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Algebraic methods for chromatic polynomials

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This work is dedicated to Jaap Seidel who made many contributions to algebraic combinatorics. Like many of us, he was happiest when the key to a problem turned out to be a matrix, whose eigenvalues and multiplicities had to be found. Although he never worked on chromatic polynomials, we think he would have liked the algebra described below.

Abstract

In this paper we discuss the chromatic polynomial of a 'bracelet', when the base graph is a complete graph K_b and arbitrary links L between the consecutive copies are allowed. If there are n copies of the base graph the resulting graph will be denoted by $L_n(b)$. We show that the chromatic polynomial of $L_n(b)$ can be written in the form

$$P(L_n(b); k) = \sum_{\ell=0}^{b} \sum_{\pi \vdash \ell} m_\pi(k) \mathrm{tr}\,(N_L^\pi)^n.$$

Here the notation $\pi \vdash \ell$ means that π is a partition of ℓ, and $m_\pi(k)$ is a polynomial that does not depend on L. The square matrix N_L^π has size $\binom{b}{\ell} n_\pi$, where n_π is the degree of the representation R^π of Sym_ℓ associated with π.

We derive an explicit formula for $m_\pi(k)$ and describe a method for calculating the matrices N_L^π. Examples are given. Finally, we discuss the application of these results to the problem of locating the chromatic zeros.

1. Introduction

The chromatic polynomials considered in this paper are associated with graphs, which we call *bracelets*, constructed in the following way. Take n copies of a *base graph*, and join certain vertices in the ith copy to certain vertices in the $(i+1)$th copy, the joins being the same for each i, and $n+1 = 1$ by convention. Although this may appear to be a rather special construction, it does have important applications. That is because the partition functions of models studied by theoretical physicists are analogues of the

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chromatic polynomial, and their models are based on infinite graphs with a lattice-like structure. Our bracelets can be regarded as finite approximations to such graphs, and by considering the behaviour as n tends to infinity we can obtain useful insights into physical phenomena. An additional bonus is the fact that the explicit formulae obtained here are well-adapted to the methods of complex function theory, so that results about the locations of the zeros of the polynomials can be deduced.

A relatively simple case occurs when we take the base graph to be the complete graph K_b, and the joins to be the matching in which each vertex in one copy of K_b is joined to the same vertex in the next copy. This gives a bracelet that we denote by $B_n(b)$. The chromatic polynomials of $B_n(2)$ and $B_n(3)$ were first calculated in 1972 [7] and 1999 [8], and the result for $B_n(4)$ has recently been obtained by two different methods [6, 9]. For the sake of illustration, and in order to convince the reader that the problem is not quite trivial, we give in full the formula for the number of k-colourings of $B_n(4)$:

$$\begin{aligned}
&(73 - 84k + 41k^2 - 10k^3 + k^4)^n \\
&\quad + (k-1)((73 - 50k + 12k^2 - k^3)^n + 3(21 - 22k + 8k^2 - k^3)^n) \\
&\quad + k(k-3)/2((31 - 11k + k^2)^n + 3(11 - 7k + k^2)^n + 2(7 - 5k + k^2)^n) \\
&\quad + (k-1)(k-2)/2(3(21 - 9k + k^2)^n + 3(5 - 5k + k^2)^n) \\
&\quad + k(k-1)(k-5)/6((7-k)^n + 3(3-k)^n) \\
&\quad + (k-1)(k-2)(k-3)/6((1-k)^n + 3(5-k)^n) \\
&\quad + k(k-2)(k-4)/3(3(6-k)^n + 2(4-k)^n + 3(2-k)^n) \\
&\quad + k^4 - 10k^3 + 29k^2 - 24k + 1.
\end{aligned}$$

This formula suggests that the terms occur in 'levels', the terms at level ℓ being of the form

$$(\text{Polynomial of degree } \ell) \times (\text{Integer})(\text{Polynomial of degree } b - \ell)^n,$$

where $b = 4$ in this example. The main result of [6] is that, for all b, the terms at level ℓ correspond to the partitions π of ℓ. Specifically, the representation R^π of Sym_ℓ associated with π gives rise to a matrix N^π with the following property: each 'polynomial of degree $b - \ell$' is an eigenvalue of N^π and the associated 'integer' is its multiplicity. For example, when $b = 4$ and $\ell = 3$ the matrix $N^{[21]}$ has eigenvalues $6 - k$, $4 - k$, $2 - k$, with multiplicities 3, 2, 3 respectively. The corresponding terms are visible in the penultimate line of the formula displayed above.

This paper begins (Section 2) with an outline of a theoretical framework that justifies the existence of formulae like the one displayed above. An explicit formula for the 'polynomial of degree ℓ' is obtained in Section 3. These results were suggested by the approach described in [14], although the proofs do not depend on the presentation in that paper. In the rest of the paper we describe techniques for calculating the complete set of polynomials that occur in the formula, using methods based on recent work in a special case [6]. We shall also explain briefly how this framework can be used to study the limiting behaviour of the zeros of chromatic polynomials.

