The chromatic polynomial of the 3 x n toroidal square lattice

1. Introduction

Let $V = \{1, 2, \ldots, b\}$ be the vertex-set of the complete graph K_b. Given an integer $n \geq 3$ and a subset L of $V \times V$, the following construction produces a graph with bn vertices. Take n disjoint copies of K_b and link them by extra edges as follows. For $i = 1, 2, \ldots, n$ and each pair $(v, w) \in L$, join vertex v in the ith copy to vertex w in the $(i+1)$th copy, with the convention that $n + 1 = 1$. We obtain a 'ring' of n copies of K_b linked by edges in the manner prescribed by L.

Examples of the construction with $b = 2$ have been discussed elsewhere [1]. In the case $b = 3$ and $L = \{(1, 1), (2, 2), (3, 3)\}$, the graph is a *toroidal square lattice graph* $\mathcal{L}_n$, with 3 squares around one circumference of the torus and n squares around the other. In this paper we shall obtain the following explicit formula for the chromatic polynomial of $\mathcal{L}_n$.

$$\begin{aligned} P(\mathcal{L}_n; z) \;=\; & (z^3 - 6z^2 + 14z - 13)^n \\ & + (z-1)\big((-z^2 + 7z - 13)^n + 2(-z^2 + 4z - 4)^n\big) \\ & + z(z-3)/2\,\big((z-5)^n + 2(z-2)^n\big) \\ & + (z-1)(z-2)/2\,\big(2(z-4)^n + (z-1)^n\big) \\ & + (z^3 - 6z^2 + 8z - 1)(-1)^n. \end{aligned}$$

The two key techniques used in the derivation of this formula are: (i) a sieve formula for the action of the compatibility operator T (Section 3), and (ii) the construction of certain invariant subspaces of T (Sections 4 and 5). Both techniques can be extended to the general case, where b is any natural number and L is any subset of $V \times V$. The resulting general theorems [2] enable us to locate the zeros of the chromatic polynomials inside specific regions of the complex plane, without having to calculate the polynomials in full.

2. The eigenfunction method

From now on we fix $b = 3$ and $V = \{1, 2, 3\}$, so that an injection $\alpha : V \to \{1, 2, \ldots, k\}$ is a (proper) k-colouring of K_3. We denote by P_k the set of all such k-colourings, and by $\mathcal{V}_k$ the vector space of real-valued functions defined on P_k. The *standard basis* for $\mathcal{V}_k$ contains, for each α in P_k, the function $[\alpha]$ defined by

$$[\alpha](\beta) = \begin{cases} 1, & \text{if } \alpha = \beta; \\ 0, & \text{otherwise.} \end{cases}$$

We say that an ordered pair (α, β) of members of P_k is *compatible* if

$$\alpha(v) \neq \beta(v) \quad \text{for all } v \in V.$$

The idea is that if two disjoint copies of K_3 are linked by edges joining corresponding vertices, then the colourings α and β combine to form a (proper) colouring of the linked graph.

We define the *compatibility matrix* $T = T(k)$ as follows. The rows and columns of T correspond to the elements of P_k, and the entries are given by:

$$T_{\alpha\beta} = \begin{cases} 1 & \text{if } (\alpha, \beta) \text{ is a compatible pair;} \\ 0 & \text{otherwise.} \end{cases}$$

It is convenient to use the same symbol T for the linear operator represented by the matrix T, with respect to the standard basis on the space $\mathcal{V}_k$.

The connection between $T(k)$ and the chromatic polynomial arises from the formula [1]:

$$P(\mathcal{L}_n; k) = \operatorname{trace}\big(T(k)^n\big).$$

So if the eigenvalues of $T(k)$ are $\lambda_1(k), \lambda_2(k), \dots, \lambda_s(k)$, with multiplicities $m_1(k), m_2(k)$, $\dots, m_s(k)$ respectively, we have

$$P(\mathcal{L}_n; k) = \sum_{r=1}^{s} m_r(k) \lambda_r(k)^n.$$

The significance of this formula is that the calculation of $P(\mathcal{L}_n; k)$ is reduced to the calculation of the eigenspaces of T.

