MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **95** (2026) 509–522
ISSN: 0340–6253
doi: 10.46793/match.95-2.19325

Closed–Form Formulas for Topological Indices of Graphs Using Recurrences

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(Received August 12, 2025)

Abstract

We show how to obtain, solving recurrences, closed-form formulas for topological indices of families of graphs obtained through the iterated application of some specific operation on a given graph.

1 Introduction

In what follows, we will deal with a finite simple connected graph $G = (V, E)$ with vertex set $V = \{1, 2, \ldots, n\}$ and edge set E. For all graph-theoretical concepts the reader can consult reference [20]. On such a graph, the Kirchhoff index is defined (see [4]) as

$$K(G) = \sum_{i<j} R_{ij}, \tag{1}$$

where R_{ij} is the effective resistance between vertices i and j when the graph is thought of as an electric network where every edge is given a unit

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resistance. This topological index has been the subject of intense scrutiny in the past few decades, and one specific goal has been to find closed-form expressions for the index in a variety of families of graphs. In that regard, several different tools have been used, such as classic results from electric networks and linear algebra (see [16] and [2], for earlier articles on the subject, and [3] and [8], for more recent ones). One approach that perhaps that has not been exploited much is the use of recurrences. In [21], they used recurrences for individual resistances between pairs of vertices, yielding many valuable results, though the values of the Kirchhoff indices based on the recurrences of the individual resistances (theorem 4.1) arguably are not given in closed form. Other works where they use recurrences to find individual effective resistances can be found in [9] and references therein. In [17] we looked at recurrences defined *directly on the Kirchhoff indices*, not on individual resistances, of some c-cyclic graphs, using the following argument: starting with a given graph G, we obtain a new graph $G^{'}$ by joining to each vertex of G a new pendant vertex with a single edge. Then it is shown with simple calculations that

$$K(G^{'}) = 4K(G) + 2n^2 + n. \tag{2}$$

Next, a family of graphs is defined recursively by choosing an initial graph G_1 to be a c-cyclic graph, for small values of c, and then defining

$$G_{n+1} = G^{'}(G_n). \tag{3}$$

With the help of (2), we can express (3) as the recurrence

$$R_{n+1} - 4R_n = 2^{2n+1} - 2^n, \tag{4}$$

where $R_n = K(G_n)$, and then we solve the recurrence using classical arguments.

In [17] we also mentioned that the operation described above is in fact $G \circ K_1$, the *corona* of G with an isolated vertex K_1. We remind the reader that the corona $G_1 \circ G_2$ of the graphs $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ is the graph that results from one copy of G_1 and $|V_1|$ copies of G_2, after joining each vertex of the i-th copy of G_2 to the i-th vertex of G_1.

Then (2) could have been found using the formula for the corona of two graphs $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$, where $n = |V_1|$ and $|V_2| = m$, found in [23]:

$$K(G_1 \text{ o } G_2) = mn^2 - mn + (m+1)^2 K(G_1) + n^2 K(G_2 + K_1). \qquad (5)$$

Here $G_2 + K_1$ is the graph resulting from joining a single vertex to all vertices of G_2 using m edges.

In this article we want to generalize the result in [17] in several directions: first, we will consider graphs other than K_1 to play the role of G_2 in (5), and G_1 will be arbitrary, not just a c-cyclic graph; also, we will consider operations other than the corona; and finally, we will consider topological indices other than the Kirchhoff index. The only limitation of our method is that we will need to obtain a linear recurrence with constant coefficients such as (4).

In general, the linear recurrence should have the form

$$c_0 R_{n+i} + c_1 R_{n+i-1} + \cdots + c_i R_n = g(n).$$

If the right side is $g(n) = 0$ we say that the equation is homogeneous and if $g(n) \neq 0$ we say that the equation is non-homogeneous. There are at least two methods of solving these recurrences, one entails using generating functions and the other, that we will follow, imitates the usual way to solve linear ordinary differential equations: first, a solution of the form $R_n = r^n$ is proposed for the homogeneous equation, leading to a problem of finding the roots $r_1, r_2, \ldots, r_i$ of the characteristic polynomial

$$c_0 r^i + c_1 r^{i-1} + \cdots + c_i = 0,$$

and then expressing the general solution to the homogeneous equation as

$$R_n = k_1 r_1^n + k_2 r_2^n + \cdots + k_i r_i^n.$$

Once this is achieved, we find a particular solution of the non-homogeneous using the method of undetermined coefficients, and finally, the general solution to the non-homogeneous equals the general solution of the homogeneous plus the particular solution to the non-homogeneous. For the remainder of this article we will only consider recurrences with $i = 1$, which in the language of ordinary differential equations would mean solving *first order* linear equations. For all details regarding this and other methods of solving recurrences, the reader is directed to reference [10].

