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CONFIGURATIONS, REGULAR GRAPHS AND CHEMICAL COMPOUNDS

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Abstract

The mathematical structures of a configuration and a regular graph and certain chemical compounds are compared. Some recursive construction methods for these structures are described. A short survey on results about configurations concludes the paper.

1. Definitions and examples

1.1. CONFIGURATIONS

DEFINITION 1.1.

A *configuration* (v_r, b_k) is a finite incidence structure with the following properties:

(a) There are v points and b lines.

(b) There are k points on each line and r lines through each point.

(c) Two different lines intersect each other at most once and two different points are connected by a line at most once.

Remark 1.2

It is easy to prove that the following conditions are necessary for the existence of a configuration (v_r, b_k):

$$(1)\quad vr = bk, \quad (2)\quad v \geq r(k-1)+1, \quad \text{and} \quad (3)\quad b \geq k(r-1)+1.$$

If $v = b$ and hence $r = k$, the configuration is called symmetric and is denoted by v_k. Configuration is abbreviated by cfz. (Plural: cfzs.; the Italian word is "configurazione".)

EXAMPLE 1.3

Figures 1, 2 and 3 show the Fano cfz.7_3, a certain blocking set free cfz.13_3 (compare [3]) and the unique cfz.$(6_2, 4_3)$, respectively.

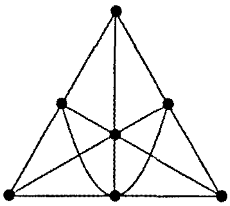


Fig. 1.

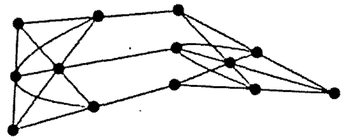


Fig. 2

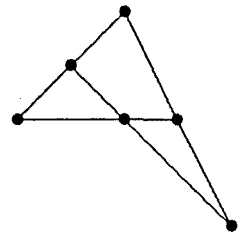


Fig. 3.

1.2. REGULAR GRAPHS

DEFINITION 1.4

An *r-regular graph* with v vertices is a graph where all vertices have degree r. Such a graph has $b = vr/2$ edges.

EXAMPLE 1.5

Figures 4, 5, and 6 show the two non-isomorphic 3-regular graphs with 6 vertices and the famous Petersen graph, one of the twenty-one 3-regular graphs with 10 vertices.

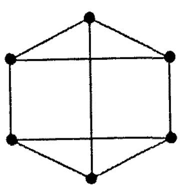


Fig. 4.

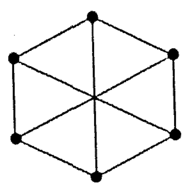


Fig. 5.

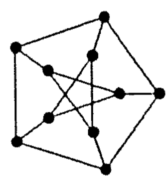


Fig. 6

1.3. CHEMICAL COMPOUNDS

In this paper, "chemical compound" is a name for the following simple model of a molecule consisting of atoms of chemical elements (such as carbon, hydrogen, . . .) and the bonds between them. The model does not describe the realization of the molecule in three-dimensional Euclidean space.

EXAMPLE 1.6

Figures 7, 8, 9, and 10 show the molecules CH_4, C_3H_6, and two possible isomers of C_6H_6.

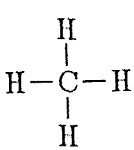


Fig. 7.

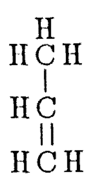


Fig. 8.

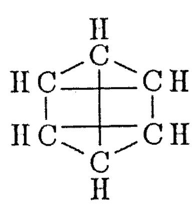


Fig. 9.

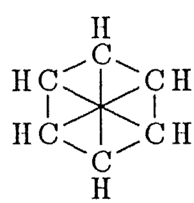


Fig. 10.

2. Some history

2.1. CONFIGURATIONS AND GRAPHS

Configurations were defined by Reye in 1876. During the period until 1910, many results were obtained (compare section 4), mainly by German, Italian, and Dutch mathematicians. After 1910, the interest in configurations and the knowledge of them decreased significantly (see [6]).

Some early results in graph theory have been obtained since 1736 (Euler and the bridges of Königsberg), but as singular results and not within a theory. These include also chemical results (e.g. Cayley and acyclic hydrocarbons).