2. The theoretical framework

We consider the situation when the base graph is a complete graph K_b, but arbitrary links between the copies are allowed. The set of links between successive copies of K_b will be denoted by L, a subset of $V \times V$, where $vw \in L$ if and only if the vertex v in one copy is joined to the vertex w in the next copy. The resulting graph will be denoted by $L_n(b)$. Thus the graphs $B_n(b)$ correspond to the choice $L = B = \{11, 22, \ldots, bb\}$.

The following basic result will be proved in this section.

Theorem 1. *The chromatic polynomial of $L_n(b)$ can be written in the form*

$$P(L_n(b); k) = \sum_{\ell=0}^{b} \sum_{\pi \vdash \ell} m_\pi(k) \operatorname{tr}(N_L^\pi)^n. \quad \square$$

Here the notation $\pi \vdash \ell$ means that π is a partition of ℓ, and $m_\pi(k)$ is a polynomial that does not depend on L. The square matrix N_L^π has size $\binom{b}{\ell} n_\pi$, where n_π is the degree of the representation R^π of Sym_ℓ associated with π.

Comparing this formula with the terminology used in the Introduction, we see that $m_\pi(k)$ must be the 'polynomial of degree ℓ'; this will be referred to as a *global multiplicity*. The trace of $(N_L^\pi)^n$ is a sum of the form $\sum \mu_i \lambda_i^n$, where μ_i is the multiplicity of the eigenvalue λ_i of N_L^π, so μ_i must be the 'integer': this will be referred to as a *local multiplicity*. It is worth noting that only in favourable cases will each individual λ_i be a 'polynomial of degree $b - \ell$', although the situation can be rescued by collecting algebraically conjugate sets of eigenvalues.

Let the vertex-set of K_b be $V = \{1, 2, \ldots, b\}$. For all $k \geq b$ let $\Gamma_k(b)$ denote the set of k-colourings of K_b (that is, injections from V to $\{1, 2, \ldots, k\}$) and let $\mathcal{V}_k$ be the vector space of complex-valued functions defined on $\Gamma_k(b)$. The canonical basis for $\mathcal{V}_k$ is the set of functions $[\alpha]$ ($\alpha \in \Gamma_k(b)$) such that $[\alpha](\beta) = 1$ if $\beta = \alpha$, and 0 otherwise.

Two colourings $\alpha, \beta \in \Gamma_k(b)$ are said to be *compatible* with a given linking set L if $\alpha(v) \neq \beta(w)$ whenever $vw \in L$. The *compatibility operator* $T = T_L(k)$ is defined (with respect to the canonical basis of $\mathcal{V}_k$) by the matrix whose entries are

$$T_{\alpha\beta} = \begin{cases} 1 & \text{if } \alpha \text{ and } \beta \text{ are compatible with } L; \\ 0 & \text{otherwise.} \end{cases}$$

It follows from a simple argument [2] that $P(L_n(b); k)$, the number of k-colourings of $L_n(b)$, is equal to the trace of $T_L(k)^n$.

The elements of the set $\Gamma_k(b)$ are just ordered b-tuples of distinct elements of the set of colours, and the symmetric group Sym_k acts in the obvious way on this set. In other words $\mathcal{V}_k$ is a $\mathbb{C}\mathrm{Sym}_k$-module, the action S being defined by

$$S(\omega)[\alpha] = [\omega\alpha] \qquad (\omega \in \mathrm{Sym}_k).$$

Clearly, if α and β are compatible with L, then so are $\omega\alpha$ and $\omega\beta$, so that

$$T_L(k)S(\omega) = S(\omega)T_L(k) \qquad \text{for all } \omega \in \mathrm{Sym}_k.$$

This means that $T_L(k)$ belongs to the centralizer algebra of S, for any linking set L.

The decomposition of S can be deduced from the standard works on representations of the symmetric group [13, Sections 4 and 14]. The irreducible submodules of S are in bijective correspondence with the partitions τ of k that satisfy $\tau \succ \gamma_{k,b}$, where the relation $\succ$ is the dominance order, and $\gamma_{k,b}$ is the partition $(k-b, 1^b)$. The condition $\tau \succ \gamma_{k,b}$ means that, for some ℓ, $(0 \le \ell \le b)$, τ is a partition in which the largest part is $k-\ell$ and the remaining parts form a partition π of ℓ. The degree (that is, dimension) of the corresponding submodule is equal to the number n_τ of standard tableaux of shape τ, and its multiplicity is equal to $\binom{b}{\ell} n_\pi$.

For our purposes it is convenient to reverse the correspondence between τ and its 'truncation' π. Given π such that $\pi \vdash \ell$ and $\ell \le b \le k$, let the parts be $\pi_1 \ge \pi_2 \ge \cdots \ge \pi_\ell$, where all the terms except π_1 can be zero. Then we define π^k to be the corresponding τ, that is the partition of k with parts $k-\ell \ge \pi_1 \ge \pi_2 \ge \cdots \ge \pi_\ell$, and write $m_\pi(k)$ instead of n_{π^k}.

Since $T_L(k)$ centralizes S, its action on $\mathcal{V}_k$ decomposes in the same way as that of S, with the degree and multiplicity interchanged (see, for example, [12]). Thus $T_L(k)$ can be represented by a matrix in which there is a diagonal block for each pair (π, ℓ) with $\pi \vdash \ell \le b$, this block consisting of $m_\pi(k)$ matrices N_L^π of size $\binom{b}{\ell} n_\pi$. It follows that

$$P(L_n(b); k) = \operatorname{tr}(T_L(k))^n = \sum_{\ell=0}^{b} \sum_{\pi \vdash \ell} m_\pi(k) \operatorname{tr}(N_L^\pi)^n.$$

This completes the proof of Theorem 1.

