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Simplified Computation of Matchings in Polygraphs*

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Matching polynomial and perfect matchings for fasciagraphs, rotagraphs and twisted rotagraphs are treated in the paper. Classical transfer matrix approach makes it possible to get recursions for matching polynomial and perfect matchings, but the order of the matrix grows exponentially in the number of the linking edges between monographs. Novel transfer matrices are introduced whose order is much lower than that in classical transfer matrices. The virtue of the method introduced is especially pronounced when two or more linking edges end in the same terminal vertex of a monograph. An example of a polyacene polygraph with extended pairings is given where a novel matrix has only 16 entries as compared to 65536 entries in the classical transfer matrix. However, all pairings are treated here on equal footing, but the method introduced can be applied to selected types of pairings of interest in chemistry.

INTRODUCTION

The π-electron interactions in conjugated systems are conveniently described by molecular graphs,[1,2] *e.g.*, interactions of six π-electrons in benzene are shown in Figure 1a, where nearest-neighbours interactions are depicted by edges. A pairwise coupling of electrons over the skeleton of the molecular graph is known in chemistry as the Kekulé structure and in mathematics as the perfect matching, and one of two such possible pairings for benzene is shown in Figure 1b. However, π-electrons could pair through space like in the Dewar, Claus or

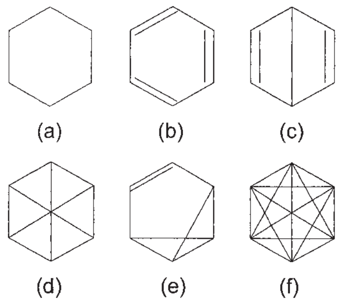

Figure 1. Molecular graph (a) of benzene with its Kekulé (b), Dewar (c), and Claus (d) structures. All structures (b)–(e) are perfect matchings of the complete graph, K_6, on six vertices (f).

* Dedicated to Dr. Edward C. Kirby in happy celebration of his 70th birthday.

** Authors to whom correspondence should be addressed. (E-mail: graovac@irb.hr, vukicevi@pmfst.hr or janez.zerovnik@imfm.uni-lj.si) other resonance structures. These new, so-called extended pairings (in further text we sometimes simply call them pairings) are described by new graphs, *i.e.,* for benzene by Figure 1c–1e, and these graphs, let us call them extended pairings graphs, differ from the original first-neighbours interactions graph shown in Figure 1a. All these extended pairings are just some of the perfect matchings of the related complete graph, *i.e*., of graph K_6 on six vertices (Figure 1f). Kekulé and other valence bond structures have played for decades an important role in organic chemistry.[3] For example, the stability of benzenoid hydrocarbons depends on the number K of Kekulé structures of the related hexagonal graphs. Also, the Dewar, Claus and other extended structures contribute, but to a smaller extent, to the stability of the bezenoid. The importance of considering the extended structures in order to get the exact valence bond solutions have been discussed in the literature.[4]

In the present paper, we study polymers that are conveniently represented by polygraphs,[5] especially those where building blocks of polymers are mutually isomorphic and where there is a uniform bonding between blocks. For such highly structured objects, efficient algorithms have been developed to compute various graph invariants.[6–8] Many of them are based on extensive use of recursions for the invariants under consideration. The number of perfect matchings, K, in polygraphs has been extensively studied so far.[9] The order of the related recursions can be lowered for special classes of polygraphs and this is especially true when two or more bonding edges terminate in a single vertex. Some attempts to lower the order of the classical transfer matrices have been already made in the literature.[10] In the present paper, we study the matching polynomial and perfect matchings in polygraphs, and develop a method to lower the order of related recursions for their computation. The method counts the total number of all extended pairings (Kekulé, Dewar, Claus and others) for a given connectivity between monographs and within a monograph, while in a special case when we adhere to the connectivity of a parent (chemical) polygraph, the method counts only the number of Kekulé structures. Here we treat all extended pairings on the same footing, but the method introduced can be later applied to separate and distinguish pairings as well.