The earliest paper in graph-theoretic language is said to be Petersen's paper of 1891 [11] called *Die Theorie der regulären graphs*, where he proves results about regular graphs.

It is easy to see that configurations (v_r, b_2) and r-regular graphs with v vertices are equivalent combinatorial structures. So it happened that some 3-regular and 4-regular graphs were enumerated already in 1889/91 in the language of configurations.

2.2. THE WORK OF JAN DE VRIES

One of the most important mathematicians who investigated configurations in those early days was Jan De Vries (born 1st March 1858 in Amsterdam, died 3rd May 1940 in Utrecht). After having studied in Amsterdam, he became a teacher of mathematics in Kampen in 1880. Most of his research on configurations was done before he became Professor of Geometry in Utrecht in 1897.

In 1889, De Vries wrote a paper [12] in which he investigated "planar configurations in which each point is incident with two lines". It is easy to see that these structures are isomorphic to regular graphs if the lines of the configuration are taken as the vertices and if the points are regarded as the edges of the graph. In fact, he determined all small 3-regular and 4-regular graphs (up to a small error, which he corrected in 1891 in [13]) at a time when Petersen published his famous paper about "The theory of regular graphs". The recursive method of De Vries is exhibited in section 3.2. For further details, see [7].

2.3. REGULAR GRAPHS AND ANNULENES

Since the papers of De Vries use the language of configurations long before graph theory became an established mathematical theory, his results were unknown to most of the graph theorists (maybe even to all of them!) until very recently. The "first" enumeration of all 3-regular graphs with 10 vertices, for example, was done by A.T. Balaban in 1966/67 [1]. His motivation was his interest in a chemical problem. Balaban wanted to determine all possible valence-isomers of the annulene $C_{10}H_{10}$.

If only those isomers are considered where each C-atom is connected to three other C-atoms and one H-atom, and in which only simple bonds are allowed, the problem of determining all such possible molecules is equivalent to the determination of all 3-regular graphs with 10 vertices.

> [1, p. 1099] A ... problem in the theory of graphs ... is to find out ... all topologically different ways of connecting $2p$ equivalent points so that each point is connected to three other points.

Compare figs. 4 and 5 with 9 and 10.

By using a computer, Balaban solved this problem in graph theory in 1966/67.

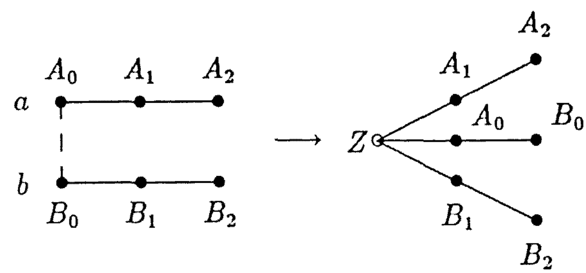
3. Recursive construction methods

3.1. V. MARTINETTI AND CONFIGURATIONS

In [10], Martinetti defined a recursive construction method in order to construct all cfzs. 11_3.

> [10, p. 1] In questa nota mi propongo di far conoscere un metodo per dedurre tutte le forme possibili di configurazioni μ_3, quando si conoscano tutte le cfz. $(\mu - 1)_3$. Applicherò in fine questo metodo per dedurre dalle note cfz.10_3 tutte le cfz.11_3 che, io credo, non furono ancora indicate.

Given a cfz. n_3. If possible, take two parallel lines $a = \{A_0, A_1, A_2\}$ and $b = \{B_0, B_1, B_2\}$ and two points, say $A_0 \in a$ and $B_0 \in b$ which are non-connected. Remove lines a and b and add a new point Z as well as the three new lines through Z: $\{Z, A_1, A_2\}$, $\{Z, B_1, B_2\}$, $\{Z, A_0, B_0\}$. One obtains a cfz. $(n + 1)_3$.



All configurations $(n + 1)_3$ which can be constructed by this method (apply it wherever you can!) are called reducible, the others are called irreducible.

Martinetti also constructed all irreducible cfzs. n_3: one series of cfz.n_3 (take $\{1, 2, 4\}$ mod(n)), one series of cfz.$(10n)_3$, the Pappus cfz.9_3 and two more cfz.10_3. See section 4.2 for the enumeration of cfz.n_3 after Martinetti.

