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Abstract

The maximum C_k-free 2-matching problem is a problem of finding a maximum simple 2-matching which does not contain cycles of length k or less in undirected graphs. The complexity of the problem varies due to k and the input graph. The case where $k = 4$ and the graph is bipartite, which is called the maximum square-free 2-matching problem in bipartite graphs, is well-solved. Previous results on this setting include min-max theorems, polynomial combinatorial algorithms, linear programming formulation with dual integrality for the weighted version, and discrete convex structure.

In this paper, we further investigate the structure of square-free 2-matchings in bipartite graphs and present new decomposition theorems. These theorems serve as an analogue of the Dulmage-Mendelsohn decomposition for matchings in bipartite graphs and the Edmonds-Gallai decomposition for matchings in nonbipartite graphs. We exhibit two canonical minimizers for the set function in the min-max formula, and a characterization of the maximum square-free 2-matchings with the aid of these canonical minimizers.

1 Introduction

For a simple undirected graph $G = (V, E)$ and a positive integer k, a subset M of E is called a *C_k-free 2-matching* if each vertex has at most two incident edges in M and M does not contain a cycle of length k or less. The *maximum C_k-free 2-matching problem* is a problem of finding a C_k-free 2-matching of maximum size for given G and k. If a C_k-free 2-matching has size $|V|$, which shall be maximum, then it is called a *C_k-free 2-factor*.

An important motivation of investigating the maximum C_k-free 2-matching problem is that it is a relaxation of the Hamilton cycle problem. Indeed, for the case $k \geq |V|/2$, a C_k-free 2-factor is exactly a Hamilton cycle. Applications of C_k-free 2-matchings also include NP-hard problems related to the Hamilton cycle problem, such as the graphic traveling salesman problem and the minimum 2-edge connected spanning subgraph problem. For these two problems, if a C_k-free 2-factor is found, then $(1 + 2/k)$-approximation immediately follows. For a more elaborated use of C_k-free 2-factors, see [5, 6, 8].

The complexity of the maximum C_k-free 2-matching problem varies due to k. As stated above, the case $k \geq |V|/2$ contains the Hamilton cycle problem and hence is NP-hard, while the case $k \leq 2$ is exactly the classical maximum simple 2-matching problem and hence is polynomially solvable.

Moreover, Papadimitriou proved NP-hardness for the case $k \geq 5$ (see [7]), whereas Hartvigsen [17] proposed a combinatorial algorithm for the case $k = 3$. The case $k = 4$ is left open.

The weighted version of the maximum C_k-free 2-matching problem is also of interest. The NP-hardness of the case $k \geq 5$ follows from that of the unweighted version, while the case $k = 2$ is the classical maximum-weight simple 2-matching problem and hence polynomially solvable. A nontrivial result is due to Vornberger [38], who proved the NP-hardness of the case $k = 4$. The maximum-weight C_3-free 2-matching problem is still open.

In bipartite graphs, C_4-free 2-matchings are often referred to as *square-free 2-matchings*, and in the present paper we mainly use this terminology. About 15 years after the above basic results, Hartvigsen [18] proposed a Tutte-type theorem characterizing bipartite graphs admitting a square-free 2-factor and a combinatorial algorithm. Király [24] gave a precise description and proof of the Tutte-type theorem and extended it to a min-max formula. Since then, the maximum C_k-free 2-matching problem for the case $k = 3, 4$ has been studied actively. Frank [13] introduced the $K_{t,t}$-free t-matching problem in bipartite graphs, which is a generalization of the square-free 2-matching problem in bipartite graphs, and presented a min-max formula. After that, a full version [19] of [18] followed, and Pap [34] also gave a combinatorial algorithm for the maximum square-free 2-matching problem in bipartite graphs, which slightly differs from Hartvigsen's algorithm and is extended to the maximum $K_{t,t}$-free t-matching problem in bipartite graphs (see also [33]). We remark here that the min-max formula in [13, 34] differs from the formula in [19, 24]. We will give a detailed comparison of these two min-max formulas in Section 3.

For the weighted version of the maximum C_k-free 2-matching problem in bipartite graphs, NP-hardness is proved for the case $k \geq 6$ by Geelen [16] and for the case $k = 4$ by Király (see [13]). On the other hand, for the case $k = 4$ and the edge weight satisfies a property that the weight is vertex-induced on every square, Makai [30] presented a linear programming formulation with dual integrality. This formulation implies polynomial solvability via the ellipsoid method, and a combinatorial algorithm for this case was given by Takazawa [36].

Discrete convex structure of the C_k-free 2-matchings was first studied by Cunningham [9], who proved that the set of the degree sequences of the C_k-free 2-matchings is a *jump system* [4] for the case $k \leq 3$, and is not necessarily a jump system for the case $k \geq 5$. We remark that this result is consistent with the polynomial solvability of the maximum C_k-free 2-matching problem. For the case $k = 4$, Cunningham conjectured that the degree sequences of the C_4-free 2-matchings form a jump system, and later this was proved by Kobayashi, Szabó and Takazawa [27]. In [27], it is also proved that the weighted square-free 2-matchings in bipartite graphs induce an *M-concave function on a constant-parity jump system* [31] if and only if the edge weight is vertex-induced on every square, which is also consistent with polynomial solvability.

