Bounds on the Chromatic Polynomial and on the Number of Acyclic Orientations of a Graph

Nabil Kahale[1], Leonard J. Schulman[2]

Abstract

An upper bound is given on the number of acyclic orientations of a graph, in terms of the spectrum of its Laplacian. It is shown that this improves upon the previously known bound, which depended on the degree sequence of the graph. Estimates on the new bound are provided.

A lower bound on the number of acyclic orientations of a graph is given, with the help of the probabilistic method. This argument can take advantage of structural properties of the graph: it is shown how to obtain stronger bounds for small-degree graphs of girth at least five, than are possible for arbitrary graphs. A simpler proof of the known lower bound for arbitrary graphs is also obtained.

Both the upper and lower bounds are shown to extend to the general problem of bounding the chromatic polynomial from above and below along the negative real axis.

[1]XEROX Palo Alto Research Center, 3333 Coyote Hill Road, CA 94304. Partially supported by the NSF under grant CCR–9404113. Most of this research was done while the author was at the Massachusetts Institute of Technology, and was supported by the Defense Advanced Research Projects Agency under Contracts N00014-92-J-1799 and N00014-91-J-1698, the Air Force under Contract F49620-92-J-0125, and the Army under Contract DAAL-03-86-K-0171.

[2]Department of Computer Science, U.C. Berkeley. Supported by an ONR graduate fellowship, grants NSF 8912586 CCR and AFOSR 89-0271, and an NSF postdoctoral fellowship.

1 Introduction

Given an undirected graph G, the number of acyclic orientations of G, $\alpha(G)$, is the number of ways in which all of its arcs can be directed without introducing directed cycles.

The number of acyclic orientations was first considered by Stanley [20] in 1973, who pointed out a remarkable characterization of this number as the value at -1 of the chromatic polynomial χ_G of the graph. Since then interest has arisen in $\alpha(G)$ in computer science, because $\log \alpha(G)$ is a lower bound on the computational complexity of various decision and sorting problems [18, 9]. Hence useful bounds on $\alpha(G)$ have been sought.

However Stanley's result does not provide an effective indication of the magnitude of $\alpha(G)$. In fact Linial has shown that the problem of exact determination of the number of acyclic orientations of a graph, is complete for the complexity class #P [13]. (More generally Jaeger, Vertigan and Welsh [10] have shown that evaluation of the Tutte polynomial of the cycle matroid of a graph is #P complete at all but nine special points; $\alpha(G)$ is the value of the Tutte polynomial at a non-special point.) This hardness result suggests that effective exact expressions for $\alpha(G)$ are an unlikely prospect, and provides additional motivation for obtaining bounds on this number.

The first bound on $\alpha(G)$, due to Fredman [11] and to Manber and Tompa [18], was the upper bound $\alpha(G) \leq \prod_{v \in G}(d_v + 1)$, where d_v represents the degree of vertex v. As noted in [9], this bound is sometimes close to the truth, as for the case of $G = K(a, b)$ with $b >> a$. In this case $\alpha(G) \sim a!(a+1)^b$. The second such result was the following lower bound, also in terms of the degree sequence of the graph [9]. Let $f(x) = (x!)^{1/x}$. Then $\alpha(G) \geq \prod_{v \in G} f(d_v + 1)$. This bound is tight in the case of the complete graph. The gap between these two bounds can be estimated from Stirling's formula, and is bounded by e^n, where n is the number of vertices in G.

We present a new upper bound on the number of acyclic orientations of a graph. We show that the degree bound $\prod_{v \in G}(d_v + 1)$ can be replaced by a spectral bound $\prod_{i=1}^{n}(\lambda_i + 1)$ where $\{\lambda_i\}$ are the eigenvalues of the Laplacian of the graph. Thus the bound is the determinant of the sum of the Laplacian of the graph and the identity matrix; or, the Kirchhoff matrix of the graph.

We also present a new approach to giving lower bounds on the number of acyclic orientations of a graph. It is known how to obtain a lower bound on this number, from the out-degree sequence of any particular orientation; the difficulty in taking advantage of this statement lies in coming up with an orientation with a desirable out-degree sequence. We show how to circumvent this difficulty using the probabilistic method.

In section 2 we show how to bound from above the number of acyclic orientations of a graph, by the number of spanning trees in a closely related graph; the latter quantity is in turn expressed in terms of the spectrum of the Kirchhoff matrix of the original graph, via the matrix-tree theorem. We then show that this bound always improves upon the degree bound of [18]. In section 3 we show that for regular graphs the determinant of the Kirchhoff matrix is asymptotically bounded by roughly $(d+1/2)^n$; and that for certain graphs, this is a nearly tight estimate of the Kirchhoff determinant. We also give an asymptotic bound, in terms of the degree sequence, on the Kirchhoff determinant in general graphs.

In section 4 we extend our study of acyclic orientations to the study of χ_G at arbitrary negative values. In section 4.1 we show that the inequality between the number of acyclic orientations and the number of spanning trees, extends to an inequality between $\det(Q + wI)$ and $(-1)^n\chi(-w)$ for $w \geq 0$, where Q is the Laplacian of a graph and χ is its chromatic polynomial. In section 4.2 we provide a simple probabilistic proof of the aforementioned lower bound on $\alpha(G)$ for arbitrary graphs. We also show how this proof extends to give a lower bound on $(-1)^n\chi_G(-w)$ for arbitrary positive w.