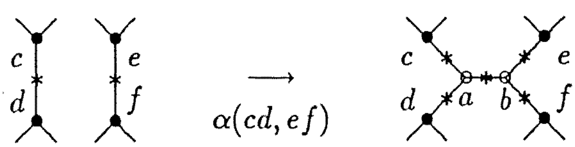
3.2. J. DE VRIES AND REGULAR GRAPHS

The recursive method of De Vries [12] can be used to construct all cfzs. (v_r, b_2) (i.e. all 3-regular graphs).

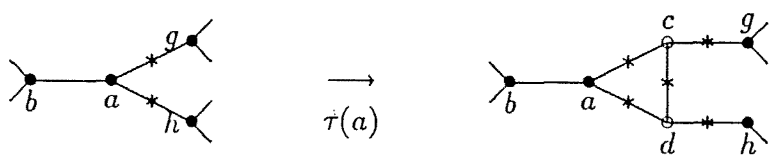
> [12, p. 387] Uit het voorgaande blijkt nu, dat de verschillende $(3n_2, 2n_3)$ door middel van drie vervormingen kunnen bepaald worden, zoodra men de overeenkomstige cf. met twee en vier lijnen minder kent.

The three transformations used by De Vries are described here in graph-theoretic notation. New vertices are denoted by ∘ instead of •. All removed or added edges are labeled with *.

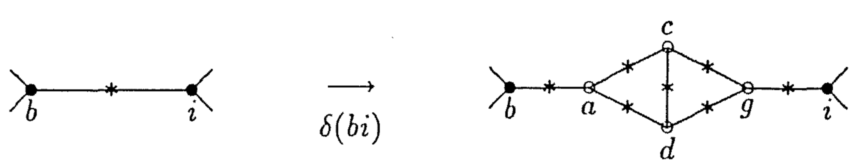
$\alpha(cd, ef)$ ("atrigonische vervorming"): Remove the edges *cd*, *ef* and add as new edges *ab*, *ac*, *ad*, *be*, *bf*, where *a* and *b* are two new vertices. The edge *ab* is not on a triangle.



$\tau(a)$ ("trigonische vervorming"): Remove the edges *ag*, *ah* and add as new edges *ac*, *ad*, *cd*, *cg*, *ch*, where *c* and *d* are two new vertices. The edge *cd* is on exactly one triangle.



$\delta(bi)$ ("ditrigonische vervorming"): Remove the edge *bi* and add as new edges *ab*, *ac*, *ad*, *cd*, *cg*, where *a*, *c*, *d*, *g* are four new vertices. The edge *cd* belongs to two triangles.



The transformations α and τ yield cubic graphs on $v + 2$ vertices and δ yields a graph on $v + 4$ vertices, if the original graph had v vertices.

De Vries also found a similar method for 4-regular graphs which, however, he could not apply because of a condition which was not true in the smallest case.

3.3. A.T. BALABAN AND ANNULENES

In [2], Balaban defined two operations in order to construct all general cubic graphs (i.e. also those with loops and multiple edges) of order $n+2$ recursively from those of order n.

Operation 1: Mark on two edges two new vertices and join them by a new edge.

Operation 2: Mark on an edge a new vertex and join it by a new edge to a new loop.

3.4. FURTHER METHODS

Two further methods are mentioned here very briefly. In 1971, Imrich [9] determined all 3-regular graphs with 10 vertices. He did not use a recursive method, but he classified all the graphs depending on how many triangles they contain. This was done without a computer. The proof needs about four pages.

Quite recently, I read the English summary of a Chinese paper by Zhang and Yang [14], who use an algorithm RGC (regular graphs counting) for determining all regular graphs with at most 12 vertices.

4. Configurations as generalized regular graphs

It is explained above that configurations with $k=2$ are equivalent to regular graphs. In this sense, configurations can be regarded as generalized regular graphs. In this section, the main results which have been obtained in configuration theory will be exhibited. The interested reader is referred to further papers which describe these results in detail (see [4–6]).

4.1. EXISTENCE

Given parameters v, r, b, k, the question arises whether cfz.(v_r, b_k) exists. Of course, the necessary conditions must hold. A very famous non-existence result says that there are no two orthogonal Latin squares of order 6. This implies the non-existence of a cfz.$(36_7, 42_6)$.

For $k=3$, the existence problem has been solved (see [4]): All cfz.(v_r, b_3) exist for which the necessary conditions hold.