Through these results, one could assert that the maximum square-free 2-matching problem in bipartite graphs is indeed a well-solved case of the maximum C_k-free 2-matching problem. Apart from bipartite graphs, in subcubic graphs C_3- or C_4-free 2-matchings become tractable as well. See [1, 2, 20, 21, 25, 26, 28, 38] for progress in subcubic graphs.

The purpose of the present paper is to deepen the theory of C_k-free 2-matchings by investigating the structure of the square-free 2-matchings in bipartite graphs. First we exhibit that the two min-max formulas in [19, 24] and [13, 34] are essentially different in a sense that a vertex set minimizing the set function in one formula is not necessarily a minimizer in the other. We then establish decomposition theorems for square-free 2-matchings in bipartite graphs, which serve as an analogue for the Dulmage-Mendelsohn decomposition for matchings in bipartite graphs [10, 11] and the Edmonds-Gallai decomposition for matchings in nonbipartite graphs [12, 14, 15]. Here we focus on the min-max formula in [19, 24], and we prove that two minimizers found by the

algorithm in [19] are canonical in some sense. With these two minimizers, we can characterize the structure of the maximum square-free 2-matchings. We can know, e.g., which vertices have degree two for every maximum square-free 2-matching, and which edges belong in some maximum square-free 2-matching. These theorems suggest that the maximum square-free 2-matching problem has similarity to the maximum matching problem in both bipartite and nonbipartite graphs.

The rest of the paper is organized as follows. In Section 2, we review basic theorems for matchings in bipartite and nonbipartite graphs, such as the min-max theorems and the Dulmage-Mendelsohn and Edmonds-Gallai decompositions. In Section 3, we compare two min-max formulas for the maximum square-free 2-matching problem in bipartite graphs, and review Hartvigsen's algorithm [19]. Our decomposition theorems for square-free 2-matchings in bipartite graphs appear in Section 4.

2 Min-max and decomposition theorems for matchings

In this section, we review the basic results of matchings in bipartite graphs and nonbipartite matchings such as the min-max formulas, the Dulmage-Mendelsohn decomposition, and the Edmonds-Gallai decomposition. For more detailed discussion, the readers are referred to [22, 29, 32, 35].

Let $G = (V, E)$ be a simple undirected graph with vertex set V and edge set E. For $X \subseteq V$, the complement of X is denoted by $\bar{X}$, i.e., $\bar{X} = V \setminus X$. For $X \subseteq V$ and $F \subseteq E$, let $F[X]$ denote the set of edges in F spanned by X. A graph $G' = (V', E')$ is a *subgraph* of G if $V' \subseteq V$ and $E' \subseteq E$. For a subgraph H of G, the vertex and edge sets of H are denoted by $V(H)$ and $E(H)$, respectively. For $X \subseteq V$, let $G[X] = (X, E[X])$, the subgraph induced by X. For $F \subseteq E$ and two disjoint vertex subsets $X, Y \subseteq V$, let $F[X, Y]$ denote the set of all edges in F connecting X and Y. Let $G[X, Y] = (X \cup Y, E[X, Y])$. If G is bipartite, we often denote $G = (V^+, V^-; E)$, where $\{V^+, V^-\}$ is a partition of V and every edge in E connects V^+ and V^-. For $X \subseteq V$, let $X^+ = X \cap V^+$ and $X^- = X \cap V^-$.

For $F \subseteq E$ and a vertex $v \in V$, the *degree* of F on v is defined as the number of edges in F incident to v and denoted by $\deg_F(v)$. A subset M of edges is called a *matching* if $\deg_M(v) \leq 1$ for each $v \in V$. For an integer vector $b \in \mathbf{Z}^V_{\geq 0}$, an edge subset $M \subseteq E$ satisfying $\deg_M(v) \leq b_v$ for each $v \in V$ is called a *b-matching*. In particular, if $\deg_M(v) \leq b_v$ for each $v \in V$, then M is called a *b-factor*. If $b_v = k$ for every $v \in V$ for an integer k, a b-matching is called a *k-matching*. For $X \subseteq V$, let $b(X) = \sum_{v \in X} b_v$.

We remark that in the literature a b-matching with the above definition is often called a simple b-matching, and in a b-matching multiplicities on edges are allowed . In the present paper, since we only discuss subsets of edges and never put multiplicities on edges, we omit the term "simple".

We begin with the classical min-max theorem for matchings in bipartite graphs of Kőnig [23]. For a graph $G = (V, E)$, $X \subseteq V$ is called a *vertex cover* if every edge in E is incident to at least one vertex in X.

Theorem 1 ([23]). *For a bipartite graph $G = (V, E)$, the maximum size of a matching is equal to the minimum size of a vertex cover.*

Theorem 1 is extended to the following min-max theorems for b-matchings in bipartite graphs and matchings in nonbipartite graphs. A component of a graph G is called *odd* if it consists of odd number of vertices, and let $o(G)$ denote the number of odd components in G. For $X \subseteq V$, $G - X$ denotes the subgraph obtained from G by deleting X and edges incident to at least one vertex in X.

