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FIBONACCI GRAPHS

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Some general properties of Fibonacci graphs are established. In addition to this a precise definition of Fibonacci graphs is given for the first time. It is previously known that the nonadjacent numbers of Fibonacci graphs can be calculated via a Fibonacci-type recurrence relation. We show here that the same is true for the independence numbers. These results provide very efficient methods for the calculation of a number of graph polynomials (characteristic, Z-counting, matching = acyclic = reference, independence = color and μ-polynomial) of Fibonacci graphs.

The theory of graph polynomials and their chemical applications has nowadays a long bibliography (for review and further references see[1-3]). One of the basic problems in this field is the calculation of the respective polynomial for a given molecular graph. The recent developement in this area goes mainly in two directions. Firstly, general computer procedures are designed and implemented, enabling an efficient calculation of various graph polynomials of arbitrary molecular graphs (see, for instance, refs. 4-6). Secondly, for particular classes of molecular graphs special calculation schemes are developed, which are based on the specific structural features characterizing the members of this class (for recent work along these lines see[7-16]).

Within the efforts of this second kind, the concept of Fibonacci graphs was put forward by one of the present authors[15,16]. For Fibonacci graphs various graph polynomials (characteristic, matching = acyclic = reference, Z-counting, independence = color, sextet and μ-polynomial) can be computed by using Fibonacci-type recurrence relations. In the present paper we shall elaborate some mathematical aspects of the Fibonacci graphs and the polynomials associated with them.

Fibonacci numbers occur in problems of Kekulé structure enumeration. The first papers where this has been observed seem to be[17,18]; for more recent work on this matter see[19-21]. Another recent application of Fibonacci numbers is in the theory of Herndon resonance energy[22].

Hosoya[23-25] was the first to introduce a graph-theoretical interpretation of the Fibonacci sequence. He namely demonstrated that the nonadjacent numbers of the path provide a representation of the Fibonacci numbers (and also that Lucas numbers are represented by the nonadjacent numbers of the cycle[25]). Although not explicitly stated, families of graphs implying Fibonacci-type recurrences have been considered by one of the present authors[26-28].

CONSTRUCTION OF FIBONACCI GRAPHS

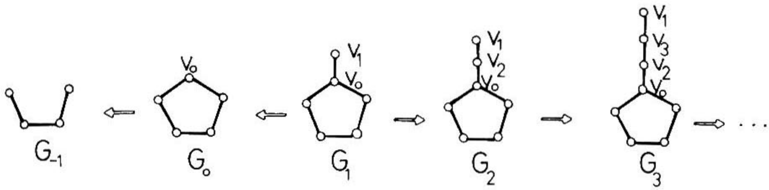
The description of Fibonacci graphs given in ref. 16 is not completely satisfactory. Therefore we provide now a more precise definition. Let $G_{-1}, G_0, G_1, G_2, \ldots$ be an infinite sequence of graphs, constructed in the following manner.

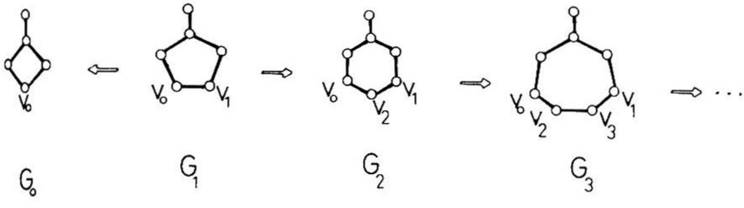
G_1 is an arbitrary graph, possessing at least one edge. Its two adjacent vertices are labeled by v_0 and v_1. For all $i \geq 1$, the graph G_{i+1} is obtained from G_i by inserting a vertex v_{i+1} on the edge connecting v_{i-1} and v_i. The graph G_0 is obtained from G_1 by identifying the vertices v_0 and v_1. The graph G_{-1} is obtained from G_1 by deleting the vertices v_0 and v_1.

DEFINITION. The (finite or infinite) set $\{G_r, G_{r+1}, \ldots, G_{r+s}\}$, $r \geq 0$, $s > r+1$, is called a set of Fibonacci graphs. Further, if either v_0 or v_1 is of degree one, then also $\{G_{-1}, G_0, \ldots, G_r\}$, $r > 0$ is a set of Fibonacci graphs.

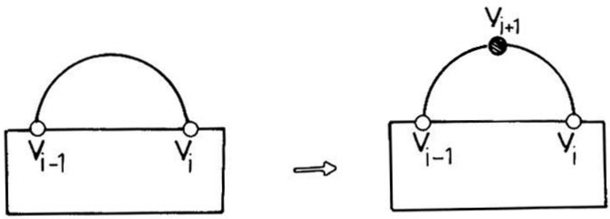
A set of Fibonacci graphs must possess at least three elements.

