RECOGNITION AND COMBINATORIAL OPTIMIZATION ALGORITHMS FOR BIPARTITE CHAIN GRAPHS

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Abstract. In this paper we give a recognition algorithm in $O(n(n + m))$ time for bipartite chain graphs, and directly calculate the density of such graphs. For their stability number and domination number, we give algorithms comparable to the existing ones. We point out some applications of bipartite chain graphs in chemistry and approach the Minimum Chain Completion problem.

Keywords: Bipartite chain graphs, weakly decomposition, recognition algorithms, combinatorial optimization algorithms

1 INTRODUCTION

A graph $G = (V, E)$ is called bipartite chain [31] if it is bipartite and for each color class the neighbourhoods of the nodes in that color class can be ordered linearly with respect to inclusion.
The class of bipartite chain graphs is also known as $2K_2$-free bipartite graphs, difference graphs [12] or bisplit graphs [10].

An undirected graph $G = (V, E)$ is a bisplit graph if its vertex set can be partitioned into a stable set and a complete bipartite graph.

A graph $G = (V, E)$ is said to be a difference graph if there exist the real numbers $a_1, a_2, \ldots, a_n$ associated with the vertices of $G$ and a positive real number $d$ such that

1. $|a_i| < d$ for $i = 1, 2, \ldots, n$;
2. distinct vertices $i$ and $j$ are adjacent if and only if $|a_i - a_j| \geq d$.

A graph is a difference graph if and only if it is $\{2K_2, C_3, C_5\}$-free [4].

In [3] an $O(nm)$ algorithm for bisplit graphs is given.

In [32] recognition algorithms for the bipartite chain graphs in polynomial time are given, using characterizations of these graphs with forbidden subgraphs; also, linear algorithms are given for independent set [13] and for domination [21].

Bisplit graphs are decomposed in 3 stable sets such that we have total adjacency between two of these stable sets [3].

In different problems from the theory of graphs, particularly in the building of some recognition algorithms, a type of partition of the set of vertices in three classes $A, B, C$ appears frequently such that $A$ induces a connected subgraph, and $C$ is totally adjacent to $B$ and totally nonadjacent to $A$. This happens, for example, when building cographs, starting from a $K_{1,2}$ and substituting the vertices with cographs. The introduction of the notion “weakly decomposition” [5, 27] and the study of its properties allows us to obtain other results of this type, such as the characterization of cographs with cotrees (result obtained by Lerchs [18], also see [15, 19], but for which we obtain an easier proof). Also, we characterize the $K_{1,3}$-free graphs and give a recognition algorithm for these graphs. Other properties are obtained for triangulated graphs.

2 PRELIMINARIES

Throughout this paper, $G = (V, E)$ is a connected, finite and undirected graph [1], without loops and multiple edges, having $V = V(G)$ as the vertex set and $E = E(G)$ as the set of edges, $(n = |V|, m = |E|)$. $\overline{G}$ is the complement of $G$. If $U \subseteq V$, by $G(U)$ or $[U]_G$ we denote the subgraph of $G$ induced by $U$. By $G - X$ we mean the subgraph $G(V - X)$, whenever $X \subseteq V$, but we simply write $G - v$, when $X = \{v\}$. If $e = xy$ is an edge of a graph $G$, then $x$ and $y$ are adjacent, while $x$ and $e$ are incident, as are $y$ and $e$. If $xy \in E$, we also use $x \sim y$, and $x \not\sim y$ whenever $x, y$ are not adjacent in $G$. If $A, B \subseteq V$ are disjoint and $ab \in E$ for every $a \in A$ and $b \in B$, we say that $A, B$ are totally adjacent and we denote by $A \sim B$, while by $A \not\sim B$ we mean that no edge of $G$ joins some vertex of $A$ to a vertex from $B$ and, in this case, we say $A$ and $B$ are non-adjacent.
The neighborhood of the vertex \( v \in V \) is the set \( N_G(v) = \{ u \in V : uv \in E \} \), while \( N_G[v] = N_G(v) \cup \{ v \} \); we denote \( N(v) \) and \( N[v] \), when \( G \) appears clearly from the context. The degree of \( v \) in \( G \) is \( d_G(v) = |N_G(v)| \). The neighborhood of the vertex \( v \) in the complement of \( G \) will be denoted by \( \overline{N}(v) \).

The neighborhood of \( S \subset V \) is the set \( N(S) = \bigcup_{v \in S} N(v) - S \) and \( N[S] = S \cup N(S) \). A graph is complete if every pair of distinct vertices is adjacent. A clique is a subset \( Q \) of \( V \) with the property that \( G(Q) \) is complete. The clique number of \( G \), denoted by \( \omega(G) \), is the size of the maximum clique.

