Upper Bound for the Coefficients of Chromatic polynomials

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Abstract

This paper describes an improvement in the upper bound for the magnitude of a coefficient of a term in the chromatic polynomial of a general graph. If $a_r$ is the coefficient of the $q^r$ term in the chromatic polynomial $P(G, q)$, where $q$ is the number of colors, then we find $a_r \leq \binom{e}{v-r} - \binom{e-g+2}{v-r-g+2} - \sum_{n=1}^{k_g-\ell_g} \sum_{m=1}^{\ell_g-1} \binom{e-g+1-n-m}{v-r-g} - \delta_{g,3} \sum_{n=1}^{k_g+\ell^{*}_{g+1}-\ell_g} \binom{e-\ell_g-g+1-n}{v-r-g}$, where $k_g$ is the number of circuits of length $g$ and $\ell_g$ and $\ell^{*}_{g+1}$ are certain numbers defined in the text.

key words: chromatic polynomial
1 Introduction

Let $G$ be a loopless graph with $v$ vertices and $e$ edges. The chromatic polynomial $P(G, q)$ counts the number of ways of coloring the vertices of $G$ with $q$ colors subject to the condition that adjacent vertices have different colors \([1, 2]\). (More generally, one may consider multigraphs $G$ with multiple edges; however, it is elementary that the chromatic polynomial for a graph with multiple edges joining two vertices $v$ and $v'$ is the same as for the graph with just one edge joining these vertices.) Besides its role in graph theory, this polynomial is of interest in statistical physics as the zero-temperature value of a certain model of cooperative phenomena and phase transitions known as the Potts model (e.g., \([5, 13]\) and references therein.). The chromatic polynomial of a graph can be calculated by means of the iterative use of the deletion-contraction theorem or equivalently, the addition-contraction theorem, which explicitly shows that it is a polynomial of maximal degree $v$ in $q$. It can be written as

\[
P(G, q) = \sum_{r=1}^{v} (-1)^{v-r} a_r q^r.
\]

Since the chromatic polynomial of a set of graphs is the product of the chromatic polynomials of each individual graph, we shall restrict our attention to a connected graph.

2 Basic Properties of $a_r$

Since the calculation of $P(G, q)$ is, in general, a \#P-hard problem \([11]\), it is useful to have bounds on the coefficients. The coefficients of a chromatic polynomial can be expressed as the sum of the number of its subgraphs which do not contain any broken circuit \([4, 8]\).

By an elementary application of the deletion-contraction theorem, it follows that the coefficients $a_r$ in eq. \((1.1)\) are positive. Furthermore, the leading terms are \([7]\)

\[
a_r = \begin{cases} \binom{e}{v-r} & \text{if } r > v - g + 1 \\
\binom{e}{v-r} - k_g & \text{if } r = v - g + 1
\end{cases}
\]

where $g$ is the girth of the graph, and $k_g$ is the number of circuits of length $g$ in the graph. In particular, $a_v = 1$ and $a_{v-1} = e$.

In practice, one finds that the $a_r$ increase monotonically as $r$ decreases from $v$, with at most two of these coefficients having the maximal value, and then the $a_r$ decrease monotonically for lower values of $r$. We can easily show that the magnitude of $a_j$ can not just increase monotonically without decreasing as follows,

**Proposition 1** The statement that $a_r \leq a_{r-1}$ $\forall 1 \leq r \leq v$ is false except for the trivial case $e = 1$. 

Proof. This statement is equivalent to

\[ a_v \leq a_{v-1} \leq a_{v-2} \leq \ldots \leq a_1. \]  \hspace{1cm} (2.2)

Here we consider the graph with \( e \geq 2 \), and therefore, \textit{a fortiori}, \( P(G, q = 1) = 0 \). However, eq. (2.2) implies

\[ P(G, q = 1) = a_v - a_{v-1} + a_{v-2} - a_{v-3} + \ldots + (-1)^{v-1}a_1 = 1 - e + a_{v-2} - a_{v-3} + \ldots + (-1)^{v-1}a_1 \neq 0. \]  \hspace{1cm} (2.3)

