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Perfect Non-Neighbor Harmonic Graphs

A. Rizwana[1*], G. Jeyakumar[2], M. Mohamed Ismail[3]

[1]Dept. Mathematics, Manonmaniam Sundaranar University, Tirunelveli-12, India
[2]Dept. of Mathematics, St.John's College, Tirunelveli – 2, India
[3]Dept. of Computer Application, the New College, Chennai-14, India

[*]Corresponding Author: rijurizwana@gmail.com, Tel.: +91-8508435629

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Abstract— Computation of topological indices is a recent research problem in mathematical and computational chemistry. Based on the number of non-neighbors of a vertex u in a graph G, non-neighbor harmonic index is defined. In this paper we compute the non-neighbor harmonic polynomial of some graphs. We develop a MATLAB program for computing the roots of the non-neighbor harmonic polynomial and hence define the perfect non-neighbor harmonic graphs.

Keywords— Graphs, non-neighbors, non-neighbor harmonic polynomial, perfect non-neighbor harmonic graphs.

I. INTRODUCTION

Chemical graph theory is a branch of mathematical chemistry which deals with the nontrivial applications of graph theory to solve molecular problems. In chemical graph theory a topological representation of a molecule is called molecular graph or chemical graph. Chemical graph serves as a convenient model for any real or abstract chemical system. Molecular graph is connected undirected graph one-to-one corresponded to structural formula of chemical compound so that vertices of the graph correspond to atoms of the molecule and edges of the graph correspond to chemical bonds between these atoms. Graph theory [1] is largely applied to the characterization of chemical structures The characterization of a molecule by an associated graph leads to a large number of powerful and useful discriminators called topological indices. In chemical graph theory a topological index is a numerical parameter mathematically derived from hydrogen-suppressed molecular graphs. A topological index is a numerical descriptor of a molecule, based on a certain topological feature of the corresponding molecular graph such as distance based, degree based [2] and both degree and distance based.

In this paper we are concerned with simple graphs, having no directed or weighted edges, and no self-loops. A graph G is an ordered pair of two sets V and E. The set $V = V(G)$ is a finite non empty set and $E = E(G)$ is a binary relation defined on V. A graph can be visualized by representing the elements of V by vertices and joining the pair of vertices u,v by an edge if and only if $uv \in E$(G). Also we denote $|V(G)| = n$ and $|E(G)| = m$. The degree of the vertex $v \in V(G)$, written $d(v)$, is the number of first neighbors of v in the underlying graph G. Many topological indices have been introduced and studied: Randic Index [3], Wiener index [4], First and Second Zagreb indices and First and Second Zagreb coindices [5,6,7,8,9] are a few examples of these concepts. For terms and definition not given in this paper refer to [10].

The paper is organized as follows, Section I contains the introduction of chemical graphs and topological indices, Section II contain the related work of harmonic index, harmonic polynomial and non-neighbor harmonic index, Section III describes results and discussion of Non-Neighbor Harmonic Polynomial (NNHP) of graphs and Perfect Non-Neighbor Harmonic graphs. Non-Neighbor Harmonic Polynomial of some standard graphs and some special types of graph is calculated and a MATLAB program is developed for computing the roots and Section IV concludes the research work with the scope for future.

II. RELATED WORK

In the 1980s, Siemion Fajtlowicz created a vertex-degree-based quantity which was re-introduced by Zhong in 2012 called Harmonic Index [11]. The harmonic index is one of the most important indices in chemical and mathematical fields. The harmonic index gives better correlations with physical and chemical properties of molecules. It is defined as

$$H(G) = \sum_{uv \in E(G)} \left[\frac{2}{d(u) + d(v)}\right]$$

The vertices that are not adjacent to a vertex $v \in V(G)$ are called non-neighbors of the vertex v. In this paper we define $\overline{d(v)}$ as the number of the non-neighbors of the vertex $v \in V(G)$, where $\overline{d(v)} = n - 1 - d(v)$. Based on the non-neighbors of the vertices of a graph *G* topological indices called Non-Neighbor Zagreb Indices and Non-Neighbor Harmonic index have been introduced [12]. The Non-Neighbor Harmonic Index is defined as

$$\overline{H(G)} = \sum_{uv \in E(G)} \left(\frac{2}{\overline{d(u)} + \overline{d(v)}} \right)$$

Non-Neighbor Harmonic Index is considered to be an important Non-Neighbor Topological Index as its values of the Path graph P_n is well correlated with the boiling point of the alkanes in Organic Chemistry.