A stable set is a subset \( X \) of vertices where every two vertices are not adjacent. \( \alpha(G) \) is the number of vertices of a stable set of maximum cardinality; it is called the stability number of \( G \). \( \chi(G) = \omega(\overline{G}) \) is called chromatic number.

If \( N[v] = V \), then \( v \) is called a dominating vertex in \( G \).

A dominating set for a graph \( G = (V, E) \) is a subset \( D \subseteq V \) such that \( \forall v \in V - D, \exists d \in D \) such that \( vd \in E \). The domination number \( \nu(G) \) is the number of vertices in the smallest dominating set for \( G \).

Let \( G = (V, E) \) be a connected graph. A subset \( A \subset V \) is called cutset if \( G - A \) is not connected.

By \( P_n \), \( C_n \), \( K_n \) we mean a chordless path on \( n \geq 3 \) vertices, a chordless cycle on \( n \geq 3 \) vertices, and a complete graph on \( n \geq 1 \) vertices, respectively.

A graph \( G \) is called \( F \)-free if none of its subgraphs is in \( F \). The Zykov sum of the graphs \( G_1, G_2 \) is the graph \( G = G_1 + G_2 \) having:

\[
V(G) = V(G_1) \cup V(G_2), \\
E(G) = E(G_1) \cup E(G_2) \cup \{uv : u \in V(G_1), v \in V(G_2)\}.
\]

A bipartite graph is a graph whose vertices can be divided into two disjoint sets \( A \) and \( B \) such that every edge connects a vertex in \( A \) to one in \( B \). That is, \( A \) and \( B \) are stable sets.

A gem graph is a graph formed by making an universal vertex adjacent to each of the four vertices of the induced path \( P_4 \) as an induced subgraph.

We call adjacent graph (\( X \)-adjacent) of a family of graphs \( \{G_x\}_{x \in V(X)} \), indexed by the set of vertices \( X \), the graph denoted \( \cup_{x \in X} G_x \) (see \([11]\), also \([8, 23]\)) where:

\[
V(\cup_{x \in X} G_x) = \bigcup_{x \in X} V(X) \times \{x\}; \\
E(\cup_{x \in X} G_x) = \bigcup_{x \in X} E(G_x) \cup \{[ax, bx']|x \neq x', xx' \in E(X), a \in V(G_x), b \in V(G_{x'})\}.
\]

For a graph \( G = (V, E) \):

- the distance \( d(u, v) \) between two vertices \( u \) and \( v \) is defined as the length of the shortest path from \( u \) to \( v \);
- the eccentricity of a vertex \( u \in V \) is \( e_G(u) = \max\{d(u, v) : v \in V\} \);
- the radius is \( r(G) = \min\{e_G(u) : u \in V\} \);
- the center \( C(G) \) of a graph \( G \) is \( C(G) = \{u \in V : r(G) = e_G(u)\} \).
When searching for recognition algorithms, a type of partition appears frequently for the set of vertices in three classes $A, B, C$, which we call a weakly decomposition, such that: $A$ induces a connected subgraph, $C$ is totally adjacent to $B$, while $C$ and $A$ are totally nonadjacent.

The structure of the paper is as follows. In Section 3 we recall a characterization of the weak component and the existence of the weakly decomposition, and give an algorithm to find one. In Section 4 we present a new characterization of the bipartite chain graphs and give a recognition algorithm. In Section 5 we give combinatorial optimization algorithms for bipartite chain graphs. In Section 6 we point out some applications of bipartite chain graphs in chemistry and approach the Minimum Chain Completion problem.

3 THE WEAKLY DECOMPOSITION

At first, we recall the notions of weakly component and weakly decomposition.

**Definition 1** ([27, 28]). A set $A \subset V(G)$ is called a weakly set of the graph $G$ if $N_G(A) \neq V(G) - A$ and $G(A)$ is connected. If $A$ is a weakly set, maximal with respect to set inclusion, then $G(A)$ is called a weakly component. For simplicity, the weakly component $G(A)$ will be denoted with $A$.

**Definition 2** ([27, 28]). Let $G = (V, E)$ be a connected and non-complete graph. If $A$ is a weakly set, then the partition $\{A, N(A), V - A \cup N(A)\}$ is called a weakly decomposition of $G$ with respect to $A$.

The name of “weakly component” is justified by the following result.

In order for the paper to be self-explained, we give below the proofs for Theorem 1 and Theorem 2, as well as the algorithm to obtain a weakly decomposition.