This contradiction disproves the statement except for the trivial case: the tree graph with only two vertices and one edge has \( P(T_2, q) = q(q-1) = q^2 - q \). \hfill \square

Recall the deletion-contraction theorem [3]-[1]: Let \( x \) and \( y \) be adjacent vertices in \( G \), and denote the edge joining them as \( xy \). Then

\[ P(G, q) = P(G - xy, q) - P(G/xy, q) \]  \hspace{1cm} (2.4)

where \( G - xy \) is the graph obtained from \( G \) by deleting the edge \( xy \), and \( G/xy \) is the graph obtained from \( G \) by deleting the edge \( xy \) and identifying \( x \) and \( y \).

If we also write

\[ P(G - xy, q) = \sum_{r=1}^{v} (-1)^{v-r}a'_r q^r \]  \hspace{1cm} (2.5)

and

\[ P(G/xy, q) = \sum_{r=1}^{v-1} (-1)^{v-1-r}a''_r q^r, \]  \hspace{1cm} (2.6)

then

\[ a_r = a'_r + a''_r \quad \text{for} \quad 1 \leq r \leq v - 1. \]  \hspace{1cm} (2.7)

3 Upper Bound on \( a_r \)

It was known that the coefficients \( a_r \)'s are bounded above by the corresponding coefficients of the complete graph with the same number of vertices, \( K_v \) [8]. However, this upper bound is sharp only for complete graphs.

An upper bound on \( a_r \) was given by Li and Tian [3] and is

\[ a_r \leq \binom{e}{v-r} - \binom{e-g+2}{v-r-g+2} + \binom{e-k_g-g+2}{v-r-g+2}. \]  \hspace{1cm} (3.1)
We improve this bound. Let us use the convention

\[
\binom{a}{b} = \begin{cases} 
1 & \text{if } b = 0 \\
0 & \text{if } b > a \text{ or } b < 0 
\end{cases} \tag{3.2}
\]

and, for some function \( f(n) \)

\[
\sum_{n=0}^{m} f(n) = 0 \quad \text{if } m < 0 . \tag{3.3}
\]

Therefore, the bound reduced to the exact values in eq. (2.1) when \( r \geq v - g + 1 \).

Let us derive a basic relation which will be used repeatedly later:

**Lemma 1** If \( a > b \geq c \geq 0, \) then

\[
-a - b \sum_{n=1}^{a-b} \binom{a-n}{c-1} . \tag{3.4}
\]

**Proof** We know

\[
\binom{b+1}{c} - \binom{b}{c-1} = \frac{(b+1)!}{c!(b+1-c)!} - \frac{b!}{(c-1)!(b-c+1)!} \\
= \frac{b!}{(c-1)!(b+1-c)!} \left[ \frac{b+1}{c} - 1 \right] \\
= \frac{b!}{(c-1)!(b+1-c)!} \frac{b+1-c}{c} \\
= \frac{b!}{c!(b-c)!} \\
= \binom{b}{c} , \tag{3.5}
\]

and the result follows if we keep on applying this relation on the positive term generated from \( \binom{b}{c} \).

Next we prove a lemma that will be used for our bound. To begin, we make a choice of a certain edge \( xy \) in \( G \) where we shall apply the deletion-contraction theorem. We then define \( \ell_{g} \) as the number of circuits in \( G \) of length \( g \) that contain this edge \( xy \).

**Lemma 2** If the number of circuits of length \( n \) in a graph \( G \) is \( k_{n} \), where \( k_{n} \geq 0, g \leq n \leq s, g \leq s \leq v, \) and the number of circuits of length \( n \) containing the edge \( xy \) is \( \ell_{n} \), then there are \( v \) vertices and \( e - 1 \) edges in graph \( G - xy \), and the number of circuits of length \( n \) is \( k'_{n} = k_{n} - \ell_{n} \). For the graph \( G/xy \), there are \( v - 1 \) vertices, and the number of edges and the number of circuits of length \( n \) are (i) \( e - 1 \) and \( k''_{n} = k_{n} - \ell_{n} + \ell_{n+1} \) if \( \ell_{3} = 0, \)
or (ii) $e - \ell_3 - 1$ and $k''_n = k_n - \ell_n + \ell_{n+1}^*$ if $\ell_3 \neq 0$, where $\ell_{n+1}^*$ is the number of circuits of length $n + 1$ which do not contain the edge $xz$ (or the edge $yz$) for any vertex $z$.

