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# On edge metric dimension of chemical chains

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**Abstract**

The fundamentals of edge metric dimension are examined in this study, along with constraints for various graph types and algorithms for quickly computing edge-resolving sets. The EMD of a graph is an uniqueness of the metric dimension, which originated from the graph's emphasis on vertex resolving sets. In this context, an edge-resolving set is a collection of vertices in which each edge of the graph can be particularly recognized by its distance from the vertices. In fields where edges must be found, such as network topology, robotic mobility, chemistry and combinatorial optimization, it is crucial.

***Subject Classification:*** *05C12, 05C76, 05C90, 68R10.*

***Keywords:*** *Resolving set, Metric basis, Metric dimension, Chemical chains.*

## 1. Introduction

Graph theory studies the relationships among objects which are represented as vertices and edges in a graph, making it one of the discrete mathematics branches involving distances, as the theory application in graphs distance is quite vast: network design, robot navigation, biochemical structure analysis, etc. In terms of measuring the ability to determine

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which edges in the graph may represent network vertices and fixing the set of reference points, known as the resolving set, the metric dimension of a graph is indeed a significant parameter.

To study the idea further, instead of vertices, edges are the distinguishing features that need to be identified in an edge metric dimension. For a given subset of vertices, which is an edge-resolving set, every edge in the graph has a distinct representation in terms of distances to selected vertices. Due to its relevance in network security, communication and transportation systems, an increasing interest has emerged. In this work, we study some theoretical aspects of the edge metric dimension, its complexity and ways of obtaining edge-resolving sets for various graph forms. A connected graph with at most one vertex connected to any two simple cycles is called cactus graph. This means that no two cycles share an edge, making the structure tree-like but with some loop.

Parachain square cactus graphs and triangular cactus graphs are particular kinds of cactus graphs, which are linked graphs where any two basic cycles share maximum one vertex. A triangular cactus graph is made up of triangle subgraphs (cycles of length 3) where each pair of cycles shares maximum one vertex; in a parachain square cactus graph the structure is made up of several square (cycle of length 4) subgraphs linked in a chain-like way. Since their restricted cycle-sharing properties enable fast algorithms for is-sues in network structures including shortest paths, coloring and reliability analysis, these charts are very important in network design, chemical graph theory and computational biology.

There are several effective methods for determining the EMD for specific types of graphs, that include trees. [1] Efficiently defined edge metric dimension for general graphs. [2] Discussed the metric dimension in graphs. [3] Talked about the EMD on few families of trees in their study. [4] Explored the EMD of prism graph. [5] Discussed convex polytopes related graph. [6] Explored graph related benzenoid tripod structure.

## 2. Parachain square cactus graph

**Theorem 1:** *Suppose EMD of parachain square cactus graph is n-1 for (n≥3).*

***Proof:*** To show that edge metric dimension of parachain square cactus graph is equal to $n$-1 for ($n$≥3), we will prove this using contradiction. Let us say that cardinality of parachain square cactus graph is $n$-1 ($n$≥3) (See Figure 1).

Let the graph have vertices given as $u_1,u_2,u_3..,v_1,v_2,v_3..,w_1,w_2,w_3..$ and the edges as $e_1, e_2,.. e_i$. To make contradictions let us suppose that $S = \{a_i,b_i\}$, for $n = 3$ that resolves all the edges, $S = \{a_i,b_i,c_i\}$, for $n = 4$ that resolves all

the edges and $S = \{a_i, b_i, c_i, d_i\}$ for $n = 5$ that resolves all the edges (See Table 1 and Table 2).