In section 5 we show how to use the probabilistic lower bound method to take advantage of a structural assumption on the graph, namely that it has no 3-cycles or 4-cycles (i.e. girth ≥ 5). In this case we can prove lower bounds for $\alpha(G)$ and for the chromatic polynomial, that are strictly stronger than those possible for an arbitrary graph. (As noted above, the general lower bound on $\alpha(G)$ is sometimes tight.) Our improvement is most significant for small-degree graphs, and we calculate the case of degree 3 in detail. Section 6 contains concluding remarks.

2 Acyclic Orientations and Spanning Trees

It will be convenient to view an acyclic orientation as the Hasse diagram of a partial order, and speak of one vertex dominating another if it precedes it in the orientation.

Form the undirected graph G' from G by adjoining a new vertex u which is connected to all the vertices of G. Let $\tau(G')$ denote the number of spanning trees of G' rooted at u (equivalently, the number of spanning trees of G'). We show that:

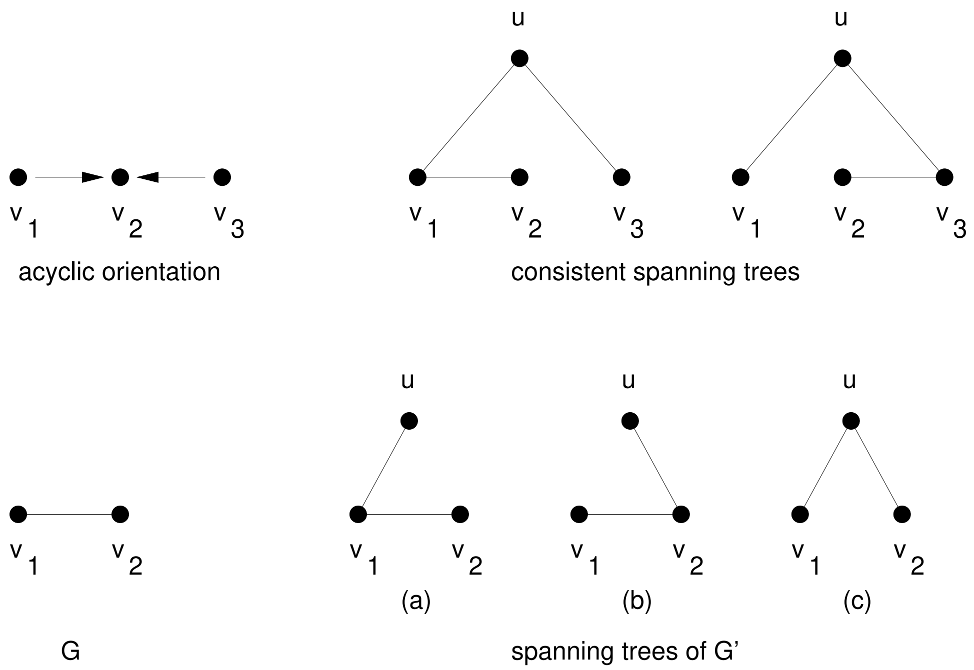
Lemma 1. *$\alpha(G) \leq \tau(G')$.*

Proof: The argument is by injection from acyclic orientations to spanning trees rooted at u. We construct the tree associated with an orientation level by level, beginning with u at level 0. In the first stage we connect every maximal vertex of the orientation to u, thus obtaining level 1 of the tree. In general at stage i we select all as yet unplaced vertices of G which are dominated only by vertices that are already in the spanning tree; and we place these vertices in level i of the tree by connecting them to a neighboring vertex which is at level $i-1$. Such a neighbor must exist else we would have placed the current vertex in the tree at an earlier stage.

Observe that if one vertex precedes another in the acyclic orientation then it will be placed at a lower level of the tree. Any pair of distinct acyclic orientations disagree on some edge vw and so their associated trees will differ as to which of the two vertices is lower. Hence no two orientations are carried to the same tree. $\square$

We comment that for two reasons this inequality is not tight. First, there are arbitrary choices in the tree construction whenever a vertex may be connected to one of several vertices at the preceding level (see Fig. 1). The proof demonstrates that the sets of trees which can be formed from different orientations are disjoint; our bound might be tightened with the help of estimates on the sizes of these sets. Second, not all spanning trees can be formed by the construction: e.g. (c) in Fig. 2. The spanning trees which can be formed are precisely those in which every level of the tree is an independent set in the graph.

We can now relate the number of acyclic orientations to the graph spectrum. The Laplacian $Q(H)$ of an undirected graph H is the symmetric matrix which for $i \neq j$, has a 0 in entry $Q(H)_{ij}$ if vertices i and j are not connected, and a -1 if they are connected; while on the diagonal, the degrees of the vertices appear in the corresponding order. Kirchhoff's matrix-tree theorem [6] establishes that the



number of spanning trees of a graph is equal to the determinant of a minor of the Laplacian in which the row and column corresponding to any vertex are omitted.

The Kirchhoff matrix $K(H)$ of an undirected graph H is defined as $Q(H)+I$, where I is the identity. Observe that the spectrum of the Kirchhoff matrix is simply shifted by 1 from that of the Laplacian. Applying the matrix-tree theorem to G' by omitting the row and column corresponding to the introduced vertex u, we obtain a bound on acyclic orientations directly in terms of the spectrum of G: $\alpha(G) \leq \det(K(G))$. Namely

Theorem 1. *The number of acyclic orientations of an undirected graph is no greater than the determinant of its Kirchhoff matrix.* □

Comparison with the Degree Bound

We now show that the bound given by Theorem 1 on the number of acyclic orientations of a graph improves upon the degree bound. In the next section we give estimates on the improvement achieved. Let d_v be the degree of vertex v.