3. A formula for the global multiplicities

For a given partition π of ℓ, there is a strictly decreasing partition σ of $\frac{1}{2}\ell(\ell+1)$, with ℓ non-zero parts given by $\sigma_i = \pi_i + \ell - i \quad (1 \le i \le \ell)$. Let

$$x_i = \frac{\sigma_i!}{\prod_{j>i}(\sigma_i - \sigma_j)}, \qquad g_\pi = x_1 x_2 \ldots x_\ell.$$

It is a standard result [13] that g_π is a divisor of $\ell!$, the quotient being the number of standard tableaux associated with π, which is also the degree n_π of the irreducible representation R^π.

Theorem 2. *If $\pi \vdash \ell$, the global multiplicity $m_\pi(k)$ is given by the formula*

$$m_\pi(k) = g_\pi^{-1}(k-\sigma_1)(k-\sigma_2)\cdots(k-\sigma_\ell).$$

Proof. According to the theory described in Section 2, the global multiplicity $m_\pi(k)$ is the number of standard tableaux associated with the augmented partition π^k of k, which has parts $k-\ell \ge \pi_1 \ge \pi_2 \ge \cdots \ge \pi_\ell$. For this partition, denote by σ^* the associated strictly decreasing partition of $1/2k(k+1)$ with k parts, and let

$$y_i = \frac{\sigma_i^*!}{\prod_{j>i}(\sigma_i^* - \sigma_j^*)}, \qquad g_{\sigma^*} = y_1 y_2 \ldots y_k,$$

so that the required number is $k!/g_{\sigma^*}$. It is easy to check by elementary algebra that

$$y_1 = \frac{k!}{(k-\sigma_1)(k-\sigma_2)\cdots(k-\sigma_\ell)};$$
$$y_i = x_{i-1} \qquad (2 \le i \le \ell+1); \qquad y_i = 1 \qquad (\ell+2 \le i \le k).$$

Thus

$$\frac{k!}{g_{\sigma^*}} = \frac{k!}{y_1 y_2 \ldots y_k} = \frac{(k-\sigma_1)(k-\sigma_2)\cdots(k-\sigma_\ell)}{x_1 x_2 \cdots x_\ell}$$
$$= \frac{1}{g_\pi}(k-\sigma_1)(k-\sigma_2)\cdots(k-\sigma_\ell). \quad \square$$

For the partitions $[\ell]$ and $[1^\ell]$, associated with the principal and alternating representations of Sym_ℓ, the formula gives

$$m_{\mathrm{pri}}(k) = m_{[\ell]}(k) = \binom{k}{\ell} - \binom{k}{\ell-1}, \qquad m_{\mathrm{alt}}(k) = m_{[1^\ell]}(k) = \binom{k-1}{\ell}.$$

4. The sieve principle

The practical problem of finding the constituent matrices N_L^π can be solved by a method based on the sieve principle. This enables us to define a set of operators $S_M(k)$, such that each $T_L(k)$ can be expressed as a linear combination of the $S_M(k)$. These operators are related to a method based on coherent algebras [14], and there are also links with the theory of Temperley–Lieb algebras [11].

Our method involves a new basis for $\mathcal{V}_k$, defined in the following way. Let P be a subset of V and let θ be a k-colouring of the subgraph of K_b induced by P. For any $\alpha \in \Gamma_k(b)$, denote by α_P the restriction of α to P. We define $[P \mid \theta]$ to be the element of $\mathcal{V}_k$ given by

$$[P \mid \theta] = \sum_{\alpha_P = \theta} [\alpha].$$

In other words, $[P \mid \theta]$ is the function that takes the value 1 on the colourings that agree with θ on P, and 0 otherwise. The *weight* of $[P \mid \theta]$ is defined to be $|\theta(P)|$ (trivially this is equal to $|P|$ when the base graph is complete).

Let $M \subseteq V \times V$ be a *matching*: equivalently, M is a triple (M_1, M_2, μ) with $M_1 \subseteq V$, $M_2 \subseteq V$ and $\mu : M_1 \to M_2$ a bijection. Define $S_M(k) : \mathcal{V}_k \to \mathcal{V}_k$ by the rule

$$S_M(k)[\alpha] = [M_2 \mid \alpha\mu^{-1}].$$

Given any linking set $L \subseteq V \times V$, consider the bipartite graph formed by two copies of V, with edges defined by L, and let $\mathcal{M}(L)$ denote the set of matchings in this graph. In other words, the matching M is in $\mathcal{M}(L)$ if M is a subset of L.

The following theorem is a generalization of the result proved in [4] and used in [6].