**Table 1**

**Comparison of vertices.**

| Cases | Vertices |
|---|---|
| $n = 3$ | $d(e_1 \mid S) = d(e_2 \mid S) = d(e_3 \mid S)$, $d(e_2 \mid S) = d(e_4 \mid S)$, $d(e_5 \mid S) = d(e_6 \mid S)$, $d(e_9 \mid S) = d(e_{10} \mid S)$, $d(e_{11} \mid S) = d(e_{12} \mid S)$, $d(e_4 \mid S) = d(e_5 \mid S)$, $d(e_3 \mid S) = d(e_4 \mid S) = d(e_6 \mid S)$, $d(e_7 \mid S) = d(e_8 \mid S) = d(e_{10} \mid S)$ |
| $n = 4$ | $d(e_3 \mid S) = d(e_4 \mid S) = d(e_5 \mid S) = d(e_6 \mid S)$, $d(e_5 \mid S) = d(e_6 \mid S)$, $d(e_7 \mid S) = d(e_8 \mid S)$, $d(e_9 \mid S) = d(e_{10} \mid S)$, $d(e_{11} \mid S) = d(e_{12} \mid S)$, $d(e_{13} \mid S) = d(e_{14} \mid S)$, $d(e_{15} \mid S) = d(e_{16} \mid S)$, $d(e_1 \mid S) = d(e_2 \mid S)$ |
| $n = 5$ | $d(e_5 \mid S) = d(e_6 \mid S)$, $d(e_7 \mid S) = d(e_8 \mid S)$ |

**Table 2**

**Comparison of vertices In general $\forall$ $n$, we obtain $r(e_{2n+3}|S) = r(e_{2n+4}|S)$.**

| Cases | Vertices |
|---|---|
| $n = 5$ | $d(e_9 \mid S) = d(e_{10} \mid S)$, $d(e_{11} \mid S) = d(e_{12} \mid S)$, $d(e_{13} \mid S) = d(e_{14} \mid S)$, $d(e_{15} \mid S) = d(e_{16} \mid S)$, $d(e_{17} \mid S) = d(e_{18} \mid S)$, $d(e_{19} \mid S) = d(e_{20} \mid S)$ |

This implies S is not a resolving set. Hence EMD is $n$, $\forall n \geq 3$.

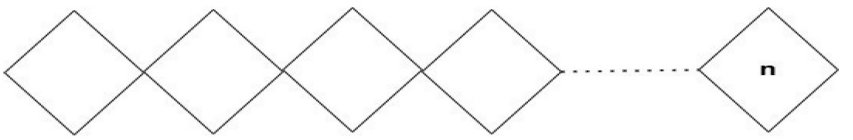



**Figure 1**

**Parachain n diagram.**

**Theorem 2:** *Let $R_z$ be a parachain square cactus graph the edge metric dimension at $n = 2$ is 2.*

***Proof:*** Let vertex subset is $S = \{w_1, v_3, w_2\}$. The minimum vertex subset is 3 that resolve all the edges (See Figure 2).

**Case 1**

$$r(e_i \mid S) = \begin{cases} (2-i,3,2) & \text{if i=1,2} \\ (4-i,2,1) & \text{if i=3,4} \\ (1,1,6-i) & \text{if i=5,6} \\ (2,0,8-i) & \text{if i=7,8} \end{cases}$$

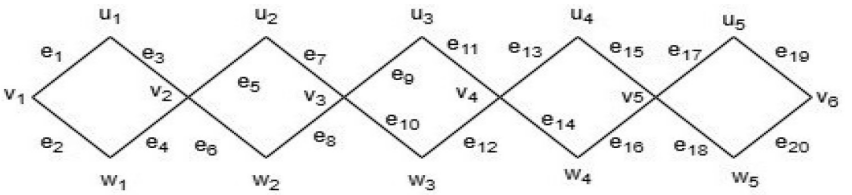



**Figure 2**

**Parachain graph $R_5$.**

**Theorem 3**: *Let $R_z$ be a parachain square cactus graph the edge metric dimension at n≥3 is n.*

***Proof:*** **Case 2:**

$$r(e_i \mid S) = \begin{cases} (2-i,2,4) & \textit{if} \text{ i=1,2} \quad \& \quad (4-i,1,3) & \textit{if} \text{ i=3,4} \\ (1,6-i,2) & \textit{if} \text{ i=5,6} \quad \& \quad (2,8-i,1) & \textit{if} \text{ i=7,8} \\ (3,1,10-i) & \textit{if} \text{ i=9,10} \quad \& \quad (4,2,12-i) & \textit{if} \text{ i=11,12} \end{cases}$$

$S = \{w_1, w_2, w_3\}$. The minimum vertex subset is 3 at $n = 3$ that resolve all the edges. Now we further find resolving set for $n = 4, 5$ and generalized them and from this we find our generalized dimension that is $n$ for n≥3.

