On Chromatic Roots with Negative Real Part

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Abstract

A chromatic root is a root of the chromatic polynomial of some graph G. E. Farrell conjectured in 1980 that no chromatic root can lie in the left-half plane, and in 1991 Read and Royle showed by direct computation that the chromatic polynomials of some graphs do have a root there. These examples, though, yield only finitely many such chromatic roots. Subsequent results by Shrock and Tsang show the existence of chromatic roots of arbitrarily large negative real part. We show that theta graphs with equal path lengths of size at least 8 have chromatic roots with negative real part

1 Introduction

The chromatic polynomial of a graph G = (V, E) is the number $\pi(G, x)$ of functions $f: V \to \{1, \ldots, x\}$ such that $uv \in E$ implies $f(u) \neq f(v)$. It is well known that $\pi(G, x)$ is a monic polynomial in x of degree |V|, whose coefficients are integers that alternate in sign. The roots of $\pi(G, x)$ are often called the chromatic roots of G, and by a chromatic root we mean a root of some chromatic polynomial. Chromatic roots have been fairly well studied [3, 5, 6, 7, 8, 13, 16], though there is still much that is not known.

It is obvious, from the fact that the coefficients alternate in sign, that no real chromatic root is negative. Based on the chromatic roots of all graphs on at most 8 vertices, the following was conjectured in 1980.

Conjecture 1.1 [10] There are no chromatic roots with negative real part.

In 1991 Read and Royle computed the chromatic polynomials of all 3-regular graphs on at most 16 vertices, noting that graphs with high girth appear to be contributing the roots with smallest real part. They proceeded to plot the chromatic roots of all 3-regular graphs of girth at least 5 on

18 vertices, and observed the following, thus providing the smallest known counterexample to the above conjecture.

Proposition 1.2 [13] There are graphs of order 18 having a chromatic root with negative real part.

They noted the same for the 3-regular graphs of girth at least 6 on 20 vertices, and girth at least 7 on 26 vertices. More recently, Shrock and Tsang [14] have shown how badly the conjecture fails by showing that as $k \to \infty$, the k-ary theta graphs (i.e. graphs formed from two vertices joined by k internally disjoint paths) had chromatic roots whose real parts tended to $-\infty$. By different techniques (namely the Hermite-Biehler and Sturm theorems on the roots of real polynomials), we show here that indeed infinitely many chromatic roots of negative real part are achievable among 3-ary theta graphs themselves. These provide examples of the smallest corank (i.e. with minimal |E| - |V| + 1).

2 Background: The Hermite-Biehler and Sturm Theorems

A polynomial f with real coefficients is $Hurwitz\ quasi-stable\ [2,15]$ if every root of f has nonpositive real part. The statement of the Hermite-Biehler Theorem proved in Gantmacher [11] is actually a criterion for deciding whether every root of a real polynomial has strictly negative real part. Wagner [15] deduced from this an analogous criterion for Hurwitz quasi-stability. It is the latter which we shall call the Hermite-Biehler Theorem. As in [15], a polynomial is standard if it is either identically zero or has positive leading coefficient, and is said to have $only\ nonpositive\ zeros$ if it is either identically zero or has all of its roots real and nonpositive. Also, if k is a field and x an indeterminate, then k[x] denotes the ring of polynomials in x with coefficients from k.

Theorem 2.1 (Hermite-Biehler) Let $P(x) \in \mathbb{R}[x]$ be standard, and write $P(x) = P_e(x^2) + xP_o(x^2)$. Set $t = x^2$. Then P(x) is Hurwitz quasi-stable if and only if both $P_e(t)$ and $P_o(t)$ are standard, have only nonpositive zeros, and $P_o(t) \prec P_e(t)$.

Roughly speaking (and made precise in [15]), the notation $P_o(t) \prec P_e(t)$ says that the roots of $P_o(t)$ 'interlace' the roots of $P_e(t)$, but we do not concern ourselves with that here. In fact, we shall only need the following.

Corollary 2.2 If either $P_e(t)$ or $P_o(t)$ has a nonreal root (and is not identically zero), then P(x) is not Hurwitz quasi-stable.

