Wiener and Hyper-Wiener Numbers in a Single Matrix

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A novel unsymmetric square matrix, CJ_u, is proposed for calculating both Wiener,[1] ***W***, and hyper-Wiener,[2] ***WW***, numbers. This matrix is constructed by using the principle of single endpoint characterization of paths.[3] Its relation with Wiener-type numbers is discussed.

INTRODUCTION

Wiener,[1] ***W***, and hyper-Wiener,[2] ***WW***, indices are the most studied topological indices, both for algebraic aspects and applications (see refs 3 and 4). They can be defined as *edge/path* (***e/p***) *contributions* to a global number, ***I***

$$\boldsymbol{I} = \boldsymbol{I(G)} = \sum\nolimits_{e/p} I_{e/p} = \sum\nolimits_{e/p} \mathbf{N}_{L,e/p}\mathbf{N}_{R,e/p} \qquad (1)$$

with

$$\mathbf{N_{L,e}} + \mathbf{N_{R,e}} = \mathbf{N(G)} \qquad (2)$$

In the above relations, $\mathbf{N_L}$, $\mathbf{N_R}$ denote the number of vertices to the left and to the right of edge/path **e/p** and the summation runs over all edges/paths in graph**.** Edge/path contributions $\boldsymbol{I_{e/p}}$ are just the entries in the Wiener matrices,[5,6] $W_\mathbf{e}$ and $W_\mathbf{p}$. Thus, ***I*** can be calculated by

$$\boldsymbol{I} = \mathbf{(1/2)}\sum\nolimits_i\sum\nolimits_j[W_{\mathbf{e/p}}]_{\mathbf{ij}} \qquad (3)$$

I being ***W*** for $W_\mathbf{e}$ and ***WW*** for $W_\mathbf{p}$. Note that numbers (*i.e.*, indices) are marked by italic letters, whereas matrices (and their entries) are marked by right letters.

The meaning of ***I*** cf. eqs 1−3 is the number of all “external” paths which include all paths of length **e/p** in graph. The above relations hold only in acyclic structures. There are also relations which extend the “edge/path contribution” definition for cycle-containing graphs.[7−9]

Distance matrix D offers a challenge for calculating these indices, for any graph, as Hosoya[10] and Diudea[3] proposed

$$\boldsymbol{I} = \mathbf{(1/2)}\sum\nolimits_i\sum\nolimits_j[D_{\mathbf{e/p}}]_{\mathbf{ij}} \qquad (4)$$

where $D_\mathbf{e}$ is just the classical D matrix and $D_\mathbf{p}$ is the “distance path” matrix.[3] The meaning of ***I*** cf. eq 4 is the number of all “internal” paths, of length **e/p**, included into all shortest paths in graph.

$D_\mathbf{p}$ matrix is defined[3] as

$$[D_p]_{ij} = \binom{[D_e]_{ij} + \mathbf{1}}{\mathbf{2}} \qquad (5)$$

so that, making ***I*** = ***WW***, eq **4** can be expanded as follows

$$\boldsymbol{WW} = \mathbf{(1/2)}\sum_i\sum_j[D_e]_{ij} + \mathbf{(1/2)}\sum_i\sum_j\binom{[D_e]_{ij}}{\mathbf{2}} \qquad (6)$$

where the former term is just the Wiener number ***W***. The latter term is the “non-Wiener” part of the hyper-Wiener number, which is denoted by Δ_D (Δ in ref 3). The corresponding Δ_D matrix is defined as

$$[\Delta_D]_{ij} = \binom{[D_e]_{ij}}{\mathbf{2}} \qquad (7)$$

Thus, eq 6 can be written as

$$\boldsymbol{WW} = \boldsymbol{W} + \Delta_D \qquad (8)$$

The meaning of Δ_D is the number of all paths larger than unity included into all shortest paths in graph. In matrix form, eq 8 can be written as

$$D_p = D_e + \Delta_D \qquad (9)$$

Starting from the meaning of Δ_D, and keeping in mind eqs 8 and 9, matrix $W_\mathbf{p}$ can be decomposed as

$$W_p = W_e + \Delta_W \qquad (10)$$

where Δ_W is defined[11] by analogy to $W_\mathbf{p}$, with the specification that path contributions $\boldsymbol{I_p}$ are calculated only on paths larger than unity (see eq 1). It is easily seen that the half sum of entries in the corresponding matrices of eq 9 equals that of entries in the matrices of eq 10. Figure 1 illustrates some of the above mentioned matrices, for the graph 234M3C5 (2,3,4-trimethylpentane).