**Case 3:**

$$r(e_i \mid S) = \begin{cases} (2-i,2,4,6) & \textit{if} \text{ i=1,2} \,\&\, (3,1,10-i,2) & \textit{if} \text{ i=9,10} \\ (4-i,1,3,5) & \textit{if} \text{ i=3,4} \,\&\, (4,2,12-i,1) & \textit{if} \text{ i=11,12} \\ (1,6-i,2,4) & \textit{if} \text{ i=5,6} \,\&\, (5,3,1,i-13) & \textit{if} \text{ i=13,14} \\ (2,8-i,1,3) & \textit{if} \text{ i=7,8} \,\&\, (6,4,2,i-15) & \textit{if} \text{ i=15,16} \end{cases}$$

Let $S = \{w_1, w_2, w_3, u_4\}$ the minimum vertex subset is 4 at $n = 4$ that resolve all the edges.

**Case 4:**

$$r(e_i \mid S)=\begin{cases} (2-i,2,4,6,8)\text{if i=1,2} & \& \quad (4-i,1,3,5,7)\text{if i=3,4} \\ (1,6-i,2,4,6)\text{if i=5,6} & \& \quad (2,8-i,1,3,5)\text{if i=7,8} \\ (3,1,10-i,2,4)\text{if i=9,10} & \& \quad (4,2,12-i,1,3)\text{if i=11,12} \\ (5,3,1,i-13,2)\text{if i=13,14} & \& \quad (6,4,2,i-15,1)\text{if i=15,16} \\ (7,5,3,1,18-i)\text{if i=17,18} & \& \quad (8,6,4,2,20-i)\text{if i=19,20} \end{cases}$$

Let $S = \{w_1,w_2,w_3,u_4,w_5\}$ the minimum vertex subset is 5 at $n = 5$ that resolve all the edges.

**Case 5:** Let $S_n = \{w_1,w_2,w_3\}$ an n = 3. We define $S_{n+1,}$ ∀n≥3. Define

$$S_{n+1}=\begin{cases} S_n \cup \{u_n; n \geq 4\} n \text{ is odd} \\ S_n \cup \{w_n; n \geq 5\} n \text{ is even} \end{cases}$$

Distance of edges of $R_n$ w.r.t $S_{n+1}$ for n dimension.