RESULTS AND DISCUSSION

Polygraphs

The notions of monograph and polygraph were introduced in chemical graph theory as a formalization of the chemical notions of monomer and polymer.[5] Polygraphs with open (closed) ends are called fasciagraphs (rotagraphs) if all monographs are isomorphic and the bonding between them is uniform throughout the polygraph. Generalized rotagraphs have been treated in the literature as well.[11]

Let us consider a general polygraph obtained by linking consecutively m building monographs. Let M_1, M_2,...,M_m be arbitrary, mutually disjoint (mono)graphs, and let X_1, X_2,.., X_m be a sequence of linking edges between monographs, *i.e.,* a sequence of sets of unordered pairs of vertices such that $X_i \subseteq V(M_i) \times V(M_i + 1)$, i = 1, 2,..., m (where index i is taken modulo m). Each pair $(x, y) \in X_i$ can be viewed as an edge joining a vertex x of $V(M_i)$ with a vertex y of $V(M_{i+1})$. Note that the edges in X_m join vertices of $V(M_m)$ with vertices of $V(M_1)$. For convenience, we also set $M_0 = M_m$. A polygraph $\Omega_m = \Omega_m(M_1, M_2,..., M_m; X_1, X_2,..., X_m)$ over monographs M_1, M_2,..., M_m is defined in the following way:

$$V(\Omega_m) = V(M_1) \cup V(M_2) \cup ... \cup V(M_m)$$
$$E(\Omega_m) = E(M_1) \cup X_1 \cup E(M_2) \cup X_2 \cup ... \cup E(M_m) \cup X_m.$$

For a polygraph Ω_m and for i = 1 2...,m we also define

$$L_i = \{u \in V(M_i) \mid \exists v \in V(M_{i+1}) : (u, v) \in X_i\},$$
$$R_i = \{u \in V(M_{i+1}) \mid \exists u \in V(M_i) : (u, v) \in X_i\}.$$

In general, $R_i \cap L_{i+1}$ need not be empty. In the special case when M_1, M_2,...,M_m are all isomorphic to a graph M (*i.e.*, all graphs M_i are disjoint copies of the monograph M) and $X_1 = X_2 = ... = X_m = X$, we call the polygraph a rotagraph and denote it by $\omega_m(M; X)$. A fasciagraph $\psi_n(G; X)$ is defined similarly as a rotagraph $\omega_m(G; X)$, except that there are no edges between the first and the last copy of the monograph M, *i.e.*, $X_m = \emptyset$. Since in a rotagraph all sets L_i and sets R_i are equal, we will denote them by L and R, respectively. The same notation will be used for fasciagraphs, keeping in mind that both L_m and $R_m = R_0$ are empty.

Let φ be an automorphism of M. It enables us to define a twisted rotagraph $\varpi^{\varphi}(M; X)$ as follows. Let $X^{\varphi} = \{(u, v) \mid u \in M_m, v \in M_1, (u, \varphi(v)) \in X\}$ while, as before, all the monographs M_i are isomorphic to M and $X_i = X$ for $1 \leq i \leq m - 1$.

Matchings on Polygraphs

Let $p(G, k)$ denote the number of k-matchings in graph G, *i.e.,* the number of ways in which k independent edges can be chosen in G. $p(G, n/2)$ is the number of perfect matchings, with the property that each vertex of the graph is an endpoint of (exactly) one edge of the matching. It is well known that $p(G, n/2)$ is the constant term of the matching polynomial which is defined as

$$\alpha(G;x)=\sum_{k=0}^{\left[\frac{n}{2}\right]}(-1)^k p(G,k)x^{n-2k}$$

where $p(G, 0) = 1$ by definition.[12–14] The set of all matchings which are subsets of the edge set E will be denoted by M (E).

