Atomic Walk Counts of Negative Order

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Atomic walk counts (*awc*'s) of order k ($k \geq 1$) are the number of all possible walks of length k which start at a specified vertex (atom) i and end at any vertex j separated by m ($0 \leq m \leq k$) edges from vertex i. The sum of atomic walk counts of order k is the molecular walk count (*mwc*) of order k. The concept of atomic and molecular walk counts was extended to zero and negative orders by using a backward algorithm based on the usual procedure used to obtain the values of *mwc*'s. The procedure can also be used in cases in which the adjacency matrix **A** related to the actual structure is singular and therefore $\mathbf{A}^{-1}$ does not exist. *awc*'s and *mwc*'s of negative order may assume noninteger and even negative values. If matrix **A** is singular, atomic walk counts of zero order may not be equal to one.

INTRODUCTION

The paper was motivated by recent reports in this journal by Rücker and Rücker[1−4] on walks in molecular graphs and their uses in structure−property studies and as measures of molecular complexity.[2,4,5] Walks are defined for labeled and connected graphs. A walk is an alternating sequence of vertices and edges beginning and ending with vertices, in which the edge is incident with the two vertices immediately preceding and following it.[6] Since we are interested in molecular graphs, it should be noted that a vertex denotes an atom, and an edge corresponds to a chemical bond in a structural formula.[7] Hydrogen atoms are not considered. As an example consider the walk starting at vertex 1 and ending at vertex 2 of ethylcyclobutane, denoted by a in Figure 1: 1-2-3-4-6-5-3-2.

Another (the shortest) walk starting at vertex 1 and ending at vertex 2 of the same structure is simply 1−2. Atomic walk count (*awc*'s) of order k and related to vertex i ($i = 1,..., N$, where N is total number of vertices in a graph) is the total number of walks of length k starting at vertex i.[8,9] A path is a walk in which each vertex is distinct.[6] Both walks and paths have been related to molecular properties.[1,2,4,8,10−12] In Figure 2 we display the *awc*'s in ethylcyclobutane graph.

Molecular walk counts (*mwc*'s) of order k are the sum of all *awc*'s of order k. In our example shown in Figure 2: $w_1 = 1 + 2 + 3 + 2 + 2 + 2 = 12$, where w is the symbol representing *mwc*'s and the subscript refers to the order.[13] In this paper walk counts of negative (and zero) order will be investigated. In the next section Razinger's algorithm used to compute *awc*'s of positive orders will be formalized. In the third section the inverse procedure will be outlined, and then several properties and finally a few applications of *awc*'s of negative order will be discussed.

FORMALIZATION OF RAZINGERS ALGORITHM FOR ENUMERATING *AWC*'S

The values of *awc*'s of the second order at vertex i are equal to the sum[8] of *awc*'s of the first order of all neighbors of i (see Figure 2). In a similar manner *awc*'s of higher order can be defined. This method for counting walks in (molecular) graphs has been discussed recently by Rücker and Rücker.[8] The procedure is based on the Morgan extended connectivities[14,15] and was first used 20 years ago by Razinger[16] and later on by Figueras.[17] Therefore we call this method Razinger's algorithm. It is equivalent with the following numerical procedure. Let **1** be an N-dimensional (column) vector, all entries of which are equal to one. Let $\mathbf{a}_k$ be a (column) vector, the entries of which are the *awc*'s of order k for all vertices. Then Razinger's algorithm[16] can formally be written as[17]

$$\mathbf{a}_k = \mathbf{A}^k\mathbf{1} = \mathbf{A}^{k-1}\mathbf{a}_1 = ... = \mathbf{A}\mathbf{a}_{k-1} \qquad (1)$$

As an illustrative example consider the adjacency matrix $\mathbf{A}_{\text{ethylcyclobutane}}$ of the ethylcyclobutane graph a, given in Figure 1.

$$\begin{matrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 1 & 0 \end{matrix}$$