$$r(e_i \mid S_{n+1})=\begin{cases} (1,\ 2,\ 4,\ 6,\ 8,\ \ldots,\ 2(n-1)) & \text{if } i\ =\ 1 \\ (0,\ 2,\ 4,\ 6,\ 8,\ \ldots,\ 2(n-1)) & \text{if } i\ =\ 2 \\ (1,\ 1,\ 3,\ 5,\ 7,\ \ldots,\ 2(n-2)+1) & \text{if } i\ =\ 3 \\ (0,\ 1,\ 3,\ 5,\ 7,\ \ldots,\ 2(n-2)+1) & \text{if } i\ =\ 4 \\ (1,\ 1,\ 2,\ 4,\ 6,\ \ldots,\ 2(n-2)) & \text{if } i\ =\ 5 \\ (1,\ 0,\ 2,\ 4,\ 6,\ \ldots,\ 2(n-2)) & \text{if } i\ =\ 6 \\ (2,\ 1,\ 1,\ 3,\ 5,\ \ldots,\ 2(n-3)+1) & \text{if } i\ =\ 7 \\ (2,\ 0,\ 1,\ 3,\ 5,\ \ldots,\ 2(n-3)+1) & \text{if } i\ =\ 8 \\ (3,\ 1,\ 1,\ 2,\ 4,\ \ldots,\ 2(n-3)) & \text{if } i\ =\ 9 \\ (3,\ 1,\ 0,\ 2,\ 4,\ \ldots,\ 2(n-3)) & \text{if } i\ =\ 10 \\ (4,\ 2,\ 1,\ 1,\ 3,\ \ldots,\ 2(n-4)+1) & \text{if } i\ =\ 11 \\ (4,\ 2,\ 0,\ 1,\ 3,\ \ldots,\ 2(n-4)+1) & \text{if } i\ =\ 12 \\ (5,\ 3,\ 1,\ 0,\ 2,\ 4,\ \ldots,\ 2(n-4)) & \text{if } i\ =\ 13 \\ (5,\ 3,\ 1,\ 1,\ 2,\ 4,\ \ldots,\ 2(n-4)) & \text{if } i\ =\ 14 \\ (6,\ 4,\ 2,\ 0,\ 1,\ 3,\ 5,\ \ldots,\ 2(n-4)+1) & \text{if } i\ =\ 15 \\ (6,\ 4,\ 2,\ 1,\ 1,\ 3,\ 5,\ \ldots,\ 2(n-4)+1) & \text{if } i\ =\ 16 \\ (7,\ 5,\ 3,\ 1,\ 1,\ 2,\ 4,\ \ldots,\ 2n-5) & \text{if } i\ =\ 17 \\ (7,\ 5,\ 3,\ 1,\ 0,\ 2,\ 4,\ \ldots,\ 2(n-5)) & \text{if } i\ =\ 18 \\ (8,\ 6,\ 4,\ 2,\ 1,\ 1,\ 3,\ \ldots,\ 2(n-5)+1) & \text{if } i\ =\ 19 \\ (8,\ 6,\ 4,\ 2,\ 0,\ 1,\ 3,\ \ldots,\ 2(n-5)+1) & \text{if } i\ =\ 20 \\ \vdots & \\ ((i-3)/2,(i-7)/2,(i-11)/2,(i-15)/2,n,1+(-1)^i/2) & \text{if } i \text{ is odd}, i \geq 21 \\ ((i-4)/2,(i-8)/2,(i-12)/2,(i-16)/2,\ n,1+(-1)^i/2) & \text{if } i \text{ is even}, i \geq 22 \end{cases}$$

### 3. Triangular chain graph

**Theorem 4:** *Let $Q_z$ be a chain triangular cactus graph the EMD at n = 2 will be 2.*

***Proof:*** Let vertex subset is $S = \{w_2, u_1, u_3\}$. The minimum vertex subset is 3 that resolve all the edges (See Figure 3).

**Case 1:**

$$r(e_i \mid S) = \begin{cases} (2,0,2) \text{if i=1} \\ (1,3=i,1) \text{if i=2,3} \\ (0,i-3,5-i) \text{if i=4,5} \\ (1,1,0) \text{if i=6} \end{cases}$$

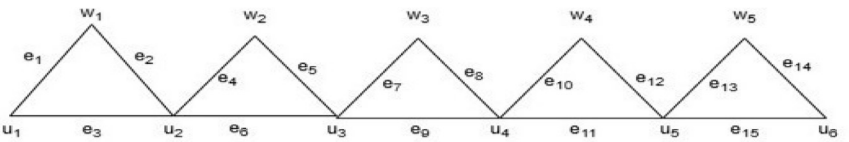



**Figure 3**

**Chain triangular cactus graph $Q_5$.**

**Theorem 5:** *The EMD of chain triangular cactus graph is n-1 for (n≥3).*

***Proof:*** To show that edge metric dimension of chain triangular cactus graph is equal to *n*-1 for (*n*≥3), we will prove contradiction. Let us say that cardinality of chain triangular cactus graph is *n*-1 (*n*≥3).

