit matchgate  $\Gamma$  with character matrix  $A$ , there is a level  $k - 1$  matchcircuit  $\Lambda$  having the same character matrix as  $\Delta$ .*

The proof for lemma 5.1-5.3 will be given in the full version.

### 5.1. Proof of theorem 3.3

*Proof.* For (1). Repeat the process in lemma 5.3 until there is no gate of bit greater than 2.

For (2). The number of matchgates used in the phases of transformation are  $O(k)$ ,  $O(k^3)$ ,  $O(k)$  and  $O(k^2)$ , respectively, so a  $k$ -bit matchgate can be simulated by  $O(k^4)$  many single and two-bit matchgates. This procedure is polynomial time computable, because there are polynomially many actions, and each action is polynomial time computable due to the fact that we compute only the edge entries. ■

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