**Theorem 1** ([27, 28]). Every connected and non-complete graph $G = (V, E)$ admits a weakly component $A$ such that $G(V - A) = G(N(A)) + G(\overline{N}(A))$.

**Proof.** Because graph $G$ is non-complete, $\alpha(G) \geq 2$, there exist the vertices $x$ and $y$, $x \neq y$, nonadjacent. Let $A_0 = \{x\}$, $B_0 = N(x)$, $C_0 = \overline{N}(x)$. We have $y \in C_0$. If $N(x) \sim \overline{N}(x)$; then $A = A_0$. Otherwise, let $x_1 \in N(x)$, $y_1 \in \overline{N}(x)$ such that $x_1 \not\sim y_1$. For $A_1 = A_0 \cup \{x_1\}$, $G(A_1)$ is connected, as $G(A_0)$ is connected and $x_1 \in N(x)$. $N(A_1) = (N(A_0) - \{x_1\}) \cup (N(x_1) \cap C_0)$. We have $y_1 \in \overline{N}(A_1)$, because $x_1 \not\sim y_1$, $y_1 \in \overline{N}(x)$ and $y_1 \not\sim A_0$. It follows that $\overline{N}(A_1) \neq \emptyset$. If $N(A_1) \sim \overline{N}(A_1)$ then $G(V - A_1) = G(N(A_1)) + G(\overline{N}(A_1))$. Let us suppose that $A_i$, $B_i = N(A_i)$, $C_i = \overline{N}(A_i)$ have been built. If $B_i \sim C_i$ then $A = A_i$. If not, let $x_{i+1} \in B_i$ and $y_{i+1} \in C_i$, with $x_{i+1} \not\sim y_{i+1}$. We denote $A_{i+1} = A_i \cup \{x_{i+1}\}$, $B_{i+1} = N(A_{i+1})$, $C_{i+1} = \overline{N}(A_{i+1})$. $G(A_{i+1})$ is connected, because $G(A_i)$ is connected and $x_{i+1} \in N(A_i)$. Also, $y_{i+1} \in \overline{N}(A_{i+1})$, because $x_{i+1} \not\sim y_{i+1}$, $y_{i+1} \in \overline{N}(A_i)$ and $y_{i+1} \not\sim A_i$. It follows that $\overline{N}(A_{i+1}) \neq \emptyset$. If $B_{i+1} \sim C_{i+1}$ then $A = A_{i+1}$ and $G(V - A_{i+1}) = G(N(A_{i+1})) + G(\overline{N}A_{i+1})$. Because $A_0 \subset A_1 \subset \ldots \subset A_i \subset \ldots \subset V$ and $|V| < \infty$. 

it follows that \( \exists p \in N \) such that \( N(A_p) \sim \overline{N}(A_p) \) and, consequently, \( A = A_p \) is a weakly component with the property specified in Theorem 1.

\[ \text{Theorem 2} \ (\cite{27, 28}). \text{ Let } G = (V, E) \text{ be a connected and non-complete graph and } A \subset V. \text{ Then } A \text{ is a weakly component of } G \text{ if and only if } G(A) \text{ is connected and } N(A) \sim \overline{N}(A). \]

\[ \text{Proof.} \text{ Let us suppose that there exists } n \in N(A) \text{ and } \pi \in \overline{N}(A) \text{ such that } n\pi \not\in E. \text{ Let } A' = A \cup \{n\} \text{ and } N' = (N(A) - \{n\}) \cup (N(n) \cap \overline{N}(A)). \text{ } G(A') \text{ is connected, } N(A') = N' \text{ and } V(G) - (A' \cup N(A')) \supseteq \{\pi\}. \text{ It follows that } N(A') \not\sim V(G) - A', \text{ contradicting the maximality of } A. \text{ Conversely, let } G(A) \text{ be connected and } N(A) \sim \overline{N}(A). \text{ We show that } G(A) \text{ is the weakly component. } \]

The next result, that follows from Theorem 1, ensures the existence of a weakly decomposition in a connected and non-complete graph.

\[ \text{Corollary 1.} \text{ If } G = (V, E) \text{ is a connected and non-complete graph, then } V \text{ admits a weakly decomposition } (A, B, C), \text{ such that } G(A) \text{ is a weakly component and } G(V - A) = G(B) + G(C). \]

Theorem 2 provides an \( O(n + m) \) algorithm for building a weakly decomposition for a non-complete and connected graph.

