1. Installing *Thorny Graph Calculator*

On the web-page http://mapmf.pmfst.hr/~vukicevi/ProjEngIndex.htm, the zip-file of the installation program of *Thorny Graph Calculator* can be found. Download this file and extract it. Then, install the program.

2. Thorny Graphs

Thorny graphs can be defined in three equivalent ways:
1) connected simple graphs with equal number of edges and vertices
2) simple graphs that contain an edge which deletion transforms them into the tree
3) connected simple graphs with the unique cycle

The example of the thorny graph is given below:
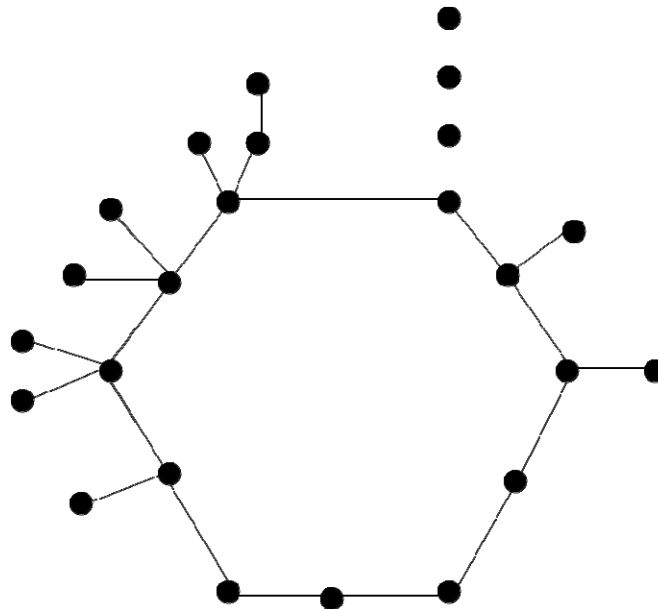
Let G be a thorny graph. Denote by a C(G) a unique cycle in G. A subthorns are connected components of graph G – C(G). A thorn is a subthorn to which a unique vertex is adjacent to an edge of that thorn is added together with a respectable edge.

In this software we restrict our attention on thorny graphs with maximal degree at most 4 that have 8 types of thorns:
- methyl-thorn
- ethyl-thorn
- propyl-thorn
- isopropyl-thorn
- butyl-thorn
- (2-methyl-propyl)-thorn
- (1-methyl-propyl)-thorn
- (1,1-dimethyl-ethyl)-thorn

That are respectively presented on the following figure:
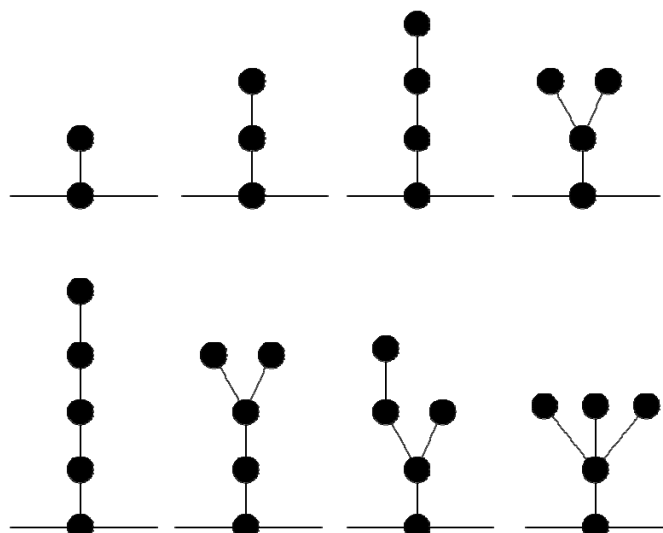
For each of these types of thorns, user of the software can prescribe if the observed thorn is allowed (by checking the corresponding box) or not by (unchecking the corresponding box). Let us illustrate this by the following example:

Suppose that methyl-thorn, propyl-thorn and butyl thorn are allowed and that ethyl-thorn, isopropyl-thorn, (2-methyl-propyl)-thorn, (1-methyl-propyl)-thorn and (1,1-dimethyl-ethyl)-thorn are not allowed, then user should check and uncheck boxes as on the following figure:

2. Indices based on edge incidence degrees.

Denote by m_{ij} the number of edges that connect vertices of degrees i and j, where $i \leq j$ are natural numbers. Since we restrict our attention on graphs with maximal degree at most 4, we may assume that $1 \leq i \leq j \leq 4$. *Indices based on edge incidence degrees* are those indices that depend solly on 10-tuple of the numbers $\left(m_{11}, m_{12}, m_{13}, m_{14}, m_{22}, m_{23}, m_{24}, m_{33}, m_{34}, m_{44} \right)$ and not on the structure of the graph. There is a large family of such indices. Here we restrict our attention on only three such indices:

- Zagreb index
- Modified Zagreb index
- Randic index.