The Harmonic Polynomial [13] of a graph *G* is defined as $H(G,x) = 2\sum_{uv \in E(G)} \left(x^{d(u)+d(v)-1}\right)$ where

$$\int_0^1 H(G,x)\,dx = \mathrm{H(G)}$$

III. RESULTS AND DISCUSSION

(A) In this section, the formula for the Non-Neighbor Harmonic Polynomial (NNHP) of graphs is given. The Non-Neighbor Harmonic polynomial is computed for some standard graphs. After computing the polynomial, MATLAB program has been developed to find the roots of the graphs with *n* vertices. Based on the roots, Perfect Non-Neighbor Harmonic graphs are defined.

The Non-Neighbor Harmonic Polynomial of a graph *G* is defined as

$$\overline{H(G,x)} = \sum_{uv \in E(G)} \left(2x^{\overline{d(u)}+\overline{d(v)}-1}\right) \text{ where}$$
$$\int_0^1 \overline{H(G,x)}\,dx = \overline{H(G)}.$$

Perfect Non-Neighbor Harmonic (PNNH) graphs are those graphs for which at least one root for the Non-Neighbor Harmonic Polynomial computed using MATLAB programming is different from zero

Non-Neighbor Harmonic Index for the Complete graph K_n is zero as each of its vertex is adjacent to all the other vertices (i.e) each of its vertex has no non-neighbors. Hence the Non-Neighbor Harmonic polynomial cannot be computed for complete graphs.

Theorem 2.1: *For a k-regular graph G,* $\overline{H(G,x)} = nkx^{2n-2k-3}$

Proof: Since *G* is a *k*-regular graph, for every vertex *u* in *G*, we have

$$\overline{d(u)} = n - 1 - d(u).$$
$$= n - 1 - k$$

Hence $\overline{H(C_n,x)} = \sum_{uv \in E(G)} 2x^{n-1-k+n-1-k-1}$
$$= nkx^{2n-2k-3}$$

Theorem 2.2: *For a cycle* $C_n (n \geq 4)$, $\overline{H(C_n,x)} = 2nx^{2n-7}$

Proof: A cycle C_n has n vertices each with degree 2. The number of non-neighbors of each vertex $v \in V(G)$ is $(n-3)$. Since there are n edges,

$$\overline{H(C_n,x)} = \sum_{uv \in E(G)} 2x^{n-3+n-3-1}$$

$$= 2nx^{2n-7}$$

Theorem 2.3: *For a path* $P_n (n \geq 4)$, $\overline{H(P_n,x)} = 4x^{2n-6} + 2(n-3)x^{2n-7}$

Proof: A path P_n with n vertices has two pendant vertices and remaining are interior vertices each with degree 2. The number of non-neighbors of the pendant vertex is $(n-2)$. The number of non-neighbors of the interior vertex is $(n-3)$. There are totally $(n-1)$ edges in which 2 are corner edges and $(n-3)$ are interior edges. Hence,

$$\overline{H(P_n,x)} = 2[2x^{n-2+n-3-1}] + (n-3)[2x^{n-3+n-3-1}]$$

$$\overline{H(P_n)} = 4x^{2n-6} + 2(n-3)x^{2n-7}$$

Theorem 2.4: *For a complete bipartite graph,* $K_{p,q}$, $\overline{H(K_{p,q},x)} = 2pqx^{p+q-3}$

Proof: A complete bipartite graph has two set of vertices, V_1 with p vertices and V_2 with q vertices. Every vertex of V_1 is adjacent to all vertices of V_2 but no vertex within V_1 is adjacent. The non-neighbors of $v \in V_1$ is $V_1 - \{v\}$. The number of non-neighbors of $v \in V_1$ is $(p-1)$. Similarly the number of non-neighbors of $v \in V_2$ is $(q-1)$. There are totally pq edges. Hence

$$\overline{H(K_{p,q},x)} = \sum_{uv \in E(G)} 2x^{p-1+q-1-1}$$
$$= 2pqx^{p+q-3}$$

Corollary 2.4.1: *For a k-regular bipartite graph* $K_{k,k}$, $\overline{H(K_{k,k},x)} = 2k^2x^{2k-3}$

