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Recursion relations for chromatic coefficients for graphs and hypergraphs

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Abstract

We establish a set of recursion relations for the coefficients in the chromatic polynomial of a graph or a hypergraph. As an application we provide a generalization of Whitney’s broken cycle theorem for hypergraphs, as well as deriving an explicit formula for the linear coefficient of the chromatic polynomial of the \( r \)-complete hypergraph in terms of roots of the Taylor polynomials for the exponential function.

1 Introduction

The chromatic polynomial \( \chi_G \) associated to a graph \( G \), introduced by Birkhoff [2], is determined by defining \( \chi_G(\lambda) \), for \( \lambda \in \mathbb{N} \), to be the number of colourings of the vertices of \( G \) with at most \( \lambda \) colours, such that no adjacent vertices are attributed the same colour [12, 19]. The definition extends to hypergraphs [5], by considering colourings such that each hyperedge contains at least two vertices with different colours. In the case of graphs, Whitney’s broken cycle theorem [3,9,10,27] provides a combinatorial interpretation to the coefficients of the chromatic polynomial \( \chi_G(\lambda) \) : if a graph \( G \) has \( n \) vertices, then the coefficient of \( \lambda^i \) is given, up to the sign \((-1)^{n-i}\), by the number of spanning subgraphs of \( G \) with \( n-i \) edges with the property of not containing as a subset any of a particular list of special subgraphs of \( G \), known as broken cycles.

In the present article, we establish a set of recursion relations for the coefficients of the chromatic polynomial of a graph or hypergraph, which allow us to express the \( i \)-th order coefficient in terms of products of linear coefficients of certain subgraphs. We similarly show that the combinatorial quantities appearing in Whitney’s theorem (as well as a natural generalization of them which covers the case of hypergraphs) also satisfy the same recursion relations (up to a sign factor). Since the two sequences are recursively defined by the same relations and it can be easily verified that they coincide on empty graphs, we obtain as a consequence a generalization

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1Whitney’s original theorem mentions broken circuits instead, but the distinction between circuits and cycles is not relevant in this context.
of the broken cycle theorem for hypergraphs. There are a number of different extensions of Whitney’s theorem to hypergraphs already present in the literature [8, 10, 11, 22]. The one we present here encompasses those known to us.

As a second application of the recursion relations, we derive an explicit formula for the linear chromatic coefficient of the \( r \)-complete hypergraphs in terms of the roots of the \((r-1)\text{th}\) Taylor polynomial of the exponential function (where the \( r \)-complete hypergraph is the hypergraph containing all possible hyperedges of cardinality \( r \)).

Whitney’s theorem implies that the coefficients of the chromatic polynomial of a graph are always integers with alternating signs. Moreover, applying the deletion-contraction principle for the chromatic polynomial [2,12,27], one can also show that they are numerically upper bounded by the corresponding coefficient for the complete graph of the same order. We show that both these facts can be obtained in a simple way as a consequence of the recursion relations we present, without using neither Whitney’s theorem nor the deletion-contraction principle.

The paper is organized as follows. In Section 2, we start by presenting the simpler case of the recursion relations for graphs, together with a new proof of Whitney’s theorem in its original form. The section will follow the same approach we will use for the general case, but since it is arguably easier we present it here for illustration of the method, but it can safely be skipped. In Section 3 we present the general case of hypergraphs, and the generalization of Whitney’s theorem. Finally in Section 4 we apply the recursion relations to obtain the formula for the linear coefficient of the \( r \)-complete hypergraph.

2 The recursion relations for graphs

In this section \( G = (V,E) \) denotes a simple graph, where \( V \) is a non-empty finite set and \( E \) is a set of unordered pairs of elements in \( V \). The members in \( V \) and \( E \) are called the vertices and edges in \( G \), respectively. The order of \( G \), i.e. the number of vertices \( |V| \), will be denoted by \( n \). By \( k(G) \) we shall denote the number of connected components of \( G \). If \( F \subseteq E \), the graph \( \bar{G}(F) \equiv (V,F) \) is called the spanning subgraph of \( G \) induced by \( F \), and we shall write \( k(F) \) for \( k(\bar{G}(F)) \). If \( V' \subset V \), the graph \( (V',E') \) where \( E' = \{ \{x,y\} \in E \mid x,y \in V' \} \) is called the subgraph of \( G \) induced by \( V' \). It will be denoted by \( G[V'] \).

Definition 2.1. Let \( \lambda \in \mathbb{N} \). A \( \lambda \)-colouring of a graph \( G = (V,E) \) is a map \( \pi : V \to \{1,2,\ldots,\lambda\} \). A \( \lambda \)-colouring is called proper if for each edge \( e = \{x,y\} \in E \) it holds that \( \pi(x) \neq \pi(y) \). We define \( \chi_G(\lambda) \) to be the number of proper \( \lambda \)-colourings of \( G \).

It is well known that the \( \chi_G(\lambda) \) is a polynomial in \( \lambda \).

Theorem 2.2. The function \( \chi_G(\lambda) \) is a polynomial, called the chromatic polynomial of \( G \), given by

\[
\chi_G(\lambda) = \sum_{i=1}^{n} a_i(G) \lambda^i, 
\]

where

\[
a_i(G) = \sum_{\substack{F \subseteq E \\text{ such that } k(F) = i \atop F \subseteq E}} (-1)^{|F|}. \tag{2.1}
\]

Proof. Define for any edge \( e \in E \) the function \( f_e \) on the set of colourings of \( G \) by

\[
f_e(\pi) = \begin{cases} 0 & \text{if } \pi \text{ is constant on } e \\ 1 & \text{otherwise.} \end{cases}
\]
\[
\chi_G(\lambda) = \sum \prod_{e \in E} f_e(\pi) = \sum \prod_{e \in E} (1 - (1 - f_e(\pi))) = \sum \sum (-1)^{|F|} \prod_{e \in F} (1 - f_e(\pi)) \\
= \sum (-1)^{|F|} \lambda^k(F).
\]

Whitney refined this result in what is known as his broken-cycle theorem [27]. Let \( \leq \) be an arbitrary linear ordering of the edge set \( E \). A broken cycle of \( G \) is then a set of edges \( F \subseteq E \) obtained by removing the maximal edge from a cycle of \( G \).