Now Sturm's Theorem [12] gives rise to a useful test for deciding whether a real polynomial has a nonreal root. We say that two consecutive terms of a sequence $s = (a_0, a_1, \ldots, a_k)$ of nonzero real numbers have a *sign* variation if they have opposite signs, and denote by $\operatorname{Var} s$ the number of sign variations of s. If s contains zero entries, then $\operatorname{Var} s$ is defined to be the number of sign variations of the subsequence of nonzero terms of s.

The Sturm sequence of a real polynomial f(t) of positive degree is f_0 , f_1, f_2, \ldots , where $f_0 = f$, $f_1 = f'$, and, for $i \geq 2$, $f_i = -\text{rem}(f_{i-1}, f_{i-2})$, where rem(g, h) denotes the remainder upon dividing g by h. The sequence is terminated at the last nonzero f_i , which is easily seen to be a constant times the greatest common divisor of f and f' (by carefully comparing the process to the Euclidean Algorithm).

Theorem 2.3 (Sturm's Theorem) Let $f(t) \in \mathbb{R}[t]$ have positive degree, and suppose (f_0, f_1, \ldots, f_k) is its Sturm sequence. Let a < b be reals that are not roots of f. Then the number of distinct roots of f in (a,b) is V(a) - V(b), where $V(c) \equiv Var(f_0(c), f_1(c), \ldots, f_k(c))$.

A proof can be found in [12]. Now we say that the Sturm sequence (f_0, f_1, \ldots, f_k) of f(t) has gaps in degree if there is a $j \leq k$ such that deg $f_j < \deg f_{j-1} - 1$. If there is a $j \leq k$ such that f_j has negative leading coefficient, then we say the Sturm sequence has a negative leading coefficient.

We shall need the following corollary to Sturm's Theorem which is not explicitly found in the literature (a similar statement, though stated incorrectly, is found in [1, p.176]).

Corollary 2.4 Let f(t) be a real polynomial whose degree and leading coefficient are positive. Then f(t) has all real roots if and only if its Sturm sequence has no gaps in degree and no negative leading coefficients.

<u>Proof</u> Let us begin with a few observations. We write f = gh, where $g = \gcd(f, f')$. Then the number of distinct roots of f is exactly $\deg h$, as the roots of g are the multiple roots of f. Consider the Sturm sequence $S_f(t) = (f_0, f_1, \ldots, f_k)$ of f. Recall that $f_0 = f$ and f_k is a (nonzero) constant times g. Then since $\deg f = \deg g + \deg h$, we have that the number of terms in $S_f(t)$ is $k+1 \leq \deg h+1$, with equality exactly when it has no gaps in degree.

We define $V(-\infty)$ and $V(\infty)$ to be, respectively, V(-M) and V(M), where M > 0 is any number large enough that all real roots of each f_i (i = 0, 1, ..., k) lie in (-M, M). It is clear that

$$V(-\infty) = \operatorname{Var}((-1)^{\deg f_0}\operatorname{lcoeff} f_0, (-1)^{\deg f_1}\operatorname{lcoeff} f_1, \dots, (-1)^{\deg f_k}\operatorname{lcoeff} f_k)$$

and

$$V(\infty) = \text{Var} (\text{lcoeff } f_0, \text{lcoeff } f_1, \dots, \text{lcoeff } f_k),$$

where lcoeff ψ denotes the leading coefficient of ψ .

All real roots of f lie in (-M, M) as $f = f_0$. Then Sturm's Theorem says that the number of distinct real roots of f is $V(-\infty) - V(\infty)$.