Corollary 2.4.2: *For a star graph* $S_k (k \geq 2)$, $\overline{H(S_k,x)} = 2kx^{k-2}$

Theorem 2.5: *For a wheel graph* $W_n (n \geq 4)$, $\overline{H(W_n,x)} = 2n[x^{2n-7} + x^{n-4}]$

Proof: A n-wheel graph W_n with $n+1$ vertices is formed by connecting a single vertex to all vertices of a cycle of length n. The vertex in the center has no non-neighbors. The remaining n vertices on the cycle each has $(n-3)$ non neighbors. Totally there are $2n$ edges in which n edges are in the cycle and n edges are between the central vertex and the cycle. Hence

$$\begin{aligned}\overline{H(W_n, x)} &= 2[nx^{n-3+n-3-1} + nx^{n-3-1}] \\ &= 2n[x^{2n-7} + x^{n-4}]\end{aligned}$$

Algorithm for finding the roots of the Non-Neighbor Harmonic Polynomial:

Let *G* be a connected simple graph with *n* vertices

Input: Number of vertices in graph *G*.

Step 1: Determine the Non-Neighbor Harmonic Polynomial of *G*.

Step 2: Determine the roots of the Non-Neighbor Harmonic Polynomial.

Step 3: Plot the figure of Non-Neighbor Harmonic Polynomial of *G*.

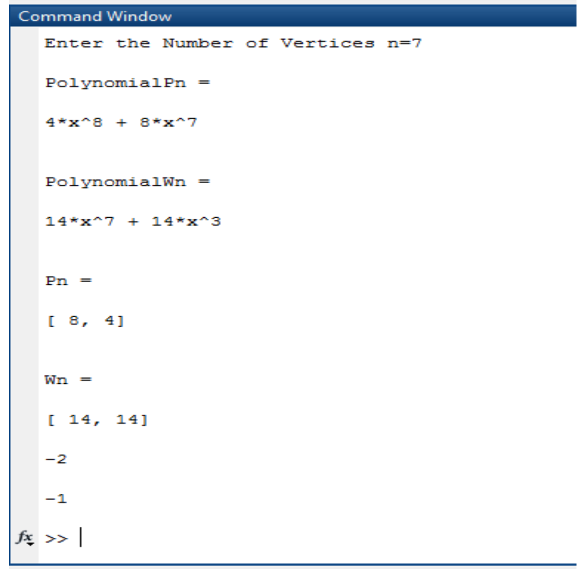
Output: Roots & Figure of the Non-Neighbor Harmonic Polynomial

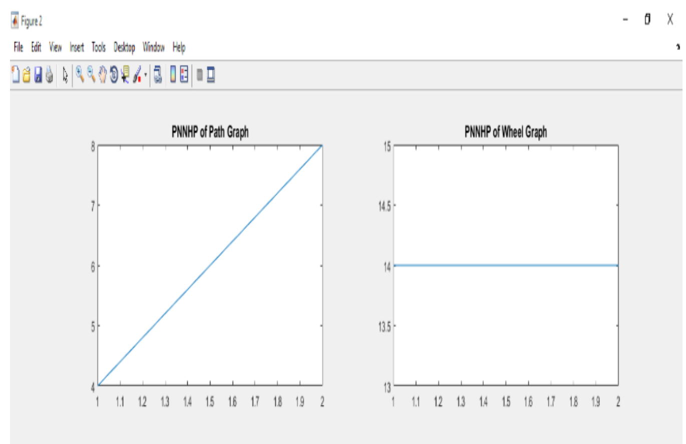
Numerical Example 1:

MATLAB Program for computing the roots of Standard Graphs:

```
clc
syms x
n=input('Enter the Number of Vertices n=');
PolynomialPn =4.*x^((2.*n)-6) + 2.*(n-3) .* x^(2.*n-7)
PolynomialWn =2.*n.*x^((2.*n)-7) + 2.*n.* x^(n-4)
Pn = coeffs(4.*x^((2.*n)-6) + 2.*(n-3) .* x^(2.*n-7))
Wn = coeffs(2.*n.*x^((2.*n)-7) + 2.*n.* x^(n-4))
Pn = fliplr(Pn);
Wn = fliplr(Wn);
z1=roots(Pn);
z2=roots(Wn);
disp(z1)
disp(z2)
figure
subplot(2,2,1)
plot(Pn)
title('PNNHP of Path Graph')
subplot(2,2,2)
plot(Wn)
title('PNNHP of Wheel Graph')
```