**Theorem 2.3** (Whitney 1932). For \( i = 1, \ldots, n \) we have that
\[
a_i(G) = (-1)^{n-i} h_i(G),
\]
where \( h_i(G) \) is the number of spanning subgraphs of \( G \) with \( n-i \) edges and containing no broken cycle.

We will establish, in the next three lemmas, a set of recursion relations for coefficients \( a_i \) and for coefficients \( h_i \), respectively. Up to a sign factor, both sets of coefficients will be shown to satisfy the same recursion relations, and by observing that they coincide on the empty graph we will obtain as a consequence an inductive proof of Theorem 2.3.

Recall, that an edge \( e \in E \) is called a bridge in \( G = (V, E) \) if \( k(E) < k(E \setminus e) \) (i.e. removing \( e \) increases the number of connected components of the graph), in which case we must have \( k(E \setminus e) = k(E) + 1 \). If \( F \subseteq E \) we say that \( e \in F \) is a bridge in \( F \) if it is a bridge in \( \overline{G}(F) \). We denote by \( B^i_e \) the collection of \( F \subseteq E \) such that \( e \) is a bridge in \( F \) and \( k(F) = i \).

**Lemma 2.4.** Let \( G = (V, E) \) be a graph with \( E \neq \emptyset \) and fix \( e \in E \). We have that
\[
a_i(G) = b^i_e(G) - b^{i-1}_e(G),
\]
where \( b^0_e(G) = 0 \) and
\[
b^i_e(G) = \sum_{F \in B^i_e} (-1)^{|F|}, \quad \forall i \geq 1.
\]

**Proof.** For each subset \( F \) of \( E \) exactly one of the following holds:

1) \( e \notin F \), 2) \( e \) is a bridge in \( F \), 3) \( e \in F \), but \( e \) is not a bridge in \( F \).

We therefore have a decompositon of the collection \( \{ F \subseteq E | k(F) = i \} \) into the three disjoint classes:

\[
A^i_e = \{ F \subseteq E | e \notin F, k(F) = i \}, \\
B^i_e = \{ F \subseteq E | e \in F, k(F) = i, k(F \setminus \{e\}) = k(F) + 1 \}, \\
C^i_e = \{ F \subseteq E | e \in F, k(F) = i, k(F \setminus \{e\}) = k(F) \}.
\]

Hence, for each \( i = 1, \ldots, n - 1 \) we have
\[
a_i = \sum_{F \in A^i_e} (-1)^{|F|} + \sum_{F \in B^i_e} (-1)^{|F|} + \sum_{F \in C^i_e} (-1)^{|F|}.
\]
Clearly, the mapping $\phi$ defined by $\phi(F) = F \cup \{e\}$ is a bijection from $A_e$ to $B_{e-1}^i \cup C_e^i$, which implies that

$$\sum_{F \in A_e} (-1)^{|F|} = \left( \sum_{F \in B_{e-1}^i} (-1)^{|F|} + \sum_{F \in C_e^i} (-1)^{|F|} \right).$$

Plugging this expression into the previous formula for $a_i$, we get

$$a_i = \sum_{F \in B_{e}^i} (-1)^{|F|} - \sum_{F \in B_{e-1}^i} (-1)^{|F|} = b_{e}^{i} - b_{e}^{i-1}$$

as desired.

\[ \blacksquare \]

Lemma 2.5. For $i = 1, 2, 3, \ldots$ we have

$$b_{e}^i(G) = - \sum_{\substack{V = V_{1} \cup \cdots \cup V_{i+1} \in \mathcal{B}_e^{i} \cup \mathcal{B}_{e-1}^{i} \ni e \in G[V_j], j=1,\ldots,i+1}} \prod_{j=1}^{i+1} a_1(G[V_j]), \quad (2.5)$$

where $V = V_1 \cup \cdots \cup V_{i+1}$ denotes any decomposition of $V$ into $i+1$ (non-empty) disjoint subsets $V_1, \ldots, V_{i+1}$.

Proof. Let $F \in B_{e}^i$ and let $G_1 = (V_1, F_1), \ldots, G_{i+1} = (V_{i+1}, F_{i+1})$ be the connected components of $G(F \setminus \{e\})$. In this way, $F$ defines a decomposition of $V$ into $i+1$ disjoint sets $V_1, \ldots, V_{i+1}$ such that $e \not\in G[V_j]$ for any $j = 1, \ldots, i+1$. Let $E_1, \ldots, E_{i+1}$ be the edge sets of the vertex induced subgraphs $G[V_1], \ldots, G[V_{i+1}]$, respectively. Note that $F$ decomposes as $F_1 \cup \cdots \cup F_{i+1} \cup \{e\}$, where $F_j \subseteq E_j$ for each $j$. Conversely, given a decomposition of $V$ into $i+1$ subsets as above such that no $G[V_j]$ contains $e$, then $F = F_1 \cup \cdots \cup F_{i+1} \cup \{e\}$ belongs to $B_{e}^i$ for any collection $F_1, \ldots, F_{i+1}$ of edge sets in $G[V_1], \ldots, G[V_{i+1}]$, respectively, such that each $(V_j, F_j)$ is connected. Hence, we can organize the sum over $F \in B_{e}^i$ by aggregating terms with the same decomposition of $V$: denoting by $k(F_j)$ the number of connected components of $(V_j, F_j)$, we have:

$$b_{e}^i(G) = \sum_{F \in B_{e}^i} (-1)^{|F|} = \sum_{\substack{V = V_{1} \cup \cdots \cup V_{i+1} \in \mathcal{B}_e^{i} \cup \mathcal{B}_{e-1}^{i} \ni e \in G[V_j], j=1,\ldots,i+1 \quad F_j \subseteq E_j, k(F_j)=1}} \prod_{j=1}^{i+1} (-1)^{1+\sum_{j=1}^{i+1} |F_j|}$$

$$= - \sum_{\substack{V = V_{1} \cup \cdots \cup V_{i+1} \in \mathcal{B}_e^{i} \cup \mathcal{B}_{e-1}^{i} \ni e \in G[V_j], j=1,\ldots,i+1 \quad F_j \subseteq E_j, k(F_j)=1}} \prod_{j=1}^{i+1} a_1(G[V_j]).$$

\[ \blacksquare \]

Note that only decompositions such that $G[V_j]$ is connected for all $j = 1, \ldots, i+1$ contribute to the right-hand side of (2.5), since $a_1$ vanishes for disconnected graphs.