Let us say few words about each of these indices:

Zagreb index

Zagreb-index is defined by

$$M_2(G) = \sum_{\{u,v\} \in E(G)} d_G(u) \cdot d_G(v),$$

where $E(G)$ is set of edges of G. Note that for each graph observed in this program, we have $\Delta(G) \leq 4$. The last formula can be reformulated as

$$M_2(G) = \sum_{1 \leq i \leq j} m_{ij} \cdot i \cdot j.$$

Modified Zagreb index

Modified Zagreb index is defined by

$${}^*M_2(G) = \sum_{\{u,v\} \in E(G)} \frac{1}{d_G(u) \cdot d_G(v)},$$

where $E(G)$ is set of edges of G. Note that for each graph observed in this program, we have $\Delta(G) \leq 4$. The last formula can be reformulated as

$${}^*M_2(G) = \sum_{1 \leq i \leq j} m_{ij} \cdot \frac{1}{i \cdot j}.$$

Randic index

Randic index is topological index defined by

$$\chi(G) = \sum_{\{u,v\} \in E(G)} \frac{1}{\sqrt{d_G(u) \cdot d_G(v)}},$$

where $E(G)$ is set of edges of G. Note that for each graph observed in this program, we have

$$\Delta(G) \le 4.$$

Denote by m_{ij} number of edges that connect vertices of degrees i and j. The last formula can be reformulated as

$$\chi(G) = \sum_{1 \le i \le j} m_{ij} \cdot \frac{1}{\sqrt{i \cdot j}}.$$

Inputting data in the computer

User can prescribe one of the following:
- Number of types of edges
- Zagreb index and number of vertices
- Modified Zagreb index and number of vertices
- Randic index and number of vertices

First, user has to select which type of data he wants to input by selecting the corresponding *radio button*:

1) If user chooses to input **Number of types of edges**, the form should look as on the following figure:

Then user inputs the values of m_{ij} using pull-down list of numbers (the value of each m_{ij} is restricted to range 0 – 250 and program can not work with larger numbers). One can note that value can be only selected by pull-down menu and can not be inputted by keyboard (this prevents the possibility of incorrect input).

2) If user chooses to input **Zagreb index and number of vertices**, the form should look as on the following figure:

Using the left-handside pull-down list of numbers user inputs the value of Zagreb index (the value of Zagreb index is restricted to 0 – 1600 and program can not work with larger numbers) and using the right-handside pull-down list of numbers user inputs the number of vertices (number of vertices is restricted to 0 – 100 and program can not work with larger numbers)

3) If user chooses to input **Modified Zagreb index and number of vertices**, the form should look as on the following figure:

Modified Zagreb index is rational number and if we restrict our attention to the graphs with maximal degree at most 4, it can be easily seen that Zagreb index can be written as the ratio of some natural number and 144. Therefore, it can be written as $x + \dfrac{y}{144}$, where x is the natural number and $0 \le y \le 143$. In this program, we restrict value of x to the range 0 – 50 and number of vertices is restricted to the range 0 – 100. Data is inputted as explained above.

4) If user chooses to input **Randic index and number of vertices**, the form should look as on the following figure:

Recall that Randic index is defined by $\chi(G) = \sum_{1 \le i \le j} m_{ij} \cdot \dfrac{1}{\sqrt{i \cdot j}}$. Since, this index works with irrational numbers, we **do not use the exact value of the Randic index**, but its approximation defined by:

$$\chi(G) = m_{11} + \frac{71}{100}m_{12} + \frac{58}{100}m_{13} + \frac{50}{100}m_{14} + \frac{50}{100}m_{22} + \frac{41}{100}m_{23} + \frac{35}{100}m_{24} + \frac{33}{100}m_{33} + \frac{29}{100}m_{34} + \frac{25}{100}m_{44}.$$

This approximation can be written as $x + \dfrac{y}{100}$, where x is the natural number and $0 \le y \le 99$.