Screenshot of Program output





Inference:

For the graph with 7 vertices, non neighbor harmonic polynomial of path graph and wheel graph is computed as $4x^8 + 8x^7, 14\,x^7 + 14x^3$ and the roots are calculated as -2 and -1 respectively**.** Roots of the Non-Neighbor Harmonic Polynomial of the Path graph P_n and the Wheel graph W_n is other than zero. Hence the path graph P_n and Wheel graph W_n are defined to be Perfect Non-Neighbor Harmonic Graphs. Also the figure of Path P_n shows a gradual increase and hence it is applicable to compute the boiling point of the alkanes. As all the roots of other standard graphs are zero, we neglect these graphs in our program.

(B) In this section, The Non-Neighbor Harmonic polynomial for some special types of graph is computed. Using the MATLAB program roots of the Non-Neighbor Harmonic polynomial and hence Perfect Non-Neighbor Harmonic graphs among these following graphs are defined.

Definition 3.1: Sunlet graph: The n-sunlet graph G on $2n$ vertices [12] is obtained by attaching n pendant edges to the cycle $C_n(n \geq 3)$.

Definition 3.2: Complete *n*-sun Graph: A n-sun graph [12] is a chordal graph G with $2n$ vertices, $n \geq 3$, whose vertex set is partitioned into two sets $W = \{w_1, w_2, \ldots, w_{n-1}\}$ and $U = \{u_0, u_2, \ldots, u_{n-1}\}$, such that $U = \{u_0, u_2, \ldots, u_{n-1}\}$, induces a cycle, W is a stable set and for all $i \in \{0, 1, 2, \ldots, n-1\}$ w_i adjacent to exactly u_i and u_{i+1}. A complete n-sun graph is a n-sun graph where $G[U]$, the subgraph induced by U is complete

Definition 3.3: Fan graph: The fan graph $f_n, (n \geq 2)$ [12] is obtained by joining all vertices of a path P_n to a further vertex, called the center, by edges. It is the graph join $P_n + K_1$.

Definition 3.4: Friendship graph: The friendship graph F_n [12] is constructed by joining n copies of cycle C_3 with a common vertex.

Theorem 3.1: *For a sunlet graph G obtained from cycle* C_n,$(n \geq 3)$,

$$\overline{H(G,x)} = 2n[x^{4n-7} + x^{4n-9}]$$

Proof: The n pendant vertices attached to C_n each has degree 1. The number of non-neighbors of each pendant vertex is $(2n-2)$. The remaining vertices lying in the cycle C_n, each has degree 3. The number of non-neighbors of the vertex $v \in V(C_n)$ is $(2n-4)$. Since there are $2n$ edges

$$\overline{H(G,x)} = 2[nx^{2n-2+2n-4-1} + nx^{2n-4+2n-4-1}$$
$$= 2n[x^{4n-7} + x^{4n-9}]$$

Theorem 3.2: *For complete n-sun graph G obtained from complete graph* $K_n(n \geq 2)$,

$$\overline{H(G,x)} = 4nx^{3n-6} + n(n-1)x^{2n-5}$$

Proof: The central vertices lying in the complete graph each has degree $(n+1)$. The non-neighbors of these central vertices is $(n-2)$. The vertex in the outer ring each has degree 2. The non-neighbors of these vertices is $(2n-3)$. There are nC_2 edges lying in the complete graph and $2n$ edges lying in the outer ring. Hence

$$\overline{H(G,x)} = 2[2nx^{2n-3+n-2-1}] + 2[\,nC_2x^{n-2+n-2-1}]$$
$$= 4nx^{3n-6} + n(n-1)x^{2n-5}$$

Theorem 3.3: *For fan graph* $f_n(n \geq 4)$, $\overline{H(f_n,x)} = 4x^{2n-6} + 4x^{n-3} + 2(n-2)x^{n-4} + 2(n-3)x^{2n-7}$

Proof: The center vertex has no non-neighbors. There are two corner vertices each of degree 2 and the number of non-neighbors of these vertices is $(n-2)$. The remaining $(n-2)$ vertices are each with degree 3. The number of non-neighbors of these remaining vertices is $(n-3)$. There are totally $2n-1$ edges. Hence

$$\begin{aligned}\overline{H(f_n,x)} &= 2[2x^{n-2+n-3-1}] + 2[2x^{n-2-1}] \\ &\quad + 2[(n-2)x^{n-3-1}] \\ &\quad + 2[(n-3)x^{n-3+n-3-1}] \\ &= 4x^{2n-6} + 4x^{n-3} + 2(n-2)x^{n-4} + 2(n-3)x^{2n-7}\end{aligned}$$

