

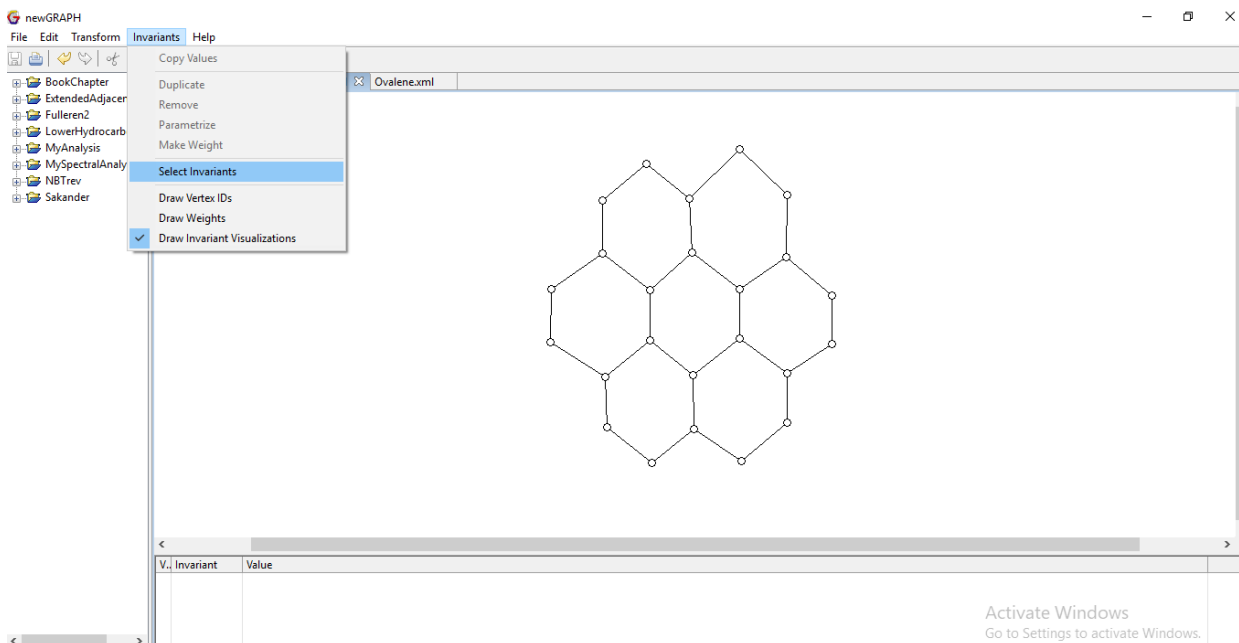
Workflow of our proposed method with a Minimal Working Example (MWE)

In this document, we will explain the working pattern of our technique to compute certain spectrum-based topological descriptors of graphs.

1. Let G be a graph for which you want to compute a spectrum-based topological index from the following list of indices:
 - i. Energy
 - ii. Estrada index
 - iii. Positive inertia index
 - iv. Negative inertia index
 - v. Nullity
 - vi. Signature

We would like to set the coronene graph as our MWE.

2. In first step, we draw graph G on newGraph and choose “Adjacency matrix” and “Vertices” as “Select Invariants” under the “Invariants” tab as follows:



-
- MATLAB R2015b
- HOME PLOTS APPS EDITOR PUBLISH VIEW
- Find Files Find Files Go To Find Files Run Section Run and Advance Run and Time
- FILE NAVIGATE EDIT BREAKPOINTS RUN
- Workspace
- Editor - C:\Users\Sakander Hayat\Desktop\Energy Estrada--UQC\Github Material\SpectrumBasedIndices.m
- graph.m teigenanalysis.m Bhmatrix.m MainPlainBh.m ModifiedSzeged.m BCN2_3.m SpectrumBasedIndices.m
- ```

1 %CIC
2 format short
3 n=24;
4 B=
5
6
7 A=
8 if
9
10 else
11
12 end
13 x=e
14 p=s
15 n=s
16 nul
17 sig
18 E=s
19 EE=

```
- Command Window
- f >>
- Evaluate Selection F9  
Open Selection Ctrl+D  
Help on Selection F1  
Cut Ctrl+X  
Copy Ctrl+C  
Paste Ctrl+V  
Select All Ctrl+A  
Wrap Comments Ctrl+J  
Comment Ctrl+R  
Uncomment Ctrl+T  
Smart Indent Ctrl+I
- Evaluate Current Section Ctrl+Enter  
Insert Section  
Insert Text Markup >  
Function Browser Shift+F1  
Function Hints Ctrl+F1  
Code Folding >
- Activate Windows  
Go to Settings to activate Windows.

- 
- The screenshot displays the MATLAB R2019b environment. The top toolbar includes tabs for HOME, PLOTS, APPS, EDITOR, PUBLISH, and VIEW. Below these are various toolbars for file operations (New, Open, Save, Find Files, Go To, Compare, Print), editing (Insert, Comment, Indent), breakpoints, running (Run, Run and Advance, Run Section, Run and Time), and navigating. The main workspace shows a project path: C:\Users\Sakander Hayat\Desktop\Energy Estrada-UQC\Github Material. Several editor windows are open, including graph.m, teigenanalysis.m, Bhmatrix.m, MainPlainBh.m, ModifiedSzeged.m, BCN2\_3.m, and SpectrumBasedIndices.m. The active window, SpectrumBasedIndices.m, contains MATLAB code for calculating spectral descriptors from a matrix B.
- ```

1 close all
2 clc
3 format short
4 n=24;
5 B= [[0, 1, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0], [1, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0], [1,
6
7
8 A= reshape(B,[n,n]);
9 if A==A'
10     disp('Matrix is Symmetric')
11 else
12     disp('Not Symmetric')
13 end
14 x=eig(A);
15 p=sum(x>0);
16 n=sum(x<0);
17 nullity=sum(x==0) ;

```
- The Command Window at the bottom shows the output of the script:
- ```

Command Window

Spectrum-related descriptors:
The energy is 34.5718
The Estrada index is 66.5600
The positive interia index is 12.0000
The negative interia index Index is 12.0000
The nullity is 0.0000
The signatur is 0.0000
fx >>

```
- An "Activate Windows" watermark is visible in the bottom right corner of the image.