3. The sieve formula

It is convenient to introduce special notation for some elements of $\mathcal{V}_k$. We shall write $[1|h]$ for the function which takes the value 1 on all the colourings that assign the colour h to vertex 1, and the value 0 otherwise. Equivalently

$$[1|h] = \sum_{\gamma(1)=h} [\gamma].$$

Similarly, we write $[12|hi]$ for the sum of all $[\gamma]$ with $\gamma(1) = h$ and $\gamma(2) = i$; and so on. If $\alpha \in P_k$ is defined by $\alpha(1) = h$, $\alpha(2) = i$, $\alpha(3) = j$ then, in this notation, $[\alpha] = [123|hij]$, and we shall further abbreviate this to $[hij]$. Finally, $u = [-|-]$ is the sum of all $[\gamma]$ without restriction, that is, the function which takes the value 1 on all colourings.

We can obtain a useful formula for the action of T by a simple application of the sieve (inclusion-exclusion) principle. Suppose we are given $\alpha = [hij]$, and we wish to list all the colourings β such that (α, β) is a compatible pair. Then we first include all colourings, then exclude those which agree with α on one vertex, and so on. It follows that the action of $T = T(k)$ on $[\alpha] = [hij]$ is given by

$$T[hij] = u - \Big([1|h] + [2|i] + [3|j]\Big) + \Big([12|hi] + [23|ij] + [13|hj]\Big) - [hij].$$

4. The principal representation

We can use the sieve formula to calculate the action of T on functions like $[1|h]$. As we shall see, it follows from these calculations that certain subspaces of $\mathcal{V}_k$ are invariant under T. To begin, we observe that since $[1|h]$ is the sum of all $[\gamma]$ for which $\gamma(1) = h$, we can write

$$[1|h] \;=\; \sum_{ij \in N(h)} [hij],$$

where the notation $ij \in N(h)$ means that the sum is taken over ordered pairs (i, j) with $i \neq j$ such that $i \neq h$ and $j \neq h$.

We have

$$T[1|h] \;=\; T\left(\sum_{ij \in N(h)} [hij]\right) \;=\; \sum_{ij \in N(h)} T[hij].$$

The sieve formula for $T[hij]$ has eight terms, and we can sum each of them over $ij \in N(h)$ as follows.

$$\begin{aligned}
\sum_{ij \in N(h)} u \;&=\; (k-1)(k-2)u \\
-\sum_{ij \in N(h)} [1|h] \;&=\; -(k-1)(k-2)[1|h] \\
-\sum_{ij \in N(h)} [2|i] \;&=\; -(k-2)(u - [2|h]) \\
-\sum_{ij \in N(h)} [3|j] \;&=\; -(k-2)(u - [3|h]) \\
\sum_{ij \in N(h)} [12|hi] \;&=\; (k-2)[1|h] \\
\sum_{ij \in N(h)} [23|ij] \;&=\; u - [2|h] - [3|h] \\
\sum_{ij \in N(h)} [13|hj] \;&=\; (k-2)[1|h] \\
-\sum_{ij \in N(h)} [hij] \;&=\; -[1|h].
\end{aligned}$$

The important point is that all the terms are linear combinations of the four functions u, $a_h = [1|h]$, $b_h = [2|h]$, and $c_h = [3|h]$. Using this notation, and collecting up the terms, we obtain

$$T(a_h) = (k^2 - 5k + 7)u - (k^2 - 5k + 7)a_h + (k - 3)b_h + (k - 3)c_h.$$

The corresponding formulae for $T(b_h)$ and $T(c_h)$ can be deduced from the symmetry of the construction. Writing $C = k^2 - 5k + 7$ and $D = k - 3$ we have

$$\begin{aligned} T(a_h) &= C(u - a_h) + D(b_h + c_h) \\ T(b_h) &= C(u - b_h) + D(a_h + c_h) \\ T(c_h) &= C(u - c_h) + D(a_h + b_h). \end{aligned}$$

Since $u = \sum_h a_h = \sum_h b_h = \sum_h c_h$, it follows that

$$T(u) = kCu - Cu + 2Du = ((k - 1)C + 2D)u = (k^3 - 6k^2 + 14k - 13)u.$$

The eigenvalue $E = k^3 - 6k^2 + 14k - 13$ is the number of 1's in each row of T, in the usual matrix representation. In other words, E represents the number of k-colourings β of K_3 such that (α, β) is a compatible pair, for any given α. Standard arguments lead to the conclusion that the eigenvalue E has multiplicity 1.

The formulae for $T(a_h)$, $T(b_h)$, and $T(c_h)$ show that the subspace of $\mathcal{V}_k$ spanned by u, a_h, b_h, c_h is invariant under T. Provided that $k > 3$ these functions are linearly independent, and the action of T on this subspace is represented by the matrix

$$\begin{pmatrix} E & 0 & 0 & 0 \\ C & -C & D & D \\ C & D & -C & D \\ C & D & D & -C \end{pmatrix}.$$

The eigenvalues of this matrix are also eigenvalues of T. Clearly, they are E and the eigenvalues of the 3×3 matrix M_1 in the lower right-hand corner. We shall refer to M_1 as the *principal representation* of T.