In this program, we restrict value of x to the range $0 - 71$ and number of vertices is restricted to the range $0 - 100$. Data is inputted as explained above.

Getting the solution

After data is inputted, user has to press the button labeled by *Is there a graph with the required properties?* After few moments (this may last even few minutes on weaker computers) computer will produce one of two possible answers "*Yes, there is.*" or "*No, there is not.*" The example is presented by the following figure:

3. Indices based on vertex degrees

Denote by n_i the number of vertices od degree i. Since we restricted our attention on the graphs with maximal degree at most 4, we may assume that $1 \le i \le 4$. *Indices based on vertex*

degrees are those indices that depend solly on 10-tuple of the numbers $\left(m_{11}, m_{12}, m_{13}, m_{14}, m_{22}, m_{23}, m_{24}, m_{33}, m_{34}, m_{44}\right)$ and not on the structure of the graph. There is a large family of such indices. Here we restrict our attention on only two such indices: Zagreb M_1 index and modified Zagreb M_1 index. Let us say few words about these indices:

Zagreb M_1 index

Zagreb M1 index is topological index defined by

$$M_1(G) = \sum_{v \in V(G)} d_G(v)^2 .$$

where *V(G)* is set of edges of G. The last formula can be reformulated as

$$\chi(G) = \sum_{1 \le i \le 4} n_i \cdot i^2 .$$

Modified Zagreb M_1 index

Modified Zagreb M1 index is topological index defined by

$$M_1(G) = \sum_{v \in V(G)} \frac{1}{d_G(v)^2} .$$

where *V(G)* is set of edges of G. The last formula can be reformulated as

$$\chi(G) = \sum_{1 \le i \le 4} n_i \cdot \frac{1}{i^2} .$$

Inputting data in the computer

First, user has to select *Indices based on vertex degree.* The form will look as on the following figure:

User can prescribe any combination of the following properties:
- Numbers of types of vertices
- Number of vertices
- Zagreb M_1 index
- Modified Zagreb M_1 index

We ilustrate this by two examples:

First example

Suppose that user wants to prescribe *Numbers of types of vertices* and *Zagreb M_1 index*. First user checks the corresponding boxes as presented on the following figure:

Then user inputs the values of n_i using pull-down list of numbers (the value of each n_i is restricted to range $0 - 250$ and program can not work with larger numbers). One can note that value can be only selected by pull-down menu and can not be inputted by keyboard (this prevents the possibility of incorrect input). After that user inputs the values of Zagreb M_1

index using pull-down list of numbers (the value of each n_i is restricted to range 1 – 1600 and program can not work with larger numbers). Again, one can note that value can be only selected by pull-down menu and can not be inputted by keyboard.

Second example

Suppose that user wants to prescribe *Number of vertices* and *Modified Zagreb* M_1 *index*. First user checks the corresponding boxes as presented on the following figure:

Modified Zagreb M_1 index is rational number and if we restrict our attention to the graphs with maximal degree at most 4, it can be easily seen that Zagreb index can be written as the ratio of some natural number and 144. Therefore, it can be written as $x + \dfrac{y}{144}$, where x is the natural number and $0 \le y \le 143$. In this program, we restrict value of x to the range 0 – 100 and number of vertices is restricted to the range 0 – 100, too. Data is inputted as explained above.

Getting the solution

After data is inputted, user has to press the button labeled by *Is there a graph with the required properties?* After few moments (this may last even few minutes on weaker computers) computer will produce one of two possible answers "*Yes, there is.*" or "*No, there is not.*" The example is presented by the following figure:

Form1

Help

○ Indices based on edge incidence degrees

● Indices based on vertex degrees

☑ Numbers of types of vertices: n1 = [4 ▼]   n2 = [5 ▼]   n3 = [7 ▼]   n4 = [5 ▼]

☐ Number of vertices:

☑ Zagreb M1 index: [115 ▼]

☐ Modified Zagreb M1 index:

Allow thorns:

☑ Methyl-thorn   ☑ Ethyl-thorn   ☐ Propyl-thorn   ☐ Isopropyl-thorn

☑ Butyl-thorn   ☐ (2-methyl-propyl)-thorn   ☐ (1-methyl-propyl)-thorn   ☐ (1,1-dimethyl-ethyl)-thorn

[Is there a graph with the required properties?]   No, there is not