The above construction is illustrated on the example of the molecular graph of fulvene. It is easy to see that in the general

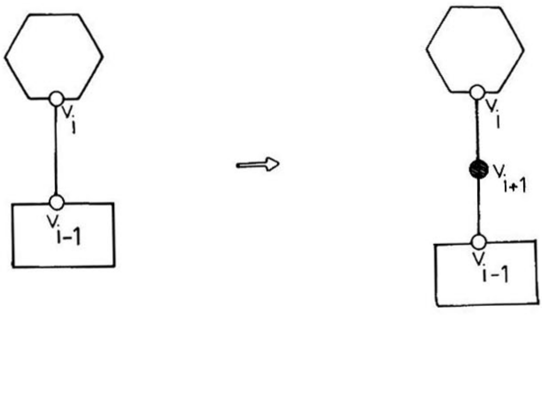




case the construction leads to two possible modes of graph-growth: an internal subdivision (a) and an external subdivision (b):



(a)



(b)

SOME PROPERTIES OF THE FIBONACCI GRAPHS

The following result has been discovered independently in refs. 15 and 28. We present it because of completeness. Ref. 15 contains detailed illustrations and applications of Theorem 1.

THEOREM 1. If G_r, G_{r+1} and G_{r+2} are Fibonacci graphs, then for all k,

$$m(G_{r+2}, k+1) = m(G_{r+1}, k+1) + m(G_r, k) \qquad (1)$$

where m(G, k) denotes the k-th nonadjacent number[23,24] of the graph G. Recall that m(G, k) is equal to the number of k-matchings of the graph G.

Let o(G, k) denote the k-th independence number of the graph G, i.e. the number of ways in which k mutually nonadjacent vertices can be selected from G. These numbers have a certain importance in theoretical chemistry[6,29-31]; in particular, if G is a Clar graph[30] then o(G, k) coincides with the k-th resonant sextet number of the corresponding benzenoid hydrocarbon[16,30,31]. Recently Balasubramanian and Ramaraj[6] considered the independence polynomial (under the name color polynomial) and pointed out several of its chemical and physical applications.

In full analogy to Theorem 1 we have the following result.

THEOREM 2. If G_r, G_{r+1} and G_{r+2} are Fibonacci graphs, then for all k,

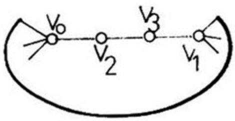
$$o(G_{r+2}, k+1) = o(G_{r+1}, k+1) + o(G_r, k) \quad . \qquad (2)$$

Proof. It is known that the independence numbers conform to the recurrence relation[6,29,30]

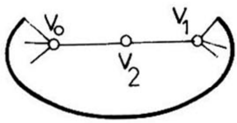
$$o(G, k+1) = o(G-v, k+1) + o(G-A_v, k) \qquad (3)$$

where v denotes a vertex of the graph G and A_v is the set containing the vertex v and all its first neighbours.

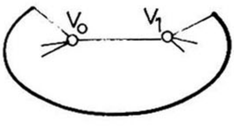
Consider the graphs G_1, G_2 and G_3:



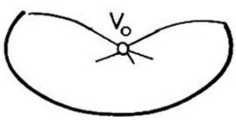
G_3



G_2



G_1



G_0

Applying (3) to the vertex v_0 of G_3 we get

$$o(G_3,\ k+1) = o(G_3-v_0,\ k+1) + o(G_3-A_{v_0},\ k) \quad . \tag{4}$$

Applying (3) to the vertex v_2 of G_3-v_0 and to the vertex v_3 of $G_3-A_{v_0}$, we further get

$$o(G_3-v_0,\ k+1) = o(G_3-v_0-v_2,\ k+1) + o(G_3-A_{v_2},\ k) \tag{5}$$

$$o(G_3-A_{v_0},\ k) = o(G_3-A_{v_0}-v_3,\ k) + o(G_3-A_{v_0}-A_{v_3},\ k-1) \ . \tag{6}$$

It is now easy to see that

$$\begin{aligned} G_3-v_0-v_2 &\simeq G_2-v_0 \quad ; \qquad G_3-A_{v_2} \simeq G_1-v_0 \\ G_3-A_{v_0}-v_3 &\simeq G_2-A_{v_0} \quad ; \qquad G_3-A_{v_0}-A_{v_3} \simeq G_1-A_{v_0} \ . \end{aligned} \tag{7}$$