CJ_U MATRIX AND ITS RELATION WITH WIENER-TYPE NUMBERS

The matrix $CJ_\mathbf{u}$ (unsymmetric Cluj matrix) is defined following the principle of single endpoint characterization of a path[3] (see also refs 5 and 12)

$$[CJ_{\boldsymbol{u}}]_{ij} = \boldsymbol{N}_{i,(i,j)} \qquad (11)$$

$$\boldsymbol{N_{i,(i,j)}} = \{u | u \in V(G);\ [D_e]_{iu} < [D_e]_{ju};\ (i,u)\cap(i,j) = \mathbf{max}\{i\}\}$$

$CJ_\mathbf{u}$ matrix is a ***square unsymmetric matrix*** of dimensions N*$\mathbf{N}$. It collects the vertices lying closer to the focused vertex **i**, but out of the shortest path **(i,j)**, or in other words, the “external” paths on the side of **i**, which include the path **(i,j)**. As it can be seen from Figure 1, all the entries in the rows of terminal vertices are equal to 1. The above definition is valid both for acyclic and cyclic graphs.[13]

Despite of its ease of construction, this matrix is extremely informative. Thus their row sums are identical to the

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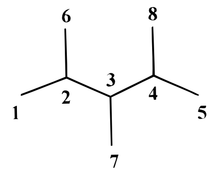

$\mathbb{D}_e$

0	1	2	3	4	2	3	4
1	0	1	2	3	1	2	3
2	1	0	1	2	2	1	2
3	2	1	0	1	3	2	1
4	3	2	1	0	4	3	2
2	1	2	3	4	0	3	4
3	2	1	2	3	3	0	3
4	3	2	1	2	4	3	0
19	13	11	13	19	19	17	19

$\mathbb{W}_e$

0	7	0	0	0	0	0	0
7	0	15	0	0	7	0	0
0	15	0	15	0	0	7	0
0	0	15	0	7	0	0	7
0	0	0	7	0	0	0	0
0	7	0	0	0	0	0	0
0	0	7	0	0	0	0	0
0	0	0	7	0	0	0	0
7	29	37	29	7	7	7	7

$\mathbb{W}_p$

0	7	5	3	1	1	1	1
7	0	15	9	3	7	3	3
5	15	0	15	5	5	7	5
3	9	15	0	7	3	3	7
1	3	5	7	0	1	1	1
1	7	5	3	1	0	1	1
1	3	7	3	1	1	0	1
1	3	5	7	1	1	1	0
19	47	57	47	19	19	17	19

$\mathbb{CJ}_u$

0	1	1	1	1	1	1	1	7
7	0	3	3	3	7	3	3	29
5	5	0	5	5	5	7	5	37
3	3	3	0	7	3	3	7	29
1	1	1	1	0	1	1	1	7
1	1	1	1	1	0	1	1	7
1	1	1	1	1	1	0	1	7
1	1	1	1	1	1	1	0	7
19	13	11	13	19	19	17	19	

Figure 1. Illustration of the matrices D_e, W_e, W_p, and CJ_u for the graph 234M3C5.

corresponding row sums in the Wiener matrix W_e

$$\mathbf{RS}(\mathrm{CJ}_{\mathbf{u}})_{\mathbf{i}} = \mathbf{RS}(\mathrm{W}_{e})_{\mathbf{i}} \tag{12}$$

Similarly, their column sums equal the corresponding column sums in the distance matrix D_e

$$\mathbf{CS}(\mathrm{CJ}_{\mathbf{u}})_{\mathbf{j}} = \mathbf{CS}(\mathrm{D}_{e})_{\mathbf{j}} \tag{13}$$

so that one can write

$$\sum\nolimits_{i}\mathbf{RS}(\mathrm{CJ}_{\mathbf{u}})_{\mathbf{i}} = \sum\nolimits_{i}\mathbf{RS}(\mathrm{W}_{e})_{\mathbf{i}} = \sum\nolimits_{j}\mathbf{CS}(\mathrm{CJ}_{\mathbf{u}})_{\mathbf{j}} = \sum\nolimits_{j}\mathbf{CS}(\mathrm{D}_{e})_{\mathbf{j}} = 2W \tag{14}$$

In other words, eqs 12−14 show the equality of sums of the "external" and "internal" paths of all paths **(i,j)** in graph, as demonstrated by Klein *et al.*[14]