Lemma 2. *The determinant of the Kirchhoff matrix of a graph G is at most $\prod_{v \in G}(d_v + 1)$.*

Proof: The number of spanning trees (rooted at u) in G' is upper bounded by $\prod_{v \in G}(d_v + 1)$ because each vertex v in G has at most $d_v + 1$ ways to choose its parent in the tree. □

(A more algebraic way of seeing this, which is useful when we more generally consider the chromatic polynomial, and the matrix $Q(H) + wI$ ($w \geq 0$) rather than $Q(H) + I$, is that the Laplacian of G is a positive semidefinite matrix, and $Q(H) + wI$ is also positive semidefinite. A standard result in linear algebra [15] is that the determinant of a positive semidefinite matrix is no greater than the product of its diagonal elements. The proof follows by applying this result to $Q(H) + wI$.)

3 Estimates on the Determinant of the Kirchhoff Matrix

We will obtain bounds on the determinant of the Kirchhoff matrix. In the case of regular graphs of degree d, these bounds will be of the form $(d+1)^n e^{-(1/2d+O(1/d^2))n}$, which is roughly $(d + 1/2)^n$. We then study the case of arbitrary graphs. The problem of estimating the determinant of the Kirchhoff matrix is related to the problem of counting the number of spanning trees of d-regular graphs. McKay [17] showed that for any family G_n of d-regular graphs,

$$\lim_{n \to \infty} \sup(\kappa(G_n))^{1/n} \leq \frac{(d-1)^{d-1}}{(d^2 - 2d)^{d/2-1}}, \tag{1}$$

where $\kappa(G_n)$ is the number of spanning trees in G_n. He also showed the existence of a family of d-regular graphs for which this bound is tight. Note that the right-hand side of Eq. 1 is equal to $d - 1/2 + O(1/d)$.

3.1 Regular Graphs

In this section we consider the case of a regular graph G of degree d. Let $\beta = d/2(d-1)$ and $\psi_d(z) = \sqrt{1 - 4(d-1)z^2}$.

Theorem 2. *The determinant of the Kirchhoff matrix of a d-regular graph on n vertices is at most $(d+1)^n \exp(-\phi(d)n)$, for a function ϕ of the form $\phi(d) = \frac{1}{2d} - \frac{1}{2d^2} + \frac{1}{12d^3} - \frac{1}{4d^4} + O(d^{-5})$.*

Proof: Our approach and calculations are similar to those in [17]. Let A be the adjacency matrix of G and $f(z) = \det(I - zA)$. Since $K(G) = (d+1)I - A$, we have $\det(K(G)) = (d+1)^n f(1/(d+1))$. In order to get the desired bound on the determinant of $K(G)$, we are going to bound $f(1/(d+1))$. A classical result [19, pages 242–243] shows that

$$\frac{f'(z)}{f(z)} = -\frac{1}{z}\sum_{l\geq 1} \mathrm{tr}(A^l)z^l. \tag{2}$$

From the definition we see that the radius of convergence of this generating function is the inverse of the largest eigenvalue of A in absolute value, which in this case is d. Note that $\mathrm{tr}(A^l)$ is the number of closed walks in G of length l. Let T^d be the infinite d-regular tree. T^d can be mapped into G in a manner that preserves edges and carries the neighbors of any vertex in T^d to distinct vertices in G. As observed in [14], it follows that $\mathrm{tr}(A^l) \geq n\rho(l)$, where $\rho(l)$ is the number of closed walks of length l in T^d starting from any vertex x. (Let $\rho(0) = 1$.) By standard generating function methods [22] (see also [17] and references therein),

$$\sum_{l\geq 0} \rho(l)z^l = \frac{1}{1 - \beta + \beta\psi_d(z)}. \tag{3}$$

Combining Eqs. 2 and 3 and integrating, we have

$$\begin{aligned}
\ln(f(\frac{1}{d+1})) &\leq -n\int_0^{1/(d+1)} \frac{du}{u}\left(\frac{1}{1-\beta+\beta\psi_d(u)} - 1\right) \\
&= -\frac{n}{2\beta - 1}\left[(1-\beta)\ln(1-\beta+\beta\psi_d(u)) - \beta\ln\left(\frac{1+\psi_d(u)}{2}\right)\right]_0^{\frac{1}{d+1}} \\
&= -n\phi(d),
\end{aligned}$$

where ϕ is defined by

$$\phi(d) = \frac{d-2}{2}\ln\left(\frac{d-2+d\psi_d(\frac{1}{d+1})}{2(d-1)}\right) - \frac{d}{2}\ln\left(\frac{1+\psi_d(\frac{1}{d+1})}{2}\right).$$

Change variables to $s = 1/d$ and note that the resulting function of s is analytic at $s = 0$, with power series

$$\frac{s}{2} - \frac{s^2}{2} + \frac{s^3}{12} - \frac{s^4}{4} + O(s^5)$$

(hence the expansion of ϕ given in the theorem). Thus $f(\frac{1}{d+1}) \leq \exp(-n\phi(d))$ as desired.