With these observations, we prove the result. If $S_f(t)$ has gaps in degree, then it has $k+1<\deg h+1$ terms, so in particular $V(-\infty)\leq k<\deg h$, and so

distinct real roots of
$$f = V(-\infty) - V(\infty)$$

 $\leq V(-\infty)$
 $< \deg h$
 $= \# \text{ distinct roots of } f$,

which implies that f has a nonreal root. If $S_f(t)$ has no gaps in degree but has a negative leading coefficient, then let j be the first i such that looeff $f_i < 0$. Then looeff $f_{j-1} > 0$ (as looeff f_0 is), and since deg $f_j = \deg f_{j-1} - 1$, we have that $(-1)^{\deg f_{j-1}} \operatorname{looeff} f_{j-1}$ and $(-1)^{\deg f_j} \operatorname{looeff} f_j$ have the same sign, so $V(-\infty) < k = \deg h$, and again f has a nonreal root.

Conversely, if $S_f(t)$ has no gaps in degree and no negative leading coefficients, then $k = \deg h$, $V(-\infty) = k$, and $V(\infty) = 0$, so

distinct real roots of
$$f = V(-\infty) - V(\infty)$$

= deg h
= # distinct roots of f ,

which says f has all real roots.

Now for c any positive real number, it is easy to see that if, on obtaining the term f_j $(0 \le j \le k)$ in the construction of the Sturm sequence (f_0, f_1, \ldots, f_k) of f(t), we were to change f_j to cf_j before continuing, then the resulting sequence would differ from (f_0, f_1, \ldots, f_k) only in that some f_i 's would now become cf_i , and so clearly that sequence could be used in place of (f_0, f_1, \ldots, f_k) when applying Theorem 2.3 or Corollary 2.4. In fact, we may perform multiplications like this at any number of steps (by repeatedly applying the above argument), and do not distinguish between the sequences so obtained, in that we consider any to be a Sturm sequence of f(t). We shall make use of this observation in Section 4.

3 Generalized Theta Graphs

One of the very few infinite families of graphs whose chromatic polynomials are known is the family of generalized theta graphs, $\Theta_{a,b,c}$, which consists exactly of two vertices u and v (called terminals) of degree 3 joined by three distinct paths of (positive) lengths a, b, and c, where no more than one of these lengths is 1 (more generally, Θ_{a_1,\ldots,a_k} is the graph with two vertices, u and v, joined by k internally disjoint paths of lengths a_1,\ldots,a_k). Thus $\Theta_{a,b,c}$ has a+b+c-1 vertices and a+b+c edges.

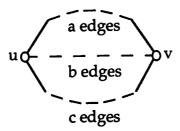


Figure 1: The graph $\Theta_{a,b,c}$.

Recall [4] that if e is an edge of a graph G, then $\pi(G,x) = \pi(G-e,x) - \pi(G \bullet e,x)$, where G-e is obtained by removing e from G, while $G \bullet e$ is obtained by identifying the ends of e. Another well known result [4] is that if two graphs G and H intersect exactly on a complete graph of order p, then $\pi(G \cup H, x) = \pi(G, x)\pi(H, x)/\pi(K_p, x)$. These allow us to derive an expression [4] for the chromatic polynomial of $\Theta_{a,b,c}$ as follows:

$$\pi(\Theta_{a,b,c},x) = \frac{\pi(C_{a+1},x)\pi(C_{b+1},x)\pi(C_{c+1},x)}{x^2(x-1)^2} + \frac{\pi(C_a,x)\pi(C_b,x)\pi(C_c,x)}{x^2} \ ,$$

where C_n is the cycle of order n, whose chromatic polynomial is well known [4] to be

$$\pi(C_n, x) = (x-1)^n + (-1)^n(x-1)$$

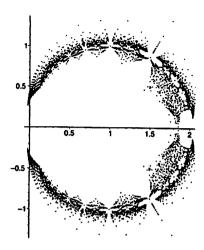


Figure 2: Chromatic roots of $\Theta_{a,b,c}$, $1 \le a \le b \le c \le 13$.

