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Bounded Autocatalytic Set and Its Basic Properties

Sumarni Abu Bakar[1,*], Noor Syamsiah Mohd Noor[1], Tahir Ahmad[2], Siti Salwana Mamat[3]

[1]College of Computing, Informatics and Media, Universiti Teknologi MARA, 40450, Shah Alam, Selangor, Malaysia
[2]Faculty of Science, Universiti Teknologi Malaysia, 81310, Skudai, Johor, Malaysia
[3]Centre of Foundation Studies, Universiti Teknologi MARA, 43800, Dengkil, Selangor, Malaysia

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Abstract Autocatalytic Set (ACS) is one of the areas of study that can be modelled using graph theory. An Autocatalytic Set (ACS) is defined as a graph, in which there is at least one incoming link for every node in the graph. Past research on ACS tremendously solved many applications including modelling complex systems through integration of ACS with fuzzy theory. Recently, a restricted form of ACS known as Weak Autocatalytic Set (WACS) was established and used to solve multi-criteria decision-making problems (MCDM), in which the related graph is transitive and involves non-cyclic triads. Though, in scenarios that occur in the real world, there exist MCDM problems, in which the related graph is intransitive, involving cyclic triads. Thus, it creates a limitation to used WACS to solve decision-making problems over cyclic triads. This paper introduced another class of ACS known as Bounded Autocatalytic Set (BACS). The concept of BACS provides the ability to represent a relation between one criterion to each other criterion, and the graph involves cyclic triads. Here, the definition of BACS is formed and introduced for the first time, and its basic properties related to edges, paths, and cycles in the form of theorem and propositions are established and presented.

Keywords Autocatalytic Set, Weak Autocatalytic Set, Graph Theory, Fuzzy Autocatalytic Set, Fuzzy Weak Autocatalytic Set

1. Introduction

The theory of an Autocatalytic Set (ACS) was firstly introduced in describing the origin of life, which was explained from a set of molecular species that catalyzed its member species [1-3]. Later, [4] portrayed the ACS as a directed graph where vertices represent species, and their catalytic relations are represented by directed edges. The formal definition of ACS is a subgraph where each node has at least one incoming link from vertices of the same subgraph [4]. The ACS is utilized in depicting the dynamical system such as in modelling a pressurized water reactor in a nuclear power generation [5]. Subsequently, [6] established another new theory from the combination of the concept of fuzzy graph and the concept of ACS called Fuzzy Autocatalytic Set (FACS). The FACS is described as a subgraph where each vertex has at least one incoming link with the membership value $\mu(e_i) \in (0,1]$, $\forall$ $(e_i) \in E$ [6]. The modelling of combustion process in clinical waste [6] and circulating fluidized bed boiler [7] are some examples of application of the concept of FACS.

Then, the ACS concept is extended to model tournament graph resultant on a new version of ACS called Weak Autocatalytic Set (WACS) [8]. The WACS is defined as a non-loop subgraph that contains a vertex with no incoming link. Several theorems which relate to ACS with potential graph and transitive tournament graph are established [9]. Later, the concept of WACS is expanded with uncertainty relationship between its vertices that is fuzzy edges that led to a new version of ACS known as Fuzzy Weak Autocatalytic Set (FWACS) [8]. The FWACS is described as a WACS where each edge, e_i has a membership value $\mu(e_i) \in (0,1]$ for $e_i \in E$. The concept of FWACS has been applied in the valorization of cultural heritage with the help of Potential Method [8].

In this study, ACS is further explored on its structure for every vertex in the graph contain incoming link from every other vertex. Its basic properties related to the edges, path, and cycles are investigated.

The paper is organized as follows. Section 2 provides preliminaries related to the study. The Bounded ACS is introduced in Section 3 and some results on its basic properties are presented.

2. Preliminaries

The idea of graph theory was pioneered by a mathematician named Leonhard Euler to solve the problem of the Königsberg bridges [10]. The problem was to locate a tour of the city where the walk path should not traverse each bridge more than once and each bridge must be totally traversed every time. Generally, the theory of graph is described as a group of nodes or points which are joined by links [11]. The graph is formally defined in Definition 1. An example of a graph with four nodes is illustrated in Figure 1.

