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Some GAP programs for computing the topological indices

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Abstract. A topological index is a numerical invariant associated with a chemical graph. In this paper we introduce some GAP programs for computing for Wiener and Hyper-wiener indices, Szeged index, Detour index, PI index and Balaban index.

Keywords: Wiener index, Szeged index, PI index, vertex-PI index
Mathematics Subject Classification (2010): 05C09, 90C35.

1 Introduction

GAP is a system for computational discrete algebra, with particular emphasis on Computational Group Theory. GAP provides a programming language, a library of thousands of functions implementing algebraic algorithms written in the GAP language as well as large data libraries of algebraic objects. See also the overview and the description of the mathematical capabilities. GAP is used in research and teaching for studying groups and their representations, rings, vector spaces, algebras, combinatorial structures, and more. The system, including source, is distributed freely. You can study and easily modify or extend it for your special use, see [23].

Topological indices are numerical valiues constructed from the associate graphs of chemical compounds. Some indices based on the distances in graph are widely used in establishing relationships between the structure of molecules and their physicochemical properties. The

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aim of this paper is to introduce some GAP program for computing the topological indices.

2 Distance matrix

Let G be a graph with vertex set $\{v_1, \cdots, v_n\}$. For arbitrary vertices u and v of graph G, the distance $d(u,v)$ is defined as the length of a minimal path connecting u and v. A distance matrix is a square matrix whose ij-entry is adistance between vertices v_i and v_j. Here, is the GAP program for distance matrix. In the function f the variable A denotes to the adjacency matrix of graph G.

```
f := function(A)
local n,b,bb,bbb,b1,bb1,bbb1,s,Ix,y,k,B,I,j;n := Length(A);
b := [];bb := [];bbb := [];b1 := [];bb1 := [];bbb1 := [];s := 0;
for x in [1..n]do
for y in [1..n]do
for k in [1..n]do
B := A^k;if B[x][y] <> 0 thenAddSet(b,k);break;fi;
od;
if y <= x then Add(bb,0); else Add(bb,b[1]);
fi;
b := []; od; Add(bbb,bb); bb := []; od;
for i in bbb do
for j in i do
s := s + j;
od; od;
Print("distanceMatrix = ","");
PrintArray(bbb + TransposedMat(bbb));Print("");
Print("WienerIndex = ",s,"");
```

3 Wiener and hyper-Wiener indices, Szeged index and detour index

Usage of topological indices in chemistry began in 1947 when Harold Wiener (the chemist) introduced Wiener index to determine correlations between physicochemical properties of organic compounds and the index of their molecular graphs. For a review, historical details and further bibliography on the chemical applications of the Wiener index see [13, 14, 25]. The Wiener index is the oldest topological index defined as follows

$$W(G) = \frac{1}{2} \sum_{x,y \in V(G)} d(x,y),$$

see [26]. Also, the hyper-Wiener index is the defined as follows:

$$W(G) = \frac{1}{2} \sum_{x,y \in V(G)} d(x,y)(d(x,y)+1),$$

Another topological index was introduced by Gutman and called the Szeged index, abbreviated as Sz [17]. Let $n(u|G)$ and $n(v|G)$ be respectively, the number of vertices of G lying closer to vertex u than to vertex v and the number of vertices of G lying closer to vertex v than to vertex u. A long time known property of the Wiener index is the formula:

$$W(G) = \sum_{xy \in E(G)} n(u|G)n(v|G),$$

which is applicable for trees. Motivated the above formula, Gutman [12] introduced a graph invariant, named as the Szeged index, defined by

$$Sz(G) = \sum_{uv \in E(G)} n(u|G)n(v|G).$$

The detour index, in contrast to the Wiener index that considers the length of the shortest path between vertices, considers the length of the longest distance between each pair of vertices. In other words, $DD(G)$ is the sum of all $dd(i,j)$, where $dd(i,j)$ is the length of the path that contains the largest number of edges between vertices i and j in graph G. This index has recently received some attention in the chemical literature, see [5] and references therein. In the following function, Wiener and hyper-Wiener indices, Szeged index and detour index are computed.