Next, we proceed to verify a similar set of recursion relations for the $h_i$. For this purpose, assume a linear ordering of the edges of the graph $G = (V, E)$ is given and let us call a set of edges $F \subseteq E$ an $i$-forest if $G(F)$ has $i$ components each of which is a tree, i.e. $G(F)$ is an acyclic graph with $k(F) = i$. Since for each tree the number of edges is one less than the number of vertices, we have that $i = k(F) = n - |F|$ for any $i$-forest $F$. Thus every spanning $i$-forest is a subgraph with $n - i$ edges. Conversely, since every cycle trivially contains a broken cycle as a subset, any subgraph of $G$ which does not contain any broken cycle is an $i$-forest, if it has $n - i$ edges. In conclusion, $h_i(G)$ is the number of spanning $i$-forests of $G$ containing no broken cycle.
Lemma 2.6. For any graph $G = (V, E)$ with a linear ordering of $E \neq \emptyset$ we have that

$$h_i(G) = c_{i-1}(G) + c_i(G),$$

where the numbers $c_i(G), i = 1, 2, 3, \ldots$, are given by

$$c_i(G) = \sum_{V=V_1 \cup \cdots \cup V_{i+1}} \prod_{j=1}^{i+1} h_1(G[V_j]).$$

and $e_{\text{max}}$ is the maximal edge of $G$, while $c_0(G) = 0$.

Proof. Let $F$ be an $i$-forest of $G$ for some $i$, and fix $e \in E$. Then exactly one of the following is true:

1. $e \notin F$, and $F \cup \{e\}$ is not a forest (i.e. adding $e$ to $F$ creates a cycle),
2. $e \notin F$, and $F \cup \{e\}$ is an $(i-1)$-forest,
3. $e \in F$, and $F \setminus \{e\}$ is a $(i+1)$-forest.

If we now choose $e = e_{\text{max}}$ and $F$ is an $i$-forest such that case 1) holds, then $F$ has a broken cycle. If we therefore consider forests which contain no broken cycle, case 1) does not occur and we can therefore decompose the set

$$E^i = \{F \subseteq E | F \text{ is a spanning } i\text{-forest with no broken cycle}\}$$

into two disjoint classes:

$$\tilde{A}_i^{e_{\text{max}}} = \{F \in E^i | e_{\text{max}} \notin F\},$$
$$\tilde{B}_i^{e_{\text{max}}} = \{F \in E^i | e_{\text{max}} \in F\}$$

and, clearly, $F \mapsto F \cup \{e_{\text{max}}\}$ is a bijection from $\tilde{A}_i^{e_{\text{max}}}$ onto $\tilde{B}_i^{e_{\text{max}}-1}$. If we now define $c_i(G) = |\tilde{B}_i^{e_{\text{max}}}|$ and recall that $h_i(G) = |E^i|$, we see that

$$h_i(G) = c_{i-1}(G) + c_i(G), \quad i = 1, 2, 3, \ldots$$

(2.8)

Note that $c_0(G) = 0$ since $E^0$ is empty. We have to show that the $c_i(G)$ given in (2.7) coincide with the ones we have just defined.

Let $F \in \tilde{B}_i^{e_{\text{max}}}$. Then $F \setminus \{e_{\text{max}}\}$ is a spanning $(i+1)$-forest and it can be written as the disjoint union of its components:

$$F \setminus \{e_{\text{max}}\} = T_1 \cup \cdots \cup T_{i+1}.$$

Let $V_j$ be the vertex set of $T_j$ and let $G_j = G[V_j]$ be the corresponding vertex induced subgraph of $G$, for each $j = 1, \ldots, i+1$. Then $T_j$ is a spanning tree of $G_j$. Since $F$ contains no broken cycle by assumption, neither does any of the $T_j$ and, in particular, $e_{\text{max}} \notin G_j$ for every $j$.

Conversely, consider a decomposition $V = V_1 \cup \cdots \cup V_{i+1}$ such that $e_{\text{max}} \notin G_j = G[V_j]$ for every $j = 1, \ldots, i+1$. If $T_j$ is a spanning tree for $G_j$ for each $j$ then $F = T_1 \cup \cdots \cup T_{i+1} \cup \{e_{\text{max}}\}$ is a spanning $i$-forest of $G$. If none of the $T_j$ contains a broken cycle, then neither will $F$. This proves the formula. \qed
As in formula (2.5) only decompositions such that all \( G[V_j] \) are connected contribute to the sum in (2.7).

Proof of Theorem 2.3. With notation as in Lemmas 2.4 and 2.6 we define

\[
\tilde{a}_i(G) = (-1)^{n-i} a_i(G) \quad \text{and} \quad \tilde{b}_i^e(G) = (-1)^{n-i} b_i^e(G)
\]

for \( i = 1, 2, \ldots, n \) and \( i = 0, 1, \ldots, n \), respectively, (where \( e = e_{\text{max}} \)). It follows from (2.6) and (2.7) that \( \tilde{a}_i \) and \( \tilde{b}_i^e \) satisfy the same recursion relations (2.3) and (2.5) as \( a_i \) and \( b_i^e \). Specialising (2.5) to \( i = 1 \) and noting that \( a_1 = b_1^e \) we get

\[
a_1(G) = - \sum_{V = V_1 \cup V_2 \in G[V_j], j=1,2} a_1(G[V_1]) \cdot a_1(G[V_2]).
\]

(2.9)

Noting that for the case of the empty graph \( \bar{G}(\emptyset) \) it holds that

\[
a_1(\bar{G}(\emptyset)) = \begin{cases} 1, & \text{if } n = 1 \\ 0, & \text{if } n > 1 \end{cases}
\]

this relation determines \( a_1(G) \) uniquely for all graphs \( G \) by induction, since the graphs \( G[V_j] \) have fewer edges than \( G \). In turn, relations (2.8) and (2.6) determine \( a_i(G) \) for \( i \geq 2 \).