Definition 1 [11]. A graph, G (V, E) consist of a set of vertices or nodes, V and a set of edges or links, E.

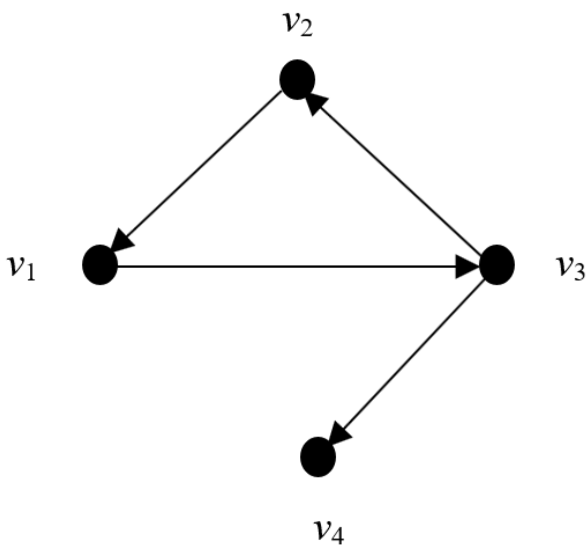


Figure 1. A graph with four nodes

Besides, a graph can be transformed into an adjacency matrix. The definition of adjacency matrix is given as in Definition 2.

Definition 2 [12]. An adjacency matrix of graph G (V, E) with n nodes, is an $n \times n$ matrix, where $a_{ij} = 1$ if E consists a directed edge from node j to node i, and $a_{ii} = 0$ if otherwise.

Thus, an adjacency matrix for the graph in Figure 1 is represented as

$$A = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix} \quad (1)$$

Several other definitions describing graph such as cyclic graph, strongly connected graph, complete symmetric digraph, Hamiltonian cycle, Hamiltonian graph which related to the study are presented as follows.

Definition 3 [13]. A cyclic graph is a graph that contains at least one graph cycle which is known as cyclic graph.

Definition 4 [14]. A strongly connected graph occurs when a path exists from vertex u to v and v to u for any two vertices.

Definition 5 [15]. A complete symmetric digraph is a digraph D (V, A) where V is a set of vertices and A is a set of arcs. A digraph D (V, A) is complete if both uv and vu $\in A$ for all $u, v \in V$.

Definition 6 [16]. A Hamiltonian cycle, also called Hamiltonian circuit, is a graph that contains a cycle (closed path) that passes through all vertices exactly once.

Definition 7 [17]. A Hamiltonian graph is a graph that possesses a Hamiltonian circuit (Hamiltonian cycle).

In the next subsection, the concept of Autocatalytic Set (ACS) is discussed briefly.

2.1. Autocatalytic Set (ACS)

The idea of an Autocatalytic Set (ACS) was firstly proposed in chemistry by Stuart A. Kauffman in 1971, in which a set of catalytic reaction peptide molecules were investigated [18]. An Autocatalytic Set also can be called a self-sustaining chemical reaction where molecules are mutually catalyzed by each other [19]. Furthermore, an Autocatalytic Set can be described as a group of entities which can be people, molecules or objects [20]. The term autocatalytic is best portrayed as catalyzed compounds or chemical reactions. A catalyst acts as an element or substance that accelerates a chemical reaction without changing its own make up. The ACS is formally defined as follows.

Definition 8 [4]. An Autocatalytic Set is a subgraph where each node has at least one incoming link from a node that belongs to the identical subgraph.

Some examples of the Autocatalytic Set (ACS) are shown in Figure 2.

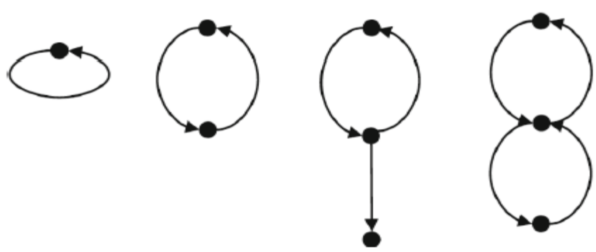


Figure 2. The Autocatalytic Sets

Subsequently, some features of ACS have been constructed in the form of theorems and lemma which are presented as follows.