It follows that $\phi(d) \sim 1/2d$ as d goes to infinity. It can also be shown that $\phi(d) \geq 1/2d - 1/2d^2$ for $d \geq 2$. (Calculation shows $\rho(2) = d$, $\rho(4) = 2d^2 - d$, $\rho(6) = d(5d^2 - 6d + 2)$. As a consequence, $\phi(d) \geq 1/2d - 1/2d^2$ for $d \geq 18$. It can be checked directly that $\phi(d) \geq 1/2d - 1/2d^2$ for any integer d, $2 \leq d \leq 18$.) $\square$

Theorem 2 is for some graphs a nearly tight bound on the determinant of the Kirchhoff matrix. For example: note that $\phi(2) = -\ln\left(\frac{3+\sqrt{5}}{6}\right)$, and so in the case of the n-cycle, the bound of the theorem is $\left(\frac{3+\sqrt{5}}{2}\right)^n$. This differs from the exact value $\left(\frac{3+\sqrt{5}}{2}\right)^n + \left(\frac{3-\sqrt{5}}{2}\right)^n - 2$ only by an additive constant. There are also graphs of high degree for which the bound is nearly tight:

Theorem 3. *For any integer $d \geq 2$, there exists a family of d-regular graphs G_n on n vertices such that* $\det(K(G_n)) = (d+1)^n \exp\left(-(\phi(d) + o(1))n\right)$.

Proof: The girth of a graph is defined as the length of its shortest cycle. Let G_n be a family of d-regular graphs such that the girth g of G_n is at least $(1 + o(1)) \ln_{d-1} n$. The existence of such a family was shown in [8]. With notation as in the proof of Theorem 2, for A the adjacency matrix of G_n, we have

$$\frac{f'(z)}{f(z)} = -\frac{1}{z}\sum_{l\geq 1} \mathrm{tr}(A^l) z^l.$$

For $l \leq g-1$ we have $\mathrm{tr}(A^l) = n\rho(l)$ since any cycle in the graph has length greater than l. On the other hand, for any l, we have $\mathrm{tr}(A^l) \leq nd^l$. Therefore, for $0 \leq z \leq 1/(d+1)$,

$$\frac{f'(z)}{f(z)} \geq -\frac{1}{z}(n\sum_{l\geq 1}\rho(l)z^l + n\sum_{l\geq g} d^l z^l),$$

from which we deduce that

$$\ln(f(\frac{1}{d+1})) \geq -n\phi(d) - nd\left(\frac{d}{d+1}\right)^{g-1} \geq -n\phi(d) - n^{1-1/(d+1)\ln(d-1)+o(1)}.$$

$\square$

Observe that if $d-1$ is prime, there exists a family of bipartite d-regular Ramanujan graphs [14, 16] of girth $(\frac{4}{3} + o(1)) \ln_{d-1} n$. Since $\mathrm{tr}(A^l) \leq 2d^l + (n -$

$2)(2\sqrt{d-1})^l$ for any nonnegative integer l, we obtain a tighter lower bound on the determinant of the Kirchhoff matrices of these graphs from the equation

$$\begin{aligned}\ln(f(\frac{1}{d+1})) &\geq -n\phi(d) - \exp\left(\left(1 - \frac{4\ln\left(\frac{d+1}{2\sqrt{d-1}}\right)}{3\ln(d-1)} + o(1)\right)\ln n\right) \\ &\geq -n\phi(d) - n^{1/3+(4\ln 2)/(3\ln(d-1))+o(1)}.\end{aligned}$$

3.2 General Graphs

The notation (v, w) refers to an ordered pair of vertices.

Theorem 4. *The determinant of the Kirchhoff matrix of a graph G is at most $\prod_{v\in G}(d_v+1)\prod_{(v,w)\in E(G)}\exp\left(-1/(2(d_v+1)(d_w+1))\right)$.*

Proof: Let Δ be the diagonal matrix indexed by the vertices of G and whose diagonal consists of the degrees of the vertices. Since $K(G) = (\Delta+I)-A$, we have $\det K(G) = \det(\Delta+I)\det(I-M)$, where $M = (\Delta+I)^{-1}A$. To prove the theorem, we need to show that $\det(I-M) \leq \prod_{(v,w)\in E(G)}\exp\left(-1/2(d_v+1)(d_w+1)\right)$.

In order to bound $\det(I-M)$ we introduce the function $h(z) = \det(I-zM)$; of course $h(1) = \det(I-M)$. As before, we have

$$\frac{-zh'(z)}{h(z)} = \sum_{l\geq 1}\mathrm{tr}(M^l)z^l. \tag{4}$$

Observing that $\mathrm{tr}(M) = 0$, we lower bound this expression by $\mathrm{tr}(M^2)z^2$. The largest eigenvalue of M is less than one in norm since the sum of the absolute values of the entries in each row is less than one. (Specifically, the sum is $d_v/(d_v+1)$ in the row corresponding to vertex v). Therefore, the radius of convergence of the generating function in Eq. 4 is greater than one. Hence, for $0 \leq z \leq 1$, we have $-h'(z)/h(z) \geq \mathrm{tr}(M^2)z$, and so by integration of h'/h from 0 to 1, we find that $h(1) \leq \exp(-\mathrm{tr}(M^2)/2)$. But $h(1) = \det(I-M)$; and by inspecting M we see that

$$\mathrm{tr}(M^2) = \sum_{(v,w)\in E(G)}\frac{1}{(d_v+1)(d_w+1)}.$$

□

By imitating the proof of Theorem 2, it is possible to get a bound on the determinant of the Kirchhoff matrix in terms of the maximum degree and the degree of each node. However, this bound is too complicated to merit inclusion here. It coincides with the bound given by Theorem 2 when the graph is regular, but it is incomparable with the bound given by Theorem 4 in general.