$CJ_{\mathbf{u}}$ matrix allows the construction of Cluj matrices $CJ_{\mathbf{e/p}}$, which, in tree graphs, are identical to the Wiener matrices $W_{\mathbf{e/p}}$

$$[\mathrm{CJ}_{\mathbf{u}}]_{\mathbf{ij}}\,[\mathrm{CJ}_{\mathbf{u}}]_{\mathbf{ji}} = [\mathrm{CJ}_{\mathbf{e/p}}]_{\mathbf{ij}} = [\mathrm{W}_{\mathbf{e/p}}]_{\mathbf{ij}} \tag{15}$$

From relation (15), the identity of the indices constructed on these matrices is straightforward

$$\boldsymbol{I} = \sum\nolimits_{i<j}[\mathrm{CJ}_{\mathbf{u}}]_{\mathbf{ij}}[\mathrm{CJ}_{\mathbf{u}}]_{\mathbf{ji}} = (1/2)\sum\nolimits_{i}\sum\nolimits_{j}[\mathrm{CJ}_{\mathbf{e/p}}]_{\mathbf{ij}} = (1/2)\sum\nolimits_{i}\sum\nolimits_{j}[\mathrm{W}_{\mathbf{e/p}}]_{\mathbf{ij}} \tag{16}$$

Thus, in acyclic structures, the $CJ_{\mathbf{u}}$ matrix allows the calculation of both ***W*** and ***WW*** numbers, either directly or by means of the symmetric matrices $CJ_{\mathbf{e/p}}$ and $W_{\mathbf{e/p}}$.

The matrix Δ_W can also be constructed according to eq 15, by imposing the restriction $|\mathbf{p}| > 1$.

Another interesting matrix, denoted Δ_{CJu}, can be obtained when definition (11) is restricted to paths larger than unity

$$[\Delta_{\mathrm{CJu}}]_{\mathbf{ij}} = [\mathrm{CJ}_{\mathbf{u}}]_{\mathrm{ij}}; \quad |(\mathbf{i},\mathbf{j})| > 1 \tag{17}$$

The half sum of its entries, Δ_{CJu}, (meaning the number of all "external" paths on the side of **i**, which include the path **(i,j)** of length larger than 1) is the "shape" part of Wiener number (see below), which can be decomposed as

$$\boldsymbol{W} = \binom{\mathbf{N}}{2} + \Delta_{CJu} \tag{18}$$

In line graphs $\mathbf{L_N}$, the quantity Δ_{CJu} shows a maximal value (see also refs 15 and 16), given by

$$\Delta_{\boldsymbol{CJu}}\,(\mathbf{L_N}) = \binom{\mathbf{N}}{3} \tag{19}$$

whose meaning is the number of all triplets in graph, thus justifying the restriction imposed to paths ($|\mathbf{p}| > 1$). In trees, any branching point decreases this quantity, as shown in refs 15−18. Let **r** be a branching vertex (i.e., a vertex of degree $\mathbf{d_r} > 2$). The number $\Delta_{\boldsymbol{CJu}}$ is given by a relation of Doyle−

Table 1. Wiener *W*, Hyper-Wiener *WW*, *and* Δ_{CJu} and the Corresponding ^2W_M Numbers in Octane Isomers[a]

graph	W	WW	Δ_{CJu}	$^2W_{De}$	$^2W_{We}$	$^2W_{CJu}$	$^2WW_{Dp}$	$^2WW_{Wp}$
C8	84	210	56	1848	2100	1596	12726	12054
2MC7	79	185	51	1628	2000	1396	9711	9829
3MC7	76	170	48	1512	1892	1284	8256	8338
4MC7	75	165	47	1476	1848	1248	7830	7815
3EC6	72	150	44	1360	1740	1136	6412	6460
25M2C6	74	161	46	1420	1900	1206	7171	7825
24M2C6	71	147	43	1312	1792	1102	6023	6536
23M2C6	70	143	42	1280	1748	1072	5772	6163
34M2C6	68	134	40	1208	1684	1004	5050	5426
3E2MC5	67	129	39	1172	1640	968	4646	4992
22M2C6	71	149	43	1316	1808	1112	6277	6779
33M2C6	67	131	39	1176	1664	978	4878	5221
234M3C5	65	122	37	1096	1648	906	4076	4700
3E3MC5	64	118	36	1072	1564	880	3916	4222
224M3C5	66	127	38	1128	1708	940	4406	5165
223M3C5	63	115	35	1032	1600	850	3653	4220
233M3C5	62	111	34	1000	1564	820	3402	3917
2233M4C4	58	97	30	868	1516	706	2521	3169

[a] M = methyl; E = ethyl.