Theorem 1 [4,21].

(i) All cycles are irreducible subgraphs, and all irreducible subgraphs are ACSs.

(ii) Not all ACSs are irreducible subgraphs and not all irreducible subgraphs are cycles.

Theorem 2 [21]. An ACS should contain a closed walk. Therefore,

(i) If a graph G has no ACS, then $\lambda_1(C) = 0$.

(ii) If a graph G has ACS, then $\lambda_1(C) \geq 1$.

Theorem 3 [21]. The subgraph of any Perron-Frobenius Eigenvector (PFE) of graph G is an ACS, if $\lambda_1(C) \geq 1$.

Lemma 1 [20]. If $G(V, E)$ is an ACS and $|V| = n$, then $|E| \leq n^2$.

Theorem 4 [20]. Any Autocatalytic Set $G(V, E)$ with n nodes has edges at most n^2 that is $|E| \leq n^2$ where $E(n)$ is a group of edges with n nodes.

In the following subsection, a Weak Autocatalytic Set (WACS) is presented.

2.2. Weak Autocatalytic Set (WACS)

A Weak Autocatalytic Set (WACS) is a new mathematical concept that is derived from a transitive tournament graph [8]. Formal definition of Weak Autocatalytic Set (WACS) is given in Definition 9. Several examples of WACS are shown in Figure 3.

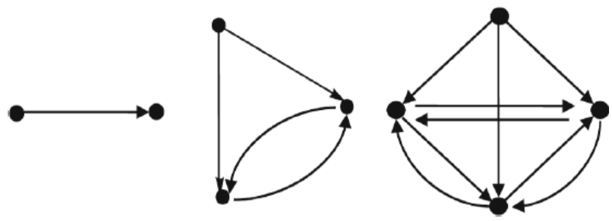


Figure 3. The Weak Autocatalytic Sets

Definition 9 [8]. A Weak Autocatalytic Set (WACS) is a non-loop subgraph that consists of a node with no incoming link.

Several features related to path and edges of Weak Autocatalytic Set (WACS) in form of theorems are deduced as follows.

Theorem 5 [9]. Every WACS is a weak connected graph.

Theorem 6 [9]. Every WACS must have at least a path, which is not closed.

Theorem 7 [9]. Let $G(V, E)$ be a WACS defined by

$$G_k \begin{cases} 0 & \text{when } i = j \text{ and } e_i \notin E \\ \mu(e_i) \in \{0,1\} & \text{when } i \neq j \text{ and } e_i \in E \end{cases} \quad \text{for } k = 1, 2, \ldots, n.$$

Consider $G = \{G_k : k = 1, 2, \ldots, n\}$ be a finite set of WACS and let $M^{n\times n}_F = \{[a_{ij}]^{n\times n} : a_{ij} \in \{0,1\}$ with $a_{ii} = 0\}$ be a square matrix. Define $f : G \rightarrow M^{n\times n}_F \ni f(G_k) = [a_{ij}]$. Then f is a bijective function.

Theorem 8 [9]. If $G(V, E)$ is a WACS and $|V| = n$, then $|E| \leq (n-1)^2$.

Theorem 9 [9]. Every WACS is a fuzzy graph.

Next subsection introduced a new type of ACS called Bounded Autocatalytic Set (BACS).

3. Bounded Autocatalytic Set (BACS)

This section presents the Bounded Autocatalytic Set (BACS). The BACS is defined formally as follows.

Definition 10. A Bounded Autocatalytic Set (BACS) is a non-loop subgraph $G(V, E)$ in which each vertex $v \in V$ has exactly $(n-1)$ incoming and $(n-1)$ outgoing links for $|V| = n$.

Some examples of BACS are illustrated in Figure 4.