Let the graph have vertices given as $w_1, w_2, w_3.., u_1, u_2, u_3..$ *and* the edges as $e_1, e_2,.. e_i$. to make contradiction let us suppose that $S = \{a_i, b_i\}$ for $n = 3$ that resolves all edges. $S = \{a_i, b_i, c_i\}$ for $n = 4$ that resolves all edges, $S = \{a_i, b_i, c_i, d_i\}$ for $n = 5$ that resolves all edges (See Table 3).

**Table 3**

**Comparison of vertices In general $\forall n$, we obtain $d(e_{3n-2} \mid S) = d(e_{3n} \mid S)$.**

| Cases | Vertices |
|---|---|
| $n = 3$ | $d(e_7 \mid S) = d(e_9 \mid S), d(e_2 \mid S) = d(e_3 \mid S) = d(e_4 \mid S) = d(e_6 \mid S), d(e_5 \mid S) = d(e_7 \mid S) = d(e_9 \mid S), d(e_5 \mid S) = d(e_6 \mid S) = d(e_7 \mid S),$ |
| $n = 4$ | $d(e_7 \mid S) = d(e_9 \mid S), d(e_8 \mid S) = d(e_{12} \mid S), d(e_5 \mid S) = d(e_7 \mid S), d(e_{10} \mid S) = d(e_{12} \mid S) = d(e_8 \mid S), d(e_2 \mid S) = d(e_3 \mid S) = d(e_4 \mid S)$ |
| $n = 5$ | $d(e_2 \mid S) = d(e_3 \mid S = d(e_4 \mid S), d(e_5 \mid S) = d(e_7 \mid S), d(e_8 \mid S) = d(e_{10} \mid S), d(e_{11} \mid S) = d(e_{13} \mid S) = d(e_{15} \mid S), d(e_{13} \mid S) = d(e_{15} \mid S), d(e_5 \mid S) = d(e_6 \mid S) = d(e_7 \mid S)$ |

This implies $S$ is not a resolving set. Hence edge metric dimension is $n$ for ($n$≥3).

**Theorem 6:** *Suppose $Q_z$ be a chain triangular cactus graph the edge metric dimension at n≥3 is n.*

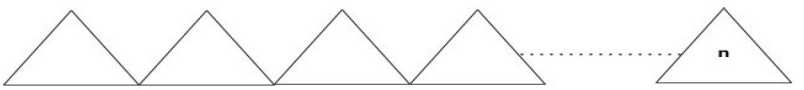



**Figure 4**

**Chain triangular cactus graph n terms.**

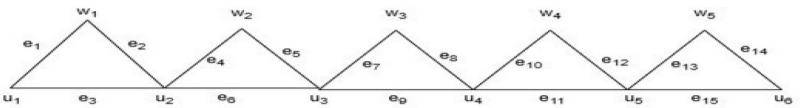



**Figure 5**

**Traingular cactus graph $Q_5$.**

***Proof:*** Let $S = \{w_2, w_3, u_1\}$. The minimum vertex subset is 3 at 3 that resolve all the edges (See Figure 4 and Figure 5).

**Case 2:**

$$r(e_i \mid S) = \begin{cases} (2,3,0)\text{if i=1} \\ (1,2,3-i)\text{if i=2,3} \\ (0,6-i,i-3)\text{if i=4,5} \\ (1,7-i,i-5)\text{if i=6,7} \\ (10-i,i-8,11-i)\text{if i=8,9} \end{cases}$$

The resolving set for $n$ = 3 should be found first, followed by the resolving set for $n$ = 4, 5 and their generalization. We further expand our dimension and establish the statement that, for $n$≥3, our dimension is $n$.

**Case 3*:***

$$r(e_i \mid S) = \begin{cases} (2,3,0,4)\text{if i=1} & \& \quad (1,2,3-i,3)\text{if i=2,3} \\ (0,6-i,i-3,7-i)\text{if i=4,5} & \& \quad (1,7-i,i-5,2)\text{if i=6,7} \\ (10-i,i-8,11-i,1)\text{if i=8,9} & \& \quad (2,1,3,1)\text{if i=10} \\ (14-i,13-i,15-i,0) & \text{if} \quad \text{i=11,12} \end{cases}$$

Let $S = \{w_2, w_3, u_1, u_5\}$. The minimum vertex subset is 4 at 4 that resolve all the edges.