It is easy to calculate the eigenvalues of M_1 by working out a determinant, but for our purposes it is useful to know the eigenfunctions as well, and these can be obtained directly from the equations. We have

$$\begin{aligned} T(a_h - b_h) &= -(C + D)(a_h - b_h) \\ T(b_h - c_h) &= -(C + D)(b_h - c_h) \\ T(a_h - c_h) &= -(C + D)(a_h - c_h). \end{aligned}$$

Thus $a_h - b_h$, $b_h - c_h$, and $a_h - c_h$ are eigenfunctions for the eigenvalue $-(C+D) = -(k-2)^2$. This result holds for each h in the range $1 \le h \le k$, but in each case the third eigenfunction is the sum of the first two, so the eigenspace of T is spanned by the $2k$ functions $a_h - b_h$ and $b_h - c_h$ $(1 \le h \le k)$. It is easily verified that the only linear relationships among these functions are the obvious ones:

$$\sum_{h=1}^{k}(a_h - b_h) = 0, \quad \sum_{h=1}^{k}(b_h - c_h) = 0,$$

and so the eigenspace has dimension $2(k-1)$.

More simple algebra shows that $k(a_h + b_h + c_h) - 3u$ is an eigenfunction for the eigenvalue $2D - C = -(k^2 - 7k + 13)$. Here there are k eigenfunctions, one for each h in the range $1 \le h \le k$, but again the sum of all of them is identically zero, so they define an eigenspace of T dimension $k-1$.

In summary, we have obtained the following eigenvalues of $T(k)$, and their multiplicities.

Eigenfunction :	u	$k(a_h + b_h + c_h) - 3u$	$a_h - b_h,\ b_h - c_h$
Eigenvalue :	$k^3 - 6k^2 + 14k - 13$	$-k^2 + 7k - 13$	$-(k^2 - 4k + 4)$
Multiplicity :	1	$k-1$	$2(k-1)$

5. The secondary representations

The results listed above yield the following partial expression for the chromatic polynomial of $\mathcal{L}_n$:

$$P(\mathcal{L}_n; k) = (k^3 - 6k^2 + 14k - 13)^n + (k-1)\big((-k^2 + 7k - 13)^n + 2(-k^2 + 4k - 4)^n\big) + r_n(k).$$

Here, $r_n(k)$ denotes a sum of terms depending on eigenvalues that will be determined in this Section. As we shall see, the contribution of $r_n(k)$ is relatively unimportant; specifically, it contains terms of degree not exceeding $n+2$. Thus the partial expression given above correctly determines the terms of the chromatic polynomial whose degree lies between $n+3$ and $3n$.

The key step is to obtain a formula for $T[12|hi]$ similar to the one for $T[1|h]$ obtained in Section 4. We do this by using the fact that $[12|hi]$ can be expressed as the sum of $[hij]$, taken over all colours j different from h and i. Writing this condition in the form $j \in N(hi)$, we have

$$T[12|hi] \;=\; T\left(\sum_{j\in N(hi)} [hij]\right) \;=\; \sum_{j\in N(hi)} T[hij].$$

Next, we calculate the sum over $j \in N(hi)$, for each of the eight terms in the sieve formula for $T[hij]$:

$$
\begin{aligned}
\sum_{j \in N(hi)} u &= (k-2)u \\
-\sum_{j \in N(hi)} [1|h] &= -(k-2)[1|h] \\
-\sum_{j \in N(hi)} [2|i] &= -(k-2)[2|i] \\
-\sum_{j \in N(hi)} [3|j] &= -(u-[3|h]-[3|i]) \\
\sum_{j \in N(hi)} [12|hi] &= (k-2)[12|hi] \\
\sum_{j \in N(hi)} [23|ij] &= [2|i]-[23|ih] \\
\sum_{j \in N(hi)} [13|ih] &= [1|h]-[13|hi] \\
-\sum_{j \in N(hi)} [hij] &= -[12|hi].
\end{aligned}
$$

We shall use the symbols u, a_h, b_h, c_h as before, and define

$$
d_{hi} = [12|hi], \quad e_{hi} = [23|hi], \quad f_{hi} = [31|hi].
$$

The terms in $T(d_{hi})$ have been calculated above. Collecting them up we obtain

$$
T(d_{hi}) \;=\; (k-3)(u-a_h-b_i+d_{hi}) + (c_h+c_i-e_{ih}-f_{ih}).
$$

Similar formulae for $T(e_{hi})$ and $T(f_{hi})$ can be written down immediately, using the symmetry.