Lemma 1. – Let e be an arbitrary edge with endpoints u and v. Then

$$\alpha(G; x) = \alpha(G - e; x) - \alpha(G - u - v; x)$$

where $G - e$ is the graph G without edge e and $G - u - v$ is the graph G without vertices u and v and all edges with endpoints u or v.

Repeated application of Lemma 1 yields[15] (for details, see Ref. 7).

Lemma 2. – Let F be an arbitrary subset of the edge set E(G). Let W be any subset of F and denote the cardinality of W by $|W|$ and the set of endpoints of W by $<W>$. Then

$$\alpha(G;x)=\sum_{W\in M(F)}(-1)^{|W|}\alpha(G-F-<W>;x).$$

Let us recall Theorem 8, from Ref. 7 which it can be proved by using Lemma 2.

Theorem 3. – The matching polynomial of a polygraph Ω_m can be expressed as

$$\alpha(\Omega_m; x) = \mathrm{tr}(T_1 \cdot T_2 \cdot \cdot \cdot T_m)$$

where $\boldsymbol{T}_i$ are matrices with elements defined as follows. For arbitrary matchings, $W_j \in$ M (X_{i-1}) and $W_k \in$ M (X_i),

$$[\boldsymbol{T}_i]_{jk}=\begin{cases}(-1)^{|W_k|}\alpha(M_i-R_j-L_k;x) & \textit{if } R_j\cap L_k=\varnothing\\ 0; & \textit{otherwise}\end{cases}$$

where $L_k = < W_k > \cap M_i$ and $R_j = < W_j > \cap M_i$.

This theorem can be expressed also in terms of matrices, which are indexed in terms of left (or right) endpoints of edges constituting the matchings rather than in terms of matchings of X_i. In the case when the number of edges in X_i is much greater than the number of its left (or right) endpoints, *i.e.,* when some linking edges end in a common vertex, the resulting matrices may be significantly smaller, thus reducing the complexity of calculations.

Before giving the alternative form of Theorem 3, we introduce notation for subsets of a set $S = \{s_1,s_2,...,s_{|S|}\}$, which will be later also used for natural encoding of its subsets. Subsets A of S are in one-to-one correspondence with integers $i(A)$, $0 \le i(A) \le 2^{|S|} - 1$, given by the rule:

$$i(A)=\sum_{k=1}^{|s|} i_k 2^{k-1},$$

where $i_k = 1 \Leftrightarrow s_k \in A$ (and $i_k = 0 \Leftrightarrow s_k \notin A$). Similarly, one can define the inverse $i \to A(i)$. Note that, as a binary number, $i(A) = (i_{|S|}i_{|S|-1}....i_2i_1)$. We will later write $S^{(i)}$ for the subset $A = A(i)$ of S.

Example. Let $S = \{s_1,s_2\ s_3\}$. Then $S^{(0)} = \emptyset$, $S^{(1)} = \{s_1\}$, $S^{(2)} = \{s_2\}$, $S^{(3)} = \{s_1,s_2\}$, $S^{(4)} = \{s_3\}$, $S^{(5)} = \{s_3,s_1\}$, $S^{(6)} = \{s_3,s_2\}$, and $S^{(2)} = S$.

In particular, we will use this notation for subsets of L_i and R_i.

Theorem 4. – The matching polynomial of a polygraph Ω_m can be expressed as

$$\alpha(\Omega_{m;}\ x) = \mathrm{tr}\ (\boldsymbol{Q}_1 \cdot \boldsymbol{Q}_2 \cdot \cdot \cdot \cdot \boldsymbol{Q}_m)$$

where $\boldsymbol{Q}_i$ are matrices with elements

$$[\boldsymbol{Q}_i]_{jk} = \alpha((M_i \cup < X_i >) - (R_{i-1}(j) \cup \overline{R_i(k)}); x),$$

and $\overline{R_i(k)} = R_i \setminus R_i(k)$ is the complement of the set $R_i(k)$ in R_i.

