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WHICH POLYNOMIALS ARE CHROMATIC? (*)

RIASSUNTO. — Vengono studiate le condizioni per cui un dato polinomio $P(\lambda)$ è i polinomio cromatico di un certo grafico G. Passiamo in esame certe condizioni note che comprendono ineguaglianze implicanti i coefficienti e le relative differenze. Viene poi dimostrato che ad un grafo G è associato un complesso simpliciale tale che i coefficienti del polinomio cromatico di G sono le sequenze simpliciali, nelle varie dimensioni, di questo complesso. Da questo fatto si traggono condizioni aggiuntive sui coefficienti e un teorema di Kruskal. Infine, si deducono delle limitazioni superiori per i coefficienti nel caso in cui G sia planare massimo.

§ 1. INTRODUCTION

Let G be a (finite, undirected) graph on n vertices and E edges (without loops or multiple edges). If λ is a positive integer, let $P(\lambda) = P(\lambda; G)$ denote the number of proper colorings of the vertices of G in λ (or fewer) colors. Then $P(\lambda)$ is a polynomial in λ of degree n

$$(1) \qquad P(\lambda) = \lambda^n - a_1 \lambda^{n-1} + a_2 \lambda^{n-2} - \cdots + (-1)^{n-1} a_{n-1} \lambda .$$

For example,

$$(2) \qquad P(\lambda; K_n) = \lambda(\lambda - 1) \cdots (\lambda - n + 1)$$

$$(3) \qquad P(\lambda; C_n) = (\lambda - 1)^n + (-1)^n (\lambda - 1)$$

where K_n is the complete graph on n vertices and C_n is an n-cycle. Also

$$(4) \qquad P(\lambda, K_{m,n}) = \sum_{\substack{l \le m \\ k \le n}} s(m, l)\, s(n, k)\, \lambda(\lambda - 1) \cdots (\lambda - k - l + 1)$$

where $K_{m,n}$ is the complete bipartite graph and $s(m, l)$ is the Stirling number of the second kind.

We are concerned here with a converse problem: given a polynomial $P(\lambda)$ in the form (1), is there a graph G such that $P(\lambda) = P(\lambda; G)$? This question is very difficult. We shall first review some known necessary conditions on $P(\lambda)$. Next we will indicate a connection between this problem and the question of characterizing the simplex counts in each dimension of a simplicial complex $\mathscr{C}$. The connecting link here is a classical theorem of H. Whitney [1] on broken circuits. With the aid of this identification of the problem, we will obtain new coefficient inequalities for the a_j in (1) which

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are necessary if P (λ) comes from a connected graph G. These unequalities will follow from a powerful theorem of J. Kruskal [2] on simplicial complexes. Additional coefficient inequalities will be found, by the same method, from results of B. Grünbaum [4], Klee [3] and others.

We then restrict the question to maximal planar graphs, and find additional coefficient restrictions which apply only to such graphs.

§ 2. Known necessary conditions

For our starting point we state the theorem of Whitney mentioned above. First, number the edges of the graph G from 1 to E in some manner. Next, from each circuit C of G delete the edge of highest index, obtaining, thereby, the broken circuit $\bar{C}$. Then we have

THEOREM 1. (Whitney [1]). *The coefficient* a_j *of the chromatic polynomial* P (λ) *in* (1) *is equal to the number of j-subsets of edges of the graph* G *which contain no broken circuit, for each* $j = 1, \cdots, n-1$.

For example, if G is the graph in fig. 1,

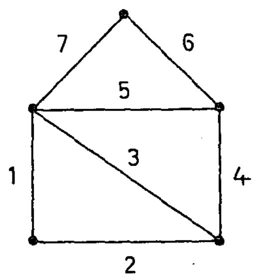
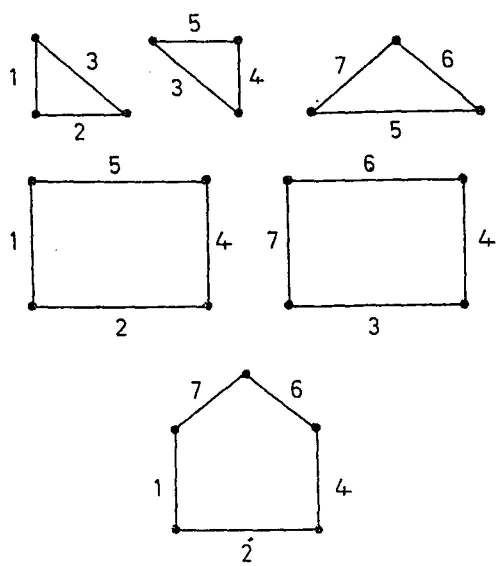