2 The results

The main idea is that if we can express the topological index T of an operation S on G, $T(S(G))$, in terms of $T(G)$ and some other parameters of G (like the number of edges or the number of vertices) in a linear way, then by the iterated application of S, we construct a sequence of graphs

$$G_1 = G,$$

$$G_{n+1} = S(G_n), \tag{6}$$

for $n \geq 1$, and then when we evaluate the index T on both sides of (6) we can find a recurrence for $T(G_n)$ that can be solved easily in a closed form. If $G_n = (V_n, E_n)$, usually we must find $|E_n|$ and/or $|V_n|$ in closed form, as a function of n, in order to solve the recurrence. In general, that is an easy task.

Example 1. If we choose $G_2 = K_2$, since $K_2 + K_1 = K_3$, we get the particular case of (5) as

$$K(G_1 \circ K_2) = 4|V_1|^2 - 2|V_1| + 9K(G_1). \tag{7}$$

Now define recursively

$$G_{n+1} = G_n \circ K_2, \tag{8}$$

for $n \geq 1$. It is clear that if V_n is the vertex set of G_n then $|V_n| = 3^{n-1}|V_1|$, and (7) and (8) imply

$$K(G_{n+1}) = K(G_n \circ K_2) = 4 \times 3^{2n-2}|V_1|^2 - 2 \times 3^{n-1}|V_1| + 9K(G_n). \quad (9)$$

And if we replace $K(G_n)$ with R_n to ease the notation, we have the recurrence

$$R_{n+1} - 9R_n = 4 \times 3^{2n-2}|V_1|^2 - 2 \times 3^{n-1}|V_1|.$$

The general solution of the homogeneous recurrence

$$R_{n+1} - 9R_n = 0$$

is simply $R_n = C9^n$, for some constant $C > 0$. To deal with a particular solution of the non-homogeneous, we split the problem in two, and find first a particular solution R_n^* to the recurrence

$$R_{n+1} - 9R_n = -2 \times 3^{n-1}|V_1|. \quad (10)$$

We propose a solution of the form $R_n^* = A3^{n-1}|V_1|$, and inserting into (10) we obtain $A = \frac{1}{3}$ and thus $R_n^* = \frac{1}{3}3^{n-1}|V_1| = 3^{n-2}|V_1|$. Now we find a particular solution R_n^{**} to the recurrence

$$R_{n+1} - 9R_n = 4 \times 3^{2n-2}|V_1|^2. \quad (11)$$

We cannot propose a solution of the form $R_n^{**} = B3^{2n-2}|V_1|^2$, because this is already a solution to the homogeneous recurrence. Therefore we propose $R_n^{**} = Bn3^{2n-2}|V_1|^2$, and inserting into (11) we get $B = \frac{4}{9}$, so that $R_n^{**} = 4n3^{2n-4}|V_1|^2$ and the general solution to the non-homogeneous is

$$R_n = C3^{2n} + 3^{n-2}|V_1| + 4n3^{2n-4}|V_1|^2. \quad (12)$$

Using the initial condition $R_1 = K(G_1)$ and inserting into (12) we find that

$$C = \frac{1}{9}\left(K(G_1) - \frac{4|V_1|^2}{9} - \frac{|V_1|}{3}\right),$$

Thus, inserting this value of C into (12), we have shown the following

Proposition 1. *If we take an arbitrary $G_1 = (V_1, E_1)$, and define recursively G_{n+1} using (8), for $n \geq 1$, then the Kirchhoff index of G_n is given by the expression*

$$K(G_n) = 4n3^{2n-4}|V_1|^2 + 3^{2n-4}\left(9K(G_1) - 4|V_1|^2 - 3|V_1|\right) + 3^{n-2}|V_1|. \tag{13}$$

In particular, if we start with $G_1 = K_3$, then we get

$$K(G_n) = (4n-3)3^{2n-2} + 3^{n-1}. \tag{14}$$

In figure 1 we illustrate the particular case $G_1 = K_3$ of proposition 1 by displaying G_3, and notice the fractal-like nature of these G_n's as n grows.

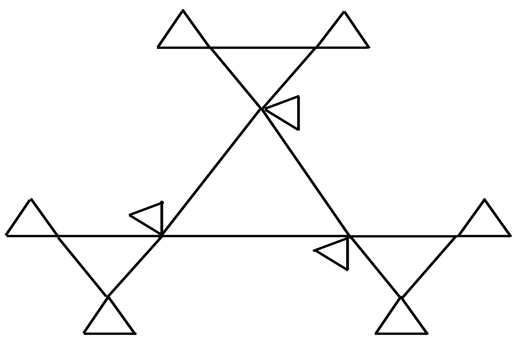

Figure 1. The graph G_3

Example 2. The multiplicative degree-Kirchhoff index is defined as

$$K^*(G) = \sum_{i<j} d_i d_j R_{ij}, \tag{15}$$

The subdivision graph of a give graph $G = (V, E)$ is the graph $S(G) = (V_{S(G)}, E_{S(G)})$ obtained by the following operation S: every edge in E is divided into two new edges with the introduction of a new vertex of degree 2, so that $|E_{S(G)}| = 2|E|$ and $|V_{S(G)}| = |V| + |E|$.