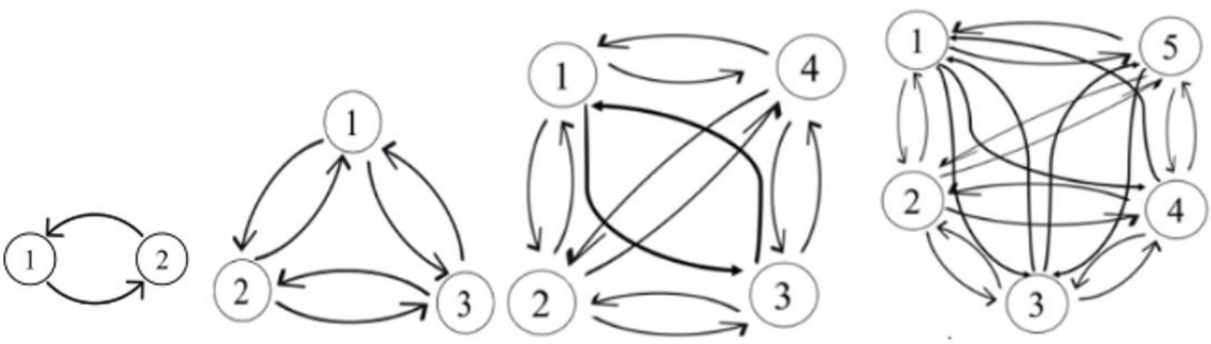


Figure 4. Examples of BACS

The analysis of number of edges, incoming and outgoing link for each node as well as closed path for the BACS graph in Figure 4 are presented in Table 1.

Table 1. Analysis of the BACS graph

Number of nodes, *V*	**Number of edges, *E***	**Incoming link for each node**	**Outgoing link for each node**	**Closed path**
2	2	1	1	2
3	6	2	2	12
4	12	3	3	44
5	20	4	4	80
n	$n(n-1)$	$(n-1)$	$(n-1)$	

If there are two nodes in the graph, then the number of edges is two. If the number of nodes is three, four and five, then the number of edges is six, twelve and twenty, respectively. Eventually, when the number of node is n, then it is expected there is $n(n-1)$ number of edges in the graph. Furthermore, if the number of nodes in the graph is two, three, four and five, then the number of incoming link and outgoing link for each node is one, two, three and four, respectively. Eventually, when the number of node is n, then the number of incoming link and outgoing link for each node is $(n-1)$.

Where does the word "Bounded" comes from? The word comes from the maximum number of incoming links for each vertex. As shown in Table 1, the number of incoming links for each node in the BACS fulfilled the following inequality.

$1 \leq |\text{incoming links}| \leq (n-1)$ for $n > 1$

Here, the number of incoming links for BACS is bounded between 1 and $(n-1)$ for $n > 1$. The following theorem, propositions and corollary present some features of BACS.

Generally, a BACS with n nodes contains a node with incoming and outgoing links. The following theorem proves that a BACS with n nodes has exactly $n(n-1)$ edges.

Theorem 10. If $G(V, E)$ is a BACS and $|V| = n$, then $|E| = n(n-1)$.

Proof. Let $G(V, E)$ be a BACS and $|V| = \{v_1, v_2, \ldots, v_n\}$. Thus, every node in G has incoming link and $|V| = n$. Hence, $|E|$ is as shown below.

$$|E| = \left| \left\{ \begin{matrix} (v_1,v_2) & (v_1,v_3) & (v_1,v_4) & \ldots & (v_1,v_n) \\ & (v_2,v_3) & (v_2,v_4) & \ldots & (v_2,v_n) \\ & & (v_3,v_4) & \ldots & (v_3,v_n) \\ & & & \ddots & \vdots \\ & & & & (v_{n-1},v_n) \end{matrix} \right\} \right| \cup \left| \left\{ \begin{matrix} & & & & (v_n,v_{n-1}) \\ & & & (v_n,v_{n-2}) & (v_{n-1},v_{n-2}) \\ & & (v_n,v_{n-3}) & (v_{n-1},v_{n-3}) & (v_{n-2},v_{n-3}) \\ & \iddots & \vdots & \vdots & \vdots \\ (v_n,v_1) & (v_{n-1},v_1) & (v_{n-2},v_1) & \ldots & (v_2,v_1) \end{matrix} \right\} \right| \tag{2}$$