Theorem 3. *Suppose that b, k, and L are given, and let $T_L(k)$ be the associated compatibility operator. Then*

$$T_L(k) = \sum_{M \in \mathcal{M}(L)} (-1)^{|M|} S_M(k).$$

Proof. For any $\alpha,\ \beta \in \Gamma_k(b)$ we shall show that

$$T_L(k)[\alpha](\beta) = \sum_{M \in \mathcal{M}(L)} (-1)^{|M|} S_M(k)[\alpha](\beta).$$

By definition $[M_2 \mid \alpha\mu^{-1}](\beta) = 1$, if and only if $\alpha\mu^{-1} = \beta_{M_2}$ for any $M \in \mathcal{M}(L)$. Let

$$W(\beta) = \{w \in V \mid \beta(w) = \alpha(v) \text{ for some } v \text{ such that } (v, w) \in L\}.$$

Then, $M_2 \not\subseteq W(\beta)$ implies $[M_2 \mid \alpha\mu^{-1}](\beta) = 0$. On the other hand, suppose that $M_2 \subseteq W(\beta)$. Then the condition $\alpha\mu^{-1} = \beta_{M_2}$ implies that there exists a unique $M \in \mathcal{M}(L)$ such that $[M_2 \mid \alpha\mu^{-1}](\beta) = 1$. Let

$$\mathcal{M}^\beta(L) = \{M \in \mathcal{M}(L) \mid [M_2 \mid \alpha\mu^{-1}](\beta) = 1\};$$

then for every $M_2 \subseteq W(\beta)$ there exists exactly one $M = (M_1, M_2, \mu) \in \mathcal{M}^\beta(L)$ and

$$\sum_{M \in \mathcal{M}(L)} (-1)^{|M|} S_M(k)[\alpha](\beta) = \sum_{M \in \mathcal{M}^\beta(L)} (-1)^{|M|}.$$

If (α, β) is compatible with L, $W(\beta)$ is empty. So $\mathcal{M}^\beta(L)$ has just one term, corresponding to $M_2 = \emptyset$, and the result is 1. On the other hand, if (α, β) is not compatible with L, $W(\beta)$ is not empty and the sum is $(1 + (-1))^{|W(\beta)|} = 0$. The result follows. $\square$

5. The constituent matrices

Theorem 3 says that the effect of T_L on a typical element $[P \mid \theta]$ is given by

$$T_L[P \mid \theta] = \sum_{M \in \mathcal{M}(L)} (-1)^{|M|} S_M[P \mid \theta].$$

Further analysis (similar to that used in [6]) leads to the following results.

Theorem 4. *For any matching M, $S_M[P \mid \theta]$ can be written as a linear combination of terms $[Q \mid \phi]$ with $\phi(Q) \subseteq \theta(P)$. Consequently, if we fix a set of colours C, the set of all $[P \mid \theta]$ with $\theta(P) \subseteq C$ spans a subspace $\mathcal{U}(C)$ of $\mathcal{V}_k$ that is invariant under every S_M, and thus invariant under T_L.* $\square$

Theorem 5. *Suppose that $\phi(Q) \subseteq \theta(P)$. Then the coefficient of $[Q \mid \phi]$ in $S_M[P \mid \theta]$ is non-zero provided that:*

(i) $\mu(P \cap M_1) \subseteq Q \subseteq M_2$, *and*

(ii) $\theta(v) = \phi(w)$ *whenever* $(v, w) \in (P \times Q) \cap M$.

When these conditions hold the coefficient is

$$(-1)^{|Q|-|P\cap M_1|} f_{|P\cup M_1|}(b, k) \qquad \text{where}$$
$$f_s(b, k) = (k - s)_{b-s} = (k - s)(k - s - 1) \ldots (k - b + 1). \quad \square$$

We proceed to examine the implications of these results. There is no loss of generality in taking $C = \{1, 2, \ldots, \ell\}$. Then we can represent the action of S_M on $\mathcal{U}(C)$ by a matrix $\hat{S}_M$, where the entry

$$(\hat{S}_M)_{[P\,|\,\theta],[Q\,|\,\phi]}$$

is the coefficient of $[Q \mid \phi]$ in $S_M[P \mid \theta]$. By listing the terms $[P \mid \theta]$ in order of their weight $|\theta(P)|$, the matrix $\hat{S}_M$ is partitioned into submatrices $U_{M,r,s}$ defined by the intersection of the rows of weight r with columns of weight s, and these submatrices are zero when $s > r$. We shall focus on the submatrix $U_{M,\ell,\ell}$, since the eigenvalues of this matrix are also eigenvalues of $\hat{S}_M$ and S_M. For the time being ℓ will be fixed and we shall write $U_M = U_{M,\ell,\ell}$.

Given any two ℓ-subsets of V, say P and Q, the rows $[P \mid \theta]$ and the columns $[Q \mid \phi]$ of U_M define a submatrix U_M^{PQ}, of size $\ell! \times \ell!$. A simple change of notation leads to an explicit formula for U_M^{PQ}. Since P is a subset of $V = \{1, 2, \ldots, b\}$ we can write $P = \{p_1, p_2, \ldots, p_\ell\}$, where $p_1 < p_2 < \cdots < p_\ell$, and given the injection $\theta : P \to C$, we can define a permutation σ in Sym_ℓ by