\[ \text{Algorithm 1 for the weakly decomposition of a graph} \ [27] \]

\[ \text{Input:} \text{ A connected graph with at least two nonadjacent vertices, } G = (V, E). \]

\[ \text{Output:} \text{ A partition } V = (A, N, R) \text{ such that } G(A) \text{ is connected, } N = N(A), A \not\sim R = \overline{N}(A). \]

\[ \text{begin} \]
\[ A := \text{any set of vertices such that } A \cup N(A) \not\supseteq V \]
\[ N := N(A) \]
\[ R := V - A \cup N(A) \]
\[ \text{while } (\exists n \in N, \exists r \in R \text{ such that } nr \not\in E) \text{ do} \]
\[ \text{begin} \]
\[ A := A \cup \{n\} \]
\[ N := (N - \{n\}) \cup (N(n) \cap R) \]
\[ R := R - (N(n) \cap R) \]
\[ \text{end} \]
\[ \text{EndWeaklyDecompositionGraph} \]

\[ \text{Remark 1.} \text{ Let } G = (V, E) \text{ be a connected, non-complete graph. If } A \text{ a weakly set then } A \not\supseteq V. \]
Proof. If \( A \) is a weakly set and \( G \) is connected it follows that \( A \neq V \) else \( N_G(A) = \emptyset \), \( V - A = \emptyset \), that is \( N_G(A) = V - A \). 

Let \( G \) be a connected graph and \( W_G = \{ A | A \) is a weakly set of \( G \} \).

Remark 2. Let \( G = (V,E) \) be a connected graph. \( W_G \) has at least an element if and only if \( G \) is not complete.

Proof. If \( G \) is not complete then there exists \( v \in V \) such that \( N_G(v) \neq V - \{ v \} \). So \( \{ v \} \) is a weakly set: \( \{ v \} \in W_G \). Conversely, let us suppose that there exists \( A \), weakly set of \( G \). Then \( N_G(A) \neq V - A \), so \( \overline{N}(A) \neq \emptyset \). It follows that \( \exists a \in A, \exists b \in \overline{N}(A) \) such that \( ab \notin E \). So \( G \) is not complete. 

Let \( W_0^G = \{ A | A \in W_G, A \) is maximal with respect to inclusion} \).

Remark 3. Let \( G = (V,E) \) be a connected, non-complete graph. If \( A \in W_0^G \) then \( A \) is cutset in \( G \).

Proof. In \( \overline{G} - A \), the sets \( R = \overline{N}(A) \) and \( N \) are nonempty sets of totally nonadjacent vertices. 

Remark 4. Let \( G = (V,E) \) be a connected, non-complete graph. If \( A \in W_0^G \) then \( N_G(A) \) is cutset in \( G \).

Proof. In \( G - A \), the sets \( R = \overline{N}(A) \) and \( A \) are nonempty sets of totally nonadjacent vertices. 

4 RECOGNITION ALGORITHMS FOR BIPARTITE CHAIN GRAPHS

In this section we characterize the bipartite chain graphs using weakly decomposition and we give a recognition algorithm based on this characterization.

Definition 3. A graph \( G = (V,E) \) is called bipartite chain if it is bipartite and for each color class the neighbourhoods of the nodes in that color class can be ordered linearly with respect to inclusion.

We give, through Theorem 3, a characterization of the bipartite chain graphs. So, the decomposition of bipartite chain graphs is in 4 stable sets. But also, \( \omega(G) = 2 \), and \( \alpha(G) \) and \( \nu(G) \) are obtained with algorithms in \( O(n+m) \) because the weakly decomposition of a graph is provided with an \( O(n+m) \) algorithm.

Theorem 3. Let \( G = (V,E) \) be a connected, non-complete graph, and \( (A,N,R) \) a weakly decomposition with \( G(A) \) the weakly component. \( G \) is a bipartite chain graph if and only if

1. \( N \) and \( R \) are stable sets
2. There exists \( B \subseteq A \) such that \( B, A - B \) are stable sets, \( B \sim N \) and \( (A - B) \not\sim N \),
\[
A - B = N_G(B) - N \text{ and } B = N_G(A - B)
\]
3. \( G(A) \) is a bipartite chain graph.

**Proof.** Let \( G \) be a bipartite chain graph and \( (A, N, R) \) a weakly decomposition with \( G(A) \) the weakly component; then \( N \sim R \). \( G(A) \) is a bipartite chain graph. If \( N \)
were not stable then \( n_1, n_2 \in N \) would exist such that \( n_1n_2 \in E \); then \( G(\{n_1, n_2, r\} \simeq C_3, \forall r \in R \). If \( R \) were not stable then \( r_1, r_2 \in R \) would exist such that \( r_1r_2 \in E \);
then \( G(\{r_1, r_2, n\} \simeq C_3, \forall n \in N \).