Fig. 1.

the circuits of G are



and the broken circuits are therefore the edge-subsets

$$12 \quad , \quad 34 \quad , \quad 56 \quad , \quad 124 \quad , \quad 346 \quad , \quad 1246 .$$

The j-subsets of edges which contain none of these are identical with with the j-subsets of edges which contain none of

$$\{1,2\} \quad , \quad \{3,4\} \quad , \quad \{5,6\}$$

whence

$$a_1 = 7$$

$$a_2 = \binom{7}{2} - 3 = 18$$

$$a_3 = \binom{7}{3} - 15 = 20$$

$$a_4 = \binom{7}{4} - 3\binom{5}{2} + 3 = 8.$$

For the graph G of five vertices, therefore,

$$P(\lambda) = \lambda^5 - 7\lambda^4 + 18\lambda^3 - 20\lambda^2 + 8\lambda = \lambda(\lambda - 1)(\lambda - 2)^3 .$$

If we now return to the general case, as corollaries we have the following necessary conditions on P (λ); in which we now suppose that G is *connected*:

C 1: $$a_j \geqq \binom{n-1}{j} \qquad (j = 1, \cdots, n-1).$$

Proof. Choose a spanning tree T of G. Number the edges of T with the $n-1$ highest labels $E, E-1, \cdots, E-n+1$, and number the remaining edges of G arbitrarily $1, 2, \cdots, E-n$. Let S be a j-subset of the edges of T. Then S contains no broken circuit. Hence a_j is at least equal to the number of such sets S.

We have also

(5) $$a_j \leqq \binom{a_1}{j} \qquad (j = 1, \cdots, n-1).$$

Proof. If $P(\lambda) = P(\lambda, G)$, then a_1 is the number of edges of G, by Theorem 1. Hence a_j cannot exceed $\binom{a_1}{j}$, the total number of j-subsets of edges of G.

Our condition C 5, below, is stronger than (5).

C 2: $$1 - a_1 + a_2 - a_3 + \cdots + (-1)^{n-1} a_{n-1} = 0 \qquad (n \geq 2).$$

Proof. If G is connected and has $\geqq 2$ vertices it must have an edge, and so cannot be properly 1-colored.

C 3: $$P(m+1) \geqq P(m) \qquad (m = 0, 1, 2, \cdots).$$

Another sort of necessary condition can be based on a result of Chvátal [5]. Let τ_k denote the number of proper colorings of G in *exactly*

k colors. Let C be one of these colorings, and let $C_1, \cdots, C_k$ be the color classes of C, with $\nu_i = \# C_i$ $(i = 1, \cdots, k)$. From each color class, C_α, choose a subset S which is neither empty nor equal to C_α. There are exactly

$$2^{\nu_\alpha} - 2$$

such subsets. Re-color the vertices of S in the $(k+1)^{st}$ color. By this construction we obtain

$$\sum_C ((2^{\nu_1} - 2) + \cdots + (2^{\nu_k} - 2))$$

$(k+1)$-colorings of G, where the outer sum extends over all exact k-colorings C. We count a fixed $(k+1)$-coloring C several times. In fact, if $C_1, \cdots, C_{k+1}$ are the color classes of C, we will count this coloring C as often as there are integers j, $1 \leqq j \leqq k$ such that $C_j \cup C_{k+1}$ is an independent set in G, therefore it will be counted $\leqq k$ times. We have then

$$\tau_{k+1} \geqq \frac{1}{k} \sum_C (2^{\nu_1} + \cdots + 2^{\nu_k} - 2k) \geqq (2^{n/k} - 2) \sum_C 1 = (2^{n/k} - 2)\, \tau_k$$

the main result of [5].