**Proof** The number of vertices and edges is clear for $G - xy$, and $G/xy$ when $\ell_3 = 0$. If $\ell_3 \neq 0$, the contraction of the edge $xy$ will result in $\ell_3$ double edges, and one of these edges can be removed from each pair without affecting the chromatic polynomial. The circuits of length $n + 1$ in $G$ which become the circuits of length $n$ in $G/xy$ and contain both edges $xy$ and $xz$ (or $yz$) are double-counted. They are the same as the circuits of length $n$ in $G$ which contain the edge $yz$ (or $xz$) but not the edge $xy$. \hfill \Box

Now the upper bound of Li and Tian can be improved with extra negative terms.

**Theorem 1** If the girth of a graph $G$ is $g$, and the number of circuits of length $g$ in the graph is $k_g$, then

$$a_r \leq \binom{e}{v-r} - \binom{e - g + 2}{v-r - g + 2} + \binom{e - k_g - g + 2}{v-r - g + 2}$$

$$- \sum_{n=1}^{k_g - \ell_g} \sum_{m=1}^{\ell_g - 1} \binom{e - g + 1 - n - m}{v-r - g} - \delta_{g,3} \sum_{n=1}^{k_g + \ell_{g+1}^* - \ell_g} \binom{e - \ell_g - g + 1 - n}{v-r - g}, \quad (3.6)$$

where, as defined above, $\ell_g$ and $\ell_{g+1}^*$ are determined by the initial choice of the edge $xy$ on which we apply the deletion-contraction theorem.

**Proof** Consider the special case $g = 3$ first. By eq. (3.1) and Lemma 2

$$a'_{r} \leq \binom{e - 1}{v-r} - \binom{(e - 1) - 3 + 2}{v-r - 3 + 2} + \binom{(e - 1) - (k_3 - \ell_3) - 3 + 2}{v-r - 3 + 2}$$

$$= \binom{e - 1}{v-r} - \binom{e - 2}{v-r - 1} + \binom{e - 2 - k_3 + \ell_3}{v-r - 1} \quad (3.7)$$

$$a''_{r} \leq \binom{e - \ell_3 - 1}{v-r - 1} - \binom{(e - \ell_3 - 1) - 3 + 2}{(v-r) - 3 + 2} + \binom{(e - \ell_3 - 1) - (k_3 - \ell_3 + \ell_4^*) - 3 + 2}{(v-r) - 3 + 2}$$

$$= \binom{e - \ell_3 - 1}{v-r - 1} - \binom{e - \ell_3 - 2}{v-r - 2} + \binom{e - k_3 - \ell_4^* - 2}{v-r - 2} \quad (3.8)$$

then by eq. (2.7) and Lemma 1,

$$a_{r} \leq \binom{e - 1}{v-r} - \binom{e - 2}{v-r - 1} + \binom{e - 2 - k_3 + \ell_3}{v-r - 1}$$

$$+ \binom{e - \ell_3 - 1}{v-r - 1} - \binom{e - \ell_3 - 2}{v-r - 2} + \binom{e - k_3 - \ell_4^* - 2}{v-r - 2}$$
\[
\begin{align*}
&= \binom{e}{v-r} - \binom{e-1}{v-r-1} - \sum_{n=1}^{k_3-\ell_3} \binom{e-2-n}{v-r-2} + \binom{e-\ell_3-1}{v-r-1} \\
&\quad - \binom{e-k_3-1}{v-r-1} + \binom{e-k_3-1}{v-r-1} - \sum_{n=1}^{k_3+\ell_3-\ell_3} \binom{e-2-n}{v-r-2} \\
&\quad + \sum_{n=1}^{k_3-\ell_3} \binom{e-\ell_3-1-n}{v-r-2} - \sum_{n=1}^{k_3+\ell_3-\ell_3} \binom{e-\ell_3-2-n}{v-r-3} \\
&\quad - \sum_{n=1}^{k_3-\ell_3} \sum_{m=1}^{\ell_3-1} \binom{e-2-n-m}{v-r-3} - \sum_{n=1}^{k_3+\ell_3-\ell_3} \binom{e-\ell_3-2-n}{v-r-3}.
\end{align*}
\]