Combining these results with those of Section 4 we see that the subspace of $\mathcal{V}_k$ spanned by the functions

$$
u, \quad a_h, b_h, c_h, \quad a_i, b_i, c_i, \quad d_{hi}, d_{ih}, e_{hi}, e_{ih}, f_{hi}, f_{ih},
$$

is invariant under T, and (provided $k > 3$) these 13 functions form a basis. Hence the action of T on this subspace is represented by a 13×13 matrix of the form

$$
\begin{pmatrix}
E & O & O & O \\
* & M_1 & O & O \\
* & O & M_1 & O \\
* & * & * & M_2
\end{pmatrix}.
$$

Here E is the eigenvalue $(k^3-6k^2+14k-13)$, representing the action of T on the subspace spanned by u, and M_1 is the 3×3 matrix, called the principal representation in Section 4. The matrix M_2 is the 6×6 matrix determined by the formulae for the action of T on the six elements $d_{hi}, d_{ih}, e_{hi}, e_{ih}, f_{hi}, f_{ih}$ of the basis. The O's represent zero matrices, and the $*$'s non-zero matrices, of the appropriate sizes.

Using the basic formulae we can express M_2 concisely in terms of the 2×2 matrices I (identity) and J (all-1), as follows:

$$M_2 = \begin{pmatrix} (k-3)I & I-J & I-J \\ I-J & (k-3)I & I-J \\ I-J & I-J & (k-3)I \end{pmatrix}.$$

In this form it is easy to check that the eigenvalues of M_2 are $k-5$, $k-4$ (twice), $k-2$ (twice), and $k-1$.

In order to determine the multiplicities of these numbers as eigenvalues of T, we return to the eigenfunction method used in Section 4. For example, let

$$w_{hi} = d_{hi} - d_{ih} + e_{hi} - e_{ih} + f_{hi} - f_{ih}.$$

Then it follows from the basic formulae that $T(w_{hi}) = (k-1)w_{hi}$. Thus we have $k(k-1)$ eigenfunctions w_{hi} for the eigenvalue $k-1$, one for each choice of the ordered pair (h,i). However there are the linear relationships

$$\sum_{i \neq h} w_{hi} = 0 \quad (1 \leq h \leq k), \qquad \sum_{h \neq i} w_{hi} = 0 \quad (1 \leq i \leq k).$$

Thus we can express all the functions w_{hk} and w_{ki} as linear combinations of the rest. Also $w_{hi} = -w_{ih}$, so the eigenspace is spanned by the set of eigenfunctions w_{hi} with h and i in the range $1 \leq h < i \leq k-1$. These eigenfunctions are linearly independepent, so the dimension of the eigenspace is $(k-1)(k-2)/2$.

In the same way we can obtain explicit eigenfunctions x_{hi}, y_{hi}, z_{hi} for the eigenvalues $k-2, k-4, k-5$, and calculate that their multiplicities are $k(k-3)$, $(k-1)(k-2)$, $k(k-3)/2$, respectively. (Similar calculations can be found in [1].)

We have now accounted for eigenvalues with total multiplicity

$$\begin{aligned} 1 + (k-1) + 2(k-1) + &(k-1)(k-2)/2 + k(k-3) + (k-1)(k-2) + k(k-3)/2 \\ &= 3k^2 - 6k + 1. \end{aligned}$$

The dimension of $\mathcal{V}_k$ is $k(k-1)(k-2)$ and so we still have to find eigenvalues with multiplicity

$$k^3 - 3k^2 + 2k - (3k^2 - 6k + 1) = k^3 - 6k^2 + 8k - 1.$$

In fact, there is only one remaining eigenvalue, -1, and its multiplicity is as stated above. The existence of the eigenvalue -1 is suggested by the formula for $T[hij]$, since $[hij]$ occurs with coefficient -1 in that formula. However, we have to explain how to get the right number of eigenfunctions.

The simplest method of showing that the multiplicity of -1 is $k^3 - 6k^2 + 8k - 1$ is to appeal to a general theory, which is based upon a pattern that has emerged in the foregoing calculations. We shall give only the outline of that theory here.