We note first, that if G is connected, the factor $\frac{k}{k-1}$ can be inserted, whence

(6) $$\tau_{k+1} \geqq \frac{k}{k-1} (2^{n/k} - 2)\, \tau_k .$$

We note next that in terms of the τ_k, the chromatic polynomial $P(\lambda)$ is

$$P(\lambda) = \sum_{k=1}^{n} \tau_k \binom{\lambda}{k}$$

and so by repeated forward differencing,

(7) $$\tau_k = \Delta^k P(0) \qquad (k = 1, \cdots, n).$$

If we put together (6) and (7) we arrive at a necessary condition for the polynomial $P(\lambda)$ to come from a connected graph G in the form

C 4: If Δ is the forward difference operator, then

(8) $$\Delta^{k+1} P(0) \geqq \left(\frac{k}{k-1}\right) (2^{n/k} - 2)\, \Delta^k P(0) \qquad (k \geqq 2).$$

This criterion can readily be checked from a difference table of values of $P(\lambda)$.

§ 3. Simplicial complexes

By a *simplicial complex* $\mathscr{C}$ we shall mean a finite collection of finite sets $S, T, \cdots$ with the property that

(9) $$S \in \mathscr{C} \quad , \quad T \subseteq S \Rightarrow T \in \mathscr{C} .$$

By a *j-simplex* of $\mathscr{C}$ we mean [1] a set $S \in \mathscr{C}$ such that $\# S = j$, and the *dimension* of $\mathscr{C}$ is the largest j such that $\mathscr{C}$ has a j-simplex. With each simplicial complex $\mathscr{C}$ we can associate a polynomial $P(\lambda) = P_{\mathscr{C}}(\lambda)$ as follows: if a_j is the number of j-simplexes of $\mathscr{C}$ then

$$P_{\mathscr{C}}(\lambda) = \lambda^n - a_1 \lambda^{n-1} + a_2 \lambda^{n-2} - \cdots + (-1)^n a_n \tag{10}$$

where $n =$ dimension $(\mathscr{C})$.

A simplicial complex $\mathscr{C}$ can be presented in at least three ways:

(a) we may list all of the sets of $\mathscr{C}$.

(b) we may list the maximal (under inclusion) sets of $\mathscr{C}$.

(c) we can make a list $\mathscr{L}$ of distinguished sets, and describe the complex $\mathscr{C}$ as the collection of all subsets of the universe which do not contain any set of the list $\mathscr{L}$. This procedure evidently describes a complex. Conversely, if $\mathscr{C}$ is given, then take $\mathscr{L}$, for instance, to be the list of all subsets which are not in $\mathscr{C}$.

THEOREM 2. *Let* $P(\lambda)$, *in* (1), *be the chromatic polynomial of a graph* G. *Then there is a simplicial complex* $\mathscr{C}$ *such that*

$$P(\lambda) = P_{\mathscr{C}}(\lambda)$$

that is, the coefficients of the chromatic polynomial are the simplex counts in each dimension of some complex $\mathscr{C}$.

Proof. The complex $\mathscr{C}$ is the collection of all edge-subsets of G which contain no broken circuit. (We shall call this complex $\mathfrak{B}(G)$, so that $P(\lambda) ; G = P_{\mathfrak{B}(G)}(\lambda)$).

The usefulness of the above result rests on the fact that the sequences $(a_1, a_2, \cdots, a_n)$ which are the simplex counts of a complex $\mathscr{C}$ have been completely characterized. Indeed, for $1 \leqq k \leqq n$, define $n_k, n_{k-1}, \cdots$ by the relation

$$a_k = \binom{n_k}{k} + \binom{n_{k-1}}{k-1} + \cdots + \binom{n_i}{i} \tag{11}$$

in which $i \geqq 1$, and $n_k, n_{k-1}, \cdots$ are uniquely defined by (11) and the condition $n_k > n_{k-1} > \cdots > n_i \geqq i$. Then define the symbol

$$a_k^{(l/k)} = \binom{n_k}{l} + \binom{n_{k-1}}{l-1} + \cdots. \tag{12}$$

Kruskal [2] and later Katona [6] had shown that the minimum (if $l < k$) or maximum (if $l > k$) value of a_l, if a_k is fixed, is exactly $a_k^{(l/k)}$. Very recently [2], J. Eckhoff and G. Wegner (to appear) have shown that these inequalities

$$a_l \geqq a_k^{(l/k)} \qquad (l < k)$$

actually characterize the simplex-count vectors of complexes completely.