$$= (-1)^n (1-x) \left[(1-x)^{n-1} - 1 \right].$$

Using this, we find

$$\pi(\Theta_{a,b,c},x) = (1/(x^{2}(x-1)^{2}))((-1)^{a+b+c+3}(1-x)^{3} [(1-x)^{a}-1] \cdot [(1-x)^{b}-1] [(1-x)^{c}-1]) + [(1-x)^{c}-1]) + (1/x^{2})((-1)^{a+b+c}(1-x)^{3} [(1-x)^{a-1}-1] \cdot [(1-x)^{b-1}-1] [(1-x)^{c-1}-1])$$

$$= ((-1)^{a+b+c}(1-x))/x^{2}) [-(1-x)^{a+b+c}-(1-x)^{a}-(1-x)^{b}-(1-x)^{c}+1+(1-x)^{a+b+c-1}+(1-x)^{a+b+c-1}+(1-x)^{a+1}+(1-x)^{b+1}+(1-x)^{c+1}-(1-x)^{2}]$$

$$= ((-1)^{a+b+c}(1-x))/x^{2}) [x(1-x)^{a+b+c-1}-x(1-x)^{a}-x(1-x)^{b}-x(1-x)^{c}+(1-x)^{c}+(1-x)^{a+b+c-1}-(1-x)^{a}-(1-x)^{a}-(1-x)^{a}-(1-x)^{b}-(1-x)^{c}+(1-x)^{a}+(1-x)^{a}+(1-x)^{a}-(1-x)^{a}-(1-x)^{a}-(1-x)^{b}-(1-x)^{c}+(1-x)^{a}+(1-x)^{a}+(1-x)^{a}-(1-x)^{a}-(1-x)^{b}-(1-x)^{c}+(1-x)^{a}+(1-x)^{a}+(1-x)^{a}-(1-x)^{a}-(1-x)^{b}-(1-x)^{c}+(1-x)^{a}+(1-x)^{a}+(1-x)^{a}+(1-x)^{a}+(1-x)^{a}-(1-x)^{a}-(1-x)^{b}-(1-x)^{c}+(1-x)^{a}$$

With this expression, we obtain the plot of the chromatic roots of all generalized theta graphs whose paths have length at most 13.

The roots clearly display some interesting, very non-random behaviour. In particular, there are zeros to the left of the imaginary axis.

4 Theta Graphs with Chromatic Roots of Negative Real Part

We restrict our attention now to the subfamily $\{\Theta_{a,a,a}: a \geq 2\}$ of generalized theta graphs whose u-v paths all have the same length. The smallest such graph having a chromatic root with negative real part is found (by direct calculation) to be $\Theta_{8,8,8}$. We can say much more.

Theorem 4.1 The graph $\Theta_{a,a,a}$ has a chromatic root with negative real part if and only if $a \geq 8$.

Proof From (1), we have

$$\pi(\Theta_{a,a,a},x) = \frac{(-1)^{3a}(1-x)}{x} \left[(1-x)^{3a-1} - 3(1-x)^a + 2 - x \right]. \tag{2}$$

Then, for $a \geq 8$, we need to show that $\pi(\Theta_{a,a,a}, -x)$ has a root with *positive* real part, i.e., that

$$\psi_a(x) \equiv (1+x)^{3a-1} - 3(1+x)^a + 2 + x \tag{3}$$

is not Hurwitz quasi-stable. So let $a \ge 8$, and expand $\psi_a(x)$ into its even and odd parts:

$$\psi_a(x) = P_e^a(x^2) + x P_o^a(x^2). \tag{4}$$

Now set $t=x^2$ (as in Theorem 2.1). Several calculations suggested that $P_e^a(t)$ always appears to have a nonreal root (for $a \geq 8$), and by Corollary 2.2, it is enough to show that this is indeed the case. To that end, it would suffice (by Theorem 2.3) to show that its Sturm sequence contains either a negative leading coefficient or gaps in degree. Our computations, however, suggest that this does not occur until close to the end of its Sturm sequence. So let us instead consider the polynomial

$$\phi_a(t) \equiv t^{\deg P_e^a(t)} P_e^a(1/t),\tag{5}$$

which clearly has a nonreal root if and only if $P_e^a(t)$ does. Moreover, we can establish the following.

Lemma 4.2 For $a \ge 14$, the Sturm sequence of $\phi_a(t)$ has as its fifth term a polynomial with negative leading coefficient.