Since it is clear that \( a_1(\bar{G}(\emptyset)) = \tilde{a}_1(\bar{G}(\emptyset)) \) and \( \tilde{a}_1(G) = \tilde{b}_1^e(G) \) it follows that \( a_i(G) = \tilde{a}_i(G) \) for all \( i \) and all graphs \( G \).

It is a well known fact that the coefficients \( a_i(G) \) alternate in sign, and that they are numerically upper bounded by the corresponding coefficients for the complete graph of equal order. We will now briefly show how this follows in a simple manner from the recursion relations of Lemmas 2.4 and 2.5 without using neither Whitney’s theorem nor the deletion-contraction principle, as a consequence of the following result.

Lemma 2.7. For any graph \( G \) of order \( n \) and any edge \( e \) of \( G \) it holds that

\[
0 \leq (-1)^{n-i} b_i^e(G) \leq (-1)^{n-i} b_i^e(K_n), \quad i = 1, \ldots, n,
\]
where \( K_n \) denotes the complete graph on \( n \) vertices. Moreover, the first inequality is sharp if and only if \( k(G) \leq i \leq n \), while the second inequality is sharp for \( 1 \leq i \leq n-1 \) unless \( G = K_n \).

Proof. We shall prove the statement by induction. Consider first the case \( i = 1 \) and note that the recursion relation (2.8) can be rewritten as

\[
d(G) = \sum_{V = V_1 \cup V_2 \in G[V_j], j=1,2} d(G[V_1]) \cdot d(G[V_2]),
\]

(2.11)

where \( d(G) = (-1)^{n-1} a_1(G) \). Since

\[
d(V, \emptyset) = \begin{cases} 1, & \text{if } |V| = 1 \\ 0, & \text{if } |V| > 1 \end{cases},
\]

it follows by induction on the number of edges in \( G \) that \( d(G) \geq 0 \) for all \( G \). If \( G \) is connected it is easy to see, by successively deleting edges in paths connecting the endpoints of \( e \), starting with
In particular, \( b \) as an equality if and only if \( b \) is sharp for \( 1 \)

Using that

**Proof.**

and non-trivial) unimodularity of the coefficients of Lemma 2.10 gives that if the second inequality of (2.14) is an equality then

For any graph \( G \) other hand, if \( G \) is disconnected, the sum in (2.11) is empty and so \( d(G) = 0 \).

Using (2.4) in the form

we get that \( (-1)^{n-i}b_i^e(G) \geq 0 \). Moreover, if \( G \) has \( k \) connected components, the sum on the right-hand side is empty if \( i < k \) whereas positive terms occur for \( k \leq i \leq n \) and hence \( (-1)^{n-i}b_i^e(G) > 0 \) in this case.

Moreover, considering \( G \) as a subgraph of \( K_n \) and comparing the formula (2.12) for \( G \) and the corresponding one for \( K_n \), we see that each summand in the former by the induction hypothesis can be bounded from above by a corresponding term in the latter, since all \( K_n[V_j] \) are complete graphs. Hence, the rightmost bound in (2.10) follows.

Finally, if \( G \) is not the complete graph, we have \( n \geq 2 \) and there is an edge \( f = \{x, y\} \) in \( K_n \) that is not an edge of \( G \). For \( i \leq n-1 \) we choose a decomposition \( V = V_1 \cup \cdots \cup V_{i+1} \) in (2.12), such that \( V_1 = \{x, y\} \) and \( V_2 = \{z\} \), where \( z \) is an endpoint of \( f \) that is not in \( V_1 \), and \( V_3, \ldots, V_{i+1} \) are arbitrary. Then \( G[V_1] \) is disconnected and therefore this term in (2.12) vanishes, while the corresponding term for \( K_n \) is strictly positive. This proves the last statement of the proposition.

**Corollary 2.8.** For any graph \( G \) with \( n \) vertices it holds for \( i = 1, 2, \ldots, n \) that

\[
0 \leq (-1)^{n-i}(a_1(G) + a_2(G) + \cdots + a_i(G)) \leq (-1)^{n-i}(a_1(K_n) + a_2(K_n) + \cdots + a_i(K_n)),
\]

and

\[
0 \leq (-1)^{n-i}a_i(G) \leq (-1)^{n-i}a_i(K_n).
\]

Moreover, in both cases the first inequality is sharp if and only if \( k(G) \leq i \leq n \), while the second inequality is sharp for \( 1 \leq i \leq n-1 \) unless \( G = K_n \).

**Proof.** Using that

\[
a_i(G) = b_i^e(G) - b_{i-1}^e(G)
\]

by (2.3) and that \( b_0^e(G) = 0 \) it follows that

\[
b_i^e(G) = a_1(G) + \cdots + a_i(G).
\]

In particular, \( b_i^e(G) \) is independent of \( e \) and (2.13) is just a rewriting of (2.10). Writing (2.15) as

\[
(-1)^{n-i}a_i(G) = (-1)^{n-i}b_i^e(G) + (-1)^{n-i+1}b_{i-1}^e(G)
\]

the inequalities (2.14) follow immediately from (2.10). Moreover, the first inequality of (2.14) is an equality if and only if \( b_i^e(G) = b_{i-1}^e(G) = 0 \) and hence if and only if \( 0 \leq i < k(G) \). Similarly, Lemma 2.10 gives that if the second inequality of (2.14) is an equality then \( b_i^e(G) = b_i^e(K_n) \) and \( b_{i-1}^e(G) = b_{i-1}^e(K_n) \) and hence \( G = K_n \). This completes the proof of the corollary.