Graver-type[18]

$$\boldsymbol{\Delta_{CJu}} = \binom{\mathbf{N}}{\mathbf{3}} - \sum_{\mathrm{r}} \binom{\mathbf{d}_{\mathrm{r}}}{\mathbf{3}} \sum_{1<\mathbf{j}<\mathbf{j}<\mathbf{k}\le \mathbf{d}_{\mathrm{r}}} \mathbf{n}_{\mathrm{i}}\mathbf{n}_{\mathrm{j}}\mathbf{n}_{\mathrm{k}} \qquad (20)$$

where $\mathbf{n_i} + \mathbf{n_j} + \mathbf{n_k} + \mathbf{1} = \mathbf{N}$ and summation runs as follows: first summation over all branching points in graph and the second one collects all $\binom{d\mathbf{r}}{3}$ triplet products around a branching point. More details about the Doyle−Graver method for calculating the Wiener number can be found in refs 15 and 16.

Combinatorial analysis of Wiener-type numbers in $\mathbf{L_N}$ graphs lead to the following relations

$$\boldsymbol{W} = \binom{\mathbf{N}}{\mathbf{2}} + \binom{\mathbf{N}}{\mathbf{3}} = \binom{\mathbf{N+1}}{\mathbf{3}} \qquad (21)$$

$$\boldsymbol{WW} = \boldsymbol{W} + \boldsymbol{\Delta} = \binom{\mathbf{N+1}}{\mathbf{3}} + \binom{\mathbf{N+1}}{\mathbf{4}} = \binom{\mathbf{N+2}}{\mathbf{4}} \qquad (22)$$

Equation 21 means that, in line graphs, ***W*** number represents the total number of vertex pairs and vertex triplets.[16] Only the number of triplets will be affected by the molecular branching (cf. eq 20) within a set of alkane isomers, whereas the number of vertex pairs remains constant. In other words, the number of vertex pairs represents the "size" term, while the number of vertex triplets is the "shape" term of the Wiener number in tree graphs. However, both the terms contribute to the correlation of ***W*** with a given molecular property (*e.g.*, the van der Waals molecular surface[19]) when a set of sets of alkanes is investigated.

At the moment, the efforts to decompose Δ (by analogy to ***W***), in the hope of finding a general relation for trees, were unsuccessful. Note that relations **(12)−(22)** are valid only in acyclic structures.

WIENER-TYPE NUMBERS OF HIGHER RANK

Walk degree, $^{e}\boldsymbol{W_i}$ (of rank **e**) of a vertex **i** (or atomic walk count[20]) is calculated as row sum of the entries in the adjacency matrix, A (raised at power **e**). Local and global invariants based on walks in graph were considered for correlating with physico-chemical properties.[20]

Weighted walk degree, $^{e}\boldsymbol{W_{M,i}}$, can be easily calculated by means of the algorithm proposed by Diudea *et al.*[21] It evaluates a local (topological) property by iterative summation of vertex contributions over all neighbors (see also refs 22 and 23). M is a square matrix used for weighting walks, and $^{e}\boldsymbol{W_{M,i}}$ has the meaning of row sum of entries in the M matrix (raised at power **e**)

$$^{e}\boldsymbol{W_{M,i}} = \sum\nolimits_{\mathrm{j}\in \mathrm{V(G)}} [\mathrm{M}^{\mathbf{e}}]_{\mathbf{ij}} \qquad (23)$$

The global value, $^{e}\boldsymbol{W_M}$, will be a ***Walk*** (or a Wiener-type) ***number of rank e***

$$^{e}\boldsymbol{W_M} = {}^{e}\boldsymbol{W_M(G)} = \mathbf{(1/2)}\sum\nolimits_{\mathrm{i}} {}^{e}W_{M,i} \qquad (24)$$

When M = $\mathrm{D_e}$ then $^{e}\boldsymbol{W_{De}}$ denotes a **Wiener-(Hosoya)** number; when M = $\mathrm{W_e}$, then $^{e}\boldsymbol{W_{We}}$ represents a **Wiener-(Wiener)** number; when M = $\mathrm{W_p}$, then $^{e}\boldsymbol{W_{Wp}}$ denotes a **hyper-Wiener-(Randić)** number. Values of $^{e}\boldsymbol{W_M}$ numbers of rank 1 and 2 are collected in Table 1.