We shall see, also, that before the fifth term in the sequence, there are neither gaps in degree nor any negative leading coefficients. However, since Lemma 4.2 tells us the leading coefficient of the fifth term is negative, we conclude that $\phi_a(t)$ has a nonreal root for $a \ge 14$, and in fact for $a \ge 8$

upon verifying the cases $8 \le a \le 13$ directly. Hence, to prove Theorem 4.1, it remains only to prove Lemma 4.2. We assume that $a \ge 14$ is *even* (the odd case is handled similarly). Then from (3), (4), and (5) we find that

$$\begin{array}{lll} \phi_a(t) & = & \left[\binom{3a-1}{2} - 3\binom{a}{2} \right] t^{\frac{3a-4}{2}} + \left[\binom{3a-1}{4} - 3\binom{a}{4} \right] t^{\frac{3a-6}{2}} \\ & + \cdots + \left[\binom{3a-1}{a} - 3\binom{a}{a} \right] t^{\frac{2a-2}{2}} + \binom{3a-1}{a+2} t^{\frac{2a-4}{2}} + \binom{3a-1}{a+4} t^{\frac{2a-6}{2}} \\ & + \cdots + \binom{3a-1}{3a-2}. \end{array}$$

Let us denote the first five terms of the Sturm sequence of ϕ_a by ϕ_a^0 (= ϕ_a), ϕ_a^1 (= ϕ_a'), ϕ_a^2 , ϕ_a^3 , and ϕ_a^4 . Then it is clear, from the form of ϕ_a and the division process, that lcoeff (ϕ_a^4) is a real valued function of a, which we shall show is always negative (for $a \ge 14$ even). We shall see that only the first 7 terms of ϕ_a are needed. To begin, we have

$$\phi_a = bt^n + ct^{n-1} + dt^{n-2} + et^{n-3} + ft^{n-4} + gt^{n-5} + ht^{n-6} + \cdots,$$

where $b = \binom{3a-1}{2} - 3\binom{a}{2}$, $c = \binom{3a-1}{4} - 3\binom{a}{4}$, ..., $h = \binom{3a-1}{14} - 3\binom{a}{14}$, and $n = \frac{3a-4}{2}$. Note that b, c, \ldots, h and n are polynomials in a with rational coefficients. Now

$$\phi'_a = bnt^{n-1} + c(n-1)t^{n-2} + d(n-2)t^{n-3} + e(n-3)t^{n-4} + f(n-4)t^{n-5} + g(n-5)t^{n-6} + h(n-6)t^{n-7} + \cdots$$

Dividing ϕ_a by ϕ'_a , we find

$$-\operatorname{rem}(\phi_{a}, \phi'_{a}) = \frac{c^{2}(n-1) - 2bdn}{bn^{2}} t^{n-2} + \frac{cd(n-2) - 3ben}{bn^{2}} t^{n-3} + \frac{ce(n-3) - 4bfn}{bn^{2}} t^{n-4} + \frac{cf(n-4) - 5bgn}{bn^{2}} t^{n-5} + \frac{cg(n-5) - 6bhn}{bn^{2}} t^{n-6} + \cdots$$

Since $bn^2 > 0$, we can (by an observation made in Section 2) clear the denominators by choosing $\phi_a^2 = bn^2 \cdot (-\text{rem}(\phi_a, \phi_a'))$. Now it turns out that $c^2(n-1) - 2bdn$ is always positive (for $a \ge 14$ even). For note that it is a polynomial in b, c, d, and n with integer coefficients, each of which (recall) are themselves polynomials in a with rational coefficients. Carrying out the substitutions in Maple, we obtain an exact expression for $c^2(n-1) - 2bdn \in \mathbb{Q}[a]$, and find that it has positive leading coefficient, and so is positive beyond its largest real root, a bound for which is obtained by applying a standard result (c.f. [9, p.197]) to the polynomial. It is then verified directly that the polynomial $c^2(n-1) - 2bdn$ is also positive for those (even) a between 14 and that bound.