By multiplying vector **1** by matrix $\mathbf{A}_{\text{ethylcyclobutane}}$ the *awc*'s of the first order will be obtained

$$\mathbf{A}_{\text{ethylcyclobutane}}\mathbf{1} = (1, 2, 3, 2, 2, 2)' = \mathbf{a}_1 \qquad (2)$$

where the prime denotes that the preceding row vector must be transposed to obtain the column vector $\mathbf{a}_1$. Other methods which may also be used to calculate *awc*'s have been reviewed recently.[9]

The use of Razinger's algorithm to obtain higher order (atomic and molecular) walk counts is straightforward. Obviously, if matrix $\mathbf{A}^{-1}$ exists, then the procedure can be inverted:

$$\mathbf{a}_{k-1} = \mathbf{A}^{-1}\mathbf{a}_k \qquad (3)$$

If eq 3 is valid, then the concept of *awc*'s can be extended to zero and negative orders.

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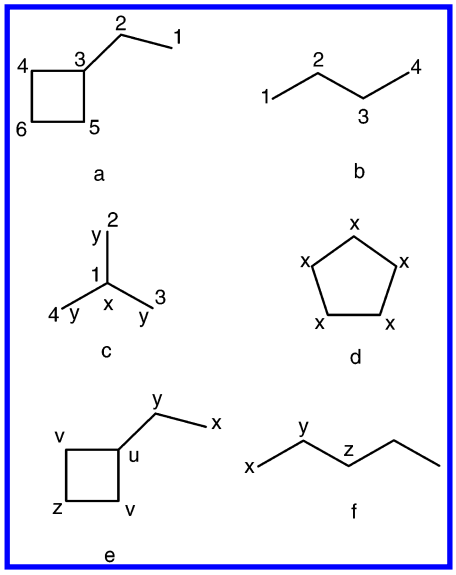

Figure 1. The numbering and types of the hydrogen-suppressed graphs which are discussed in this paper.

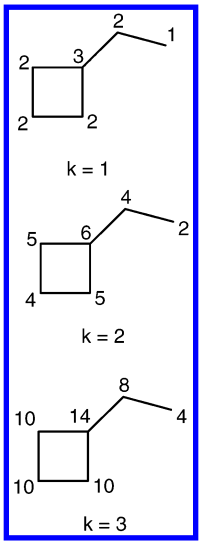

Figure 2. Atomic walk counts of the first, second, and third orders in the ethylcyclobutane graph.

In this paper we show that the procedure can be reversed even if **A** is singular, i.e., matrix **A** has no inverse. (Matrix **A** is singular if its determinant is equal to zero, or, equivalently, if one of the eigenvalues of **A** is zero.) In this case the zero-order vector of *awc*'s is sometimes not equal to **1** ($\mathbf{a}_0 \neq \mathbf{1}$). Virtual walk counts (with $k < 0$) are usually noninteger numbers. In full analogy to the case $k = 1$, *awc*'s of order -1 will be referred to as *virtual* valences. In the next section three subclasses of the inverse procedure will be investigated.

THE INVERSE PROCEDURE

Case 1. The *first* (and the simplest) case is when the inverse of the adjacency matrix does exist. Consider butane (Figure 1, structure b) as an example. $\mathbf{A}_{\text{butane}}$ (left) and $\mathbf{A}_{\text{butane}}^{-1}$ (right) are listed below.

$$\begin{array}{cccc} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{array} \qquad \begin{array}{cccc} 0 & 1 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ -1 & 0 & 1 & 0 \end{array}$$

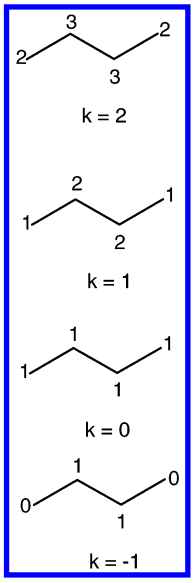

Figure 3. Hydrogen suppressed graph of butane with *awc*'s of order $k = 2$, 1, 0, and -1.

The *mwc* of order -1 is equal to 2. The calculation of *awc*'s (and *mwc*'s) of order $k < 1$ is straightforward and is summarized in Figure 3.