No distinct vertices would exist in \( N \) with distinct neighbors in \( A \). If \( n, n' \in N \)
would exist such that \( n_b \not= n'_b \), where \( n_b, n'_b \in A \) and \( nn_b, n'n'_b \in E \) then if \( b \not= b' \),
then \( G(\{n_b, n, r, n'_b\}) \simeq C_5, \forall r \in R \) else \( G(\{n_b, n, n'_b\}) \simeq 2 \cdot K_2 \).

So, \( \forall n_1, n_2 \in N \) we have either:

a) \( N(n_1) \cap A \supset N(n_2) \cap A \) or
b) \( N(n_1) \cap A = N(n_2) \cap A \).

We suppose that a) holds. Let \( x \) from \( A \) be adjacent only to \( n_1 \) and \( y \) from \( A \) be
adjacent both to \( n_1 \) and \( n_2 \). Because \( G(A) \) is connected it follows that there is \( P_{xy} \).
If \( xy \in E \) then \( G(\{x, y, n_1\}) \simeq C_3 \). If \( xy \not\in E \) then either \( x \) and \( y \) have a common
neighbor \( b \) in \( A \) and then \( G(\{b, x, n_2, r\}) \simeq 2 \cdot K_2 \) or \( x \) and \( y \) have different neighbors
in \( A \) (let them be \( b_1x \in E \) and \( b_2y \in E \)) and then \( G(\{b_1, x, n_2, r\}) \simeq 2 \cdot K_2, \forall r \in R \).
So a) does not hold. Therefore, \( N(n_1) \cap A = N(n_2) \cap A, \forall n_1, n_2 \in N \). Then \( \exists B \subset A \) so that \( B = N(n) \cap A, \forall n \in N \), which means \( B = N_G(N) \cap A \) and \( B \sim N \),
\( A - B \not\sim N \).

Because \( G \) is connected and \( N = N_G(A) \) it follows that \( B \not= \emptyset \).

If \( B = N(n) \cap A \) were not stable then \( b_1, b_2 \in N(n) \cap A \) would exist such that \( b_1b_2 \in E \); then \( G(\{b_1, b_2, n\}) \simeq C_3 \). Because \( G(A) \) is connected and \( B \) is stable set, it follows that \( A - B \not= \emptyset \).

Because \( A - B \subset A \not\sim R \), it follows that \( A - B \not\sim R \).

If \( A - B \) were not stable then \( a_1, a_2 \in A - B \) would exist such that \( a_1a_2 \in E \).
Then, because \( A - B \not\sim R \cup N \), it follows that \( G(\{a_1, a_2, n, r\}) \simeq 2K_2, \forall n \in N, \forall r \in R \).
Because \( A - B \) is stable set, \( G(A) \) is connected; it follows that \( \forall a \in A - B \),
\( \exists b \in B \) such that \( ab \in E \), so \( A - B = N_G(B) - N \). Because \( G(A) \) is connected and \( B \) is stable set, it follows that \( B = N_G(A - B) \).

We suppose that i), ii) and iii) hold. Immediately follows that \( G \) does not contain either \( 2 \cdot K_2 \), or \( C_3 \), or \( C_5 \), which means that \( G \) is bipartite chain graph.

Theorem 3 provides the following recognition algorithm for bipartite chain graphs.

**Recognition algorithm for bipartite chain graphs**

**Input:** A connected, non-complete graph \( G = (V, E) \).

**Output:** An answer to the question: “Is \( G \) bipartite chain?”
begin
L := \{G\}
while (L \neq \emptyset) do
Let H be in L
1. Determine the degree of each vertex
2. Determine a weakly decomposition \((A, N, R)\) with \(N \sim R\) for H
3. Determine \(B = N_H(N) - R\) and \(C = A - B\)
4. Let: \(r = |R|; nr = |N|; b = |B|;\)
5. If \((\exists v \in R\) such that \(d_G(v) \neq nr)\) then \(G\) is not bipartite chain
else
  if \((\exists v \in N\) such that \(d_G(v) \neq b + r)\) then
    \(G\) is not bipartite chain
else
  Put \([A]_H\) in L
6. \(G\) is bipartite chain
end.
EndRecognitionAlgorithmForBipartiteChainGraphs
So the entire execution is in \(O(n(n + m))\) time.