4 Bounds on the Chromatic Polynomial at Negative Values

In this section we bound χ_G from above and below along the negative real axis. The results of this section are stated most naturally in terms of the function $\bar{\chi}_G(w) = (-1)^n \chi_G(-w)$ (where χ_G is the chromatic polynomial of G), which we therefore study along the positive real axis. Note in particular that $\bar{\chi}_G(1) = \alpha(G)$.

4.1 Upper Bound on $\bar{\chi}_G$

The matrix-tree theorem extends to the case in which edges are assigned arbitrary weights. If, in the construction of section 2, we assign weight w (rather than 1) to all the edges incident to the new vertex u, we find that the coefficient of w^{n-j} in the polynomial $\det(Q + wI)$ is equal to the number of rooted spanning forests of G with j edges. It is known that the coefficient of w^{n-j} in $\bar{\chi}_G(w)$ is equal to the number of j-edge subgraphs which contain no "broken circuits"; the latter is a condition which, in particular, implies that the subgraphs are forests [5, page 69]. Hence for nonnegative w, all the terms of $\det(Q+wI)$ and $\bar{\chi}_G(w)$ are nonnegative, and each term in $\det(Q + wI)$ is at least as large as the corresponding term in $\bar{\chi}_G(w)$. Therefore we have the following extension of Theorem 1:

Theorem 5. *For all $w \geq 0$, $\bar{\chi}_G(w) \leq \det(Q + wI)$.*

□

There are two sources of slack in each of the inequalities on the coefficients, which give rise to the above theorem. The first is that the coefficient in the chromatic polynomial enumerates only certain kinds of j-edge forests; the second is that it enumerates unrooted forests, whereas $\det(Q + wI)$ enumerates rooted forests. The latter consideration introduces a factor of at least $j + 1$ (typically more) into the coefficient inequality. In particular a sharper inequality on $\bar{\chi}_G(w)$ is $\bar{\chi}_G(w) \leq \sum a_j w^j$, where a_j is the number of j-edge spanning forests of G.

No effective expression is known for the $\{a_j\}$. In fact, calculating their sum is #P-complete, since the number of spanning forests in a graph is equal to the value of the Tutte polynomial at the point $(2,1)$, which is not one of the special points mentioned in the introduction. (In the case of the complete graph Takács has given an exact expression for the number of spanning forests [21].) However these numbers do have the following interesting interpretation:

For each acyclic orientation σ of G, define $h(\sigma) = (h(v_1), h(v_2), \ldots, h(v_n))$, where the v_i's are the vertices of G and $h(v_i)$ is the outdegree of vertex v_i. Let P be the convex hull in $\mathcal{R}^n$ of the vectors $h(\sigma)$, where σ ranges over the acyclic orientations of G. The number of spanning forests of G is the number of integer points in P. More generally [19, Exercise 4.32], the number of spanning forests with j edges is the coefficient of w^j in the Ehrhart polynomial $i(P, w)$.

The inequality noted above can therefore be expressed as $\bar{\chi}_G(w) \leq i(P, w)$.

Recently, Annan [4] gave a fully polynomial randomised approximation scheme for calculating the number of forests in a dense graph.

4.2 Lower Bound on $\bar{\chi}_G$

We begin by showing a new, simpler proof of the lower bound of [9] for the number of acyclic orientations in a graph. Then we show how an extension of this proof technique bounds $\bar{\chi}_G$ from below anywhere on the positive real axis.

Let G be an arbitrary graph; let $f(x) = (x!)^{1/x}$ (as defined previously). We use the following lemma, implicit in [9].

Lemma 3. *Let an acyclic orientation of a graph G be given, and for each vertex v let $\delta(v)$ denote the out-degree of vertex v. Then $\alpha(G) \geq \prod_{i=1}^{n}(\delta(v_i) + 1)$.* □

Theorem 6 ([9]) $\alpha(G) \geq \prod_{v \in G} f(d_v + 1)$.

Proof: If a permutation of the vertices of G is chosen uniformly at random among all permutations, and the acyclic orientation on G is induced from this permutation, then for each vertex v, $\delta(v)$ is uniformly distributed in the set $\{0, 1, \ldots, d_v\}$. Therefore,

$$\begin{aligned}
\mathrm{E}\left[\ln\left(\prod_{v \in G}(\delta(v) + 1)\right)\right] &= \sum_{v \in G} \mathrm{E}\left[\ln(\delta(v) + 1)\right] \\
&= \sum_{v \in G} \frac{1}{d_v + 1} \sum_{j=0}^{d_v} \ln(j + 1)
\end{aligned}$$

$$
\begin{aligned}
&= \sum_{v \in G} \ln(f(d_v+1)) \\
&= \ln\left(\prod_{v \in G} f(d_v+1)\right)
\end{aligned}
$$

Hence there exists an acyclic orientation for which $\prod_{v \in G}(\delta(v)+1) \geq \prod_{v \in G} f(d_v+1)$. $\square$

We now extend this proof to $\bar{\chi}_G$. For arbitrary $x > 0$ and nonnegative integer k, let $F(x,k) = (x \cdot (x+1) \cdots (x+k-1))^{1/k}$.