Case 2. Matrix $\mathbf{A}^{-1}$ does not exist, and $\mathbf{a}_0 = \mathbf{1}$. Trimethylmethane (Figure 1, structure c) is an example of the *second* case for which matrix $\mathbf{A}^{-1}$ does not exist since **A** contains three identical rows (and columns):

$$\begin{array}{cccc} 0 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{array}$$

Let us denote the zero-order *awc* count of the branching vertex 1 by x_0—instead of using $\mathbf{a}_0(1)$—and similarly the zero-order *awc*'s of the end-vertices by y_0, whereas x_1 and y_1 are the usual first order *awc*'s (Figure 1, structure c). Then we can write for the branching vertex

$$x_1 = 3 = 3y_0 \tag{4}$$

and

$$y_1 = 1 = x_0 \tag{5}$$

for each end-vertex. The solution of this system of equations is trivial: $x_0 = y_0 = 1$. Let us repeat the same procedure for $k = -1$

$$x_0 = 1 = 3y_{-1} \tag{6}$$

$$y_0 = 1 = x_{-1} \tag{7}$$

and therefore $x_{-1} = 1$ and $y_{-1} = 1/3$. The same procedure can be repeated for any $k < 0$. Results are summarized in Figure 4.

A graph in which every vertex has the same degree D is called a regular graph of degree D.[6] Consider as an example the cyclopentane graph[18] (Figure 1, structure d): the contributions of all vertices are identical. Therefore

$$x_1 = 2 = 2x_0 \tag{8}$$

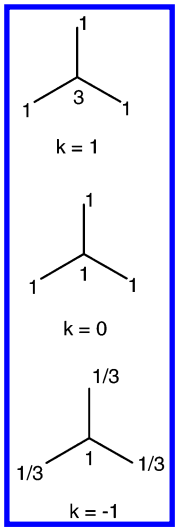

Figure 4. Hydrogen suppressed trimethylmethane graph with *awc*'s of order $k = 1$, 0, and -1.

and therefore $x_0 = 1$. Consequently

$$x_{-k} = 1/2^k \tag{9}$$

In general for any regular graph of degree m ($k > 0$).

$$x_{-k} = 1/m^k \tag{10}$$

Case 3. Matrix $\mathbf{A}^{-1}$ does not exist, and $\mathbf{a}_0 \neq \mathbf{1}$. The graph of ethylcyclobutane (Figure 1, structure e) will serve as an example to illustrate the problems encountered with this type of structure. Let us again express the degrees (i.e. first-order walks) in terms of zero-order walks:

$$x_1 = 1 = y_0 \tag{11}$$

$$y_1 = 2 = x_0 + u_0 \tag{12}$$

$$u_1 = 3 = y_0 + 2v_0 \tag{13}$$

$$v_1 = 2 = u_0 + z_0 \tag{14}$$

$$z_1 = 2 = 2v_0 \tag{15}$$

From eqs 11 and 15, $y_0 = 1$ and $v_0 = 1$, and eq 13 does not fix any new parameter. Equations 12 and 14 are not sufficient to determine the remaining three parameters x_0, u_0, and z_0, but eqs 12 and 14 can also be expressed in terms of parameters x_{-1}, u_{-1}, and z_{-1}:

$$y_1 = 2 = 2y_{-1} + 2v_{-1} \tag{16}$$

$$v_1 = 2 = y_{-1} + 4v_{-1} \tag{17}$$

yielding $y_{-1} = 2/3$ and $v_{-1} = 1/3$. From these (using eqs 12 and 14) $x_0 = y_{-1} = 2/3$, $u_0 = 4/3$, and $z_0 = 2/3$. The same procedure can be repeated for orders -1, -2, etc. (see Figure 5). *n*-Pentane (Figure 1, structure f) belongs also to this class, with $x_0 = 2/3$, $y_0 = 1$, $z_0 = 4/3$, $x_{-1} = 1/3$, $y_{-1} = 2/3$, and $z_{-1} = 2/3$.