For this index and this operation, the following relation was found in [22]:

$$K^*(S(G)) = 8K^*(G) + 2|E|(2|E| - 2|V| + 1). \tag{16}$$

If $G_1 = (V_1, E_1)$ is arbitrary and we define the sequence of graphs G_{n+1}, $n \geq 1$, as in (6), it is easy to see that

$$|E_n| = |E_1|2^{n-1}$$

and

$$|V_n| = |V_1| + |E_1|(2^{n-1} - 1).$$

If we use these facts in (16), then we get the recurrence

$$R_{n+1} - 8R_n = 2|E_n|(2|E_n| - 2|V_n| + 1) = |E_1|(2|E_1| - 2|V_1| + 1)2^n, \tag{17}$$

where $R_n = K^*(G_n)$.

Very much as in example 1, the solution to the homogeneous is $R_n = C8^n$ for some constant $C > 0$. As for the non-homogeneous, we have a simpler case than in example 1, because we only need to look for a particular solution of the form $R_n^* = A2^n$, and inserting into (17) we get

$$A = -\frac{|E_1|}{6}(2|E_1| - 2|V_1| + 1).$$

Then the general solution to the non-homogeneous is

$$R_n = C8^n - \frac{|E_1|}{3}(2|E_1| - 2|V_1| + 1)2^{n-1}. \tag{18}$$

Using the initial condition $R_1 = K^*(G_1)$ in (18) we identify the constant as

$$C = \frac{1}{8}\left[K^*(G_1) + \frac{|E_1|}{3}(2|E_1| - 2|V_1| + 1)\right],$$

and plugging this value of C back into (18) finishes the proof of the following

Proposition 2. *If $G_1 = (V_1, E_1)$ is an arbitrary graph, and we define recursively G_{n+1} for $n \geq 1$ using (6) and the subdivision as the operation S, then the multiplicative degree-Kirchhoff index of G_n is given by the expression*

$$K^*(G_n) = K^*(G_1)8^{n-1} + \frac{8^{n-1} - 2^{n-1}}{3}|E_1|(2|E_1| - 2|V_1| + 1).$$

Remark. Proposition 2 was shown in [22] with a different proof.

For our next example, we will look at a simple case which can be solved with bare hands calculations, but that we nevertheless include as an instance where the recurrence is homogeneous.

Example 3. The forgotten topological index or F-index is defined as

$$F(G) = \sum_{v \in V} d_v^3.$$

The tensor product of two graphs $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ is defined as the graph $G_1 \times G_2$ with vertex set $V_1 \times V_2$ and (u, x) adjacent to (v, y) if and only if $(u, v) \in E_1$ and $(x, y) \in E_2$. For this product, it is not difficult to get that (see [5])

$$F(G_1 \times G_2) = F(G_1)F(G_2). \tag{19}$$

We can define an operation S on all graphs G by fixing G_2, and considering $S(G) = G \times G_2$. Then we define recursively G_{n+1} as in (6), for $n \geq 1$, and if we take the F index on both sides of (6) we get

$$F(G_{n+1}) = F(G_n \times G_2) = F(G_n)F(G_2),$$

which can be rewritten, taking $R_n = F(G_n)$ as

$$R_{n+1} - F(G_2)R_n = 0.$$

This simple homogeneous recurrence has the general solution $R_n = CF(G_2)^n$, for some $C > 0$, and using the initial condition $R_1 = F(G)$ we can easily identify the constant C and see that we have shown the following

Proposition 3. *For any G, and the graphs G_n defined by (6), with the operation S being the tensor product with the fixed graph G_2 we have*

$$F(G_n) = F(G)F(G_2)^{n-1},$$

for $n \geq 1$.

Our last example deals with one of the pioneering topological indices, the first Zagreb index. This example has the added difficulty that the closed-form expression for the number of edges of the n-th graph needs itself solving a recurrence.

Example 4. The first Zagreb index is defined as

$$M_1(G) = \sum_{v \in V} d_v^2. \tag{20}$$

The composition $G[H]$ of graphs $G = (V_1, E_1)$ and $H = (V_2, E_2)$ is the graph with vertex set $V_1 \times V_2$ and (u_1, v_1) is adjacent with (u_2, v_2) whenever u_1 is adjacent with u_2 or $u_1 = u_2$ and v_1 is adjacent with v_2.