Theorem 2. *Let $G = (V, E)$ be a bipartite graph and $b \in \mathbf{Z}^V$. The maximum size of a simple b-matching in G is equal to*

$$\min_{X \subseteq V} \{b(\bar{X}) + |E[X]|\}. \tag{1}$$

Theorem 3 (Tutte-Berge formula [3, 37])**.** *The maximum size of a matching in a graph $G = (V, E)$ is equal to*

$$\frac{1}{2} \min_{X \subseteq V} \{|V| + |X| - o(G - X)\}. \tag{2}$$

Call an edge *admissible* if it belongs to some maximum matching. For $X \subseteq V$, let $\Gamma(X)$ denote the set of vertices in $V \setminus X$ adjacent to at least one vertex in X, i.e., $\Gamma(X) = \{v \in V \setminus X \mid \exists u \in X, uv \in E\}$. The Dulmage-Mendelsohn decomposition [10, 11] characterizes the structure of maximum matchings and minimum vertex covers in bipartite graphs. Among the rich structure of the Dulmage-Mendelsohn decomposition, we focus on the following statements, which are extended in the following sections.

Theorem 4. *For a bipartite graph $G = (V, E)$, let $D \subseteq V$ be the set of vertices which are not covered by at least one maximum matching in G. Then, the following statements hold.*

(i) *$X_1 = \bar{D}^+ \cup \Gamma(D^+)$ and $X_2 = \Gamma(D^-) \cup \bar{D}^-$ are minimum vertex covers.*

(ii) *For an arbitrary minimum vertex cover Y, it holds that $X_2^+ \subseteq Y^+ \subseteq X_1^+$ and $X_1^- \subseteq Y^- \subseteq X_2^-$.*

(iii) *Each edge in $E[\bar{X}_1^+, X_1^-]$ and $E[X_2^+, \bar{X}_2^-]$ is admissible.*

(iv) *$G[X_1^+ \setminus X_2^+, X_2^- \setminus X_1^-]$ has a perfect matching.*

(v) *$M \subseteq E$ is a maximum matching in G if and only if it is composed of a maximum matching in $G[\bar{X}_1^+, X_1^-]$, a maximum matching in $G[X_2^+, \bar{X}_2^-]$, and a perfect matching in $G[X_1^+ \setminus X_2^+, X_2^- \setminus X_1^-]$.*

Indeed, the Dulmage-Mendelsohn decomposition includes a finer decomposition of $G[X_1^+ \setminus X_2^+, X_2^- \setminus X_1^-]$, distributive lattice structure. For details, see, e.g., [22, 29, 32].

The Edmonds-Gallai decomposition [12, 14, 15] characterizes a minimizer of (2) which is canonical in some sense, and the structure of maximum matchings in nonbipartite graphs. A component Q in a graph G is called *factor-critical* if $Q - \{v\}$ admits a perfect matching for each vertex v in Q.

Theorem 5 (Edmonds-Gallai decomposition [12, 14, 15]; see also [29])**.** *For a graph $G = (V, E)$, let $D \subseteq V$ be the set of vertices which are not covered by at least one maximum matching, $A \subseteq V \setminus D$ be the set of vertices adjacent to at least one vertex in D, i.e., $A = \Gamma(D)$, and $C = V \setminus (D \cup A)$. Then the following statements hold.*

(i) *Each component in $G[D]$ is factor-critical.*

(ii) *$G[C]$ has a perfect matching.*

(iii) *In the bipartite graph obtained from G by deleting the vertices in C and edges in $E[A]$ and by contracting each component of $G[D]$ to one vertex, for each $X \subseteq A$ it holds that $|\Gamma(X)| > |X|$.*

(iv) *If M is a maximum matching in G, then M contains a matching of size $(|V(Q)| - 1)/2$ in each component Q of $G[D]$ and a perfect matching of $G[C]$, and matches all vertices of A with vertices in distinct components of $G[D]$.*

(v) *The maximum size of a matching in G is equal to $(|V| + |A| - o(G[D]))/2$.*

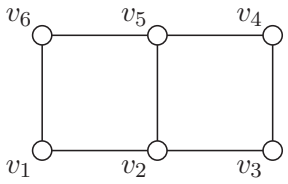

Figure 1: $Z_1 = \{v_1, v_2, v_3, v_4, v_5, v_6\}$ minimizes (3) and not (4), whereas $Z_2 = \{v_1, v_2, v_3, v_4, v_6\}$ minimizes (4) and not (3).

3 Min-max theorems and algorithms for square-free 2-matchings in bipartite graphs

In the sequel, we work on b-matchings in bipartite graphs, where $b_v \in \{0, 1, 2\}$ for each vertex v. For a bipartite graph $G = (V, E)$ and $b \in \{0, 1, 2\}^V$, a *square* is a subgraph forming a cycle of length four, and a b-matching in G is called *square-free* if it does not contain a cycle of length four. Recall that we never put multiplicities on edges in dealing with b-matchings, and note that a b-matching with $b \in \{0, 1, 2\}^V$ is a vertex-disjoint collection of cycles and paths, and the shortest length of a cycle in a bipartite graph is four.