5 COMBINATORIAL OPTIMIZATION ALGORITHMS
FOR BIPARTITE CHAIN GRAPHS

In this section we calculate the density, give \(O(n+m)\) algorithms to compute stability number, domination number, and calculate the center and the radius of these graphs.

In [4], the authors study the Dominating Set problem with measure functions, which is extended from the general Dominating Set problem.

In [16], the authors present results which allow us to compute the independence numbers of special graphs.

In [22], the authors study independence and domination in path graph of trees.

A path graph is defined as follows. Let \(G\) be a graph, \(k \geq 1\) and \(P_k\) be the set of all paths of length \(k\) in \(G\). The vertex set of path graph \(P_k(G)\) is the set \(P_k\). Two vertices of \(P_k(G)\) are joined by an edge if and only if their intersection is a path of length \(k - 1\), and their union forms either a cycle or a path of length \(k + 1\).

Using Theorem 3 we obtain the following consequence.

Consequence 1. Let \(G = (V, E)\) be a connected, non-complete graph, and \((A, N, R)\) a weakly decomposition with \(G(A)\) as the weakly component. If \(G\) is a bipartite chain graph then
1. \(\omega(G) = 2\)
2. \(\alpha(G) = \max\{|A| - |B| + |N|, |A| - |B| + |R|, |B| + |R|\}\)

Proof. We have: \(\alpha(G(A)) = \max\{|A| - |B|, |B|\}; \alpha(G(R)) = |R|; \alpha(G(A \cup N)) = \max\{\alpha(G((A - B) \cup B)), \alpha(G(A - B)) + \alpha(G(N))\} = \max\{|A| - |B|, |B|, |A| -
\(|B| + |N|\). So, \(\alpha(G) = \max\{\alpha(G(A \cup N)), \alpha(G(A)) + \alpha(G(R))\} = \max\{\max\{|A| - |B|, |B|, |A| - |B| + |N|\}, \max\{|A| - |B|, |B| + |R|\}\} = \max\{|A| - |B| + |N|, |A| - |B| + |R|, |B| + |R|\}. \]

Facility location analysis deals with the problem of finding optimal locations for one or more facilities in a given environment [17]. Location problems are classical optimization problems with many applications in industry and economy. Spatial location of the facilities often takes place in the context of a given transportation, communication, or transmission system.

The aim of this problem could be to determine a location that minimizes the maximum distance to any other location in the network. Another type of location problems optimizes a “minimum of a sum” criterion, which is used in determining the location for a service facility like a shopping mall, for which we try to minimize the total travel time.

**Consequence 2.** Let \(G = (V, E)\) be a connected graph, non-complete and \((A, N, R)\) a weakly decomposition with \(G(A)\) as the weakly component. If \(G\) is a bipartite chain graph then \(N \cup B\) is a dominating set and \(\nu(G) = |N| + |B|\). Also, the radius is 2 and the center is \(N \cup B\).

**Proof.** Because the distance between any vertex in \(R\) and any vertex in \(A - B\) is 3 and the distance between any other two vertices is at the most 2 it follows that:

\[
\begin{align*}
  e_G(u) &= 3, \quad \forall u \in R \cup (A - B); \\
  e_G(u) &= 2, \quad \forall u \in N \cup B; \\
  r(G) &= 2; \\
  C(G) &= N \cup B.
\end{align*}
\]

6 SOME APPLICATIONS OF BIPARTITE CHAIN GRAPHS IN CHEMISTRY

In this section we point out some applications of bipartite chain graphs in chemistry and approach the Minimum Chain Completion problem.

In [20], the authors discussed the challenges specific to the development of computational chemistry software.

The Wiener index was introduced in 1947 by Horold Wiener [29] and is defined as the sum of distance between all pairs of vertices in \(G\):

\[
W(G) = \sum_{u,v \in V} d_G(u, v).
\]

The theoretical framework is especially well elaborated for the Wiener index of trees [7].
The Wiener index is a graphical invariant that has found extensive application in chemistry [25].

The distance-counting polynomial was introduced [14] as:

$$H(G, x) = \sum_k d(G, k)x^k,$$

with $d(G, 0) = |V(G)|$ and $d(G, 1) = |E(G)|$, where $d(G, k)$ is the number of pair vertices lying at distance $k$ to each other. This polynomial was called Wiener, by its author Hosoya, in the more recent literature [11, 26].