$$\sigma(i) = \theta(p_i) \quad (i = 1, 2, \ldots, \ell).$$

Clearly the correspondence between θ and σ is a bijection, so we can denote $[P \mid \theta]$ by $[P, \sigma]$, and $[Q \mid \phi]$ by $[Q, \tau]$, for suitable $\sigma, \tau \in \mathrm{Sym}_\ell$. Furthermore, we can consider U_M^{PQ} as a matrix whose rows and columns correspond to the members of Sym_ℓ, the entries being

$$(U_M^{PQ})_{\sigma\tau} = (U_M)_{[P,\sigma][Q,\tau]}.$$

If M does not satisfy condition (i) of Theorem 5, U_M^{PQ} is the zero matrix. On the other hand, suppose that condition (i) is satisfied; in particular this means that $|P \cap M_1| = |(P \times Q) \cap M|$. Then, translating condition (ii) into a condition on σ and τ we obtain

$$(U_M^{PQ})_{\sigma\tau} = \begin{cases} (-1)^{\ell - |P \cap M_1|} f_{|P \cup M_1|}(b, k) & \text{if } \sigma(i) = \tau(j) \text{ whenever} \\ & \quad (p_i, q_j) \in (P \times Q) \cap M; \\ 0 & \text{otherwise.} \end{cases}$$

Let $X(\rho)$ be the permutation matrix representing ρ in the regular representation of Sym_ℓ on itself; that is, $X(\rho)_{\sigma\tau}$ is 1 if $\sigma = \tau\rho$ and 0 otherwise. Define

$$F_M^{PQ} = \{\rho \in \mathrm{Sym}_\ell \mid (p_i, q_j) \in (P \times Q) \cap M \Longrightarrow \rho(i) = j\}.$$

Since F_M^{PQ} is a coset of the pointwise stabiliser of a set of size $|P \cap M_1|$, it follows that $|F_M^{PQ}| = (\ell - |P \cap M_1|)!$. The formula for U_M^{PQ} when condition (i) holds can now be written as

$$U_M^{PQ} = (-1)^{\ell - |P \cap M_1|} f_{|P \cup M_1|}(b, k) \sum_{\rho \in F_M^{PQ}} X(\rho).$$

Denote by U_M^π the matrix obtained from U_M when $X(\rho)$ is replaced by $R^\pi(\rho)$. Thus U_M^π is partitioned into blocks $(U_M^\pi)^{PQ}$, of size $n_\pi \times n_\pi$, defined by

$$(U_M^\pi)^{PQ} = \begin{cases} (-1)^{\ell-|P\cap M_1|} f_{|P\cup M_1|}(b,k) \sum_{\rho\in F_M^{PQ}} R^\pi(\rho) & \text{if } \mu(P\cap M_1) \\ & \quad \subseteq Q \subseteq M_2; \\ O & \text{otherwise.} \end{cases}$$

It can be shown that every eigenvector of U_M^π with eigenvalue λ can be lifted to n_π linearly independent eigenvectors of U_M with the same eigenvalue (see [6, Theorem 3]). A simple counting argument now shows that every eigenvalue of U_M is an eigenvalue of some U_M^π.

The constituents of the compatibility matrix T_L can now be defined by the analogue of the formula obtained in Theorem 3:

$$N_L^\pi = \sum_{M\in\mathcal{M}(L)} (-1)^{|M|} U_M^\pi.$$

It will be seen that, for a given b and L, and a given level ℓ, the procedure requires a non-trivial amount of calculation. Fortunately, in some cases explicit formulae can be obtained, and examples are given in the following section. For the sake of orientation, we can deal with the case $\ell = 0$ directly. In this case $\mathcal{U}(\emptyset)$ is the one-dimensional space spanned by the element u that takes the value 1 on every colouring. Simple direct arguments show that $S_M(k)(u) = \kappa_M(k)u$, where $\kappa_M(k)$ is the number of $\beta \in \Gamma_k(b)$ such that $\alpha(v) = \beta(w)$ whenever $(v,w) \in M$. In fact

$$\kappa_M(k) = (k-|M|)_{b-|M|} = f_{|M|}(b,k),$$

which agrees with the general formula given above. Similarly

$$T_L(u) = \sum_{M\in\mathcal{M}(L)} (-1)^{|M|} S_M(k)(u) = \lambda_L(k)u,$$

where $\lambda_L(k) = \sum(-1)^{|M|} f_{|M|}(b,k)$ is the number of β such that α and β are compatible with L. Clearly $\lambda_L(k)$ is the unique eigenvalue at Level 0.

6. The case $b = 3$ with arbitrary links

When $b = 3$ the number of matchings M (as defined in Section 4) with $|M| = 0, 1, 2, 3$ is 1, 9, 18, 6 respectively. In this section we shall determine the matrices $U_M = U_{M,\ell,\ell}$ for all these matchings and all $\ell \leq 3$. The results are sufficient to give the constituents N_L^π of T_L, for any linking set L. Two typical examples will be given.

At level $\ell = 0, 1, 2, 3$ the matrix $U_{M,\ell,\ell}$ has size 1, 3, 6, 6, and the blocks U_M^{PQ} are of size 1, 1, 2, 6. Note that if $|M| < \ell$ the condition $Q \subseteq M_2$ cannot hold, and all the blocks are zero.