3.1 Min-max theorems and optimality criteria

In a graph, a component consisting of an edge (resp., a square) is called a *edge-component* (resp., square-component). For $Z \subseteq V$, denote the number of square-components in $G[Z]$ by $c(Z)$, and the total number of isolated vertices, edge-components and square-components in $G[Z]$ by $q(Z)$. For the maximum square-free 2-matching problem in bipartite graphs, the following two min-max theorems are established.

Theorem 6 ([19, 24])**.** *Let $G = (V, E)$ be a bipartite graph and $b \in \{0, 1, 2\}^V$. The maximum size of a square-free b-matching in G is equal to*

$$\min_{Z \subseteq V} \{b(\bar{Z}) + |Z| - q(Z)\}. \tag{3}$$

Theorem 7 ([13, 34])**.** *Let $G = (V, E)$ be a bipartite graph and $b \in \{0, 1, 2\}^V$. The maximum size of a square-free b-matching in G is equal to*

$$\min_{Z \subseteq V} \{b(\bar{Z}) + |E[Z]| - c(Z)\}. \tag{4}$$

Intuitively, Theorem 6 is close to Theorem 3, as well as Theorem 7 resembles Theorem 2. By putting $b_v = 2$ for each $v \in V$ and $X := \bar{Z}$ in (3), we obtain

$$b(\bar{Z}) + |Z| - q(Z) = 2|X| + |\bar{X}| - q(\bar{X}) = |V| + |X| - q(\bar{X}),$$

which is similar to (2).

Theorems 6 and 7 indeed differ from each other in that a minimizer of (3) does not necessarily minimize (4), and vice versa. See Figure 3.1 for an example, where $b_v = 2$ for each vertex v. Observe that the maximum size of a square-free b-matching is six, $Z_1 = \{v_1, v_2, v_3, v_4, v_5, v_6\}$ attains six in (3) and seven in (4), and $Z_2 = \{v_1, v_2, v_3, v_4, v_6\}$ attains six in (4) and seven in (3).

An advantage of Theorem 7 is that it is extended to a min-max theorem for the maximum $K_{t,t}$-free t-matching problem in bipartite graphs [13], and further to a linear programming formulation with dual integrality for the weighted $K_{t,t}$-free t-matching problem in bipartite graphs, where the edge weight is vertex-induced on each $K_{t,t}$ [30, 36]. On the other hand, in this paper we establish a structure theorem (Theorem 11), which is based on Theorem 6 and reveals the existence of some sort of canonical minimizers of (3), as with Theorem 4.

Theorem 6 implies optimality criteria for maximum square-free b-matchings in G and minimizers of (3). For an arbitrary square-free b-matching M in G and an arbitrary $Z \subseteq V$, it holds that

$$\begin{aligned} |M[Z]| &\leq |Z| - q(Z), \\ |M[Z, \bar{Z}]| + 2|M[\bar{Z}]| &\leq b(\bar{Z}). \end{aligned}$$

Thus, if M is a maximum square-free b-matching and Z minimizes (3), it holds that

$$|M[Z]| = |Z| - q(Z), \tag{5}$$
$$|M[Z, \bar{Z}]| = b(\bar{Z}), \tag{6}$$
$$M[\bar{Z}] = \emptyset. \tag{7}$$

Equation (5) further implies that

(*) the components in $G[Z]$ are either a single vertex, a single edge or a single cycle, and moreover, all edges in $E[Z]$ except one edge from each square-component belong to M.

Also, Equations (6) and (7) imply that

$$\deg_M(v) = \deg_{M[Z,\bar{Z}]}(v) = b(v) \quad \text{for each } v \in \bar{Z}. \tag{8}$$

3.2 Hartvigsen's algorithm

For the maximum square-free 2-matching problem in bipartite graphs, there are three algorithms, due to Hartvigsen [19], Pap [34] and Takazawa [36], respectively, and they slightly differ from each others. In this paper we discuss Hartvigsen's algorithm [19], since the minimizer Z of (3) found by the algorithm in [19] plays a key role in our decomposition theorem. It is also noteworthy that this minimizer Z of (3) found by the algorithm in [19] is a minimizer of (4) as well, while the minimizers of (4) implied in [34] and [36] do not necessarily minimize (3).

