COMP 3031 Assignment 3

PROLOG Programming

Fall 2020

Due: 5PM on Nov 20 Friday

Instructions

- There are five problems in this assignment. Each problem counts for 2 points.
- This is an individual assignment. You can discuss with others and search online resources, but your submission should be your own code.
- Write your prolog program according to the specification, with the same predicate name and number of arguments as specified. Write all your solutions in a single file named "ass3.pl". In this file, put down your **name, ITSC account, and student ID** as a ***comment*** (surrounded by "/*" and "*/") on the first line.
- Submit your code through Canvas before the deadline.
- **No** late submissions will be accepted.
- Your submission will be run on a lab 2 machine with the following command in swipl: ?- [ass3].
  Please make sure your submission is executable. If it is not, a significant number of points will be deducted.

NOTE: We will perform code similarity checks. In case a submission is confirmed to have code similarity issues, we will deduct partial marks or full marks on a case-by-case basis.

PART I:

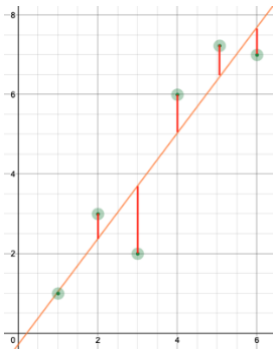
Question 1.

Define a /2 predicate `linear_regression (A, B)` to represent the regression line $y = Ax + B$ that is of the **least-squares** for a set of points (x_i, y_i). The regression line on a set of points is of the least-squares if the sum of the squares of the vertical deviations from each data point to the line is the **minimal** out of all possible lines.

We will give the set of points in two /1 facts, `xs` and `ys`, where x_i, and y_i are corresponding elements of the list in `xs` and `ys`. Example facts and query:

```
xs([1, 2, 3, 4, 5.06, 6]).
ys([1, 3, 2, 6, 7.23, 7]).

?- linear_regression(A, B).
A = 1.3298931176836508,
B = -0.29625817640294727.
```



You can check the correctness of your program output up to four digits accuracy as well as learn more about linear regression and the least-square method at the following web pages:
https://ncalculators.com/statistics/linear-regression-calculator.htm
https://en.wikipedia.org/wiki/Simple_linear_regression

Question 2.
Write a predicate `interesting(X)` to represent **all** interesting vertices X, if any, in a given undirected graph. In other words, after issuing the query `interesting(X)`, we can get all interesting vertices one by one by keeping typing ';' until all answers are returned.
A vertex is **interesting** if it satisfies the following three conditions:

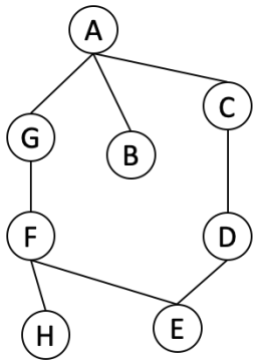
(1) It is sparse, i.e., its degree is less than or equal to 2.
(2) It is connected to at least two dense vertices (vertices whose degrees are greater than 2), and its shortest paths to its two closest dense vertices are of the same length.
(3) Its shortest path length to its two closest dense vertices is the shortest among all other sparse vertices that satisfy condition (2).

Example:
In the graph given by facts `edge`, vertex A and F are dense, and B, C, D, E, G, and H are sparse. B, C, E, H are not interesting vertices, because their shortest paths to their two closest dense vertices A and F are not of equal length. G is an interesting vertex in this graph, of which the shortest path is of length 1 to A and F. D is not interesting, because its shortest path length to A and F is 2, which is greater than length 1 of G.

Example facts and query:

```
edge('A', 'C').
edge('A', 'B').
edge('A', 'G').
edge('C', 'D').
edge('D', 'E').
edge('E', 'F').
edge('F', 'H').
edge('F', 'G').

?- interesting(X).
X = 'G'.
```

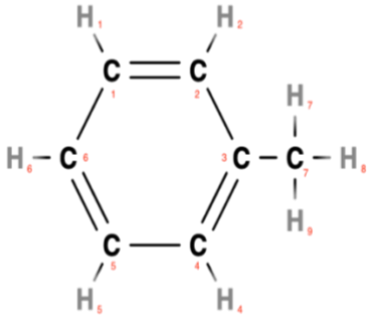


PART II:

We represent the structure of a chemical compound in the following /3 predicate:

```
atom_elements(name_of_atom, element_type, bonded_atoms)
```