It should be noted that the inequality (2.13) can also easily be deduced from the (highly non-trivial) unimodularity of the coefficients of \( \chi_G \) [14,19] and the fact that \( a_1 + a_2 + \cdots + a_n = 0 \).
Remark 2.9. The alternating sign property of the $a_i$ plays a role, for the special case $i = 1$, in the Mayer expansion for the hard-core lattice gas in statistical mechanics (also known as the cluster expansion of the polymer partition function) [13, 20, 23]. Briefly, the model is defined by a finite set $\Gamma$ which plays the role of the “single-particle” state space, a list of complex weights $w = (w_\gamma)_{\gamma \in \Gamma}$, and an interaction $W : \Gamma \times \Gamma \to \{0, 1\}$, which is symmetric and satisfies $W(\gamma, \gamma) = 0$ for all $\gamma \in \Gamma$. Given a multiset $X = \{\gamma_1, \ldots, \gamma_n\}$ of elements of $\Gamma$ (where each $\gamma_i$ can appear more than once), we define the simple graph $G[X] \subseteq K_n$ as the graph on $n$ vertices such that $i$ is adjacent to $j$ if $i \neq j$ and $W(\gamma_i, \gamma_j) = 0$. A subset $X$ of $\Gamma$ is said to be independent if $G[X]$ has no edges. The partition function is then given by

\[ Z_G(w) = \sum_{\gamma \in \Gamma} \left( \prod_{\gamma \in X} w_\gamma \right) \prod_{\{\gamma, \gamma\}' \subseteq X} W(\gamma, \gamma') = \sum_{X \subseteq \Gamma} \prod_{\gamma \in X} w_\gamma, \tag{2.16} \]

which is the (generalized) independent-set polynomial of $G[\Gamma]$ (the standard independent-set polynomial is given when $w$ is taken to be constant) [20]. The Mayer expansion gives a formal series expansion for $\log Z_G$ [13, Proposition 5.3]:

\[ \log Z_G(w) = \sum_{n \geq 1} \frac{1}{n!} \sum_{\gamma_1, \ldots, \gamma_n \in \Gamma} a_1(G[\gamma_1, \ldots, \gamma_n]) \prod_{i=1}^n w_{\gamma_i}. \tag{2.17} \]

The alternating sign property of $a_1$ implies in particular that the coefficient of order $n$ of $\log Z_G(w)$, seen as a polynomial in the variables $(w_\gamma)_{\gamma \in \Gamma}$, has sign $(-1)^{n-1}$. This holds in greater generality [20, Proposition 2.8], and has important implications for proving the convergence of the formal series (2.17) [17].

3 The recursion relations for hypergraphs

Let $H$ be a hypergraph, that is $H = (V, E)$ where $V$ is a finite non-empty set of vertices and $E$ is a set of subsets of $V$, called edges. We assume all edges have cardinality at least 2 (i.e. $H$ has no loops) and will denote $|V|$ by $n$.

A hypergraph $H' = (V', E')$ is a subgraph of $H$ if $V' \subseteq V$ and $E' \subseteq E$. If $E' = \{e \in E \mid e \subseteq V'\}$ we call $H'$ the subgraph spanned by $V'$ and denote it by $H[V']$. If $V' = \bigcup_{e \in E'} e$ we call $H'$ the subgraph spanned by $E'$ and denote it by $H(E')$. Finally, in case $V = V'$ we call $H'$ a spanning subgraph of $H$ and denote it by $H(E')$.

Two different vertices $x, y \in V$ are called neighbours in $H$ if $x, y \in e$ for some $e \in E$. A vertex $x$ is connected to a vertex $y$ if either $x = y$ or there exists a finite sequence $x_1, x_2, \ldots, x_k$ of vertices such that $x_i$ and $x_{i+1}$ are neighbours for $i = 1, \ldots, k - 1$ and $x_1 = x$ and $x_k = y$. Clearly, connectedness is an equivalence relation on $V$. Calling the equivalence classes $V_1, \ldots, V_N$ and letting $E_i$ be the set of edges containing only vertices of $V_i$, we have that $H_i = (V_i, E_i)$ is a hypergraph and $V = \bigcup_{i=1}^N V_i, \quad E = \bigcup_{i=1}^N E_i.$
If \( N = 1 \) we call \( H \) connected. Evidently, \( H_1, \ldots, H_N \) are connected. They are called the connected components of \( H \) and their number is denoted by \( k(H) \). Again, we shall use the notation \( k(F) \) for \( k(H(F)) \).

**Definition 3.1.** Let \( \lambda \in \mathbb{N} \). A \( \lambda \)-colouring of a hypergraph \( H = (V, E) \) is a map \( \pi : V \to \{1, 2, \ldots, \lambda\} \). A \( \lambda \)-colouring is called proper if for each edge \( e \in E \) there exist vertices \( x, y \in e \) such that \( \pi(x) \neq \pi(y) \). We define \( \chi_H(\lambda) \) to be the number of proper \( \lambda \)-colourings of \( H \).

Repeating the proof of Theorem 2.2 we obtain

**Theorem 3.2.** The function \( \chi_H \) is a polynomial, called the chromatic polynomial of \( H \), given by

\[
\chi_H(\lambda) = \sum_{F \subseteq E} (-1)^{|F|} \lambda^{k(F)}.
\]

Thus, the coefficients \( a_i(H) \), \( i = 1, 2, 3, \ldots, n \), of \( \chi_H \) are given by the same formula (2.1) as for graphs.

Now, fix \( e \in E \) and let

\[
A_i^e = \{ F \subseteq E \mid e \notin F, k(F) = i \}
\]

\[
B_{i,j}^e = \{ F \subseteq E \mid e \in F, k(F) = i, k(F \setminus \{e\}) = j \}.
\]

Note that \( B_{i,j}^e = \emptyset \) if \( i > j \) and, if \( F \in A_i^e \), then \( F \cup \{e\} \in B_{i,j}^e \) for some \( j \leq i \) yielding a bijective correspondence between \( A_i^e \) and \( \bigcup_{j \leq i} B_{i,j}^e \). Hence, we have

\[
\sum_{F \in A_i^e} (-1)^{|F|} = -\sum_{j=1}^i \sum_{F \in B_{i,j}^e} (-1)^{|F|}. \tag{3.1}
\]

Using

\[
a_i = \sum_{F \in A_i^e} (-1)^{|F|} + \sum_{j=1}^n \sum_{F \in B_{i,j}^e} (-1)^{|F|} \tag{3.2}
\]

it follows that

\[
a_i = \sum_{j > i} b_{i}^{e,j} - \sum_{j < i} b_{i}^{e,i}, \tag{3.3}
\]

where

\[
b_{i}^{e,j} = \sum_{F \in B_{i,j}^e} (-1)^{|F|}. \tag{3.4}
\]

In particular, we have

\[
a_1 = \sum_{j=2}^n b_{1}^{e,j}. \tag{3.5}
\]