Let us briefly sketch the algorithm. Let $G = (V^+, V^-; E)$ be a bipartite graph and let M be an arbitrary square-free 2-matching in G. In the algorithm, we augment M with the aid of alternating paths. Let $b_v = 2$ for each $v \in V^+ \cup V^-$, $U^+ = \{u \in V^+ \mid \deg_M(u) < b_v\}$ and $U^- = \{v \in V^- \mid \deg_M(v) < b_v\}$. We execute the breadth-first search (BFS) to find a path P from U^+ to U^- such that P starts with an edge in $E \setminus M$, and edges in $E \setminus M$ and in M lie alternately in P. In the BFS, if we reach an edge $e \in E \setminus M$ and a square S such that $\{e\} = E(S) \setminus M = E(S) \cap E(P_e)$, where P_e is the path from U^+ to e obtained in the BFS, we shrink S in the following manner. Let $V(S) = \{v_1^+, v_2^+, v_1^-, v_2^-\}$, where $v_1^+, v_2^+ \in V^+$ and $v_1^-, v_2^- \in V^-$. Then identify v_1^+ and v_2^+ to obtain a new vertex v_S^+, and v_1^- and v_2^- to obtain v_S^-. All edges in $E(S)$ are deleted, and edges incident to v_1^+ or v_2^+ (resp., v_1^- or v_2^-) are connected to v_S^+ (resp., v_S^-). Denote the resulting bipartite graph by $\tilde{G} = (\tilde{V}^+, \tilde{V}^-; \tilde{E})$, and reset $b \in \{1, 2\}^{\tilde{V}^+ \cup \tilde{V}^-}$ by

$$b_v := \begin{cases} 1 & \text{if } v = v_S^+ \text{ or } v = v_S^- \text{ for some shrunk square } S, \\ b_v & \text{otherwise.} \end{cases} \tag{9}$$

Now the objective becomes to find a maximum square-free b-matching in $\tilde{G}$. We remark that multiple edges connecting the same pair of vertices may appear in $\tilde{G}$, but M should contain at most one of those edges. Note also that shrunk squares are vertex-disjoint, even if repeated shrinking of squares are executed.

If an alternating path P from U^+ to U^- without such an edge e and a square S is found, then we update $M := M \triangle E(P)$, which is a square-free 2-matching with $|M'| = |M| + 1$.

After augmentation, we execute expanding of each shrunk square, which is the reverse operation of shrinking of a square. Let $\tilde{M}$ be a square-free b-matching in $\tilde{G}$. Then, it is not difficult to see that we can obtain a square-free 2-matching M in G by adding exactly three edges from each shrunk square to $\tilde{M}$.

An entire description of the algorithm is as follows.

Algorithm Square-free

Input: A bipartite graph $G = (V^+, V^-; E)$.

Output: A maximum square-free 2-matching $M \subseteq E$, and $Z \subseteq V$ minimizing both (3) and (4).

Step 0: Set $M = \emptyset$ and $\tilde{G} = G$.

Step 1: In $\tilde{G}$, define b by (9) and let $U^+ = \{u \in \tilde{V}^+ \mid \deg_M(u) < b_u\}$ and $U^- = \{v \in \tilde{V}^- \mid \deg_M(v) < b_v\}$. Construct an auxiliary directed graph $\tilde{G}_M$ from $\tilde{G}$ by orienting the edges in $E \setminus M$ from $\tilde{V}^+$ to $\tilde{V}^-$ and the edges in M from $\tilde{V}^-$ to $\tilde{V}^+$. Execute the BFS from U^+ in $\tilde{G}_M$. For an edge e, denote the path from U^+ to e obtained by the BFS by P_e. If an edge $e \in \tilde{E} \setminus M$ and a square S such that $\{e\} = \tilde{E}(S) \setminus M = \tilde{E}(S) \cap \tilde{E}(P_e)$ are found, then go to Step 2. If a path P from U^+ to U^- without such an edge e and a square S is found, then go to Step 3. Otherwise go to Step 4.

Step 2 (Shrinking): Shrink S and go to Step 1.

Step 3 (Augmentation): Update $M := M \triangle \tilde{E}(P)$, expand all shrunk squares, and then go to Step 1.

Step 4 (Termination):

Obtaining M. Expand all shrunk squares and return M.

Obtaining Z. Let $R \subseteq \tilde{V}^+ \cup \tilde{V}^-$ be the set of vertices reachable from U^+ in $\tilde{G}_M$, and let $Z = (\tilde{V}^+ \cap R) \cup (\tilde{V}^- \setminus R)$.

For each $v \in \tilde{V}^- \setminus R$ which is not contained in any shrunk square, if there exist two edges in M connecting $\tilde{V}^+ \cap R$ and v, then reset $Z := Z \setminus \{v\}$. For each $v_S^- \in \tilde{V}^- \setminus R$ of a shrunk square S, if there exists one edge in $\tilde{M}$ connecting $\tilde{V}^+ \cap R$ and v_S^-, then reset $Z := Z \setminus \{v_S^-\}$. (We remark that $v_S^+ \in Z$ always holds.)

In expanding each shrunk square S, reset Z by

$$Z := \begin{cases} (Z \setminus \{v_S^+, v_S^-\}) \cup V^+(S) \cup V^-(S) & \text{if } v_S^- \in Z, \\ (Z \setminus \{v_S^+, v_S^-\}) \cup V^+(S) & \text{if } v_S^- \notin Z. \end{cases}$$

After expanding all shrunk squares, return Z.

As is proved in [19], the output M is a maximum square-free 2-matching and Z minimizes (3). It is also not difficult to check that Z minimizes (4) as well.