So moving on to the next term in the Sturm sequence, we divide ϕ'_a by ϕ^2_a , and find

$$-\operatorname{rem}(\phi_a', \phi_a^2) = \frac{u}{(c^2(n-1) - 2bdn)^2} t^{n-3} + \frac{v}{(c^2(n-1) - 2bdn)^2} t^{n-4} + \frac{w}{(c^2(n-1) - 2bdn)^2} t^{n-5} + \cdots,$$

where

$$u = -(c^{2}(n-1) - 2bdn) (d(n-2) (c^{2}(n-1) - 2bdn) -bn (ce(n-3) - 4bfn)) + (cd(n-2) - 3ben) (c(n-1) (c^{2}(n-1) - 2bdn) -bn (cd(n-2) - 3ben)),$$

$$v = -(c^{2}(n-1) - 2bdn) (e(n-3) (c^{2}(n-1) - 2bdn) -bn (cf(n-4) - 5bgn)) + (ce(n-3) - 4bfn) \cdot (c(n-1) (c^{2}(n-1) - 2bdn) - bn (cd(n-2) - 3ben)),$$

and

$$w = -(c^{2}(n-1) - 2bdn) (f(n-4) (c^{2}(n-1) - 2bdn) -bn (cg(n-5) - 6bhn)) + (cf(n-4) - 5bgn) + (cf(n-4) - 5bgn) (c(n-1) (c^{2}(n-1) - 2bdn) -bn (cd(n-2) - 3ben)).$$

Multiplying by the positive number $(c^2(n-1)-2bdn)^2$, we choose

$$\phi_a^3 = ut^{n-3} + vt^{n-4} + wt^{n-5} + \cdots$$

Again, we have verified (with the aid of Maple) that indeed u is always positive (for $a \ge 14$ even). So let us move on to the fifth term in the Sturm sequence. Dividing ϕ_a^2 by ϕ_a^3 , we find

$$-\operatorname{rem}(\phi_a^2, \phi_a^3) = \frac{1}{u^2} \left(v((cd(n-2) - 3ben) u - (c^2(n-1) - 2bdn) v) - u((ce(n-3) - 4bfn) u - (c^2(n-1) - 2bdn) w) \right) t^{n-4} + \cdots$$

Multiplying by the positive number u^2 , we choose

$$\phi_a^4 = \left(v((cd(n-2) - 3ben) u - (c^2(n-1) - 2bdn) v) - u((ce(n-3) - 4bfn) u - (c^2(n-1) - 2bdn) w) \right) t^{n-4} + \cdots$$

We denote by lcoeff (ϕ_a^4) the coefficient of t^{n-4} in ϕ_a^4 (no confusion arises in doing so, as we are about to see that this coefficient is never zero, and so really is the leading coefficient of ϕ_a^4). So lcoeff (ϕ_a^4) is a polynomial in b, c, \ldots, h , and n with integer coefficients. Substituting (once again) our expressions for b, c, \ldots, h as polynomials in a with rational coefficients, we obtain an exact expression for lcoeff $(\phi_a^4) \in \mathbb{Q}[a]$, the first few terms of which are approximately

$$-342.7311661a^{70} + 22877.24435a^{69} - 718377.3180a^{68} + \cdots$$

In particular, the first term is negative, and so lcoeff (ϕ_a^4) is negative for a sufficiently large, which is what we want. Applying a standard result (c.f. [9, p.197]) to the polynomial lcoeff (ϕ_a^4) , we obtain 134 as a bound on its largest real root, and so the proof of Lemma 4.2 for a even is completed by verifying directly that lcoeff (ϕ_a^4) is also negative for $a = 14, 16, 18, \ldots, 134$.

We mentioned that the proof for a odd is similar. There we find

lcoeff
$$(\phi_a^4) \approx -342.7311661a^{70} + 21277.83225a^{69} - 617481.3554a^{68} + \cdots,$$

in which case an analysis like the previous paragraph is carried out.

This completes the proof of Lemma 4.2, and so of Theorem 4.1.

We remark that the smallest generalized theta graphs having a chromatic root with negative real part are $\Theta_{4,5,5,5,5}$ and $\Theta_{5,6,6,6}$, each of order 21.

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