For this composition and the first Zagreb index it is known that (see [12])

$$M_1(G[H]) = |V(H)|^3 M_1(G) + |V(G)| M_1(H) + 8|V(H)||E(H)||E(G)|. \tag{21}$$

In the particular case that $H = K_2$, equation (21) simplifies to

$$M_1(G[K_2]) = 8M_1(G) + 2|V(G)| + 16|E(G)|. \tag{22}$$

It is also mentioned in [12] that

$$|V(G[H])| = |V(G)| \times |V(H)|$$

and

$$|E(G[H])| = |E(G)||V(H)|^2 + |E(H)||V(G)|.$$

For the particular case $H = K_2$ this means

$$|V(G[K_2])| = 2|V(G)| \quad \text{and} \quad |E(G[K_2])| = 4|E(G)| + V(G). \tag{23}$$

Now we define the operation S on any graph G as

$$S(G) = G[K_2], \tag{24}$$

and then we define recursively G_{n+1} as in (6), for $n \geq 1$. If we take the M_1 index on both sides of (6) we get, using (22), that

$$M_1(G_{n+1}) = M_1(G_n[K_2]) = 8M_1(G_n) + 2|V(G_n)| + 16|E(G_n)|. \tag{25}$$

It is easy to see, using (23) that

$$|V(G_n)| = |V(G_1)|2^{n-1}, \tag{26}$$

for $n \geq 1$. As for $|E(G_n)|$, we use (23) to establish the recurrence

$$|E(G_{n+1})| = 4|E(G_n)| + |V(G_n)| = 4|E(G_n)| + |V(G_1)|2^{n-1},$$

for $n \geq 1$. Using $B_n = |E(G_n)|$, this recurrence can be written as

$$B_{n+1} - 4B_n = |V(G_1)|2^{n-1},$$

and we solve it in the usual way: the solution to the homogeneous is

$B_n = C4^n$, for some $C > 0$, and for the non-homogeneous, the choice $B_n^* = A2^{n-1}$ yields $A = -\frac{1}{2}|V(G_1)|$ so that the general solution to the non-homogeneous is

$$B_n = C4^n - |V(G_1)|2^{n-2}. \tag{27}$$

using the initial condition $B_1 = |E(G_1)|$ in (27) yields $C = \frac{1}{4}|E(G_1)| + \frac{1}{8}|V(G_1)|$, and plugging back into (27) we get

$$|E(G_n)| = 2^{2n-2}|E(G_1)| + 2^{2n-3}|V(G_1)| - 2^{n-2}|V(G_1)|. \tag{28}$$

Now, substituting (26) and (28) into (25) and denoting $R_n = M_1(G_n)$ we obtain the recurrence

$$R_{n+1} - 8R_n = (4|E(G_1)| + 2|V(G_1)|)2^{2n} - 3|V(G_1)|2^n. \tag{29}$$

The homogeneous equation has the solution $R_n = C8^n = C2^{3n}$ for some $C > 0$. For the non-homogeneous part, we split the problem of finding a particular solution into two right sides, with the proposed particular solutions being $R_n^* = A2^{2n}$ and $R_n^{**} = D2^n$, and we notice that, as opposed to the situation in example 1, neither one of these is a solution of the homogeneous, so no further fixing (multiplying by n) is needed.

Plugging R_n^* into (29) produces $A = -|E(G_1)| - \frac{1}{2}|V(G_1)|$. Plugging R_n^{**} into (29) produces $D = \frac{1}{2}|V(G_1)|$. Hence, the general solution to the non-homogeneous is

$$R_n = C8^n + (-|E(G_1)| - \frac{1}{2}|V(G_1)|)2^{2n} + \frac{1}{2}2^n|V(G_1)|. \tag{30}$$

Using the initial condition $R_1 = M_1(G_1)$ in (30) yields $C = \frac{1}{8}(M_1(G_1) + 4|E(G_1)| + |V(G_1)|)$. Replacing this value of C back into (30) finishes the proof of the following

Proposition 4. *For any G, and the graphs G_n defined by (6), with the operation S being the composition with the fixed graph K_2 we have*

$$M_1(G_n) = (M_1(G_1) + 4|E(G_1)| + |V(G_1)|)8^{n-1}$$

$$+(-|E(G_1)| - \frac{1}{2}|V(G_1)|)2^{2n} + |V(G_1)|2^{n-1},$$

for $n \geq 1$.

Final remark. We have shown how to find closed-form expressions for a variety of topological indices applied to some families of graphs built through the iterated application of some specific operation on a given graph. The main difficulties of the method are usually found when dealing with the non-homogeneous part of a linear recurrence with constant coefficients. The potential range of applications of this idea is very wide, judging by the abundance of references concerning the values of different indices on different graph operations, such as those mentioned previously in this article and [1], [6], [7], [11], [13], [14], [15], [18], [19], etc.

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