Theorem 7. *For all $w > 0$, $\bar{\chi}_G(w) \geq \prod_{v \in G} F(w, d_v+1)$.*

Proof: Let v be a vertex of G, and let (v,w) be an edge of G. By $G - v$ we denote the graph remaining after v and all incident edges have been deleted; by $G - (v,w)$ we denote the graph remaining after the edge (v,w) has been deleted; and by $G/(v,w)$ we denote the contraction of G by (v,w), i.e. the graph in which v and w have been identified into a single vertex whose neighborhood is the union of their neighborhoods in G.

Our proof relies upon the following:

Lemma 4. *For all $w \geq 0$, $\bar{\chi}_G(w) \geq (d_v + w)\bar{\chi}_{G-v}(w)$.*

Proof: For any edge e in G, $\bar{\chi}_G$ satisfies the contraction-deletion identity [20]

$$\bar{\chi}_G = \bar{\chi}_{G/e} + \bar{\chi}_{G-e}. \tag{5}$$

If $e_1, \ldots, e_{d_v}$ are the edges incident to vertex v, then we can expand this identity to obtain

$$
\begin{aligned}
\bar{\chi}_G = \bar{\chi}_{G/e_1} + \bar{\chi}_{(G-e_1)/e_2} + \bar{\chi}_{(G-e_1-e_2)/e_3} + \cdots + \bar{\chi}_{(G-e_1-e_2-\cdots-e_{d_v-1})/e_{d_v}} \\
+ \bar{\chi}_{G-e_1-e_2-\cdots-e_{d_v}}.
\end{aligned} \tag{6}
$$

Now we make two observations. First, if u is an isolated vertex of a graph H, then $\bar{\chi}_H = w\bar{\chi}_{H-u}$. Hence in particular for the last term of (6) we have $\bar{\chi}_{G-e_1-e_2-\cdots-e_{d_v}} = w\bar{\chi}_{G-v}$.

Second, $\bar{\chi}_G$ is, for positive w, monotone in the edges of the graph. (This can for instance be seen from the identity (5) and from the positivity of $\bar{\chi}_G$ for positive w.) Therefore each of the terms $\bar{\chi}_{G/e_1}, \bar{\chi}_{(G-e_1)/e_2}, \ldots, \bar{\chi}_{(G-e_1-e_2-\cdots-e_{d_v-1})/e_{d_v}}$ in (6) is at least as great as $\bar{\chi}_{G-v}$.

Combining these observations we find that $\bar{\chi}_G \geq (d_v + w)\bar{\chi}_{G-v}$. $\square$

As a result, if an acyclic orientation of the vertices of G is given and the $\{\delta(v)\}$ are as defined above, then $\bar{\chi}_G(w) \geq \prod_v(\delta(v)+w)$. The remainder of the proof now proceeds just as for the case of acyclic orientations, by considering the expectation of $\ln \prod_v(\delta(v) + w)$ over uniformly selected permutations of the vertices. $\square$

Note that both the upper and lower bounds on $\bar{\chi}_G(w)$ given in theorems 5 and 7 are asymptotic to w^n as w goes to infinity.

5 Improved Lower Bound for degree 3, girth ≥ 5

We show that in certain cases it is possible to improve the lower bound on the chromatic polynomial of a graph along the negative real axis (and in particular, the number of acyclic orientations), by modifying the probabilistic argument given in the previous section.

In a complete graph the analysis of that argument is tight, and there is no variation in the random variable $\sum_v \ln(\delta(v) + 1)$ used to lower bound $\alpha(G)$ (or more generally in the random variable $\sum_v \ln(\delta(v) + w)$ used to lower bound $\bar{\chi}_G$); but in other graphs there will be some variation and the inequality based on the expectation of this variable, will be strict. Hence under suitable assumptions on G, improvement in the bound can be sought. In this section we show how the absence of small cycles in the graph is enough to provide a stronger lower bound. Unfortunately the improvement provided by this method degrades for large degree graphs, so we restrict ourselves to describing the method for degree 3 graphs, where the improvement is substantial.

If, given a graph, we could exhibit the existence of an acyclic orientation in which many of its vertices had approximately balanced in-degrees and out-degrees, then using lemma 3 we could demonstrate a strong lower bound on $\bar{\chi}_G$ and on the number of acyclic orientations of the graph. In general however we do not know how to do this, and instead describe a method of sampling acyclic orientations, which tends to produce orientations with more balanced in-degrees and out-degrees, than result from the straightforward method of section 4.2 in which we sampled uniformly among linear orders. However, for large d, the girth assumption by itself will not yield a lower bound on the number of acyclic orientations substantially better than the one in subsection 4.2 (using the outdegrees approach). Indeed, it is easy to show (see, e.g., [2, page 122]) that, if the second largest eigenvalue of a d-regular graph is much smaller than d, in every acyclic orientation of the graph the outdegrees will be essentially uniformly distributed between 0 and d. In the case of non-bipartite d-regular Ramanujan graphs, for example, $\prod_{v\in G}(\delta_v+1) = ((d+o(d))/e)^n$, for any acyclic orientation.