(1) This is slightly at variance with the usual topological definition.

(2) I am indebted to Professor Grünbaum for this reference.

Hence our next necessary condition is

$C\,5$: *The coefficients of the chromatic polynomial* (1) *satisfy the relations*

$$a_l \geqq a_k^{(l/k)} \qquad (k = 1, \cdots, n-1\,;\, l < k). \tag{13}$$

Further progress along these lines must await refinements of (13) which hold for complexes which have the special properties of $\mathfrak{B}$ (G), which do not hold for complexes in general. In this direction, we observe that the $\mathfrak{B}$ (G) complexes are special in that all of thier structure is determined by the top dimension $n-1$, which is the content of the following

LEMMA. *Let* G *be a connected graph. Then* $\mathfrak{B}$ (G) *is a homogeneous simplicial complex, i.e., every simplex of dimension* $d < n-1$ *is a subset of some simplex of top dimension* $n-1$ (*spanning tree with no broken circuit*).

Proof. Let S be a d-subset of edges of G with no broken circuit, where $d < n-1$. We must extend S to a $(d+1)$-subset of the same type. Let T denote the set of all edges e of G such that one endpoint of e is incident with S and the other endpoint is not.

Now T is nonempty, for otherwise the edges of G — S would fall into two classes: (I) those which, if adjoined to S, would complete a circuit of G. (II) those which are disjoint from S. But (II) is empty or G would be disconnected. Hence all edges not in S complete a circuit, and S is a spanning tree, a contradiction.

Now adjoin to S the highest numbered edge, e^*, of T. Evidently $S \cup e^*$ contains no circuit. Suppose it contains a broken circuit, and let f be the " missing edge ". Then f has a higher number than e^*, yet $f \in T$, a contradiction, whence $S \cup e^*$ contains no broken circuit, as claimed.

As questions for further investigation, we ask:

(I) What is the characterization, analogous to (13), of the simplex counts of a *homogeneous* complex?

(II) Which abstract complexes can arise as a $\mathfrak{B}$ (G) for some graph G and edge-numbering of G? (Professor Brylawski has kindly supplied an example where different edge-numberings yield non-isomorphic complexes).

We observe finally that the conditions (C 1)-(C 5) are not sufficient. Three polynomials which satisfy all of them and yet are not graphical are

$$\lambda^5 - 5\lambda^4 + 10\lambda^3 - 8\lambda^2 + 2\lambda, \qquad \lambda^5 - 7\lambda^4 + 20\lambda^3 - 26\lambda^2 + 12\lambda,$$

$$\lambda^5 - 8\lambda^4 + 26\lambda^3 - 37\lambda^2 + 18\lambda.$$

§ 4. DISJOINT GENERATORS

In this section we consider a special class of graphs G, namely those which share with the graph of fig. 1 the property that the chromatic polynomial can be calculated from a set of *pairwise disjoint* broken circuits.

A set S of broken circuits of G will be said to *generate* $\mathfrak{B}$ (G) if

(a) $\mathfrak{B}$ (G) is the collection of all edge-subsets of G which contain no broken circuits in S and

(b) No set in S contains any other.

The family of graphs which we study here are the graphs G for which the complex $\mathfrak{B}$ (G) has a set S of *pairwise disjoint* generators. These graphs are quite special, indeed we will see that they are all 3-chromatic.

LEMMA. *Let* $S_1, \cdots, S_l$ *be pairwise disjoint subsets of a set* S, *where* $\# S = n$, $\# S_i = \nu_i$ $(i = 1, \cdots, l)$. *Let* a_j^* *denote the number of* j*-subsets of* S *which contain none of the* S_i *as a subset. Then*

$$\sum_{j \geq 0} a_j^* x^j = (1 + x)^{n - \nu_1 - \cdots - \nu_l} \prod_{i=1}^{l} \{(1 + x)^{\nu_i} - x^{\nu_i}\}. \tag{14}$$