Theorem 3.4: *For friendship graph* $F_n(n \geq 2)$,$\overline{H(F_n,x)} = 2n[x^{4n-5}] + 4n[x^{2n-3}]$

Proof: The common vertex in the center has no non-neighbors. The remaining $2n$ vertices have degree 2. The number of non-neighbors of these remaining vertices is $(2n-2)$. There are totally $3n$ edges. Hence

$$\overline{H(F_n,x)} = 2[nx^{2n-2+2n-2-1}] + 2[2nx^{2n-2-1}]$$
$$= 2n[x^{4n-5}] + 4n[x^{2n-3}]$$

Example 2:

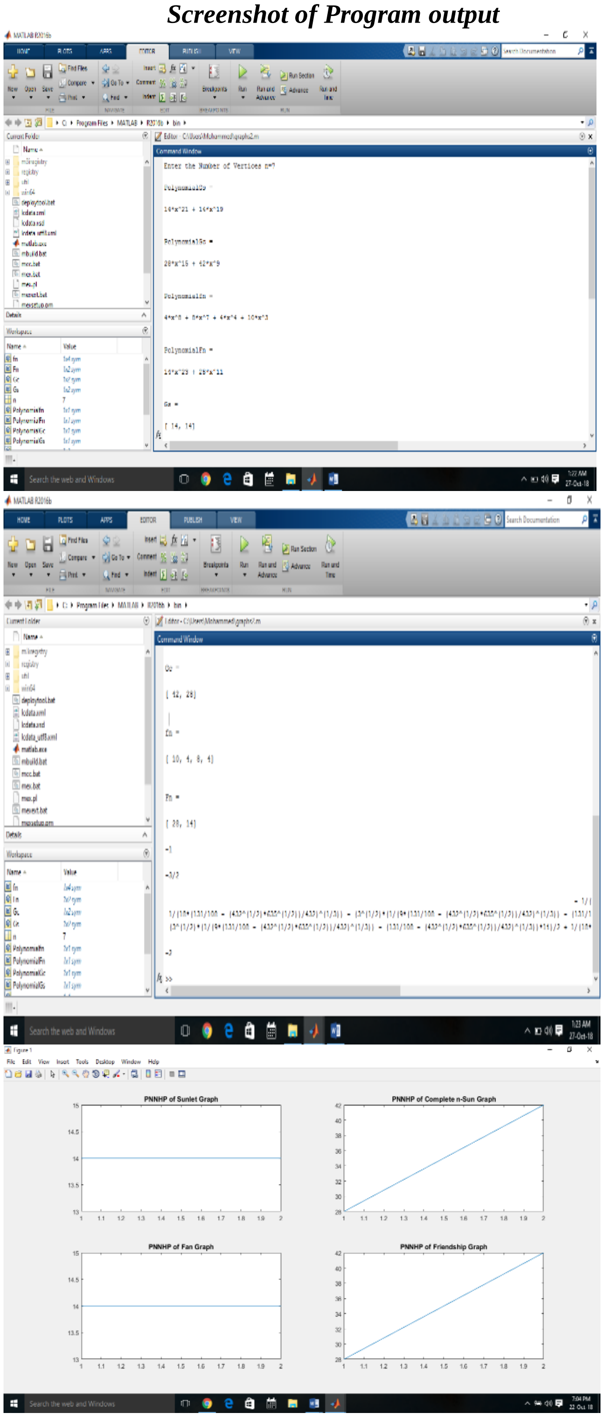
MATLAB Program for computing the roots of some special Graphs:

```
clc
syms x
n=input('Enter the Number of Vertices n=');
PolynomialGs= 2.*n.*x^((4.*n)-7) + 2.*n.* x^((4.*n)-9)
PolynomialGc= 4.*n.*x^((3.*n)-6) + n.*(n-1) .* x^(2.*n-5)
Polynomialfn= 4.*x^((2.*n)-6) +4.*x^(n-3)+2.*(n-2) .* x^(n-
4)+ 2.*(n-3) .* x^(2.*n-7)
PolynomialFn= 2.*n.*x^((4.*n)-5) + 4.*n.* x^((2.*n)-3)
Gs = coeffs(2.*n.*x^((4.*n)-7) + 2.*n.* x^((4.*n)-9))
Gc = coeffs(4.*n.*x^((3.*n)-6) + n.*(n-1) .* x^(2.*n-5))
fn = coeffs(4.*x^((2.*n)-6) +4.*x^(n-3)+2.*(n-2) .* x^(n-4)+
2.*(n-3) .* x^(2.*n-7))
Fn = coeffs(2.*n.*x^((4.*n)-5) + 4.*n.* x^((2.*n)-3))
Gs = fliplr(Gs);
Gc = fliplr(Gc);
fn = fliplr(fn);
Fn = fliplr(Fn);
z1=roots(Gs);
z2=roots(Gc);
z3=roots(fn);
z4=roots(Fn);
disp(z1)
disp(z2)
disp(z3)
disp(z4)
figure
subplot(2,2,1)
plot(Gs)
title('PNNHP of Sunlet Graph')
subplot(2,2,2)
plot(Gc)
title('PNNHP of Complete n-Sun Graph')
```



```
subplot(2,2,3)
plot(Gs)
title('PNNHP of Fan Graph')
subplot(2,2,4)
plot(Gc)
title('PNNHP of Friendship Graph')
```