Level 0. As explained at the end of Section 5, when $|M| = 0, 1, 2, 3$ respectively U_M is the 1×1 matrix

$$k(k-1)(k-2), \qquad (k-1)(k-2), \qquad (k-2), \qquad 1.$$

There is only the principal representation and hence $U_M^{\mathrm{pri}} = U_M$.

Level 1. Here $U_\emptyset$ is zero. When $|M| \geq 1$, U_M is the 3×3 matrix with entries $(U_M)_{pq} = U_M^{PQ}$, $P = \{p\}$, $Q = \{q\}$. Condition (i) of Theorem 5 becomes

$$q \in M_2 \qquad \text{and} \qquad p \in M_1 \Longrightarrow (p, q) \in M.$$

Condition (ii) is automatically satisfied, so $F_M^{pq} = \mathrm{Sym}_1 = \{id\}$. Thus the matrix U_M is given by

$$(U_M)_{pq} = \begin{cases} (k - |M|)_{3-|M|} & \text{if } q \in M_2, \text{ and } (p, q) \in M; \\ -(k - |M| - 1)_{2-|M|} & \text{if } q \in M_2, \text{ and } p \notin M_1; \\ 0 & \text{if } q \notin M_2 \text{ or } p \in M_1 \text{ and } (p, q) \notin M. \end{cases}$$

As in the previous case we have only the principal representation and hence $U_M^{\mathrm{pri}} = U_M$. For example

$$U_{11}^{\mathrm{pri}} = \begin{pmatrix} (k-1)(k-2) & 0 & 0 \\ -(k-2) & 0 & 0 \\ -(k-2) & 0 & 0 \end{pmatrix}, \qquad U_{11,\,22}^{\mathrm{pri}} = \begin{pmatrix} k-2 & 0 & 0 \\ 0 & k-2 & 0 \\ -1 & -1 & 0 \end{pmatrix},$$

$$U_{11,\,22,\,33}^{\mathrm{pri}} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Level 2. Here U_M is a 6×6 matrix partitioned into blocks U_M^{PQ} of size 2×2. Each block is either the all-zero matrix O, or a multiple of I or $J - I$, where J is the all-one matrix. All blocks are O if $|M| < 2$. Assume $P = \{p_1, p_2\}$ with $p_1 < p_2$ and $Q = \{q_1, q_2\}$ with $q_1 < q_2$. For $|M| \geq 2$ let

$$F_M(P, Q) = \begin{cases} I & \text{if } (p_1, q_1) \in M \text{ or } (p_2, q_2) \in M; \\ J - I & \text{if } (p_1, q_2) \in M \text{ or } (p_2, q_1) \in M. \end{cases}$$

Then the entries of U_M are given by

$$U_M^{PQ} = \begin{cases} (k - |M|)_{3-|M|} \quad F_M(P, Q) & \text{if } Q \subseteq M_2 \text{ and } P \subseteq M_1 \text{ and } \mu(P) = Q; \\ -F_M(P, Q) & \text{if } Q \subseteq M_2 \text{ and } P \nsubseteq M_1; \\ O & \text{if } Q \nsubseteq M_2 \text{ or } P \subseteq M_1 \text{ and } \mu(P) \neq Q. \end{cases}$$

For example

$$U_{11,\,22} = \begin{pmatrix} (k-2)I & O & O \\ -I & O & O \\ -(J-I) & O & O \end{pmatrix}, \qquad U_{11,\,33} = \begin{pmatrix} O & -I & O \\ O & (k-2)I & O \\ O & -I & O \end{pmatrix},$$

$$U_{11,\,22,\,33} = \begin{pmatrix} I & O & O \\ O & I & O \\ O & O & I \end{pmatrix}.$$

Here we have the principal and alternating representation of Sym_2 and the matrices U_M^{pri} and U_M^{alt} are obtained as follows. For U_M^{pri} we replace in U_M the matrices I, $J - I$ and O by 1, 1 and 0. For U_M^{alt} we replace in U_M the matrices I, $J - I$ and O by 1, -1 and 0.

Level 3. The only non-zero cases are when $|M| = 3$. In these cases U_M is a 6×6 matrix with a single block U_M^{PQ}, corresponding to $P = Q = \{123\}$. Condition (i) is automatically satisfied, and it is easy to show that $F_M^{PQ} = \{\mu\}$, so $U_M = X(\mu)$. Thus $U_M^\pi = R^\pi(\mu)$. Here, apart from the principal and alternating representations we have the representation corresponding to the partition [21], and $U_M^{\mathrm{pri}} = 1$, $U_M^{\mathrm{alt}} = \mathrm{sign}(\mu)$, while $U_M^{[21]}$ is a 2×2 matrix.