Consider \( g > 3 \) and choose the edge \( xy \) so that the girth of \( G/xy \) is \( g-1 \) and the number of circuits of length \( g-1 \) is \( \ell_g \). By eq. (3.1) and Lemma 2

\[
a'_r \leq \binom{e-1}{v-r} - \binom{(e-1) - (g+2)}{(v-r) - (g+2)} = \binom{e-1}{v-r} - \binom{e-g+1}{v-r-g+2} + \binom{e-k_g + \ell_g - g+1}{v-r-g+2} \tag{3.10}
\]

\[
a'_g \leq \binom{e-1}{v-1-r} - \binom{(e-1) - (g-1) + 2}{(v-1) - r - (g-1) + 2} = \binom{e-1}{v-1-r} - \binom{e-g+2}{v-r-g+2} + \binom{e-\ell_g - g+2}{v-r-g+2} \tag{3.11}
\]

therefore,

\[
a_r \leq \binom{e-1}{v-r} - \binom{e-g+1}{v-r-g+2} + \binom{e-k_g + \ell_g - g+1}{v-r-g+2} + \binom{e-1}{v-r-1} - \binom{e-g+2}{v-r-g+2} + \binom{e-\ell_g - g+2}{v-r-g+2} \\
= \binom{e}{v-r} - \binom{e-g+2}{v-r-g+2} - \sum_{n=1}^{k_g-\ell_g} \binom{e-g+1-n}{v-r-g+1} \\
+ \binom{e-k_g - g+2}{v-r-g+2} - \binom{e-k_g - g+2}{v-r-g+2} + \binom{e-\ell_g - g+2}{v-r-g+2} \tag{3.12}
\]
\[
\begin{align*}
&= \left( \frac{e}{v-r} \right) - \left( \frac{e-g+2}{v-r-g+2} \right) + \left( \frac{e-k_g-g+2}{v-r-g+2} \right) \\
&\quad - \sum_{n=1}^{k_g-\ell_g} \left( \frac{e-g+1-n}{v-r-g+1} \right) + \sum_{n=1}^{k_g-\ell_g} \left( \frac{e-\ell_g-g+2-n}{v-r-g+1} \right) \\
&= \left( \frac{e}{v-r} \right) - \left( \frac{e-g+2}{v-r-g+2} \right) + \left( \frac{e-k_g-g+2}{v-r-g+2} \right) \\
&\quad - \sum_{n=1}^{k_g-\ell_g} \sum_{m=1}^{\ell_g-1} \left( \frac{e-g+1-n-m}{v-r-g} \right) .
\end{align*}
\]

(3.12)

It is obvious that this bound of \(a_r\) is reduced to the Li-Tian bound in eq. (3.1) when \(k_g = \ell_g = 1\), and is optimized if we choose the edge \(xy\) so that the magnitude of the summation \(S\), where

\[
S = \sum_{n=1}^{k_g-\ell_g} \sum_{m=1}^{\ell_g-1} \left( \frac{e-g+1-n-m}{v-r-g} \right)
\]

is as large as possible. By Lemma 1, we can rewrite the bound as

\[
a_r \leq \left( \frac{e}{v-r} \right) - \left( \frac{e-g+2}{v-r-g+2} \right) + \left( \frac{e-\ell_g-g+2}{v-r-g+2} \right) - \left( \frac{e-g+1}{v-r-g+2} \right) \\
+ \left( \frac{e-k_g+1}{v-r-g+2} \right) - \delta_{g,3} \left[ \left( \frac{e-\ell_g-g+1}{v-r-g+1} \right) \right] \\
- \left( \frac{e-k_g-1}{v-r-g+1} \right) .
\]

(3.14)

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