Theorem 8. *Let M and Z be outputs of* Algorithm Square-free. *Then, M is a maximum square-free 2-matching in G, and Z minimizes both* (3) *and* (4).

4 Decomposition theorems for square-free 2-matchings in bipartite graphs

In this section, we describe our main contribution, structure theorems for square-free 2-matchings in bipartite graphs. Denote the minimizer of (3) obtained by Algorithm Square-free by Z_1. By replacing the roles of V^+ and V^- in Algorithm Square-free, we obtain another minimizer of (3), denoted by Z_2. We begin with showing a property of Z_1 and Z_2, which is stronger than (*).

Proposition 9. *For $i = 1, 2$, it holds that*

- *the components in $G[Z_i]$ is either a single vertex, a single edge, or a single square, and*
- *for an arbitrary maximum square-free 2-matching M, all edges in $E[Z_i]$ except for one edge from each square-component belong to M.*

Proof. We only discuss Z_1, since the same argument applies to Z_2. Since Z_1 and an arbitrary maximum square-free 2-matching M satisfy the property (*), it suffices to prove that $G[Z_1]$ does not have a cycle of length at least six. Suppose to the contrary that $G[Z_1]$ has such a cycle Q. Denote the maximum square-free 2-matching found by Algorithm Square-free by M^*. Then we have that $V^+(Q) \subseteq Z_1$ and $E(Q) \subseteq M^*$. This implies that the vertices in $V^-(Q)$ cannot belong to Z_1 (see Step 4 of Algorithm Square-free) regardless of whether Q contains shrunk squares or not, a contradiction. □

In the sequel, we denote the graph and square-free b-matching at the last stage of Algorithm Square-free, for which neither shrinking nor augmentation is executed, by $\tilde{G} = (\tilde{V}^+, \tilde{V}^-; \tilde{E})$ and $\tilde{M}$. For $X \subseteq V$, let $\tilde{X}$ denote the subset of $\tilde{V}$ corresponding to X.

We are now ready describe our decomposition theorems. Following the notation of the Edmonds-Gallai decomposition, define $D, A, C \subseteq V$ by

$$D = Z_1^+ \cup Z_2^-, \quad A = \bar{Z}_1^- \cup \bar{Z}_2^+, \quad C = V \setminus (D \cup A).$$

First, the following theorem characterizes the vertex set D.

Theorem 10. *It holds that*

$$D = \{u \in V \mid \exists \textit{maximum square-free 2-matching } M \textit{ such that } \deg_M(u) \leq 1\}.$$

Proof. We only discuss the vertices in V^+. The arguments straightforwardly apply to the vertices in V^-.

By (8), $\deg_M(u) = 2$ holds for each $u \in \bar{Z}_1^+$ and an arbitrary maximum square-free 2-matching M. We next show that, for each $u \in Z_1^+$, there exists a maximum square-free 2-matching M such that $\deg_M(u) \leq 1$.

Let $u \in Z_1^+$ be a vertex which is not contained in any shrunk square in $\tilde{G}$. In $\tilde{G}_{\tilde{M}}$, there exists a path P from U^+ to u. Let $\tilde{M}' = \tilde{M} \triangle \tilde{E}(P)$ to have $\deg_{\tilde{M}'}(u) \leq 1$. By expanding all shrunk squares, we obtain another maximum square-free 2-matching M' from $\tilde{M}'$ with $\deg_{M'}(u) \leq 1$.

If $u \in Z_1^+$ is shrunk into v_S^+ for some square S in $\tilde{G}$, let P be a path from U^+ to v_S^+ in $\tilde{G}_{\tilde{M}}$. Again let $\tilde{M}' = \tilde{M} \triangle \tilde{E}(P)$ to have $\deg_{\tilde{M}'}(v_S^+) = 0$, and we can expand all shrunk squares to obtain a maximum square-free 2-matching M' from $\tilde{M}'$ satisfying $\deg_{M'}(u) \leq 1$. □

The following theorem corresponds to Theorem 4 (ii), and suggests that the minimizers Z_1 and Z_2 are canonical.

Theorem 11. *For an arbitrary set $Y \subseteq V$ minimizing* (3)*, it holds that $Z_1^+ \subseteq Y^+ \subseteq Z_2^+$ and $Z_2^- \subseteq Y^- \subseteq Z_1^-$.*

Proof. We first prove that $Z_1^+ \subseteq Y^+$. For $u \in Z_1^+$, by Theorem 10 there exists a maximum square-free 2-matching M satisfying $\deg_M(u) \leq 1$. On the other hand, by (8), we have that $\deg_M(v) = 2$ for every $v \in \bar{Y}$. Thus, $u \in Y$ follows.

Next we prove that $Y^- \subseteq Z_1^-$. Suppose to the contrary that there exists $v \in Y^- \setminus Z_1^-$.