Although the overall sums in graph of the "internal" and "external" paths are identical, they count distinct quantities. This fact is reflected in the entries of the corresponding matrices and results in different walk numbers of rank higher than one. Thus, any tree-graph shows $^{1}\boldsymbol{W_{De}} = {}^{1}\boldsymbol{W_{We}} = {}^{1}\boldsymbol{W}$ and $^{1}\boldsymbol{W_{Dp}} = {}^{1}\boldsymbol{W_{Wp}} = {}^{1}\boldsymbol{WW}$ but different walk numbers of rank two $^{2}\boldsymbol{W_M}$ (see Table 1). As a consequence, the composition of ***WW*** (eq 8) is not maintained between the corresponding walk numbers of rank 2 (*i.e.*, $^{2}\boldsymbol{W_{Dp}} \neq {}^{2}W_{De} + {}^{2}W_{\Delta D}$ or $^{2}\boldsymbol{W_{Wp}} \neq {}^{2}W_{We} + {}^{2}W_{\Delta W}$).

Walk numbers showed[3] good correlation with some physico-chemical properties of alkanes, such as the octane number and van der Waals areas.

The novel matrix $\mathrm{CJ_u}$ can be operated by the $^{e}\boldsymbol{W_M}$ algorithm[21] to give its walk numbers the $^{1}\boldsymbol{W}_{\mathrm{CJu}}$ and $^{2}\boldsymbol{W}_{\mathrm{CJu}}$. Now, it is easy to write eq 14 in walk number terms

$$^{1}\boldsymbol{W_{CJu}} = {}^{1}\boldsymbol{W_{We}} = {}^{1}\boldsymbol{W_{De}} = {}^{1}\boldsymbol{W} \qquad (25)$$

As it can be seen from Table 1, the walk numbers of rank 2 are different for the three matrices. In addition to the $^{e}\boldsymbol{W_M}$ algorithm, numbers $^{2}\boldsymbol{W_M}$ cam be obtained either by making square of the corresponding M matrices or by calculating the unsymmetric super-matrix $W_{(M^1M^2M^3)}$,[3,24] defined as

$$[W_{(M_1M_2M_3)}]_{ij} = {}^{[M_2]_{ij}}\boldsymbol{W}_{M_{1,i}}[M_3]_{ij} \qquad (26)$$

The half sum of entries in such a matrix provides various ${}^e\boldsymbol{W}_M$ numbers, function of matrix combinations:

$$(CJ_{\mathbf{u,r}}, 1, CJ_{\mathbf{u,r}}) \text{ and } (W_{\mathbf{e}}, 1, W_{\mathbf{e}}) \text{ give } {}^2\boldsymbol{W}_{We}$$

$$(CJ_{\mathbf{u,c}}, 1, CJ_{\mathbf{u,c}}) \text{ and } (D_{\mathbf{e}}, 1, D_{\mathbf{e}}) \text{ give } {}^2\boldsymbol{W}_{De}$$

$$(CJ_{\mathbf{u,r}}, 1, CJ_{\mathbf{u,c}}) \text{ and } (CJ_{\mathbf{u,c}}, 1, CJ_{\mathbf{u,r}}) \text{ give } {}^2\boldsymbol{W}_{CJu}$$

where $CJ_{\mathbf{u,r}}$ and $CJ_{\mathbf{u,c}}$ indicate that the algorithm runs on rows and columns, respectively, and 1 is a square matrix with entries $[1]_{ij} = 1$. The number ${}^2\boldsymbol{W}_{CJu}$ represents the mean of the half sum of entries in the matrix product, to the left and to the right, of matrices $W_{\mathbf{e}}$, and $D_{\mathbf{e}}$. It is an additional proof that the matrix $CJ_{\mathbf{u}}$ contains the information of the both matrices. Properties of the super-matrix $W_{(M^1M^2M^3)}$ will be discussed in a future paper.[24]

CONCLUSIONS

Unsymmetric characterization of paths enables the construction of unsymmetric square matrices.[3] When the considered property is the number of vertices lying to one part of one of the endpoints of a path, it results in a matrix denominated $CJ_{\mathbf{u}}$. This matrix can be used for construction of other (symmetric) matrices, $W_{\mathbf{e}}$, $W_{\mathbf{p}}$, Δ_W, and $\Delta_{CJ\mathbf{u}}$, and for calculating the corresponding walk numbers (or Wiener-type numbers), which can be used as topological descriptors in correlating studies.[3,4,15]

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