Case 4:

$$r(e_i \mid S) = \begin{cases} (2,3,5,0,5)\text{if i=1} & \& \quad (1,2,4,3-i,4)\text{if i=2,3} \\ (0,6-i,8-i,i-3,8-i)\text{if i=4,5} & \& \quad (1,7-i,3,i-5,3)\text{if i=6,7} \\ (2,0,2,3,2)\text{if i=8} & \& \quad (i-8,1,2,i-7,2)\text{if i=9,10} \\ (3,2,1,4,1)\text{if i=11} & \& \quad (i-10,i-11,13-i,i-9,1)\text{if i=12,13} \\ (18-i,17-i,i-14,19-i,0) & \text{if} \quad \text{i=14,15} \end{cases}$$

Let $S = \{w_2, w_3, w_5, u_1, u_8\}$. The minimum vertex subset is 5 at dimension 5 that resolve all the edges. Hence proved that the edge metric dimension for triangular chain cactus graph is $n$ for $n \geq 3$.

For n dimension of $Q_n$

Let $S_n = \{w_2, w_3, u_1\}$ for $n = 3$. Define $S_n = \{w_2, w_3, u_1\} \cup \{u_{n+1} | n \geq 4\} \cup \{w_k | 5 \leq k \leq n\}$, $n \geq 4$.

$$r(e_i \mid S_n) = \begin{cases} (2,3,0,n,5,6,7,\ldots,n) & \text{if } i=1 \\ (1,2,1,n-1,4,5,6,\ldots,n-1) & \text{if } i=2 \\ (1,2,0,n-1,4,5,6,\ldots,n-1) & \text{if } i=3 \\ (0,2,1,n-1,4,5,6,\ldots,n-1) & \text{if } i=4 \\ (0,1,2,n-2,3,4,5,\ldots,n-2) & \text{if } i=5 \\ (1,1,1,n-2,3,4,5,\ldots,n-2) & \text{if } i=6 \\ (1,0,2,n-2,3,4,5,\ldots,n-2) & \text{if } i=7 \\ (2,0,3,n-3,2,3,4,\ldots,n-3) & \text{if } i=8 \\ (1,1,2,n-3,2,3,4,\ldots,n-3) & \text{if } i=9 \\ (2,1,3,n-3,2,3,4,\ldots,n-3) & \text{if } i=10 \\ (3,2,4,n-4,1,2,3,\ldots,n-4) & \text{if } i=11 \\ (2,3,0,n-4,1,2,3,\ldots,n-4) & \text{if } i=12 \\ (3,2,4,n-4,0,2,4,6,\ldots,n-4) & \text{if } i=13 \\ (4,3,5,n-5,0,1,2,3,\ldots,n-5) & \text{if } i=14 \\ (3,2,4,n-5,1,1,2,3,\ldots,n-5) & \text{if } i=15 \\ (4,3,5,n-5,1,0,2,3,\ldots,n-5) & \text{if } i=16 \\ \vdots & \\ (i-12,i-13,i-11,n-s,\ldots,n-s) & \text{if } i \geq 17, s \geq 6 \end{cases}$$

Hence the edge metric dimension for triangular chain cactus graph $Q_n$ is n, $\forall n \geq 3$.

## Application

Its applications can be seen in areas of network discovery and verification explored by [7]. Landmarks in graphs is discussed by [8], image processing by [9]. The strong resolving graph and the strong metric dimension of cactus graphs is discussed by [10-18].

## Conclusion

Both chemical cactus chains has an EMD $n$ for $n \geq 3$. These results demonstrate the distinct chemical structures and their EMD offers important insight within their potential reactivity or stability in the graph theory and engineering field.

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