In other words, the entries of matrix $\boldsymbol{Q}_i$ are the matching polynomials of the monograph M_i plus (some of) the edges of X_i without some vertices of R_{i-1} and R_i. The set of vertices missing at R_i must be compatible (*i.e.,* complement) with the corresponding structure of Q_{i+1}. Analogous considerations hold also for L_i and L_{i+1}.

If the polygraph is a fasciagraph, rotagraph or twisted rotagraph, then this theorem implies that:

$$\alpha(\psi_m;x)=Q^m_{0,0}$$

$$\alpha(\omega_m;x)=\mathrm{tr}(Q^m)=\sum_{i=0}^{2^{|R|}} Q_{ii}$$

$$\alpha(\omega^{\varphi}_m;x)=\sum_{i=0}^{2^{|R|}} Q^m_{i,\varphi(i)}.$$

For $x = 0$, the above formulae give the number of perfect matchings in a rotagraph, fasciagraph and twisted rotagraph. Depending on the connectivity of the underlying polygraph, the formulae give the number of all extended pairings or only of Kekulé structures. More precisely, if the Kekulé structures are to be counted, the benzenoid rings are presented by 6-cycles and if all extended pairings are to be counted, the benzene rings are presented by complete graphs with 6 vertices.

Application: Computation of the Number of Kekulé and Extended Pairing Structures

In this section, we derive formulae for the number of perfect matchings for fasciagraphs, rotagraphs and twisted rotagraphs. Let us first consider polyacene and its related fasciagraph (Figure 2a), rotagraph (Figure 2b) and twisted rotagraph (Figure 2c).

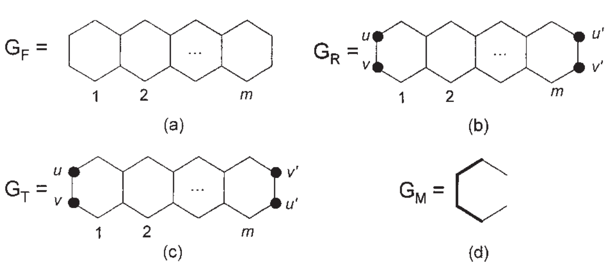

Figure 2. Polyacene fasciagraph (a), rotagraph (b), twisted rotagraph (c) with *m* repeating monographs (d). In rotagraph (b) and twisted rotagraph (c) vertex′ is identified with *u* and *v*′ is identified with *v*.

The corresponding monograph G_M on four vertices (drawn in heavy lines) is depicted together with two linking edges (drawn in light lines) in Figure 2d. The classical transfer matrix is of the order 2^l, where l stands for the number of linking edges. The transfer matrix introduced here is of the order 2^v, where v is the smaller of the numbers of left and right terminal vertices. As for polygraphs depicted in Figure 2, $l = v = 2$, both classical and here introduced transfer matrices are of the same order. Our transfer matrix for monograph G_M reads as:

$$\boldsymbol{Q}(\mathrm{G_M}) = \begin{bmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

It is easy to compute that

$$\boldsymbol{Q}(\mathrm{G_M})^m = \begin{bmatrix} 1 & 0 & 0 & m \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

Note that G_F is a fasciagraph plus a different monograph, and hence the formula reads:

$$\mathrm{K(G_F) = Q(G_M)}^m + \mathrm{Q(G_M)}^m$$

After simple computation, we get:

$$\mathrm{K\ (G_F)} = n + 1.$$

Similarly for K (G_R) and K (G_T) one obtains:

$$\mathrm{K(G_R)} \equiv \alpha(\omega_m;\ x) = \mathrm{tr(Q(G_M)}^m) = 4.$$

$$\mathrm{K(G_T)} \equiv \alpha(\omega_m^{\varphi};x) = \mathrm{Q(G_M)}^{m}_{0,0} + \mathrm{Q(G_M)}^{m}_{1,2} + \mathrm{Q(G_M)}^{m}_{2,1} + \mathrm{Q(G_M)}^{m}_{3,3} = 2,$$