**Theorem 4.** Let $G = (V, E)$ be a connected, non-complete graph, and $(A, N, R)$ a weakly decomposition with $G(A)$ the weakly component. If $G$ is bipartite chain graph, $d$ is the number of common neighbours in $B$ for all pairs of vertices in $A - B$ and $ad$ ($nad$) is the number of vertices $x$ in $A - B$, $y$ in $B$, adjacent (non-adjacent), then

1. the Wiener polynomial is

$$H(G, x) = [2(|A| - |B|)(|A| - |B| - 1) - 4d|x^4 + [3(|A| - |B|)|R| + nad]x^3
\quad + |R|(|R| - 1) + 2|B||R| + |N|(|N| - 1) + 2(|A| - |B|)|N|
\quad + |B|(|B| - 1) + 2d|x^2 + (|N||R| + |N||B| + ad)x + |V|$$

2. the Wiener index is

$$W(G) = |R|(|R| - 1) + |N||R| + 2|B||R| + 3(|A| - |B|)|R| + |N|(|N| - 1)
\quad + |N||B| + 2(|A| - |B|)|N| + |B|(|B| - 1) + ad + 3nad
\quad + 2((|A| - |B|)(|A| - |B| - 1) - d).$$

**Proof.** Let $G = (V, E)$ be a connected, non-complete graph, and $(A, N, R)$ a weakly decomposition with $G(A)$ the weakly component. Because $G$ is a bipartite chain, it follows that:

- $N$ and $R$ are stable sets
- there exists $B \subseteq A$ such that $B$, $A - B$ are stable sets, $B \sim N$ and $(A - B) \not\sim N$, $A - B = N_G(B) - N$ and $B = N_G(A - B)$
- $G(A)$ is a bipartite chain graph.

Let $d$ be the number of common neighbours in $B$ for all pairs of vertices in $A - B$.

Considering the distances between all pairs of vertices we have:

$$\sum_{u \in R, v \in R} d(u, v) = 2(|R| - 1)|R|/2$$
$$\sum_{u \in R, v \in N} d(u, v) = |N||R|$$
\[
\sum_{u \in R, v \in B} d(u, v) = 2|B||R|
\]
\[
\sum_{u \in R, v \in A - B} d(u, v) = 3(|A| - |B|)|R|
\]
\[
\sum_{u \in N, v \in N} d(u, v) = 2|N|(|N| - 1)/2
\]
\[
\sum_{u \in N, v \in B} d(u, v) = |N||B|
\]
\[
\sum_{u \in A - B, v \in A - B} d(u, v) = 2d + 4(|A| - |B|)(|A| - |B| - 1)/2 - d).
\]

So, the Wiener polynomial is
\[
H(G, x) = [2(|A| - |B|)(|A| - |B| - 1) - 4d]x^4 + [3(|A| - |B|)|R|
+ 3nad]x^3 + [|R|(|R| - 1) + 2|B||R| + |N|(|N| - 1) + 2(|A| - |B|)|N|
+ |B|(|B| - 1) + 2d]x^2 + (|N||R| + |N||B| + ad)x + |V|
\]

and the Wiener index is
\[
W(G) = |R|(|R| - 1) + |N||R| + 2|B||R| + 3(|A| - |B|)|R|
+ |N|(|N| - 1) + |N||B| + 2(|A| - |B|)|N| + |B|(|B| - 1)
+ ad + 3nad + 2(|A| - |B|)(|A| - |B| - 1) - d).
\]

In what follows, we approach the Minimum Chain Completion problem. A graph is \((P_5, \text{gem})\)-free, when it does not contain \(P_5\) or a gem. In [2] the authors present \(O(n^2)\) time recognition algorithms for \((P_5, \text{gem})\)-free graphs.

In [9] the authors give approximation algorithms for two variants of the Minimum Chain Completion problem, where a bipartite graph \(G = (U, V, E)\) is given, and the goal to find the minimum set of edges \(F\) that need to be added to \(G\) such that the bipartite graph \(G' = (U, V, E')\) \((E' = E \cup F)\) is a chain graph.

In [9] the authors discuss the following two variants:

**Total Minimum Chain Completion (T-mcc).** Given a bipartite graph \(G = (U, V, E)\), find the minimum set of edges \(F\) that need to be added to \(G\) such that the bipartite graph \(G' = (U, V, E')\), where \(E' = E \cup F\), is a chain graph. The value of the solution is \(|E'|\).
Additional Minimum Chain Completion (A-mcc). Given a bipartite graph \( G = (U,V,E) \), find the minimum set of edges \( F \) that need to be added to \( G \) such that the bipartite graph \( G'' = (U,V,E'' \cup F) \), where \( E'' = E \cup F \), is a chain graph. The value of the solution is \(|F|\).

Since the A-mcc problem is NP-hard [30], so is the T-mcc problem.