Here and later the symbol $\simeq$ denotes the isomorphism of the respective two graphs. Bearing in mind the isomorphisms (7), the relations (5) and (6) become

$$o(G_3-v_0,\ k+1) = o(G_2-v_0,\ k+1) + o(G_1-v_0,\ k) \tag{8}$$

$$o(G_3-A_{v_0},\ k) = o(G_2-A_{v_0},\ k) + o(G_1-A_{v_0},\ k-1) \ . \tag{9}$$

Substituting (8) and (9) back into (4) we obtain

$$\begin{aligned} o(G_3,\ k+1) = &\{o(G_2-v_0,\ k+1) + o(G_2-A_{v_0},\ k)\} + \\ &+ \{o(G_1-v_0,\ k) + o(G_1-A_{v_0},\ k-1)\} \ . \end{aligned}$$

Since by (3),

$$o(G_2-v_0,\ k+1) + o(G_2-A_{v_0},\ k) = o(G_2,\ k+1)$$

and

$$o(G_1-v_0,\ k) + o(G_1-A_{v_0},\ k-1) = o(G_1,\ k)$$

it is immediately seen that Theorem 2 holds for $r = 1$. By a completely analogous argument Theorem 2 is proved also for $r > 1$.

In order to verify Theorem 2 for r = 0, apply (3) to the vertices v_0, v_1 and v_2 of G_2 and to the vertex v_0 of G_1. This yields:

$$o(G_2,\ k+1) = o(G_2-v_0-v_2,\ k+1) + o(G_2-A_{v_2},\ k) + \\ + o(G_2-A_{v_0}-v_1,\ k) + o(G_2-A_{v_0}-A_{v_1},\ k-1)$$

and

$$o(G_1,\ k+1) = o(G_1-v_0,\ k+1) + o(G_1-A_{v_0},\ k) \quad .$$

We have further

$$G_2-v_0-v_2 \simeq G_1-v_0 \quad ; \quad G_2-A_{v_2} \simeq G_0-v_0$$

$$G_2-A_{v_0}-v_1 \simeq G_1-A_{v_0} \quad ; \quad G_2-A_{v_0}-A_{v_1} \simeq G_0-A_{v_0}$$

where the structure of the graph G_0 is presented on the previous figure. Therefore,

$$o(G_2,\ k+1) - o(G_1,\ k+1) = o(G_0-v_0,\ k) + o(G_0-A_{v_0},\ k-1) = \\ = o(G_0,\ k) \quad .$$

Thus we see that Theorem 2 is true also for r = 0.

If v_1 is a vertex of degree one, then obviously,

$$G_1-v_1 \simeq G_0 \quad ; \quad G_1-A_{v_1} \simeq G_1-v_0-v_1 \simeq G_{-1}$$

and consequently

$$o(G_1,\ k+1) = o(G_0,\ k+1) + o(G_{-1},\ k)$$

which shows that Theorem 2 holds also for r = -1, provided v_1 (or, what is the same, v_0) is of degree one.

This completes the proof of Theorem 2. ⌑

As it is well known, the nonadjacent numbers m(G, k) are the coefficients of the Z-counting and of the matching = acyclic = reference polynomial. The independence numbers are coefficients of the independence = color polynomial and, if G is a Clar graph, of the sextet polynomial. (For more details on this matter and further references see[16].) Therefore Theorems 1 and 2 relate the matching and the independence polynomials of Fibonacci graph.

We now point at some general properties of graph polynomials whose coefficients conform to relations analogous to (1) and (2).

Let $I(G, k)$ be a graph invariant depending on a certain parameter k (not necessarily an integer!). Let $F(G, x)$ be a graph function defined as

$$F(G) = F(G, x) = \sum_k I(G, k)\, x^k \qquad (10)$$

with summation going over all relevant values of the parameter k. (When necessary, the summation in (10) can be replaced by integration.)

LEMMA 1. Let $G_0, G_1, G_2, \ldots$ be a sequence of graphs. If for any three consecutive members of this sequence the relation

$$I(G_{r+2}, k+1) = I(G_{r+1}, k+1) + I(G_r, k) \qquad (11)$$

holds, then also

$$F_{r+2} = F_{r+1} + x\, F_r \qquad (12)$$

where for the sake of brevity we write F_r instead of $F(G_r, x)$.

Formula (12) is equivalent to

$$\begin{pmatrix} F_{r+1} \\ F_r \end{pmatrix} = \begin{pmatrix} 1 & x \\ 1 & 0 \end{pmatrix} \begin{pmatrix} F_r \\ F_{r-1} \end{pmatrix} = \begin{pmatrix} 1 & x \\ 1 & 0 \end{pmatrix}^r \begin{pmatrix} F_1 \\ F_0 \end{pmatrix} .$$

Proof. Substitute (11) into (10). ¤

LEMMA 2a. If the relation (12) holds for all $r = 0,1,2,\ldots,$ then $F_r = F(G_r, x)$ can be presented in the form

$$F_r = (2\cos t)^{-r}\,\{A\exp(irt) + B\exp(-irt)\} =$$
$$= (2\cos t)^{-r}\,\{(A+B)\cos rt + i(A-B)\sin rt\}$$

where A and B are pertinent functions (independent of r), which can be determined from the initial conditions (say, from the knowledge of F_0 and F_1) and where $x = -(2\cos t)^{-2}$ and $i = \sqrt{-1}$.