Case 1: v is reachable from U^+ in $\tilde{G}_{\tilde{M}}$. If v does not belong to any shrunk square in $\tilde{G}$, then let $e = uv \in E$ be the last edge of a shortest path from U^+ to v. By the above argument, we have that $u \in Z_1^+ \subseteq Y^+$, and hence $e \in E[Y] \setminus M$, which implies that e is the unique edge out of M in a square-component S in $G[Y]$ by the property (*). Since $v \notin Z_1$, by (8) we have that $\deg_M(v) = 2$, which implies that there exists one edge in M, say tv, not belonging to $E(S)$. Since S is a square-component in $G[Y]$, we have that $t \notin Y$. On the other hand, since $v \in V^-$ is reachable from U^+, we have that $t \in V^+$ is also reachable, and hence $t \in Z_1 \subseteq Y$, a contradiction.

If v is shrunk into v_S^- for some square S, then we have that v_S^+ is reachable. Again let $uv \in E$ be the last edge of a shortest path from U^+ to v_S^-, and let $V^+(S) = \{u_0, u_1\}$ and $V^-(S) = \{v, v_0\}$. Note that u, u_0, u_1 are distinct and $u, u_0, u_1 \in Z \subseteq Y$. If $V^-(S) \subseteq Y$, then the unique edge in $E(S) \setminus M$ is contained in a component which is not a square in $G[Y]$, contradicting to (*). Thus we have that $v_0 \notin Y$. Then the component in $G[Y]$ containing v does not satisfy (*).

Case 2: v is not reachable from U^+ in $\tilde{G}_{\tilde{M}}$. Since $v \notin Z_1^-$, v is removed from Z_1 in Step 4 of Algorithm Square-free. Suppose that v does not belong to any shrunk square in $\tilde{G}$. We have that $\deg_{M[Z_1^+, \{v\}]}(v) = 2$, and hence $\deg_{M[Y]}(v) = 2$ since $Z_1^+ \subseteq Y^+$. Thus, by (*), v belongs to a square S or a cycle Q of length at least six in $G[Y]$. In the former case, S should be shrunk, a contradiction. In the latter case, we have that $V(Q) \subseteq Y$ and $E(Q) \subseteq M$ by (*), and then in $\tilde{G}_{\tilde{M}}$ the vertices in $V(Q)$ is not reachable from U^+, a contradiction.

If v is shrunk into v_S^- for some square S, a similar arguments as in Case 1 leads to a contradiction.

The same arguments prove $Y^+ \subseteq Z_2^+$ and $Z_2^- \subseteq Y^-$. □

Finally, the following theorem is a counterpart of the Dulmage-Mendelsohn decomposition for matchings in bipartite graphs (Theorem 4) and the Edmonds-Gallai decomposition for matchings in nonbipartite graphs (Theorem 5).

Theorem 12. *The following statements hold.*

(i) *The components in $G[D]$ and $G[D, C]$ is either a single vertex, a single edge, or a single square.*

(ii) *Every edge in $E[D, A]$ is admissible.*

(iii) *Shrink the squares in $G[D]$ and $G[D, C]$ in the same manner as in* Algorithm Square-free *to obtain a new graph $G' = (V', E')$, denote the vertex subsets of V' corresponding to D, C by D', C', and define $b' \in \{1, 2\}^{D' \cup C'}$ by*

$$b'_v = \begin{cases} 1 & \text{if } v = v_S^+ \text{ or } v = v_S^- \text{ for some shrunk square } S, \\ & \quad \text{or } v \text{ belongs to an edge-component in } G[D] \text{ or } G[D, C], \\ 2 & \text{otherwise.} \end{cases}$$

Then,

(a) *for arbitrary $X \subseteq A$, it holds that $b'(\Gamma(X) \cap D') > 2|X|$, and*

(b) *$G'[C']$ has a b'-factor.*

(iv) *An arbitrary maximum square-free 2-matching M in G is composed of the following edges:*

(a) *in $G[D]$ and $G[D, C]$, M contains the single edge of each edge-component, and exactly three edges from each square-component;*

(b) *for $u \in A$, M contains two edges connecting u and distinct components in $G[D]$; and*

(c) *in $G[C]$, $M[C]$ corresponds to a b'-factor in $G'[C']$.*

(v) *Both $D \cup C^+$ and $D \cup C^-$ minimize both* (3) *and* (4).

Proof. Assertion (v) directly follows from $D \cup C^- = Z_1$ and $D \cup C^+ = Z_2$.

We next prove (i) and (iv)(a). It suffices to deal with $G[D] = G[D^+, D^-]$ and $G[D^+, C^-]$. Let M^* be the maximum square-free 2-matching found by Algorithm Square-free. By Proposition 9, it suffices to prove that $G[Z_1]$ does not have a square intersecting both D^- and C^-. Suppose to the contrary that $G[Z_1]$ has such a square S. Then, S is not shrunk in $\tilde{G}$, and by (*) one vertex $v \in \tilde{V}^-(S)$ has two incident edges in M^* connecting v and $\tilde{V}(S)^+ \subseteq D^+$. Then v should belong to A^- (see Step 4 of Algorithm Square-free), a contradiction.

Assertion (iv)(b) is now straightforward from (6) and Assertions (i) and (iv)(a).