We shall determine a weakly decomposition \((A,N,R)\) with \(N \sim R\) for \(G\). If \(G\) is a bipartite chain graph the \(G\) is a gem-free graph. \([A]_G\) is \(2K_2\)-free if and only if \(G - R\) is \(P_5\)-free. It follows from [2] that there exists an \(O(n^2)\) time recognition algorithms for \((P_5, \text{gem})\)-free graphs.

An algorithm for the Minimum Chain Completion problem tests, for every \(i \in A - B\), for every \(j \in A - B\), if \(((N(i) - N(j)) \neq \emptyset)\) and \((N(j) - N(i)) \neq \emptyset\) and then adds \((i,k)\) to \(E\) (where \(k \in (N_G(j) - N_G(i)) \cap B\)).

The possible \(2K_2\) in \([A]_G\) are eliminated, which means that \([A]_G\) becomes, from a bipartite graph, a bipartite chain graph.

The test \(((N(i) - N(j)) \neq \emptyset)\) and \((N(j) - N(i)) \neq \emptyset\) means that the vertices \(i\) and \(j\) in \(A - B\) have uncommon neighbours in \(B\). By adding the edge \((i,k)\), where \(k\) is a neighbour of \(j\) and is not a neighbour of \(i\) in \(B\), the vertices \(i\) and \(j\) in \(A - B\) have a common neighbour in \(B\).

Let \(ni\) be the number of neighbours (that, clearly, belong to \(B\)) of \(i\) in \(A - B\).

Let \(nj\) be the number of neighbours (that, clearly, belong to \(B\)) of \(j\) in \(A - B\).

The number of distinct paths of length \(2\) between \(i\) and \(j\) (paths that, clearly, go through \(B\)) – let this be \(nc\).

Then the test \(((N(i) - N(j)) \neq \emptyset)\) and \((N(j) - N(i)) \neq \emptyset\)) can be replaced with the test \(((ni - nc > 0)\) and \((nj - nc > 0)\)).

A cut, vertex cut, or separating set of a connected graph \(G\) is a set of vertices whose removal renders \(G\) disconnected. The connectivity or vertex connectivity \(k(G)\) is the size of a smallest vertex cut. A graph is called \(k\)-connected or \(k\)-vertex-connected if its vertex connectivity is \(k\) or greater. A vertex cut for two vertices \(u\) and \(v\) is a set of vertices whose removal from the graph disconnects \(u\) and \(v\). The local connectivity \(k(u,v)\) is the size of a smallest vertex cut separating \(u\) and \(v\).

In [1] we can find the following result.

**Theorem 5** (Menger’s theorem). Let \(G\) be an undirected graph, and let \(u\) and \(v\) be nonadjacent vertices in \(G\). Then, the maximum number of pairwise-internally-disjoint \((u,v)\)-paths in \(G\) equals the minimum number of vertices from \(V(G) - \{u,v\}\) whose deletion separates \(u\) and \(v\).

By Menger’s theorem, for any two vertices \(u\) and \(v\) in a connected graph \(G\), the numbers \(k(u,v)\) can be determined efficiently using the max-flow min-cut algorithm. The Edmonds-Karp algorithm is an implementation of the Ford-Fulkerson method for computing the maximum flow in a flow network in \(O(nm^2)\). It is asymptotically slower than the relabel-to-front algorithm, which runs in \(O(n^3)\), but it is often faster in practice for sparse graphs. The algorithm was first published by a Russian
scientist, Yefim (Chaim) Dinic, in 1970 [6] and independently by Jack Edmonds and Richard Karp in 1972 [8] (discovered earlier). Dinic’s algorithm includes additional techniques that reduce the running time to $O(n^2 m)$.

So the algorithm for the minimum chain completion problem becomes:

**Algorithm – Minimum Chain Completion**

**Input:** A connected, non-complete graph $G = (V, E)$.

**Output:** The transformation of $G$ from bipartite graph to bipartite chain graph

```
begin
  For every $i \in A - B$
    For every $j \in A - B$
      If $((ni - nc > 0) \text{ and } (nj - nc > 0))$ then
        add $(i, k)$ to $E$ (where $k \in (N_G(j) - N_G(i)) \cap B$)
  end.

EndMinimumChainCompletion
```

The complexity is $O(n^2)$

7 CONCLUSIONS AND FUTURE WORK

In this paper we give an efficient recognition algorithm for bipartite chain graphs and some combinatorial optimization algorithms, based on weakly decomposition. We point out some applications of bipartite chain graphs in chemistry and approach the Minimum Chain Completion problem. Our future research will focus on recognition algorithms for weak-bisplit graphs.

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