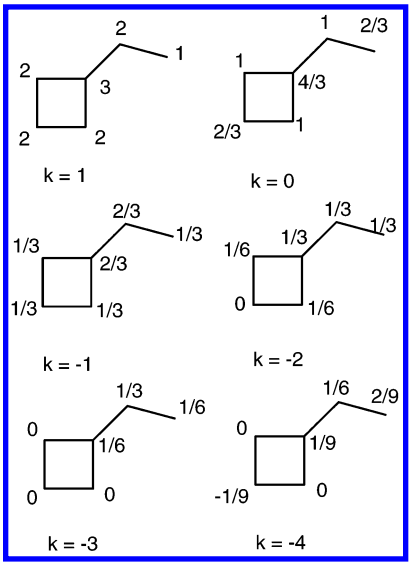

Figure 5. Hydrogen suppressed graph of ethylcyclobutane with *awc*'s of order $k = 1$, 0, -1, and -2.

The fact whether $\mathbf{a}_0$ is equal or not to **1** can only be decided in the knowledge of the actual adjacency matrix.

PROPERTIES OF WALK COUNTS OF NEGATIVE ORDER

For any matrix **A** the Cayley-Hamilton theorem[19] holds

$$\mathbf{A}^N + a_1\mathbf{A}^{N-1} + a_2\mathbf{A}^{N-2} + ... + a_{N-1}\mathbf{A} + a_N\mathbf{I} = 0 \tag{18}$$

where **I** denotes the unit matrix and coefficients a_i ($1 \leq i \leq N$) are identical with the coefficients of the polynomial

$$\lambda^N + a_1\lambda^{N-1} + a_2\lambda^{N-2} + ... + a_{N-1}\lambda + a_N = 0 \tag{19}$$

and λ is an eigenvalue of matrix **A**, i.e., the solution of the secular equation $|\mathbf{A} - \lambda\mathbf{I}| = 0$. Multiplying eq 18 by $\mathbf{A}^{-1}$ and expressing $\mathbf{A}^{-1}$ in terms of the remaining matrices we obtain

$$\mathbf{A}^{-1} = -(\mathbf{A}^{N-1} + a_1\mathbf{A}^{N-2} + ... + a_{N-1}\mathbf{I})/a_N \tag{20}$$

In analogy to the example listed in the Introduction, it is easy to extend the concept of *mwc* to zero and negative orders: for any $k \leq 0$, w_k is equal to the sum of diagonal and one-half of the off diagonal entries of matrix $\mathbf{A}^k$. If $\mathbf{A}^{-1}$ exists then from this definition and eq 20 it follows that

$$w_{-1} = -(w_{N-1} + a_1w_{N-2} + a_2w_{N-3} + ... + a_{N-1}w_0)/a_N \tag{21}$$

Equation 21 is not valid if the adjacency matrix is singular (when $a_N = 0$). Note also that in all cases (i.e. irrespectively whether A is singular or not) it holds that

$$\mathbf{A1} = \mathbf{Aa}_0 = \mathbf{a}_1 \tag{22}$$

and

$$\mathbf{1'a}_0 = \mathbf{a}_0'\mathbf{a}_0 \tag{23}$$

Consider ethylcyclobutane (Figure 5) as an example: $\mathbf{1'a}_0$ = (1, 1, 1, 1, 1, 1)(2/3, 1, 4/3, 1, 1, 2/3)′ = 17/3 = (2/3, 1,

4/3, 1, 1, 2/3)(2/3, 1, 4/3, 1, 1, 2/3)′ = $\mathbf{a}_0'\mathbf{a}_0$. From eqs 22 and 23 it follows that

$$\mathbf{1}'\mathbf{a}_k = \mathbf{a}_0'\mathbf{a}_k \quad (24)$$

It follows from eq 1 that for any (positive) m and n

$$\mathbf{a}_m'\mathbf{a}_n = (\mathbf{A}^m\mathbf{1})'(\mathbf{A}^n\mathbf{1}) = \mathbf{1}'\mathbf{A}^m\mathbf{A}^n\mathbf{1} = \mathbf{1}'\mathbf{A}^{m+n}\mathbf{1} = \mathbf{1}'\mathbf{a}_{m+n} = w_{m+n} \quad (25)$$

because **A** is symmetric. Note that the equation

$$\mathbf{a}_m'\mathbf{a}_n = w_{m+n} \quad (26)$$

holds for $m,n \leq 0$, even if $\mathbf{A}^{-1}$ does not exist. As an example consider ethylcyclobutane with $m = 1$ and $n = -2$ (Figures 2 and 5):

$$\mathbf{a}_1'\mathbf{a}_{-2} = (1*1/3 + 2*1/3 + 3*1/3 + 2*1/6 + 2*1/6 + 2*0) = 8/3 = w_{-1} \quad (27)$$