$f := function(n)$
$local\ d1,i1,j1,x2,xx1,s1,p1,a1,b1,aa1,n1,str,ff,s,zz,v,xx,sts,h,i,j,y,y1,y2,y3,yy,yyy,ww,$
$d,dd,iii,jjj,n2,m,ii,ss,rr,nn,a,r,l,p,x,x1,u,v1,q,sss,qq,l1,ll;s1 := 0;$
$p1 := [];n1 := 0;qq := 0;l1 := [];ll := [];$
$for\ i1\ in[1..n]do$
$s1 := s1 + 2^i1;\ Add(p1,s1);$
$od;$
$a1 := [];b1 := [];aa1 := [];x2 := [];xx1 := [];$
$for\ i1\ in[2..5]\ do\ Add(aa1,[1,i1]);\ od;$
$for\ i1\ in\ p1\ do$
$for\ j1\ in[i1..2 * i1 + 1]\ do$
$Add(a1,j1);Add(a1,2 * j1 + 2);Add(b1,j1);Add(b1,2 * j1 + 3);$
$Add(aa1,a1);Add(aa1,b1);a1 := [];b1 := [];$
$od;$
$od;$
$ww := [];l := [];p := 0;u := 0;v1 := [];sss := 0;$
$for\ iin\ [1..n]\ do\ Add(ww,0);Add(ww,1);$
$od;$
$str := [];ff := [];y := [0,0];y1 := [0,1];y2 := [0,2];y3 := [0,3];yyy := [];$
$s := 1;v := [];xx := [];sts := [];$
$while\ s <= Length(ww)\ do$
$Add(v,s);s := s + 1;$

```
od;
h := Combinations(v);;
Sort(h,function(v,w)returnLength(v) < Length(w);end);
s := 1;r := 1;
while s <= Length(h)do
whiler <= Length(h[s])do
Add(str,ww[h[s][r]]);r := r + 1;
od;
Add(sts,str);s := s + 1;r := 1;
if Length(str) <= nandLength(str) >= 1then
AddSet(xx,str);fi;
str := [];
od; for i in xx do
for j in i do
Add(y,j);Add(y1,j);Add(y2,j);Add(y3,j);
od;
Add(yyy,y);Add(yyy,y1);Add(yyy,y2);Add(yyy,y3);
y := [0,0];y1 := [0,1];y2 := [0,2];y3 := [0,3];od;
Add(yyy,[0,0]);Add(yyy,[0,1]);Add(yyy,[0,2]);Add(yyy,[0,3]);Add(yyy,[0]);
Sort(yyy,function(v,w)returnLength(v) < Length(w);end);
dd := [];
for x in yyy do
d := [];
for x1 inyyy do
n2 := Length(x);m := Length(x1);
if n < m then nn := n2;
else
nn := m;fi;
for iiin[1..nn]do
if x[ii] <> x1[ii]then
ii := ii − 1; break;fi;
od;
ss := n2 + m − (2 ∗ ii);Add(d,ss); od;
Add(dd,d);
od;
v1 := [];Add(v1,4);
for i in [2..2^(n + 2) − 3] do
Add(v1,3);
od;
for i in [2^(n + 2) − 2..2^(n + 3) − 3]do
Add(v1,1);
```

```
od; Print("NumberOfVertixesis :",Length(v1),"");
for i in dd do
for j in i do
p := p + j;
od;
od;
for j in [1..Length(dd)] do
for i in [1..Length(dd)] do
if j < i then
qq := qq + (dd[j][i]) * (dd[j][i] + 1);fi;
od;
od;
Print("HyperWienerIndex = ",qq,"");
Print("DetourIndex = "); return(p/2); end;
```

4 PI index

By the reason of the coincidence of Wiener and Szeged indices, in the case of trees, the authors in [16,18] introduced another Szeged/Wiener-like topological index, called Padmakar-Ivan index, abbreviated as PI. This new index, denoted by $PI(G)$, is defined on the ground of non-equidistant edges $m(e|G)$:

$$PI(G) = \sum_{uv \in E(G)} m(u|G) + m(v|G).$$

It turned out the PI index has similar discriminating power as the other two indices and in many cases it gives better results. As we already mentioned, the Szeged index incorporates the distribution of vertices of a molecular graph, while the PI index does this for edges. Hence it seems that a combination of both could give good results in QSRP/QSAR studies.