Example 1. The graphs $B_n(b)$ are obtained when the linking set is $B = \{11, 22, \ldots, bb\}$. The chromatic polynomial of $B_n(3)$ was first calculated in 1999 [8], and many terms for $B_n(b)$ in general are now known [6]. The basic equation is

$$T_B = S_\emptyset - (S_{11} + S_{22} + S_{33}) + (S_{11,\,22} + S_{11,\,33} + S_{22,\,33}) - S_{11,\,22,\,33}$$

from which it follows that

$$N_B^\pi = U_\emptyset^\pi - (U_{11}^\pi + U_{22}^\pi + U_{33}^\pi) + (U_{11,\,22}^\pi + U_{11,\,33}^\pi + U_{22,\,33}^\pi) - U_{11,\,22,\,33}^\pi.$$

At Level 0 we get the 1×1 matrix

$$N_B^{\mathrm{pri}} = k(k-1)(k-2) - 3(k-1)(k-2) + 3(k-2) - 1,$$

and thus the eigenvalue $k^3 - 6k^2 + 14k - 13$. At Level 1 we get the 3×3 matrix

$$N_B^{\mathrm{pri}} = \begin{pmatrix} -k^2+5k-7 & k-3 & k-3 \\ k-3 & -k^2+5k-7 & k-3 \\ k-3 & k-3 & -k^2+5k-7 \end{pmatrix}$$

with eigenvalues $-k^2 + 7k - 13$ and $-k^2 + 4k - 4$ (twice). At Level 2 we get the 3×3 matrices

$$N_B^{\mathrm{pri}} = \begin{pmatrix} k-3 & -1 & -1 \\ -1 & k-3 & -1 \\ -1 & -1 & k-3 \end{pmatrix} \quad \text{and} \quad N_B^{\mathrm{alt}} = \begin{pmatrix} k-3 & -1 & 1 \\ -1 & k-3 & -1 \\ 1 & -1 & k-3 \end{pmatrix}$$

with respective eigenvalues $k-5$ and $k-2$ (twice), and $k-1$ and $k-4$ (twice). At Level 3 we have $F_M^{PQ} = \{id\}$ and hence the eigenvalue -1 with local multiplicity 1, 1 and 2 corresponding to the three representations.

The global multiplicities $m_\pi(k)$ are:

π	$\ell = 0$	$\ell = 1$	$\ell = 2$	$\ell = 3$
$[\ell]$	1	$k-1$	$k(k-3)/2$	$k(k-1)(k-5)/6$
$[1^\ell]$	–	–	$(k-1)(k-2)/2$	$(k-1)(k-2)(k-3)/6$
$[21]$	–	–	–	$k(k-2)(k-4)/3$

Example 2. When the linking set is $H = \{12, 13, 21, 23, 31, 32\}$, the resulting graph $H_n(3)$ is a *cyclic octahedron*. The name is suggested by the fact that in the case $n = 2$ the graph reduces to the regular octahedron, $K_{2,2,2}$. The calculations for $H_n(3)$ were done by *ad hoc* methods in [3], and here we shall describe how the results fit into our

general framework. There are 1, 6, 9, 2 matchings $M \in \mathcal{M}(H)$ with $|M| = 0, 1, 2, 3$ respectively. Taking the appropriate alternating sum at Level 0 we get the 1×1 matrix

$$N_H^{\text{pri}} = k(k-1)(k-2) - 6(k-1)(k-2) + 9(k-2) - 2,$$

and thus the eigenvalue $k^3 - 9k^2 + 29k - 32$. At Level 1 we get the 3×3 matrix N_H^{pri} with entries $2k - 6$ on the diagonal and $-k^2 + 7k - 13$ elsewhere. The eigenvalues are $-2(k-4)^2$ and $k^2 - 5k + 7$ (twice). At Level 2 we get the 3×3 matrices

$$N_H^{\text{pri}} = \begin{pmatrix} k-4 & k-5 & k-5 \\ k-5 & k-4 & k-5 \\ k-5 & k-5 & k-4 \end{pmatrix} \quad \text{and}$$

$$N_H^{\text{alt}} = \begin{pmatrix} k-4 & -(k-3) & k-3 \\ -(k-3) & k-4 & -(k-3) \\ k-3 & -(k-3) & k-4 \end{pmatrix}$$

with respective eigenvalues $3k - 14$ and 1 (twice), and $k - 2$ and $-2k - 7$ (twice). At Level 3, we get the 6×6 matrix $-(X(123) + X(132))$, and collapsed matrices N_H^{pri}, N_H^{alt} and $N_H^{[21]}$, of size 1×1, 1×1 and 2×2 respectively. The first two matrices are just (-2), so -2 is an eigenvalue with local multiplicity 1 in each case. The matrix $N_H^{[21]}$ is the identity matrix of size 2, so it has eigenvalue 1 (twice). The respective global multiplicities do not depend on L and hence are equal to the ones given in the previous example. These results imply that the chromatic polynomial of $H_n(3)$ is

$$\begin{aligned} P(H_n(3); k) = {} & (k^3 - 9k^2 + 29k - 32)^n \\ & + (k-1)((-2(k-4)^2)^n + 2(k^2 - 5k + 7)^n) \\ & + (1/2)k(k-3)((3k-14)^n + 2) \\ & + (1/2)(k-1)(k-2)((k-2)^n + 2(-2k+7)^n) \\ & + (1/6)k(k-1)(k-5)(-2)^n \\ & + (1/6)(k-1)(k-2)(k-3)(-2)^n \\ & + (1/3)k(k-2)(k-4)(2). \end{aligned}$$

7. Location of chromatic zeros

Because $P(G; k)$ is a polynomial function of k, it is usual to consider it as a function of a complex variable. This is particularly appropriate in statistical mechanics, where the focus is on the *thermodynamic limit* $\lim_{n\to\infty} P(G_n; z)^{1/v_n}$, v_n being the number of vertices of G_n. The thermodynamic limit is generally not analytic in the entire complex plane, and its singularities depend on the limiting behaviour of the zeros of $P(G_n; z)$ as $n \to \infty$. The framework described in this paper is well-adapted for investigating this behaviour.