DISCUSSION

The solution of the "downward recursion" problem delineated in this paper is not complete: still an algorithm applicable to all types of structures should be created. Clearly, if matrix **A** is nonsingular, one may conveniently choose $\mathbf{A}^{-1}$ to perform this task. For the case that **A** is singular we still wish that a step toward $\mathbf{a}_{m-1} = \mathbf{A}^{(-)}\mathbf{a}_m$ is achieved, where $\mathbf{A}^{(-)}$ denotes some generalized inverse to **A**. For positive m this task is achieved if $\mathbf{A}^{(-)}$ does not admix null and nonnull spaces of **A**, whence since the $\mathbf{a}_m$ for positive m must have no component in the null space of **A**, it is seen that the part of $\mathbf{A}^{(-)}$ may be chosen in any way one wishes. One convenient way to choose this null-space part of $\mathbf{A}^{(-)}$ is as null and then take the nonnull space part of $\mathbf{A}^{(-)}$ to be the inverse of **A** on its restriction to this nonnull space. Then $\mathbf{A}^{(-)}$ is the Moore-Penrose generalized inverse[20] of **A**.

This construction readily indicates when $\mathbf{a}_0$ defined by the downward recursion (as $\mathbf{A}^{(-)}\mathbf{a}_1$) is distinct from the vector **1** with all components equal to 1. One has $\mathbf{a}_0 \neq \mathbf{1}$ if and only if **1** has no component in the null-space of **A**. Thence $\mathbf{a}_0 = \mathbf{1}$ not only when **A** is nonsingular but also for many singular cases, such as cyclobutane, cyclooctane, methylcyclobutane, propane, trimethylmethane (Figure 1), 2-methylbutane, and 2,3-dimethylbutane. It seems that our solution is *not* an instance of the Moore-Penrose inversion, as $\mathbf{a}_0 \neq \mathbf{1}$ is a legitimate solution. In fact, although equation $\mathbf{a}_1 = \mathbf{A1}$ is always valid, replacement of the left-hand variables by 1 in eqs 11−15 would inevitably lead to contradictory equations, which have no solution at all.

To obtain *awc*'s and *mwc*'s of negative orders, calculator programs have been created (separately for each molecule considered), which solve the respective backward recursion equations, like (4)−(7) and (11)−(17). Figure 5 displays the walk counts of ethylcyclobutane of order $k = 1, 0, -1, -2, -3$, and -4. The corresponding *mwc*'s are as follows: 12, 17/3, 8/3, 4/3, 2/3, and 7/18, respectively. The *mwc*'s obtained for $k = -5, -6, \ldots, -10$ are 4/18, 1/6, 1/9, 11/108, 2/27, and 2/27, respectively. The values of the *mwc*'s, except for case $k = -10$, decrease. Later on with decreasing values of k the corresponding *mwc*'s may also increase, e.g. $w_{-17} = 13/486 = 0.026748971$, and $w_{-18} = 1/36 = 0.027777777$.

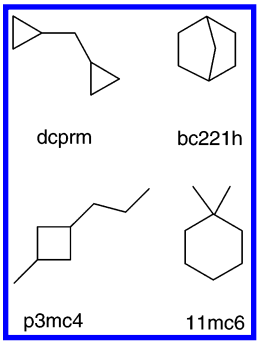

Figure 6. Two pairs of structures (in Rücker's and Rücker's notation:[1] dcprm, bc221h and p3mc4, 11mc6) with equal values of *twc*'s.