Proof. In order to construct a j-subset of S which contains no S_i, we choose $r_1 < \nu_1$ elements of $S_1, \cdots, r_l < \nu_l$ elements of S_l, which can be done in

$$\binom{\nu_1}{r_1} \binom{\nu_2}{r_2} \cdots \binom{\nu_l}{r_l}$$

ways, and the remaining $j - (r_1 + \cdots + r_l)$ elements can be chosen in

$$\binom{n - \nu_1 - \cdots - \nu_l}{j - r_1 - \cdots - r_l}$$

ways, from which

$$a_j^* = \sum_{\substack{r_1 + \cdots + r_l + t = j \\ 0 \leq r_i < \nu_i}} \binom{\nu_1}{r_1} \binom{\nu_2}{r_2} \cdots \binom{\nu_l}{r_l} \binom{n - \nu_1 - \cdots - \nu_l}{t}$$

and the generating function (14) follows at once.

If the complex $\mathfrak{B}$ (G) has pairwise disjoint generators, then it follows from the Lemma that the chromatic polynomial of G is

$$P(\lambda) = \lambda^n \left(1 - \frac{1}{\lambda}\right)^E \prod_{i=1}^{l} \left\{1 - \frac{1}{(1 - \lambda)^{\nu_i}}\right\} \tag{16}$$

where E is the number of edges of G, n is the number of vertices of G, and ν_i is the number of edges in the i^{th} broken circuit in the set of l generators.

Since P (λ) is completely factored in (16) we can read off its zeros, which are at $\lambda = 1 - \omega$ where ω runs through the ν_i^{th}-roots of unity $(i = 1, \cdots, l)$. Hence if some ν_i is even, G is 3-chromatic, while if all ν_i are odd, G is 2-chromatic (bipartite).

Now consider a graph G which need not have a generating set of pairwise disjoint broken circuits. Suppose we select, from among the broken circuits of G, a subset $\bar{S}$ of them, and consider the complex $\bar{\mathfrak{B}}$ which is generated by $\bar{S}$. Evidently, in every dimension the number of simplexes in $\mathfrak{B}(G)$ will be at most equal to the corresponding number in $\bar{\mathfrak{B}}$, *i.e.*, we will have found upper bounds for the coefficient of $P(\lambda; G)$.

In particular, let G be a maximal planar graph. Among the broken circuits of G we can select $\bar{S}$ to be a subset consisting of pairwise disjoint broken circuits each of which contains exactly two edges. Such broken circuits consist of two of the bounding edges of some face. We will call them *broken face boundaries*. Suppose there are exactly τ such broken circuits in S. Then by the remarks in the preceding paragraph and equation (16) with $l = \tau$, $\nu_1 = \cdots = \nu_\tau = 2$, the coefficients a_j of the chromatic polynomial of G are dominated by the corresponding coefficients a_j^* of the function

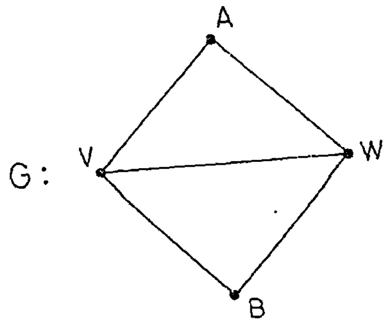
$$P^*(\lambda) = \lambda^n \left(1 + \frac{1}{\lambda}\right)^E \left(1 - \frac{1}{(1+\lambda)^2}\right)^\tau \tag{17}$$

$$= \lambda^{n-E+\tau} (\lambda + 1)^{E-2\tau} (\lambda + 2)^\tau .$$

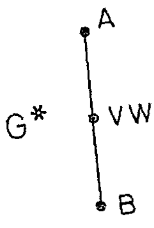
For the sharpest estimates we want τ to be as large as possible. In that direction we have

THEOREM 3. *For a maximal planar graph* G *of* F *faces we can number the edges of* G *so that there will be* F/2 *pairwise disjoint broken face boundaries.*