**Proposition 3.3.** For \( i < j \) it holds that

\[
b_{i}^{e,j} = -\sum_{V_1 \cup \cdots \cup V_j = V} \prod_{k=1}^j a_1(H[V_k]), \tag{3.6}
\]

where the sum is over all decompositions of \( V \) into \( j \) (non-empty) disjoint subsets such that \( e \) intersects exactly \( j - i + 1 \) of them.
Proof. Let $F \in \mathcal{B}^{i,j}_e$. Then $\bar{H}(F)$ has $i$ components $C_1, \ldots, C_i$, whereas $\bar{H}(F \setminus \{e\})$ has $j$ components $H_1 = (V_1, F_1), \ldots, H_j = (V_j, F_j)$ which are connected spanning subgraphs of $H[V_1], \ldots, H[V_j]$, respectively. Indeed, we have $e \in C_m \equiv (V', F')$ for some $m = 1, \ldots, i$, and $(V', F' \setminus \{e\})$ then has $j - i + 1$ components which together with $\{C_1, \ldots, C_{m-1}, C_{m+1}, \ldots, C_i\}$ make up $\{H_1, \ldots, H_j\}$, and $e$ intersects exactly those $V_k$ which originate from $C_m$ by deleting $e$.

On the other hand, given a decomposition $V_1 \cup \cdots \cup V_j$ of $V$ and connected spanning subgraphs $H_1 = (V_1, F_1), \ldots, H_j = (V_j, F_j)$ of $H[V_1], \ldots, H[V_j]$, respectively, such that $e$ intersects exactly $j - i + 1$ of $V_1, \ldots, V_j$, we get that $F_1 \cup \cdots \cup F_j \cup \{e\} \in \mathcal{B}^{i,j}_e$ and the mapping $\psi$ defined by

$$\psi(\{H_1, \ldots, H_j\}) = F_1 \cup \cdots \cup F_j \cup \{e\}$$

is a bijection onto $\mathcal{B}^{i,j}_e$.

Since

$$(1) (-1)^{|F_1 \cup \cdots \cup F_j \cup \{e\}|} = - \prod_{k=1}^j (-1)^{|F_k|},$$

the claim follows upon noting that $a_1(H[V']) = 0$ if $H[V']$ is not connected. \hfill \square

Setting $i = 1$ and summing over $j$ in (3.6) we get

$$a_1(H) = - \sum_{j=0}^n \sum_{V_1 \cup \cdots \cup V_j = V} (-1)^j \prod_{k=1}^j a_1(H[V_k]) \quad (3.7)$$

which determines $a_1(H)$ inductively for any hypergraph $H$, since $H[V_1], \ldots, H[V_j]$ all have fewer edges than $H$ and we obviously have

$$a_1(\bar{H}(\emptyset)) = \begin{cases} 1 & \text{if } |V| = 1 \\ 0 & \text{if } |V| > 1. \end{cases} \quad (3.8)$$

Once $a_1$ is known we obtain $b^{i,j}_e(H)$ for any $H$ from (3.5) and consequently $a_i(H)$ from (3.3). Hence, equations (3.3), (3.6) and (3.8) determine all $a_i$ (as well as all $b^{i,j}_e$).

We will now present a generalization of Whitney’s broken cycle theorem for hypergraphs.

**Definition 3.4.** Let $H = (V, E)$ be a hypergraph and fix some linear ordering $\leq$ of $E$. A non-empty set $F \subseteq E$ is called broken-cyclic in $H$ with respect to $\leq$ if it fulfils the following property

$$(\star) \quad H(F) \text{ is connected and there exists an edge } e_0 \subseteq \bigcup_{f \in F} f \text{ such that } e_0 > \max F.$$  

**Lemma 3.5.** Assume $H = (V, E)$ is a hypergraph with connected components $H_1(V_1, E_1), \ldots, H_N = (V_N, E_N)$. Then $F \subseteq E$ is broken-cyclic in $H$ if and only if $F \subseteq E_i$ and $F$ is broken-cyclic in $H_i$ for some $i = 1, \ldots, N$, with ordering of edges inherited from that of $H$.

**Proof.** If $F$ is broken-cyclic in $H$ then $H(F)$ is connected and hence is a subgraph of some $H_i$. Consequently, if $e_0 \subseteq \bigcup_{f \in F} f$ it is an edge of $H_i$ and it follows that $F$ is broken-cyclic in $H_i$.

The converse, that a set of edges $F$ which is broken-cyclic in $H_i$ is also broken-cyclic in $H$, is obvious. \hfill \square
From now on \( H = (V, E) \) is a fixed hypergraph with some linear ordering \( \leq \) on \( E \) and \( D \) is some subset of \( 2^E \) consisting of broken-cyclic subsets in \( H \) with respect to \( \leq \). Moreover, if \( H' = (V', E') \) is a subgraph of \( H \) it will be assumed that \( E' \) is ordered with respect to the restriction of \( \leq \) to \( E' \).

We define
\[
E_D = \{ F \subseteq E \mid A \not\subseteq F \text{ for all } A \in D \}
\]
(3.9)
and set
\[
a_{i,D} = \sum_{F \in E_D} (-1)^{|F|},
\]
(3.11)
for \( i = 1, 2, 3, \ldots, n \). Note that \( a_i = a_{i,\emptyset} \).

We may now formulate the following version of the broken-cycle theorem.

**Theorem 3.6.** For any set \( D \) of broken-cyclic subsets of edges in a hypergraph \( H \) it holds that
\[
a_i = a_{i,D}
\]
(3.12)
for all \( i \).