Theorem 8. *Let G be a 3-regular graph G on n vertices, without 3-cycles or 4-cycles (i.e. of girth ≥ 5). Let $w \geq 0$. Then*

$$\bar{\chi}_G(w) \geq (w^{1/8}(w+1)^{3/8}(w+2)^{3/8}(w+3)^{1/8})^n.$$

In particular

$$\alpha(G) \geq (2^{3/8}3^{3/8}4^{1/8})^n \cong 2.328^n$$

In comparison the lower bound of section 4.2 is $\alpha(G) \geq (2^{1/4}3^{1/4}4^{1/4})^n \cong 2.213^n$.

Proof: Denote the neighbors of v by v_1, v_2, v_3; and denote the remaining neighbors of v_1 by $v_{1,1}, v_{1,2}$, the remaining neighbors of v_2 by $v_{2,1}, v_{2,2}$, and the remaining neighbors of v_3 by $v_{3,1}, v_{3,2}$.

At each vertex v select a random variable x_v independently, uniformly in $[-1,1]$. Let $y_u = x_u + \sum_{(w,u)\in E(G)} x_w/2$. The values $\{y_u\}$ induce an order on the vertices of G. (Observe that if we used the values $\{x_u\}$ to induce the order, then the distribution on orders would be uniform, as in section 4.2.) Now

$$y_v > y_{v_1} \iff x_v + x_{v_2} + x_{v_3} - x_{v_1} - x_{v_{1,1}} - x_{v_{1,2}} > 0$$

$$y_v > y_{v_2} \iff x_v + x_{v_1} + x_{v_3} - x_{v_2} - x_{v_{2,1}} - x_{v_{2,2}} > 0$$

$$y_v > y_{v_3} \iff x_v + x_{v_1} + x_{v_2} - x_{v_3} - x_{v_{3,1}} - x_{v_{3,2}} > 0$$

Observe by symmetry that $P(y_v > y_{v_1}) = P(y_v > y_{v_2}) = P(y_v > y_{v_3}) = 1/2$. Further, by symmetry:

(a) The probabilities $P(y_v > y_{v_1}, y_{v_2}, y_{v_3})$ and $P(y_v < y_{v_1}, y_{v_2}, y_{v_3})$ are equal. Denote this quantity a.

(b) All of the probabilities $P(y_{v_i} > y_v > y_{v_j}, y_{v_k})$ and $P(y_{v_i}, y_{v_j} > y_v > y_{v_k})$ (for i, j, k ranging over all permutations of $1, 2, 3$) are equal. Denote this quantity b.

Therefore $2a + 6b = 1$.

Note that $P(y_v > y_{v_2}, y_{v_3}) = a + b$, while $P(y_{v_2} > y_v > y_{v_3}) = 2b$. We will exhibit an isometry of the portion of the sample space corresponding to the event $y_v > y_{v_2}, y_{v_3}$, with the portion corresponding to the event $y_{v_2} > y_v > y_{v_3}$; it will then follow that $a = b$, and consequently that $a = b = 1/8$.

Thus, in fact, the events $\{y_v > y_{v_i}\}_i$ are independent. (Locally, as if the process oriented the edges of the graph independently at random.)

The isometry is given by the following "signed permutation" map from the variables $x_v, ..., x_{v_{3,2}}$ to the variables $x'_v, ..., x'_{v_{3,2}}$:

$$\begin{array}{rcl} x'_v & = & x_{v_2} \\ x'_{v_1} & = & -x_{v_3} \\ x'_{v_2} & = & x_v \\ x'_{v_3} & = & -x_{v_1} \\ x'_{v_{1,1}} & = & x_{v_{1,1}} \\ x'_{v_{1,2}} & = & x_{v_{1,2}} \\ x'_{v_{2,1}} & = & -x_{v_{2,1}} \\ x'_{v_{2,2}} & = & -x_{v_{2,2}} \\ x'_{v_{3,1}} & = & x_{v_{3,1}} \\ x'_{v_{3,2}} & = & x_{v_{3,2}} \end{array}$$

It is readily verified that this map is an isometry of the sample space regions described.

Hence:

$$P(\mathrm{rank}(y_v) \in \{y_v, y_{v_1}, y_{v_2}, y_{v_3}\} = 1) = 1/8$$

$$P(\mathrm{rank}(y_v) \in \{y_v, y_{v_1}, y_{v_2}, y_{v_3}\} = 2) = 3/8$$

$$P(\mathrm{rank}(y_v) \in \{y_v, y_{v_1}, y_{v_2}, y_{v_3}\} = 3) = 3/8$$

$$P(\mathrm{rank}(y_v) \in \{y_v, y_{v_1}, y_{v_2}, y_{v_3}\} = 4) = 1/8$$

The theorem now follows by substituting these probabilities in place of $1/4 = 1/(d_v + 1)$ in the proof of section 4.2. □

6 Concluding remarks

1. An upper bound on the determinant of the Kirchhoff matrix can be computed directly for some graphs. For example, the determinant of the

Kirchhoff matrix of the d-dimensional hypercube [12] is at most $(d+1)^{2^d}\exp\left(-2^d\left(\frac{1}{2d}-\frac{1}{4d^2}+O(d^{-3})\right)\right)$. This bound beats the one given in Theorem 2. This is due to the fact that the hypercube has many cycles of length 4, which implies that $\mathrm{tr}(A^l) > \rho(l)$ for even l greater than or equal to 4. However, since the number of spanning trees of any connected d-regular graph on n vertices [1] is at least $(d-o(d))^n$, the same lower bound holds on the determinant of the Kirchhoff matrix of any d-regular graph on n vertices. Thus, our approach will not yield an upper bound on the number of acyclic orientations much better than the degree bound, for any regular graph with large degree.