Screenshot of Program output



Inference:

For the graph with 7 vertices, non neighbor harmonic polynomial of Sunlet graph, Complete *n*- Sun graph, Fan Graph and Friendship Graph is computed. The roots are calculated for each polynmial respectively using MATLAB program. Roots of the Non-Neighbor Harmonic Polynomial of Sunlet graph, Complete *n*- Sun graph, Fan Graph and Friendship Graph is other than zero. Hence the Sunlet graph, Complete *n*- Sun graph, Fan Graph and Friendship Graph are defined to be Perfect Non-Neighbor Harmonic Graphs.

IV. CONCLUSION AND FUTURE SCOPE

In this paper MATLAB programming is used extensively to find the roots of the non-neighbor harmonic polynomial and hence it is able to define the perfect non neighbor harmonic graphs. As future work, we can apply MATLAB programming to compute the non-neighbor harmonic index of various graphs.

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Authors Profile

Ms.A.Rizwana completed Bachelor of Science from Sadakathullah Appa College, affiliated to Manonmaniam Sundaranar University, Tirunelveli-12, Tamilnadu in 2006 and Master of Science from Sarah Tucker College, affiliated to Manonmaniam Sundaranar University in 2008. She completed her Master of Philosophy from St.Xaviers College (Autonomous) in 2009. She is currently pursuing Ph.D and working as Head & Assistant Professor in Department of Mathematics (Unaided), Sadakathullah Appa College (Autonomous) since 2014. She has cleared her State Eligibility Test (SET)-Tamilnadu in 2016. She has published more than 5 research papers in reputed international journals and presented several papers in national and international conferences. Her main research work focuses on Topological Indices in Chemical Graph Theory. She has 8 years of teaching experience and 4 years of Research Experience..

Dr.G.Jeyakumar is working as Associate Professor and Head, Department of Mathematics, St.John's College, Affiliated to Manonmaniam Sundaranar University, Tirunelveli. He completed his Undergraduate, Postgraduate and M.Phil in Mathematics from Manonmaniam Sundaranar University, Tirunelveli, Tamilnadu. He has completed his PhD from Alagappa University, Karaikudi. He has involved in various academic activities. He has more than 10 research publications in reputed journals. He has presented several research papers in national and international conferences. He has guided more than 5 research scholars in which two of them have completed their Doctoral degree. He has got 34 years of teaching experience. His area of specialization is Graph Labeling in Graph Theory..

Dr. M. Mohamed Ismail is currently working as Assistant Professor, Department of Computer Applications in The New College, Chennai. He has completed M.Sc Information Technology in Bharathidasan university and Ph.D. Information Technology in Manonmaniam Sundaranar University, Tirunelveli. He has more than 10 research publications in journals. He has attended many national and international seminars, conferences and presented numerous research papers. He has been involved in the software development of various optical and astronomical instruments. His current interests are Adaptive Optics, Virtual Reality, Image Processing, Artificial Intelligence and Cryptography.