**Proof.** Let \( e = \max E \). Defining the sets
\[
A_{i,e,D} = A_i \cap E_D, \quad B_{i,j,e,D} = B_{i,j} \cap E_D,
\]
we have the decomposition
\[
E_D = A_{i,e,D} \cup \left( \bigcup_{j \geq i} B_{i,j,e,D} \right)
\]
(3.14)
into disjoint subsets. Moreover, since \( e \) is maximal in \( E \) it does not belong to any broken-cyclic subset in \( H \) and therefore the mapping \( \varphi \) defined by \( \varphi(F) = F \cup \{ e \} \) is a bijection from \( A_{i,e,D} \) onto \( \bigcup_{j \leq i} B_{i,j,e,D} \). Thus, defining
\[
b_{i,e,D} = \sum_{F \in B_{i,j,e,D}} (-1)^{|F|},
\]
(3.15)
the same arguments as those leading to relation (3.3) imply
\[
a_{i,D} = \sum_{j > i} b_{j,e,D} - \sum_{j < i} b_{j,i,e,D}.
\]
(3.16)

We next argue that the analogue of (3.6) also holds. Let \( F \in B_{i,j,e,D} \) and consider the corresponding connected components \( H_1 = (V_1, F_1), \ldots, H_N = (V_j, F_j) \) of the subgraph \( H[\{ F \setminus \{ e \}\}] \) (see the proof of Proposition 3.3). For \( A \in D \) we have by Lemma 3.5 that \( A \subseteq F \) if and only if \( A \subseteq F_k \) for some \( k = 1, \ldots, j \). Defining
\[
D_k = D \cap 2^{E_k},
\]
(3.17)
where \( E_k \) denotes the edgeset of \( H[V_k] \), this means that \( A \not\subseteq F \) for all \( A \in D \) if and only if \( A \not\subseteq F_k \) for all \( A \in D_k \) and all \( k = 1, \ldots, j \). Observe that any \( A \in D_k \) is broken-cyclic in \( H[V_k] \)
Proposition 3.7. Assume theorems of [8, 10, 22] and those quoted for hypergraphs in [11] as to mixed hypergraphs [25]. Since the vertices of edges in $A$ belong to $V_k$ and hence $H(A) = H[V_k](A)$. We conclude that $F \in B_{e,D}^{i,j}$ if and only if $F_k \in A_{e,D_k}(H[V_k])$ for all $k = 1, \ldots, j$.

As in the proof of Proposition 3.3 we obtain, conversely, from any decomposition $V_1 \cup \cdots \cup V_j = V$ and connected, spanning subgraphs $H_1 = (V_1, F_1), \ldots, H_j = (V_j, F_j)$ of $H_1 = H[V_1], \ldots, H_j = H[V_j]$ such that $A \not\subseteq F_k$ for all $A \in D_k$ and all $k = 1, \ldots, j$, and such that $e$ intersects exactly $j - i + 1$ of the sets $V_1, \ldots, V_j$, that $F = F_1 \cup \ldots F_j \cup \{e\}$ belongs to $B_{e,D}^{i,j}$. Hence we obtain the desired relation

$$b_{e,D}^{i,j}(H) = - \sum_{V_1 \cup \cdots \cup V_j = V}^{(i)} \prod_{k=1}^{j} a_{1,D_k}(H[V_k]),$$

where one should note that $D_k$ depends solely on $V_k$ and $D$ for a given $H$.

Having established equations (3.10) and (3.18) the claimed equality of $a_i$ and $a_{i,D}$ follows by induction on the number of edges since, if $E = \emptyset$, we must have $D = \emptyset$ and so

$$a_{i,D}(\tilde{H}(\emptyset)) = a_i(\tilde{H}(\emptyset)), \quad i = 1, 2, 3, \ldots \quad (3.19)$$

The following Propositions 3.7 and 3.8 show that Theorem 3.6 contains the broken cycle theorems of [8, 10, 22] and those quoted for hypergraphs in [11].

Proposition 3.7. Assume $H' = (V', F')$ is a $\delta$-cycle in $H = (V, E)$ in the sense of [22], i.e. $H'$ is a minimal subgraph of $H$ such that $F \neq \emptyset$ and $k(H') = k(H' - e)$ for all $e \in F$. Then $F \setminus \{\max F\}$ is broken-cyclic in $H$ according to Definition 3.4.

Proof. Since $H'$ is minimal it follows that $k(H') = k(H' - e) = 1$ for all $e \in F$. In particular, $H' - \max F$ is connected and equals $H'(F \setminus \{\max F\})$ with vertex set $V'$. Hence, $\max F \subseteq \bigcup_{f \in F \setminus \{\max F\}} f$ and, of course, $\max F > \max(F \setminus \{\max F\})$. □

Proposition 3.8. Let $C = x_1 e_1 x_2 e_2 \ldots x_n e_n x_1$ be a cycle in $H$ in the sense of [1], i.e. $x_1, \ldots, x_n$, resp. $e_1, \ldots, e_n$, are pairwise distinct vertices, resp. edges, in $H$ such that $x_i \in e_i-1 \cap e_i$ for $i = 1, \ldots, n$ (with $e_0 \equiv e_n$). Setting $F = \{e_1, \ldots, e_n\}$ we have that $F \setminus \{\max F\}$ is broken-cyclic in $H$ provided

$$\max F \subseteq \bigcup_{f \in F \setminus \{\max F\}} f,$$

which in particular holds if $\max F$ has cardinality 2.

Proof. It is clear that $H(F \setminus \{\max F\})$ is connected and that (3.20) ensures that we may use $e_0 = \max F$ in Definition 3.4.

If $\max F = e_k$ has cardinality 2 then $e_k = \{x_k, x_{k+1}\} \subseteq e_{k-1} \cup e_{k+1} \subseteq \bigcup_{f \in F \setminus \{e_k\}} f$. □

Alternating sign properties of the $a_i$ for hypergraphs such as the ones described in Section 2 for graphs have been demonstrated in some specific cases, see e.g. [8]. To what extent analogues of (2.14) can be obtained in the general case of hypergraphs is not clear. We should mention on this topic that the deletion-contraction principle has been extended to hypergraphs [29] as well as to mixed hypergraphs [25].
4 An application: the first chromatic coefficient for complete hypergraphs

As a last topic we show that the recursion relations of Section 3 can be used to derive the value of $a_1$ for complete hypergraphs. Let $K^r_n$ be the $r$-complete hypergraph of order $n$, i.e. the edge set of $K^r_n$ consists of all $r$-subsets of its vertex set $V = \{1, 2, \ldots, n\}$. Note that if $r = 2$, then $K^2_n$ is the complete graph $K_n$ and the result is well known (see e.g. [12]).