Thus,

$$|E| = \left[\sum_{j=2}^{n} |(v_1,v_j)| + \sum_{j=3}^{n} |(v_2,v_j)| + \sum_{j=4}^{n} |(v_3,v_j)| + \cdots + 2 + 1 \right] + \left[1 + 2 + \cdots + \sum_{j=4}^{n} |(v_j,v_3)| + \sum_{j=3}^{n} |(v_j,v_2)| + \sum_{j=2}^{n} |(v_j,v_1)| \right] \tag{3}$$

Consequently,

$$\begin{aligned} |E(n)| &= \binom{n}{2} + \binom{n}{2} \\ &= 2\binom{n}{2} \\ &= 2\left(\frac{n!}{2!(n-2)!} \right) \\ &= \frac{n!}{(n-2)!} \\ &= \frac{n(n-1)(n-2)!}{(n-2)!} \\ &= n(n-1). \end{aligned} \tag{4}$$

Thus, $|E| = n(n-1)$. Hence, a BACS with n nodes has exactly $n(n-1)$ edges.

Next proposition shows that every BACS is an ACS.

Proposition 1. Every BACS is an ACS. (Trivial case)

Proof. Let $G(V, E)$ be a BACS. By definition of BACS, every node in G has $(n-1)$ incoming links for $n > 1$. This served the definition of ACS saying that every vertex must have at least one incoming link from the vertices of the same subgraph. Hence, every BACS is an ACS.

Figure 5 represents the relation between Bounded Autocatalytic Set (BACS) and Autocatalytic Set (ACS).

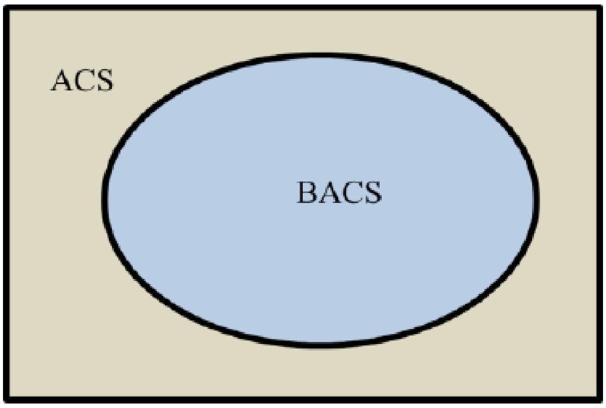


Figure 5. BACS is an ACS

Proposition 2. Every BACS has exactly one cycle between any pair of vertices in the graph.

Proof. Suppose $G(V, E)$ is a BACS with adjacency matrix $A = \begin{pmatrix} a_{11} & \cdots & a_{1n} \\ \vdots & \ddots & \vdots \\ a_{n1} & \cdots & a_{nn} \end{pmatrix}$ with $a_{ij} \neq 0$ for $i, j = 1, 2, 3, \ldots, n$.
Next, consider the sequence $a_{ij} \rightarrow a_{si} \rightarrow a_{ts} \rightarrow \ldots \rightarrow a_{pl} \rightarrow a_{jp}$.

We know that

a_{ij} indicates there exists a link from j to i

a_{si} indicates there exists a link from i to s

a_{ts} indicates there exists a link from s to t

$\vdots$

a_{pl} indicates there exists a link from l to p

a_{jp} indicates there exists a link from p to j.

Since all the link are connected and the path starts and ends at the same point (vertex), therefore the sequence in the form of $a_{ij} \rightarrow a_{si} \rightarrow a_{ts} \rightarrow \ldots \rightarrow a_{pl} \rightarrow a_{jp}$ forms a cycle.