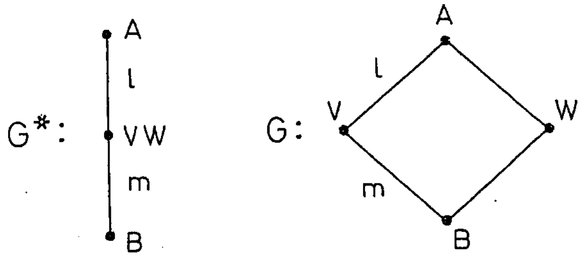
Proof. This is clearly true if $F = 2$. Suppose true for graphs of $2, 4, \cdots, F-2$ faces, and let G have F faces. Choose a pair of adjacent faces of G



as shown, and create a new graph, G*, by identifying V and W



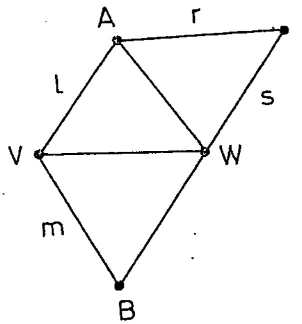
Suppose the two edges of G^* shown acquire the numbers l, m. Then in G, G^* we have the configurations



where the assignment of l, m to the left or right member in G is arbitrary.

Consider first the case where one, at least, say (A, VW), of the edges of G^* shown is not involved in any broken circuit in G^*. Number edges AW, VW, BW with numbers $E - 1$, $E - 2$, E respectively. This creates a new broken circuit, consisting of edges AV, VW, which is disjoint from all others, and does not destroy any previously existing broken circuits. Hence in G we have $F/2$ such circuits.

Otherwise, both (A, VW) and (B, VW) in G^* belong to broken circuits. Then in G, the edges l and m, say belong to broken circuits inherited from G^*. AW and BW do not belong to any such. Suppose AW is not the third side of a broken face boundary. Then we number AW, VW, BW with numbers $0, -1, E - 2$ respectively, obtaining a new circuit (AW, VW) and destroying no old one. Finally, if AW is the third side of some broken circuit, then in G we have the picture



where we know that $l > r$, $l > s$ because r, s is a broken circuit in G^*. Renumber each edge whose label x satisfies $l \leq x \leq E - 3$ with the label $x + 2$. Number edges AW, VW, BW with labels $l, l + 1$, E respectively. It is easy to check that this renumbering, which produces one new broken face boundary, does not disturb any previously existing one.

THEOREM 4. *Let*

$$P(\lambda) = \lambda^n - a_1 \lambda^{n-1} + a_2 \lambda^{n-2} - \cdots$$

be the chromatic polynomial of a maximal planar graph. The coefficients of P (λ) *are dominated by the corresponding coefficients of*

$$\lambda^{-(n-4)}\,[(\lambda+1)(\lambda+2)]^{n-2},$$

and, explicity, we have

$$a_j \leqq \sum_{k=0}^{\min(j,n-2)} \binom{n-2}{j-k}\binom{n-2}{k}\,2^k \qquad (j=1,\cdots,n-1). \tag{18}$$

Proof. By Theorem 3 we can apply (17) with $\tau = \frac{F}{2} = n-2$. The right hand side of (17) becomes simply

$$\lambda^{-(n-4)}\,[(\lambda+1)(\lambda+2)]^{n-2},$$

whose coefficients appear in (18).

It is instructive, to get an idea of the sharpness of this bound, to deal with the case $j = n-2$, where (18) becomes

$$a_{n-2} \leq \sum_{k=0}^{n-2} \binom{n-2}{k}^2 2^k = (-1)^n\,P_{n-2}(-3)$$

where $P_n(x)$ is the usual Legendre polynomial. For large n,

$$(-1)^n\,P_{n-2}(-3) \sim An^b\,(3+\sqrt{2})^n = An^b\,(5.82\cdots)^n$$

which may be compared with the universal upper bound given by condition C 2 above:

$$a_{n-2} \leqq \binom{3n-6}{n-2} \sim An^b\,(6.75)^n.$$

The first three inequalities (18), when compared with the actual values of a_1, a_2, a_3, are

$$(j=1) \quad 3n-6 \leqq 3n-6$$

$$(j=2) \quad \frac{n-2}{2}(9n-28) \leqq \frac{n-2}{2}(9n-23)$$

$$(j=3) \quad \frac{(n-2)(3n-8)(3n-11)}{2} \leqq \frac{(n-2)(n-3)(9n-24)}{2}.$$

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