where φ is the automorphism that interchanges *u* and *v*, where $\mathrm{Q(G_M)}_{0,0}$, $\mathrm{Q(G_M)}_{1,2}$, $\mathrm{Q(G_M)}_{2,1}$ and $\mathrm{Q(G_M)}_{3,3}$ are the numbers of perfect matchings in G_M, G_M – (left *v*) – (right *u*), G_4 – (left *u*) – (right *v*) and G_M – (left *u* and *v*) – (right *u* and *v*), respectively. The real virtue of the method introduced is illustrated for polygraphs depicted in Figure 3.

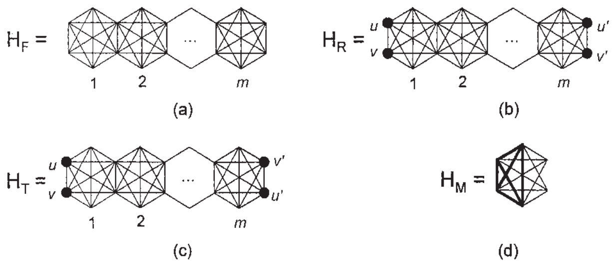

Figure 3. Polyacene with extended pairings fasciagraph (a), rotagraph (b), twisted rotagraph (c) with *m* repeating monographs (d). In rotagraph (b) and twisted rotagraph (c) vertex *u*′ is identified with *u* and *v*′ is identified with *v*.

The classical transfer matrix is here of the order 2^l, where $l = 8$, *i.e.*, it is of the order 256 and has 65536 entries. The cardinalities of left and right terminal vertices are four and two. Therefore, $v = 2$ and the transfer matrix introduced here is of the order $2^2 = 4$, *i.e.,* it has only 16 entries, and it reads:

$$\boldsymbol{Q}(\mathrm{H_M}) = \begin{bmatrix} 3 & 0 & 0 & 12 \\ 0 & 3 & 3 & 0 \\ 0 & 3 & 3 & 0 \\ 1 & 0 & 0 & 2 \end{bmatrix}.$$

It is easy to compute that

$$\boldsymbol{Q}(\mathrm{H_M})^m = \begin{bmatrix} \frac{3}{7}(-1)^m + \frac{4}{7}6^m & 0 & 0 & -\frac{12}{7}(-1)^m + \frac{12}{7}6^m \\ 0 & \frac{1}{2}6^m & \frac{1}{2}6^m & 0 \\ 0 & \frac{1}{2}6^m & \frac{1}{2}6^m & 0 \\ \frac{1}{7}(-1)^m + \frac{1}{7}6^m & 0 & 0 & \frac{4}{7}(-1)^m + \frac{3}{7}6^m \end{bmatrix}$$

Therefore,

$$\mathrm{K(H_F) = Q(H_4)}^m_{00} + \mathrm{Q(H_4)}^m_{03}\ .$$

After simple computation, we get

$$K(H_F) = \left(\frac{3}{7}\cdot(-1)^m + \frac{4}{7}\cdot 6^m\right) + \left(-\frac{12}{7}\cdot(-1)^m + \frac{12}{7}\cdot 6^m\right) =$$

$$\frac{16}{7}\cdot 6^m - \frac{9}{7}\cdot(-1)^m$$

Similarly for $K(H_R)$ and $K(H_T)$ one obtains:

$$K(H_R) \equiv \alpha(\omega_m; x) = \mathrm{tr}(Q(H_M)^m) = 2 \cdot 6^m + (-1)^m.$$

$$K(H_T) \equiv \alpha(\omega^{\mu}_{0,0}\mu; x) =$$
$$Q(H_M)^m_{0,0} + Q(H_M)^m_{1,2} + Q(H_M)^m_{2,1} + Q(H_M)^m_{3,3} =$$
$$2 \cdot 6^m + (-1)^m$$

where f is an automorphism that interchanges u and v and where notation for $Q(M)_{00}$, $Q(H_M)_{1,2,}$ $Q(H_M)_{2,1}$, and $Q(H_M)_{3,3}$ follows the above one for G_M.