Moreover, if $i = s = t = \ldots = l = p$, then $a_{jp} = a_{ij}$ which indicates that there exists a link from i to j. Thus, the sequence $a_{ij}\, a_{si}\, a_{ts} \ldots a_{pl}\, a_{jp}$ is reduced to $a_{ij}\, a_{ji}$ for $i \neq j$. This shows that there exists exactly one cycle between any pair of vertices in the graph.

The following propositions are shown to prove that BACS is a strongly connected graph and a complete symmetric digraph.

Proposition 3. Every BACS is a strongly connected graph.

Proof. Let $G(V, E)$ be a BACS with n vertices. If u and v are two arbitrary vertices in G, therefore by Proposition 2, there exists exactly one cycle between u and v which means there exists a path from vertex u to v and v to u. Thus, by Definition 4, every BACS is a strongly connected graph.

Proposition 4. Every BACS is a complete symmetric digraph.

Proof. Let $G(V, E)$ be a BACS. Thus, each vertex in G has an incoming and outgoing link from every other vertex in the same graph. Thus, there are two opposite edges for every two vertices, say, from u to v and from v to u. Hence, by Definition 5, every BACS is a complete symmetric digraph.

Next, proposition and corollary are shown to prove that BACS has at least a Hamiltonian cycle and it is a Hamiltonian graph.

Proposition 5. Every BACS has at least a Hamiltonian cycle.

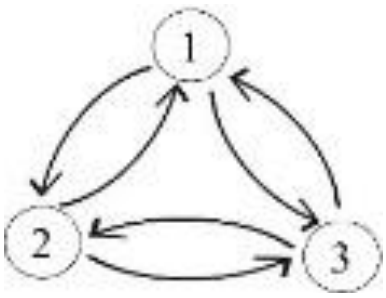
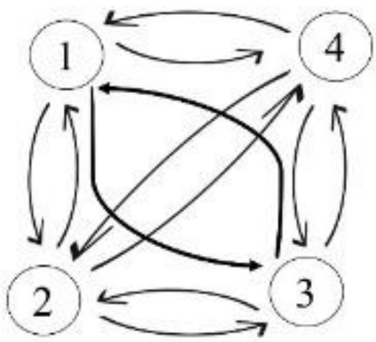
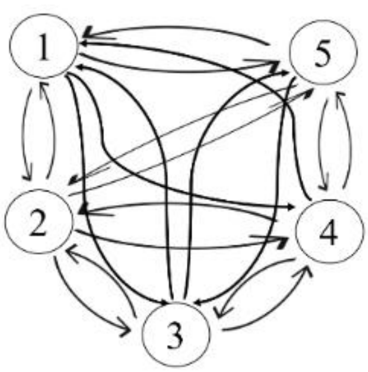
Proof. Let $G(V, E)$ be a BACS with n vertices. Suppose u and v are two arbitrary nodes in BACS, then there exists a walk from u to v in a sequence of $u = u, u_1, u_2, \ldots, u_j = v$. Since by Proposition 2, there exists exactly one cycle between any pair of vertices in the graph, then there exists a walk from v to u. Thus, a closed walk $u = u, u_1, u_2, \ldots, u_j = v, u$ is created. Hence, by Definition 6, it shows that every BACS has at least a Hamiltonian cycle.

Corollary 1. Every BACS is a Hamiltonian graph.

Proof. Let $G(V, E)$ be a BACS. From Proposition 5, every BACS has at least a Hamiltonian cycle. Thus, by Definition 7, every BACS is a Hamiltonian graph.

Table 2 illustrates the analysis of number of nodes, edges and Hamiltonian cycles for some BACS graphs in Figure 6. When there are two nodes in the graph, the number of edges is two, and it has one Hamiltonian cycle. If there are three nodes in the graph, then the number of edges is six, with two Hamiltonian cycles. Furthermore, if the graph has four nodes, the number of edges is twelve, with six Hamiltonian cycles. Lastly, if there are five nodes in the graph, then the number of edges is twenty, and has twenty-four Hamiltonian cycles. In addition, the Hamiltonian cycles are calculated by selecting an initial node first and then each circuit (cycle) will be counted n times rather than just once.