Nevertheless this series of *mwc*'s of increasing negative orders seems to converge with the limit being equal to zero. Note that a similar series related to some other graph may also diverge. The graph of 1-methyl-3-propylcyclobutane—see structure p3mc4 in Figure 6—is an example: $w_0 = 8$, $w_{-1} = 4$, $w_{-2} = 20/7$, $w_{-3} = 2$, $w_{-4} = 124/49$, $w_{-5} = 784$, $w_{-6} = 1256$, and $w_{-7} = 8428$. We just mention that for positive orders k with increasing values of k, the value of *mwc*'s also rapidly increases.

The *awc*'s of zero order are in cases 1 and 2 identical for all vertices. According to this result there exists only a single walk of length zero for each vertex. However, this plausible result does not hold for structures belonging to case 3, where for some i $\mathbf{a}_0(i) \neq 1$ (Figure 5). Even more surprisingly $\mathbf{a}_0(i)$ may assume noninteger (and for negative orders even negative) values (Figure 5). The interpretation of these noninteger (and negative) *awc*'s has not yet been accomplished, but it seems that the concept of *awc*'s has to be extended in order to account for such cases. A consequence of such an interpretation atomic (and molecular) walk counts of positive order would constitute a special case of such an extended concept.

To account for the branching, Rücker and Rücker proposed a new invariant, the total walk count,[8] which has been defined as follows[21]

$$t = \Sigma w_k \quad (28)$$

where t denotes the total walk count (*twc*) and the summation has to be performed from $k = 1$, through $k = N-1$. We defined the analogue of t performing the summation from $k = -1$, through $k = -N+1$ (this index will be denoted by t'), and we tried to find out whether t' discriminates molecules in cases where *twc*'s are identical. Molecules with identical values of *twc*'s were found in Rücker's and Rücker's paper[1] and are depicted in Figure 6. (The denotation is due to Rücker and Rücker.[1]) Both pairs of structures, dcprm and bc221h ($t = 1974$)[22a] and p3mc4 and 11mc6 ($t = 3658$),[22b] have identical values of *twc*'s. The first pair of these structures (dcprm and bc221h) cannot be discriminated by using t' since all first neighbors have the same degree. However, the second pair of structures, p3mc4 and 11mc6 (Figure 6), can be discriminated, because $t' = 20.845482$ and $t' = 6.137000$, respectively.

awc's of 0th order are in most cases noninformative; therefore, *awc*'s of order $k = -1$ were considered. These figures, in full analogy with case $k = 1$, will be called *virtual* valences (VVs). The VVs of butane, trimethylbutane, and

ethylcyclobutane are shown in Figures 3−5, respectively, and are also listed for *n*-pentane and cyclopentane (in section "The Inverse Procedure"). In analogy with valences in ethylcyclobutane the VV of vertex 1 is still lower than the corresponding value at vertex 2. The VVs of vertex 2 and vertex 3 are equivalent. Vertices 4 and 6 being equivalent at $k = 1$, remain equivalent at $k = -1$. A similar tendency can be observed for the other examples: if i and j are adjacent vertices, and degree(i) ≥ degree(j) then VV(i) ≥ VV(j). It has to be noted that in a series of unsaturated molecules *no* correlation between *awc*'s of orders 0, −1 and −2 and several quantum chemical indices (frontier orbital density, superdelocalizability, π-electron charges, free valence indices as calculated by using the simple Hückel approach) could be detected; however, this conclusion might be altered if all-valence electron methods were used in a series of saturated hydrocarbons.

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(13) Usually the *abbreviation mwc* and the corresponding mathematical symbol w_k are not set apart, and *mwc* may refer to both concepts. In the present work we have discriminated these two denotations. Similar remarks hold for *awc*'s and *twc*'s.
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(21) Originally eq 28 was given as[8] $t = (1/2)\Sigma w_k$. This formula reflected the fact that most walks in graphs occur in pairs. However, later it has been found[3] that there exits palindromic self-returning walks. Note that palindromic self-returning walks are self-reversed and consequently do not appear in pairs. Thus, in the present report we used the above formula without factor 1/2.
(22) This value was in the paper by Rücker and Rücker[1] 987(a) (and 1829(b)) since in that paper they used formula $t = (1/2)\ \Sigma w_k$.

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