2. For a d-regular graph, the lower bound provided by Lemma 3 never exceeds $(d/2+1)^n$. This is because the average value of the outdegrees is $d/2$. By choosing a particular acyclic orientation of the d-dimensional hypercube, it can be shown [12] that the number of acyclic orientations of the d-dimensional hypercube is at least $(d/2+3/4+O(d^{-1}))^{2^d}$. Similarly, for even d, the number of acyclic orientations of the Cayley graph of Z_n with respect to the generators $\{1,-1,2,-2,\ldots,d/2,-d/2\}$ is at least $(d/2+1)^{n-d/2}$. Using a different approach, it can be shown [3] that the number of acyclic orientations of a d-regular complete bipartite graph is at least $(d/(e\ln 2)+O(\ln d))^{2d}$, with $e\ln 2 = 1.88\ldots$. By considering the union of such graphs, it follows that for any integer $d \geq 3$, there exists a family of d-regular graphs on n vertices having at least $(d/1.88\ldots+O(\ln d))^n$ acyclic orientations. Whether there exist d-regular graphs having at least $(d-o(d))^n$ acyclic orientations, for large d and large n, is an open question.

Acknowledgements

Thanks to N. Linial and R. Stanley for helpful consultations, and to N. Alon and an anonymous referee for several suggestions that improved the paper.

References

[1] N. Alon, The number of spanning trees in regular graphs, Random Structures & Algorithms **1** (1990), no. 2, 175–181.

[2] N. Alon and J. H. Spencer, The Probabilistic Method, Wiley Verlag, 1991.

[3] N. Alon and N. Kahale, personal communication, August 1993.

[4] J. D. Annan, *A randomized approximation algorithm for counting the number of forests in dense graphs*, Combinatorics, Probability and Computing **3** (1994), no. 3, 273–283.

[5] N. Biggs, Algebraic Graph Theory, Cambridge University Press, 1974.

[6] J. A. Bondy and U. S. R. Murty, Graph Theory and Applications, American Elsevier, 1976.

[7] H. Chernoff, "A measure for asymptotatic efficiency of tests of a hypothesis based on the sum of observations," Ann. Math. Statist. **23** (1952), 493–507.

[8] P. Erdös and H. Sachs, *Regulare Graphe gegebener Taillenweite mit minimaler Knotenzahl*, Wiss. Z. Univ. Halle-Wittenberg, Math.-Nat. **12** (1963), no. 3, 251–258.

[9] W. Goddard, C. Kenyon, V. King and L. J. Schulman, *Optimal Randomized Algorithms for Local Sorting and Set-Maxima*, SIAM J. Computing **22** (1993), no. 2, 272–283. Also in "Optimal Randomized Algorithms for Local Sorting and Set-Maxima," W. Goddard, V. King and L. Schulman, Proc. Twenty Second Annual ACM Symp. on Theory of Computing (1990), 45–53.

[10] F. Jaeger, D. L. Vertigan and D. J. A. Welsh, On the Computational Complexity of the Jones and Tutte Polynomials, Proceedings of the Cambridge Philosophical Society, vol. 108 (1990), 35–53.

[11] R. Graham, F. Yao, and A. Yao, "Information Bounds are Weak in the Shortest Distance Problem", J. ACM 27 (1980), 428–444.

[12] N. Kahale. *Expander Graphs.* PhD thesis, Massachusetts Institute of Technology, September 1993. MIT Laboratory for Computer Science, Technical Report MIT/LCS/TR-591.

[13] N. Linial, Hard enumeration problems in geometry and combinatorics, SIAM J. on Algebraic and Discrete Methods, 7 (1986), 331–335.

[14] A. Lubotzky, R. Phillips, and P. Sarnak, *Ramanujan graphs*, Combinatorica **8** (1988), no. 3, 261–277.

[15] M. Marcus and H. Minc, A Survey of Matrix Theory and Matrix Inequalities, Prindle Weber and Schmidt 1964, Dover 1992, §II.4.1.7 114.

[16] G. A. Margulis, *Explicit group-theoretical constructions of combinatorial schemes and their applications to the design of expanders and concentrators*, Problemy Peredači Informacii **24** (1988), no. 1, 51–60.

[17] B. D. McKay, *Spanning trees in regular graphs*, Euro. J. Combinatorics **4** (1983), 149–160.

[18] U. Manber and M. Tompa, *The Effect of Number of Hamiltonian Paths on the Complexity of a Vertex-Coloring Problem*, SIAM J. Comp. **13** (1984), 109–115.

[19] R. P. Stanley. Enumerative Combinatorics, Wadsworth & Brooks/Cole, 1986.

[20] R. P. Stanley, *Acyclic Orientations of Graphs*, Discrete Mathematics **5** (1973), 171–178.

[21] L. Takács, On the Number of Distinct Forests, SIAM J. Disc. Math, Vol. 3 No. 4, Nov. 1990, 574-581.

[22] J. S. Vitter and P. Flajolet, Handbook of Theoretical Computer Science, Vol. A: Algorithms and Complexity, MIT press (edited by J. Van Leeuwen), 1990, 433–524.