The following example represents the compound ***toluene***. It is resulted from bonding a benzene (***C6H6***) and a ***CH3*** group. The graph contains 15 vertices, including seven ***C*** atoms and eight ***H*** atoms, and 15 edges, including eight ***C-H*** edges and seven ***C-C*** edges.



```
atom_elements(h1,hydrogen,[c1]).
atom_elements(h2,hydrogen,[c2]).
atom_elements(h4,hydrogen,[c4]).
atom_elements(h5,hydrogen,[c5]).
atom_elements(h6,hydrogen,[c6]).
atom_elements(h7,hydrogen,[c7]).
atom_elements(h8,hydrogen,[c7]).
atom_elements(h9,hydrogen,[c7]).
atom_elements(c1,carbon,[c2,c6,h1]).
atom_elements(c2,carbon,[c1,c3,h2]).
atom_elements(c3,carbon,[c2,c7,c4]).
atom_elements(c4,carbon,[c3,c5,h4]).
atom_elements(c5,carbon,[c4,c6,h5]).
atom_elements(c6,carbon,[c1,c5,h6]).
atom_elements(c7,carbon,[c3,h7,h8,h9]).
```

Question 3.

CH3 is a structure consisting of one ***C*** atom bound with three ***H*** atoms. Define a predicate `ch3(X)` in which `X` is a list containing all C atoms that belong to the ***CH3*** structures given in `atom_elements`. The order of the elements in the list is unimportant.

Example query on the given compound *toluene*:

```
?- ch3(X).
X=[c7].
```

Question 4.

Define a predicate `c6ring(X)` in which X represents a list containing all six-***C***-atom rings in the given `atom_elements`. Each six-***C***-atom ring is a list containing the six ***C*** atoms that form the ring. The order of the *C* atoms in the list is unimportant, so each six-***C***-atom ring occurs **exactly once** in the list of rings.

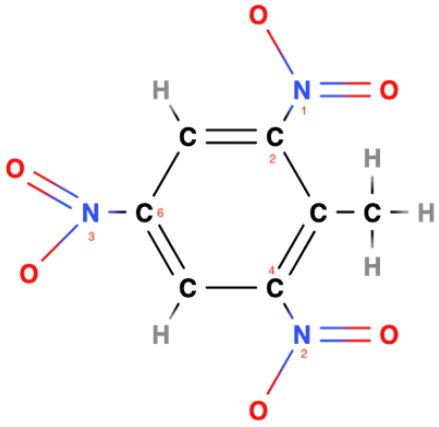
Example query on the given compound *toluene*:

```
?- c6ring(X).
X= [[c1,c2,c3,c4,c5,c6]].
```

Question 5.

The compound ***2,4,6-Trinitrotoluene (TNT)***, shown in the following figure, is formed with the ***H*** atom at ***C2***, ***C4*** and ***C6*** of the benzene ring replaced with an ***NO2*** structure. The structure ***NO2*** consists of one ***N*** atom bound with two ***O*** atoms.

Define a predicate `tnt(X)` in which `X` is a list containing all TNT structures. Each TNT structure is represented as a list containing all six ***C*** atoms on the ring, of which three ***C*** atoms, at position 2,4,6 on the ring respectively, are each represented as a list containing itself and the ***NO2*** structure it is bound to. The order of the six ***C*** atoms in the list is unimportant, and each TNT structure occurs **exactly once** in the list of TNT structures.



The facts that give the example *2,4,6-Trinitrotoluene* figure:

```
atom_elements(h1,hydrogen,[c1]).
atom_elements(n1,nitrogen,[o1, o2, c2]).
atom_elements(o1,oxygen,[n1]).
atom_elements(o2,oxygen,[n1]).
atom_elements(n2,nitrogen,[o3, o4, c4]).
atom_elements(o3,oxygen,[n2]).
atom_elements(o4,oxygen,[n2]).
atom_elements(h5,hydrogen,[c5]).
atom_elements(n3,nitrogen,[o5, o6, c6]).
atom_elements(o5,oxygen,[n3]).
atom_elements(o6,oxygen,[n3]).
atom_elements(h7,hydrogen,[c7]).
atom_elements(h8,hydrogen,[c7]).
atom_elements(h9,hydrogen,[c7]).
atom_elements(c1,carbon,[c2,c6,h1]).
atom_elements(c2,carbon,[c1,c3,n1]).
atom_elements(c3,carbon,[c2,c7,c4]).
atom_elements(c4,carbon,[c3,c5,n2]).
atom_elements(c5,carbon,[c4,c6,h5]).
atom_elements(c6,carbon,[c1,c5,n3]).
atom_elements(c7,carbon,[c3,h7,h8,h9]).
```

Example query on the *2,4,6-Trinitrotoluene*:

```
?- tnt(X).
X = [[c1, [c2, n1, o1, o2], c3, [c4, n2, o3, o4], c5,
[c6, n3, o5, o6]]] .
```