Proof. The general solution of the recurrence relation (12) is of the form[32]

$$F_r = A(\lambda_1)^r + B(\lambda_2)^r$$

where λ_1 and λ_2 are the solutions of the auxiliary equation $\lambda^2 = \lambda + x$. Hence,

$$\lambda_{1,2} = \{1 \pm (1 + 4x)^{1/2}\}/2 = (2\cos t)^{-1}\,(\cos t \pm i\sin t) =$$
$$= (2\cos t)^{-1}\exp(\pm it)$$

where the substitution $x = -(2\cos t)^{-2}$ has been made. Lemma 2a follows now straightforwardly. ⌑

LEMMA 2b. If the relation (12) holds for all $r = 0,1,2,\ldots,$ then F_r can be represented in the form

$$F_r = (2\cos t)^{-r}\{2\,F_1(\cos t)\frac{\sin rt}{\sin t} - F_0\,\frac{\sin(r-1)t}{\sin t}\}$$

where $x = -(2\cos t)^{-2}$.

Proof. Lemma 2b follows from Lemma 2a when the initial conditions ($r = 0$ and $r = 1$) are explicitly taken into account. ⌑

LEMMA 3. Let us denote $f_r = F_r$ in the special case when $F_0 = F_1 = 1$. Then

$$f_r = (2 \cos t)^{-r} \sin(r+1)t/\sin t \qquad (13)$$

where $x = -(2 \cos t)^{-2}$.

Proof. Substitute $F_0 = F_1 = 1$ into Lemma 2b and perform appropriate trigonometric transformations. ∎

LEMMA 4. If the relation (12) holds for all $r = 0,1,2,\ldots$, then F_r can be presented in the form

$$F_r = F_1 f_{r-1} + x F_0 f_{r-2} \quad . \qquad (14)$$

Proof. Combine Lemma 2b with eq. (13). ∎

It is instructive to summarize Lemmas 1-4 in the following way:

THEOREM 3. Let $G_0, G_1, G_2, \ldots$ be a sequence of graphs, having the property (11) for all $r=0,1,2,\ldots$, and let $F(G)$ be defined via (10). Then the recurrence relation (12) is obeyed and its general solution is of the form (14), where the function f_r is defined via (13).

Bearing in mind that the Z-counting and the independence polynomial of a graph G with n vertices and m edges are defined as

$$\zeta(G, x) = \sum_{k=0}^{m} m(G, k)\, x^k$$

and

$$\omega(G, x) = \sum_{k=0}^{n} o(G, k)\, x^k$$

respectively, we arrive at the following consequences of Theorems 1, 2 and 3.

COROLLARY 3.1. If $G_0, G_1, G_2, \ldots$ are Fibonacci graphs, then all the results given in Lemmas 1-4 and in Theorem 3 apply to the Z-counting polynomial $\zeta(G, x)$. One has to set $F_r = \zeta(G_r, x)$ and to choose f_r to be the Z-counting polynomial of the path with r vertices.

COROLLARY 3.2. If $G_0, G_1, G_2, \ldots$ are Fibonacci graphs then all the results given in Lemmas 1-4 and in Theorem 3 apply to the independence polynomial $\omega(G, x)$. One has to set $F_r = \omega(G_r, x)$ and to choose f_r to be the independence polynomial of the path with r-1 vertices.

The matching polynomial is related to the Z-counting polynomial via[33]

$$\alpha(G, x) = x^n \zeta(G, -x^{-2}) \quad .$$

Then Corollary 3.1 can be reformulated as follows.

COROLLARY 3.3. If $G_0, G_1, G_2, \ldots$ are Fibonacci graphs, then

$$\alpha(G_r, x) = A \exp(irt) + B \exp(-irt) =$$

$$= (A+B)\cos rt + i(A-B)\sin rt$$

and

$$\alpha(G_r, x) = \alpha(G_1)\frac{\sin rt}{\sin t} - \alpha(G_0)\frac{\sin(r-1)t}{\sin t}$$

where A and B are pertinent functions independent of r, $x = 2 \cos t$ and $\sin(r+1)t/\sin t$ is the matching polynomial of the path with r vertices.

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