Table 2. Number of nodes, edges, and Hamiltonian cycles of BACS for n = 2, 3, 4, and 5

Graph	Number of Nodes, V	Number of Edges, E	Hamiltonian Cycles	Number of Hamiltonian Cycles
	2	2	1-2-1	1
	3	6	1-2-3-1 1-3-2-1	2
	4	12	1-2-3-4-1, 1-4-3-2-1 1-2-4-3-1, 1-3-4-2-1 1-4-2-3-1, 1-3-2-4-1	6
	5	20	1-2-3-4-5-1, 1-5-4-3-2-1 1-3-4-5-2-1, 1-2-5-4-3-1 1-4-5-3-2-1, 1-2-3-5-4-1 1-5-2-3-4-1, 1-4-3-2-5-1 1-5-4-2-3-1, 1-3-2-4-5-1 1-4-2-3-5-1, 1-5-3-2-4-1 1-3-5-2-4-1, 1-4-2-5-3-1 1-2-5-3-4-1, 1-4-3-5-2-1 1-2-4-3-5-1, 1-5-3-4-2-1 1-3-2-5-4-1, 1-4-5-2-3-1 1-4-3-5-2-1, 1-2-5-3-4-1 1-5-3-2-4-1, 1-4-2-3-5-1	24
	n	$n(n-1)$		$(n-1)!$

These relations and features are summarized in Figure 6.

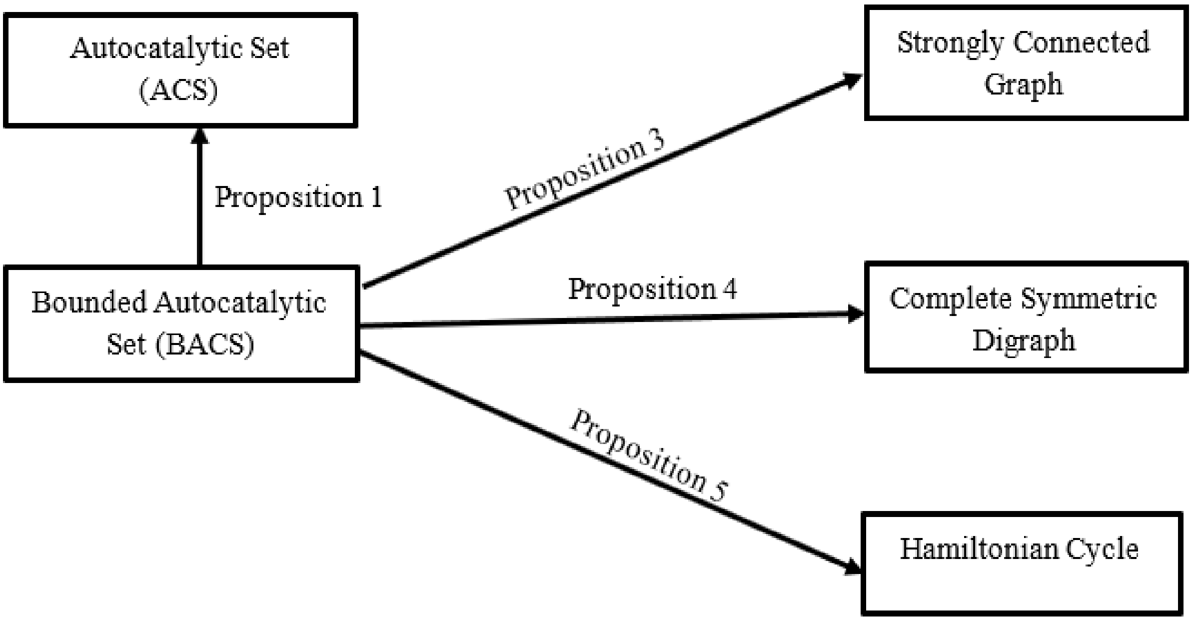


Figure 6. Some relations and features with respect to BACS

4. Conclusion

A new concept of Autocatalytic Set (ACS), namely Bounded Autocatalytic Set (BACS), is introduced in this paper. Several findings in the form of theorem, propositions and corollary pertaining to path and cycle are presented.

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