We shall calculate $a_1(K^r_n)$ for $r \geq 2$ and $n \geq 1$ making use of (3.7), which in this case takes the form

$$a_1(K^r_n) = \sum_{j=2}^{r} \sum_{1 \leq k_1 \leq \cdots \leq k_j} N^r_{k_1, \ldots, k_j} \sum_{s_1, \ldots, s_j \geq 0} \binom{n-r}{s_1 + \cdots + s_j} \cdot a_1(K^r_{k_1+s_1}) \cdot \cdots \cdot a_1(K^r_{n_j+s_j}),$$

(4.1)

where $N^r_{k_1, \ldots, k_j}$ denotes the number of partitions of $\{1, \ldots, r\}$ into $j$ sets of size $k_1, \ldots, k_j$ and $\binom{n-r}{s_1 + \cdots + s_j}$ is the standard multinomial coefficient.

Note also that we obviously have

$$\chi_{K^r_n}(\lambda) = \begin{cases} \lambda^n & \text{if } 0 \leq n < r \\ \lambda^n - \lambda & \text{if } n = r \end{cases},$$

(4.2)

so that, in particular,

$$a_1(K^r_n) = \begin{cases} 1 & \text{if } n = 1 \\ 0 & \text{if } n = 2, 3, \ldots, r-1 \\ \cdots \end{cases},$$

(4.3)

(while $a_1(K^r_n) = -1$).

**Theorem 4.1.** For $r \geq 2$ and $n \geq 1$ it holds that

$$a_1(K^r_n) = -(n-1)! \mu_{r-1}(n),$$

(4.4)

where

$$\mu_r(n) = \sum_{i=1}^{r} R_i^n$$

(4.5)

and $R_1, \ldots, R_r$ denote the roots of the $r$'th Taylor polynomial $E_r$ of $\exp$.

**Proof.** Fix $r \geq 2$. We introduce the generating function $g(x)$ given by

$$g(x) = \sum_{n=0}^{\infty} \frac{a_1(K^r_{n+1})}{n!} x^n$$

(4.6)

and rewrite equations (4.1)-(4.3) as

$$g^{(r-1)}(x) = -\sum_{j=2}^{r} \sum_{1 \leq k_1 \leq \cdots \leq k_j} N^r_{k_1, \ldots, k_j} g^{(k_1-1)}(x) \cdot \cdots \cdot g^{(k_j-1)}(x)$$

(4.7)

with initial condition

$$g(0) = 1, \quad g'(0) = g''(0) = \cdots = g^{(r-2)}(0) = 0.$$
Given two $C^\infty$-functions $\psi$ and $\varphi$ of a real variable we recall the formula

$$
(\psi \circ \varphi)^{(r)}(x) = \sum_{j=1}^{r} \sum_{1 \leq k_1 \leq \cdots \leq k_j \leq k_1 + \cdots + k_j = r} N_{k_1, \ldots, k_j}^r \psi^{(j)}(\varphi(x))\varphi^{(k_1)}(x) \cdots \varphi^{(k_j)}(x),
$$

which is easy to verify by induction. For $\psi = \exp$ this gives

$$
\exp(-\varphi(x)) (\exp \circ \varphi)^{(r)}(x) = \sum_{j=1}^{r} \sum_{1 \leq k_1 \leq \cdots \leq k_j \leq k_1 + \cdots + k_j = r} N_{k_1, \ldots, k_j}^r \varphi^{(k_1)}(x) \cdots \varphi^{(k_j)}(x).
$$

Setting $g = \varphi'$ in (4.7) and using $N_{1,1,\ldots,1} = 1$ it follows that $\varphi$ satisfies

$$(\exp \circ \varphi)^{(r)}(x) = 0,$$

and hence that $\exp \circ \varphi$ equals a polynomial $P$ of degree at most $r - 1$. Thus

$$
g(x) = \frac{P'(x)}{P(x)}.
$$

The initial conditions are easily seen to imply that $P = E_{r-1}$ and consequently

$$
g(x) = \frac{E_{r-1}'(x)}{E_{r-1}(x)} = \sum_{i=1}^{r-1} \frac{1}{x - R_i},
$$

which gives the claimed result. 

Remark 4.2. For $r = 2$ we have $R_1 = -1$ and we get from Theorem 4.1 the known result

$$
a_1(K_n) = a_1(K_n^2) = (-1)^{n-1}(n-1)!. 
$$

By inserting this value into (2.5), we obtain an expression for $a_i(K_n)$ for all $i$. It should be noted though that the value of $a_i(K_n)$ is equal to $s(n,i)$, where $s(n,i)$ denotes the signed Stirling numbers of the first kind.

Remark 4.3. For $r = 3$ the roots of $E_2$ are $R_{\pm} = -1 \pm i$ which gives

$$
a_1(K_n^3) = (-1)^{n-1}(n-1)! \left( 2^{1-\frac{n}{2}} \cos \frac{n\pi}{4} \right). 
$$

For the calculation of $a_1(K_n^r)$ for larger values of $r$ one may use the results available in the literature for the moment function $\mu_r(n)$. In particular, the value of $\mu_r(n)$ was computed for $n \leq 2(r+1)$ [28, Theorem 7], which gives the following expression for $a_1(K_n^r)$, expanding the one given in (4.3)

$$
a_1(K_n^r) = \begin{cases} 
1 & \text{if } n = 1 \\
0 & \text{if } 2 \leq n \leq r - 1 \\
(-1)^{n-r+1} \binom{n-1}{r-1} & \text{if } r \leq n \leq 2r - 1 \\
-[1 + (-1)^r] \binom{2r-1}{r} & \text{if } n = 2r 
\end{cases}
$$
In [28] it was also shown that, once $\mu_r(n)$ is known for $r$ consecutive values of $n$, then it is possible to recursively determine the value of $\mu_r(n)$ for every $n$. This recursive formula for $\mu_r(n)$, when expressed in terms of $a_1(K^r_{j+m})$, reads as:

$$\sum_{j=0}^{r-1} \binom{r-2+m}{r-1-j} a_1(K^r_{j+m}) = 0, \quad \forall m \in \mathbb{N}. \tag{4.12}$$

On a more general note, the properties of the zeros of the Taylor polynomials of exp have been intensively investigated, starting from the work of Szegö [21] and Dieudonné [7], who showed that the points $\frac{2\pi i}{r}$ accumulate, as $r$ goes to infinity, on a closed curve contained in the unit circle, now known as the Szegö curve. See also [4, 6, 15, 16, 18, 24, 26, 28] for further developments.

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References