Denote by $(k)_r$ the 'falling factorial' $k(k-1)\dots(k-r+1)$, with the usual convention $(k)_0 = 1$. Define polynomials $p_s(k)$ inductively as follows:

$$p_0(k) = 1, \quad p_s(k) = (k)_s - \sum_{r=1}^{s} \binom{s}{r} p_{s-r}(k).$$

An explicit formula for $p_s(k)$ follows by inversion:

$$p_s(k) = \sum_{r=0}^{s} (-1)^{s-r} \binom{s}{r} (k)_r.$$

The relevance to our specific problem is that the numbers

$$\binom{3}{0} p_0(k) = 1, \qquad \binom{3}{1} p_1(k) = 3(k-1),$$
$$\binom{3}{2} p_2(k) = 3(k^2 - 3k + 1), \quad \binom{3}{3} p_3(k) = k^3 - 6k^2 + 8k - 1,$$

are the total multiplicities of the eigenvalues of degree $3, 2, 1, 0$ respectively. Note also that the definition implies that the sum of these numbers is $k(k-1)(k-2)$, the dimension of $\mathcal{V}_k$.

Given any subset X of $V = \{1, 2, 3\}$ we define a corresponding subspace $W(X)$ of $\mathcal{V}_k$, as follows. $W(\emptyset)$ is the 1-dimensional subspace spanned by u; $W(v)$ is the subspace spanned by all functions of the form $[v|h]$; $W(vw)$ is the subspace spanned by all functions of the form $[vw|hi]$, and $W(123)$ is whole space $\mathcal{V}_k$.

Let Y_3 be the kernel of the homomorphism $W(123) \to W(12) + W(23) + W(13)$ defined by $[hij] \mapsto [12|hi] + [23|ij] + [13|hj]$. Similarly let $Y(vw)$ be the kernel of the analogous homomorphism $W(vw) \to W(v) + W(w)$, and let $Y(v)$ be the kernel of $W(v) \to W(\emptyset)$. Finally, let $Y_2 = Y(12) \oplus Y(23) \oplus Y(13)$, $Y_1 = Y(1) \oplus Y(2) \oplus Y(3)$, and $Y_0 = W(\emptyset)$.

With these definitions it can be shown that the dimension of Y_s is $\binom{3}{s} p_s(k)$, and $\mathcal{V}_k = Y_3 \oplus Y_2 \oplus Y_1 \oplus Y_0$. The calculations in Sections 4 and 5 effectively provide bases for Y_0, Y_1, and Y_2. For example, the $3(k-1)$ functions $[1|h] - [1|1]$, $[2|i] - [2|2]$, and $[3|j] - [3|3]$ form a basis for Y_1. Turning to Y_3, for each function $[hij]$, we can choose a suitable ξ such that $[hij]' = [hij] - \xi$ is in Y_3. Furthermore,

$$T[hij]' = -[hij]' + \text{other terms},$$

where the other terms are elements of $Y_2 \oplus Y_1 \oplus Y_0$, and hence we can add suitable multiples of them to $[hij]'$ and obtain an eigenfunction for the eigenvalue -1. The construction shows that the dimension of the space Y_3 is $p_3(k)$.

In summary, the eigenvalues of $T(k)$ and their multiplicities are as given in the following table.

Eigenvalue	Multiplicity
$k^3 - 6k^2 + 14k - 13$	1
$-(k^2 - 4k + 4)$	$2(k-1)$
$-(k^2 - 7k + 13)$	$k-1$
$k-5$	$k(k-3)/2$
$k-4$	$(k-1)(k-2)$
$k-2$	$k(k-3)$
$k-1$	$(k-1)(k-2)/2$
-1	$k^3 - 6k^2 + 8k - 1$

6. Conclusion

The eigenvalues and multiplicities listed above lead directly to the formula for $P(\mathcal{L}_n; z)$ given in the Introduction. Because we know that the answer is a polynomial function, we need have no qualms about replacing the integer k by a complex variable z. Nervous readers can check that the formula evaluates to zero when $z = 0, 1, 2$ (as it should), even though the arguments given above are vacuous when $k = 0, 1, 2$, because the set P_k is empty.

There are a number of possible uses of this result. In statistical mechanics, explicit formulae for chromatic polynomials have suggested results about the location of zeros of partition functions [3,4], as well as helping to understand the behaviour of the 'thermodynamic limit' [5,6]. From a purely mathematical standpoint, the calculations given here provide a clear guide to formulating general theorems [2]. These theorems reveal that the form of the chromatic polynomial is largely independent of the choice of the linking set L (as defined in the Introduction).

References

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