We then prove (iii)(b) and (iv)(c). Since $C^+ \subseteq Z_2^+$ and $C^- \subseteq Z_1^-$, it follows from (8) that $\deg_M(v) = 2$ for an arbitrary vertex $v \in C$ and a arbitrary maximum square-free 2-matching M. Since $M[A, C] = \emptyset$ by (iv)(b), Assertions (iii)(b) and (iv)(c) follow from (iv)(a).

Next we prove (iii)(a). It suffices to consider $X \subseteq A^- = \bar{Z}_1^-$. From (iv)(a) and (iv)(b), it is clear that $b'_u \geq |\tilde{M}[\{u\}, X]|$ for each $u \in \Gamma(X) \cap D'$. Suppose that there exists a shortest path P from U^+ to $\tilde{X}$ in $\tilde{G}_{\tilde{M}}$. Denote the last edge of P by uv, where $u \in \tilde{V}^+$ and $v \in \tilde{V}^-$. Then we have that $b_u > |\tilde{M}[\{u\}, \tilde{X}]|$, which implies that $b'(\Gamma(X) \cap D')$ is strictly larger than $2|X|$. Suppose that P does not exist, i.e., all vertices in X are deleted from Z in Step 4. In this case, $b'_u > |\tilde{M}[\{u\}, \tilde{X}]|$ holds for each $u \in \Gamma(X) \cap D'$, since u is reachable from U^+, i.e., $u \in U^+$ or u has an extra edge in M reaching u from U^+, and thus the assertion follows.

Finally we prove (ii). We show that an edge $e \in E[Z_1^+, V^- \setminus Z_1^-]$ is admissible. The same argument applies to edges in $E[V^+ \setminus Z_2^+, Z_2^-]$.

Suppose that $e = uv \in \tilde{E}$, i.e., e does not belong to shrunk squares, where $u \in \tilde{V}^+$ and $v \in \tilde{V}^-$. If $e \in \tilde{M}$, then, from $\tilde{M}$, we obtain a maximum square-free 2-matching containing e by expanding all shrunk squares. If $e \in \tilde{E} \setminus \tilde{M}$, let P be a shortest path from U^+ to u in $\tilde{G}_{\tilde{M}}$, and let $\tilde{M}' = \tilde{M} \triangle \tilde{E}(P)$. Then, from $\tilde{M}'$, we obtain a maximum square-free 2-matching M' in G such that $e \in E \setminus M'$, $\deg_{M'}(u) \leq 1$ and $\deg_{M'}(v) = 2$ by expanding all shrunk squares. By adding e to M' and deleting one of edges incident to v from M', we obtain another maximum square-free 2-matching M'' (we can choose the deleted edge so that M'' does not contain a square).

Suppose that e does not appear in $\tilde{E}$, i.e., $e \in E(S)$ for some shrunk square S Let P be a path from U^+ to v_S^+. Then $\tilde{M}' = \tilde{M} \triangle \tilde{E}(P)$ is a new square-free b-matching satisfying $|\tilde{M}'| = |\tilde{M}|$ and $\deg_{\tilde{M}'}(v_S^+) = 0$. Now it is not difficult to see that we can add e to $\tilde{M}'$ in expanding S. □

Here let us describe how Assertions (i) and (iv)(a) in Theorem 12 relates to Theorems 4 and 5. In Assertion (i) in Theorem 12, the components in $G[D]$ are analogue to the components in $G[D]$ in Theorems 4 and 5, which are factor-critical (in Theorem 4, every component in $G[D]$ consists of a single vertex). For a component Q which is either a single vertex, an edge-component or a

square-component, the maximum size of a square-free 2-matching in Q is equal to $|V(Q)|-1$, while the maximum size of a matching in a factor-critical component Q' is $(|V(Q')|-1)/2$. In particular, if Q is a square-component, for every pair of $u^+ \in V^+(Q)$ and $u^- \in V^-(Q)$ there exists a maximum square-free 2-matching M_Q in Q satisfying $\deg_{M_Q}(u^+) = \deg_{M_Q}(u^-) = 1$ and $\deg_{M_Q}(v) = 2$ for $v \in V(Q) \setminus \{u^+, u^-\}$. This would correspond to the fact that a factor-critical component Q' admits a perfect matching in $Q' - \{v\}$ for each vertex v in Q'. Moreover, by Assertion (iv)(a), an arbitrary maximum square-free 2-matching contains a maximum square-free 2-matching in each component in $G[D]$, as is the case for a maximum matching and the factor-critical components in $G[D]$ in Theorem 5 (iv).

The components in $G[D, C]$ appear in neither the Dulmage-Mendelsohn nor the Edmonds-Gallai decomposition. For edge-components in $G[D, C]$, however, their counterpart indeed exists in bipartite b-matchings, which corresponds to the term $|E[X]|$ in (1). The square-components in $G[D, C]$ are specific to square-free 2-matchings, but again are analogue to the edge-components in $G[X]$ in Theorem 2 in a sense that each square-component S contains three edges from an arbitrary maximum square-free 2-matching by Assertion (iv)(a) and thus it can be shrunk and dealt with just as an edge-component.

With the above analogy in mind, for the other assertions in Theorem 12 it is not difficult to find their counterparts in Theorems 4 and 5.

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