The following program computes the PI index of a connected graph.

```
M := (AdjacencyMatrix)
e := [];q := 0;h := [];o := 0;uu := 0;
for i in [1..Length(M)]do
for j in [1..Length(M)]do
if M[i][j] = 1 then
AddSet(e,Set([i,j]));
fi;
od;
od;
B := [];
for b in e do
for bb in e do
```

```
if Intersection(b,bb) = []then
if ((M[b[1]][bb[1]] = M[b[2]][bb[2]]) and((M[b[1]][bb[1]] + 1 = M[b[1]][bb[2]])
and (M[b[2]][bb[2]] + 1 = M[b[2]][bb[1]]))) or ((M[b[1]][bb[2]] = M[b[2]][bb[1]])
and ((M[b[1]][bb[2]] + 1 = M[b[1]][bb[1]]) and (M[b[2]][bb[1]] + 1 = M[b[2]][bb[2]])))or
((M[bb[1]][b[1]] = M[bb[1]][b[2]]) and (
(M[bb[1]][b[1]] <= M[bb[2]][b[1]]) and (M[bb[1]][b[1]] <= M[bb[2]][b[2]])))or
((M[bb[2]][b[1]] = M[bb[2]][b[2]]) and (
(M[bb[2]][b[1]] <= M[bb[1]][b[2]]) and (M[bb[2]][b[1]] <= M[bb[1]][b[1]])))
then
AddSet(B,bb);
fi;fi;AddSet(B,b);
od;
Print("x",Length(e) − Length(B),"");
q := q + 1;Add(h,Length(B));
B := [];
od;
Print("");Print("Numberofedgeis : ",q,"");Print("");Sort(h);
g := [];gg := [];
Print("PIPolynomial = ");
for i in h do
for j in h do
if j = i then
Add(g,j);fi;od;AddSet(gg,g);g := [];od;
for i in [1..Length(gg) − 1]do
Print(Length(gg[i]),"x");Print(Length(e) − gg[i][1]);Print(" + ");
uu := uu + Length(gg[i]) ∗ (Length(e) − gg[i][1]);
od;
a := Length(gg);
Print(Length(gg[a]),"x");Print(Length(e) − gg[a][1],"");
uu := uu + Length(gg[a]) ∗ (Length(e) − gg[a][1]);
Print("");Print("PIIndex = ",uu,"");
```

5 Balaban index

Balaban index is a distance-based topological index. It was introduced by Alexandru T. Balaban over 30 years ago [3,4]. Let G be a graph on n vertices and m edges. For $x \in V(G)$, the transmission of x is defined as $w(x) = \sum_{y \in V(G)} d_G(x,y)$. Balaban index $J(G)$ of a graph G is defined as

$$J(G) = \frac{m}{m-n+2} \sum_{uv \in E(G)} \frac{1}{\sqrt{w(u).w(v)}}.$$

$M := (AdjacencyMatrix)$
$n := Length(M); e := []; d := []; t := 0; dd := [];$
$foriin[1..n]do$
$forjin[i+1..n]do$
$ifM[i][j] = 1then$
$Add(e,[i,j]);$
$fi;$
$od;$
$od;$
$m := Length(e); s := 0;$
$foriin[1..n]do$
$forjinM[i]do$
$s := s + j;$
$od;$
$Add(d,s);$
$s := 0;$
$od;$
$forainedoAdd(dd,d[a[1]]);od;$
$foriinddoforjinddot := t + (1/(Sqrt(i*j)));od;od;$
$Print("");$
$Print("BalabanIndex = ",(m/(m-n+2))*t);Print("");$
$Print("");$

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