The same seems to be true also for $k=4$. No case of non-existence has been found and the "most difficult" of all these configurations have already been constructed.

There is no cfz.22_5 (see [4]), although the necessary conditions hold.

4.2. ENUMERATION

For those parameter sets for which a configuration exits, the question arises whether there are "essentially different" configurations. More precisely, the question is: How many non-isomorphic configurations (v_r, b_k) are there?

This question has been answered, e.g. for the following cfzs. For further details and references, see [4].

Cfz.(v_r, b_k)

Symm. cfz.	Number	Non-symm. cfz.	Number
7_3	1	$(9_4, 12_3)$	1
8_3	1	$(13_6, 26_3)$	2
9_3	3	$(15_7, 35_3)$	80
10_3	10	$(12_5, 20_3)$	5
11_3	31	$(14_6, 28_3)$	787
12_3	229	$(12_4, 16_3)$	574
13_3	2036		
14_3	21399		

The enumeration of all cfzs.11_3 was already achieved in 1887 by Martinetti, of course without the use of a computer. Instead, he created his recursive method described in section 3.1 and applied it with success. The determination of all cfzs.12_3 was tried in 1895 by D. von Sterneck. However, he did not obtain the correct result. By using his own method (not Martinetti's method), he missed exactly one configuration, a fact which was not discovered until 1988. During the last years, I combined the method of Martinetti and a computer and could determine all cfzs.12_3, 13_3, and 14_3 (see [4]).

The determination of all cfzs.$(12_4, 16_3)$ in 1990 was the last step of a more than 150 year old history of constructions of such configurations. After some singular constructions until about 1955 and after about 200 further constructions in Czechoslovakia after that (which, however, remained nearly unknown, being published in Czechoslovak journals in Czech or German), the problem could be solved by using combinatorial relations between configurations, graphs, and Steiner systems.

4.3. ADDITIONAL PROPERTIES

Until now, not many configurations have been really drawn in this paper with "real points" and "real lines", e.g. in the Euclidean plane. The so-called realizability of such a combinatorial structure is, however, but one out of many interesting properties. In the following, this property will be discussed, while some other properties such as blocking sets or divisibility can only be mentioned.

Also the question whether the abstract points of a cfz. can be located in the plane such that those points which belong to the same abstract line are, in fact, collinear in the real plane is about as old as the question of configurations itself. It was known shortly after their construction in 1881 that exactly one of all the ten configurations 10_3 cannot be drawn in the plane. On the other hand, the Desargues cfz. 10_3 can be drawn "quite easily".

A more sophisticated question is whether a configuration can be realized in the plane choosing coordinates of the points in the plane with certain restrictions. For example, the configuration 21_4 of Grünbaum and Rigby is not realizable with rational coordinates (see [8]), but it is with real coordinates.

4.4. ISOMORPHISM PROBLEM

A big problem in combinatorial mathematics is whether two structures (e.g. graphs, designs or configurations) are isomorphic or not. In figs. 11–13, three graphs are exhibited but, in fact, they all describe the same graph.

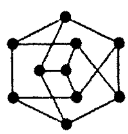


Fig. 11.

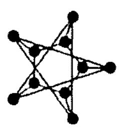


Fig. 12.

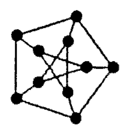


Fig. 13.

A graph is simply defined by saying which of its vertices are connected by an edge (and which are not). Thus, the above graph (of course, the Petersen graph) can be described by its 15 edges: 03, 06, 09, 15, 17, 19, 24, 25, 26, 35, 38, 48, 49, 67, 78. Applying a permutation on {1, 2, . . . , 10} to this set of 15 edges produces another graph. Since, however, these graphs can only be dstinguished by their notation, they are isomorphic.

An equivalent problem is a somehow "reasonable" name for a configuration or a design. Of course, this also arises in chemistry for finding canonical names for (especially) aromatic hydrocarbons. As far as I know, this problem has been solved in principle, but I doubt that it can really be solved for large molecules. Since computing time (even on a very large computer) is limited, there is a need for finding a normalized notation for a cfz. in a relatively short time. For references, see [4].

5. Conclusion

This short paper could only mention very briefly some facts and examples, I hope, however, that the similar concepts in combinatorial theory and mathematical chemistry will enable a good cooperation in the future.

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