CONCLUSIONS

A method based on novel transfer matrices has been developed. It enables computation of matching polynomials and perfect matchings in fasciagraphs, rotagraphs and twisted rotagraphs. It is especially suited for a situation where two or more bonding edges between monographs terminate in a single vertex. The procedure is illustrated on polyacene with an extended pairings polygraph where the transfer-matrix has only 16 entries compared to 65536 entries in a classical transfer matrix. Here, all the matching pairings are treated on the same footing, although the method developed could be used to separate pairings as well.

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REFERENCES

1. A. Graovac, I. Gutman, and N. Trinajstić, *Topological Approach to the Chemistry of Conjugated Molecules*, Lecture Notes in Chemistry 4, Springer-Verlag, New York, 1977.
2. N. Trinajstić, *Chemical Graph Theory*, CRC Press, Boca Raton, FL.1983, 2nd Edn., 1992.
3. I. Gutman and O. E. Polansky, *Mathematical Concepts in Organic Chemistry*, Springer-Verlag, Berlin, 1986.
4. N. Flocke, T. G. Schmalz, and D. J. Klein, *Chem. Phys. Lett.* **298** (1998) 71–78.
5. O. E. Polansky and N. N. Tyutyulkov, *MATCH Commun. Math. Comput. Chem.* **3** (1977) 149–223.
6. A. Graovac, O. E. Polansky, and N. N. Tyutyulkov, *Croat. Chem. Acta* **56** (1983) 325–356.
7. D. Babić, A. Graovac, B. Mohar, and T. Pisanski, *Discrete Appl. Math.* **15** (1986) 11–24.
8. M. Juvan, B. Mohar, A. Graovac, S. Klavžar, and J. Žerovnik, *J. Chem. Inf. Comp. Sci.* **35** (1995) 834–840.
9. A. Graovac, D. Babić, and M. Strunje, *Chem. Phys. Lett.* **123** (1986) 433–436.
10. H. J. Broesma and Li Xueliang, *Discrete Appl. Math.* **46** (1993) 79–86.
11. T. Pisanski, A. Žitnik, A. Graovac, and A. Baumgartner, *J. Chem. Inf. Comp. Sci.* **34** (1994) 1090–1093.
12. C. D. Godsil and I. Gutman, *J. Graph Theory* **5** (1981) 137–144.
13. J. Aihara, *J. Am. Chem. Soc.* **98** (1976) 2750–2758.
14. I. Gutman, M. Milun, and N. Trinajstić, *J. Am. Chem. Soc.* **99** (1977) 1692–1704.
15. E. J. Farrell and J. Combin. *Theory* (Ser. B) **27** (1979) 75–86.

SAŽETAK

Pojednostavljeni račun sparivanja u poligrafovima

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U radu se razmatraju polinomi sparivanja i savršena sparivanja u fascia- i rotagrafovima te izvijenim rotagrafovima. Iako klasični postupak transfer matrice omogućava izvođenje rekurzija za polinom sparivanja i savršena sparivanja, red ove matrice eksponencijalno raste s brojem veza među monografovima. Ovdje su uvedene nove transfer matrice čiji je red mnogo niži od onoga za klasične transfer matrice, i to posebice kada jedna ili više veza među monografovima završava u jednom te istom čvoru. Postupak je ilustriran na primjeru poliacenskih poligrafova gdje ovdje uvedena matrica ima samo 16 elemenata u usporedbi s 65536 elemenata klasične transfer matrice. Iako se ovdje uvedeni postupak primjenjuje istovremeno na sva moguća sparivanja u poligrafovima, on je otvoren za primjenu na odabrana sparivanja od posebnoga kemijskoga interesa.