An elementary result about the location of the zeros is Rouché's theorem [15, p. 218]. For example, consider the roots of $P(H_n(3); z) = 0$. There are $3n$ roots and their sum is $9n$, so the centroid is at the point 3 and it is convenient to put $w = z - 3$. The chromatic polynomial reduces to

$$(w^3 + 2w + 1)^n + Q_n(w),$$

where $Q_n(w)$ is a polynomial of degree $2n + 1$. The zeros of $w^3 + 2w + 1$ are (approximately)

$$-0.4534, \qquad 0.2267 + 1.4677i, \qquad 0.2267 - 1.4677i,$$

which lie in the disc $|w| \leq 1.4852$. It follows from Rouché's theorem that all the zeros of $(w^3 + 2w + 1)^n + Q_n(w)$ lie in the disc $|w| \leq R$, provided that $R > 1.4852$ and $|w^3 + 2w + 1|^n \geq |Q_n(w)|$ on the circle $|w| = R$. Since the degree of $Q_n(w)$ is $2n + 1$, it is clear that a suitable value of R can be found: for example $R = 3$ suffices. Thus all the roots lie in the disc $|z| \leq 6$, where the relevance of the number 6 is that it is the degree of $H_n(3)$. The important general result of Sokal [16] gives a weaker conclusion in this case.

More detailed information about the roots follows from the theorem of Beraha et al. [1]. Their result says that the limit points of the zeros of a sequence of polynomials of the form

$$P_n(z) = \sum_{i=1}^{s} m_i(z)\lambda_i(z)^n,$$

are the points ζ lying on the curves where two of the terms $\lambda_i(\zeta)$ are of equal modulus and dominate the other terms (together with some isolated points, which need not concern us).

In the case of the cyclic octahedra, the polynomials (expressed as functions of $w = z-3$) are

$$\lambda_A = w^3 + 2w + 1, \quad \lambda_B = -2(w-1)^2, \quad \lambda_C = w^2 + w + 1,$$
$$\lambda_D = 3w - 5, \quad \lambda_E = w + 1, \quad \lambda_F = -2w + 1, \quad \lambda_G = -2, \quad \lambda_H = 1.$$

In fact, one of the three eigenvalues $\lambda_A, \lambda_B, \lambda_D$ always dominates the other five. This means that the limiting behaviour of the roots is determined by these three.

Denote by Γ_{AB} the curve defined by the equation $|\lambda_A| = |\lambda_B|$, and so on. Then Γ_{AB} and Γ_{BD} are simple closed curves intersecting in two points

$$t, \bar{t} = 0.9971\ldots \pm 1.6284\ldots i.$$

Γ_{AD} is another simple closed curve, which necessarily contains t and $\bar{t}$.

The portions of these curves that satisfy the domination condition are the arc of Γ_{AD} that joins t and $\bar{t}$ and lies entirely in the half-plane Re $w > 0$, and the arcs of Γ_{AB} and Γ_{BD} that join t and $\bar{t}$ and do not lie entirely in the half-plane Re $w > 0$. Note that these arcs all lie in the half-plane Re $z > 0$.

These arcs divide the complex plane into three regions: a crescent-shaped region containing $w = 0$, in which λ_D dominates; another crescent-shaped region contiguous with the first, in which λ_B dominates, and the remainder of the complex plane, in which λ_A dominates. Apart from some isolated points, such as $z = 0$ $(w = -3)$, the limit points of the chromatic roots of the graphs $H_n(3)$ lie on the parts of $\Gamma_{AB}, \Gamma_{AD}, \Gamma_{BD}$ that bound these regions.

Although all the discussion here has concerned the case when the base graph is complete, similar results and methods hold more generally. For example, the proof of Theorem 3 remains valid when the base graph G and the linking set L satisfy the following condition: for each $w \in V$ the set of $v \in V$ such that $(v, w) \in L$ is a complete subgraph of G. This observation covers many of the results obtained by Shrock and his colleagues (see [10] and the references given there). We end with one example.

This condition stated above holds for the family of *generalised dodecahedra* D_n. Here G is a path with vertex-set $V = \{1, 2, 3, 4\}$ (1 and 4 being the end-vertices), and $L = \{11, 32, 44\}$. In this case the resulting graph is a cubic graph D_n with $4n$ vertices, and in particular D_5 is the graph of the regular dodecahedron. The chromatic polynomial $P(D_n; k)$ was obtained in full by Chang [9]. It can be written in the form

$$\operatorname{tr}(T_0(k))^n + (k-1)\operatorname{tr}(T_1(k))^n + (k^2-3k+1)\operatorname{tr}(T_2(k))^n + (k^3-6k^2+8k-1),$$

where the square matrices $T_\ell(k)$ $(\ell = 0, 1, 2)$ have size 3, 6, 4 respectively. Chang's result can also be obtained by the algebraic methods described here, and the zeros of $P(D_n; k)$ can be investigated by techniques based on the Beraha–Kahane–Weiss theorem [5].

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