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A Matrix Method for Chromatic Polynomials

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The chromatic polynomials of certain families of graphs can be expressed in terms of the eigenspaces of a linear operator. The operator is represented by a matrix, which is referred to here as the compatibility matrix. In this paper complete sets of eigenfunctions are obtained for several related families, and the results are used to provide information about the location of the zeros of the associated chromatic polynomials. A number of uniform features are observed, and these are explained in terms of general properties of the underlying construction.

1. THE CHROMATIC POLYNOMIALS OF THE CYCLIC LADDERS

The *cyclic ladder* L_n is the graph with $2n$ vertices $v_1, v_2, ..., v_n, w_1, w_2, ..., w_n$, joined by edges in the following way. Each of the sets $v_1, v_2, ..., v_n$, and $w_1, w_2, ..., w_n$ forms a cycle of length n, and in addition v_i is joined to w_i for $i = 1, 2, ..., n$.

The *chromatic polynomial* of a graph G is the polynomial function $P(G; z)$ of the complex variable z such that, for each non-negative integer k, $P(G; k)$ is the number of proper colourings of G when k colours are available.

A formula for the chromatic polynomial of L_n was published [6] in 1972. It is

$$P(L_n; z) = (z^2 - 3z + 3)^n + (z-1)\{(1-z)^n + (3-z)^n\} + (z^2 - 3z + 1).$$

This formula was obtained by using the deletion-contraction method. The technique was formalised and extended in [7]. The key idea is to obtain a *transfer matrix* $M(z)$ that represents the effect on the chromatic polynomial of adjoining one copy of a basic graph. Iterating this process n times corresponds to taking the nth power of $M(z)$. The chromatic polynomial of the resulting graph can be expressed as a linear combination of the eigenvalues of $M(z)^n$, which are the nth powers of the eigenvalues of $M(z)$.

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The coefficients can be found by comparison with the chromatic polynomials for small values of n. Thus, for the graph L_n, the eigenvalues are z^2-3z+3, $1-z$, $3-z$, and 1, and the coefficients are 1, $z-1$, $z-1$, and z^2-3z+1.

In [2] an alternative method was used to compute the chromatic polynomials of any family $\{G_n\}$ of graphs that can be constructed in a manner similar to the cyclic ladders. It is based on a different kind of transfer matrix, which we shall refer to as the *compatibility matrix* (the details will be given in Section 2). The main result is that $P(G_n; k)$ an be written as the trace of the nth power of a matrix $T(k)$, and hence as the sum of the nth powers of its eigenvalues, with "coefficients" equal to the multiplicities of the eigenvalues.

Recently there has been a renewal of interest in these matters, partly due to links with statistical physics [8, 13–16]. This has highlighted the fact that the compatibility matrix method has not been fully explored: indeed, there has not even been a study of the eigenfunctions of $T(k)$ for the cyclic ladders. In this paper complete sets of eigenfunctions will be found, not only for the cyclic ladders, but also for other related families. This is the beginning of a program that has identified several more general features of the compatibility matrix [5].

The method can be used to study the location of the zeros of the chromatic polynomial. Since there is no good way of finding the chromatic number of a graph, any information on the zeros provided by a general theory is potentially useful. We recall [6] two properties of $P(L_n; z)$. The first is the observation that the zeros of $P(L_n; z)$ appear to cluster around certain curves in the complex plane. This observation has been explained by Read and Royle [12], using a general result of Beraha, Kahane and Weiss [1]. Another property of $P(L_n; z)$, proved in [6], is that all its zeros lie in the disc $|z| < 3$. It is now possible to calculate explicitly the chromatic polynomials of graphs of moderate size [11, 12], and the experimental evidence lends weight to the conjecture [6] that a wide-ranging generalisation of Brooks' theorem may hold: specifically, there may be constants c_d such that the zeros of the chromatic polynomial of any regular graph with degree d lie in the disc $|z| < c_d$. A proof of this conjecture has recently been announced [13], with $c_d = 8d$ approximately. In Section 4 of this paper it will be shown that our results about the eigenspaces of $T(k)$ can be used to study the location of zeros.

2. THE COMPATIBILITY MATRIX

A *graph scheme* [3] is a pair (B, J), where B is a graph with vertex-set V_B, and J is a subset of $V_B \times V_B$. Let P_k denote the set of proper vertex-colourings of B with k colours. We say that two colourings α, β in P_k are *compatible* with respect to J if

$$(v, w) \in J \Rightarrow \alpha(v) \neq \beta(w).$$

The idea is that if two copies of B are linked by edges, joining a vertex v in the first copy to w in the second copy whenever $(v, w) \in J$, then using α to colour the first copy of B and β to colour the second copy results in a proper colouring of the entire graph.

For each integer $n \geqslant 2$ let $\mathscr{C}_n(B, J)$ denote the graph formed as follows. Take n disjoint copies of B and, for $i = 1, 2, ..., n$ join vertex v in the ith copy to w in the $(i+1)$th copy if and only if $(v, w) \in J$. (Here, by convention, $n+1=1$). For example, the cyclic ladder L_n is obtained by taking B to be the complete graph K_2 with $V_B = \{a, b\}$, and $J = \{(a, a), (b, b)\}$.

For a given graph scheme (B, J) and a given k, the *compatibility matrix* $T = T(k)$ is the matrix with rows and columns indexed by the elements of P_k, and

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

THEOREM. *Let $T(k)$ be the compatibility matrix for the graph scheme (B, J). Then*

$$P(\mathscr{C}_n(B, J); k) = \operatorname{trace}[T(k)^n].$$

Proof. Let $\alpha, \beta, ..., \nu$ be n colourings belonging to P_k. The product

$$T_{\alpha\beta} T_{\beta\gamma} \cdots T_{\nu\alpha}$$

is 1 precisely when we obtain a proper colouring of $\mathscr{C}_n(B, J)$ by colouring the first copy of B using α, the second copy using β, and so on. Thus the total number of proper colourings is

$$\begin{aligned} P(\mathscr{C}_n(B, J); k) &= \sum_{\alpha, \beta, ..., \nu} T_{\alpha\beta} T_{\beta\gamma} \cdots T_{\nu\alpha} \\ &= \sum_{\alpha} (T^n)_{\alpha\alpha} \\ &= \operatorname{trace} T^n. \quad \blacksquare \end{aligned}$$

COROLLARY. *Suppose that the matrix $T(k)$ has eigenvalues $\lambda_1(k), \lambda_2(k), ..., \lambda_s(k)$, with multiplicities $m_1(k), m_2(k), ..., m_s(k)$. Then*

$$P(\mathscr{C}_n(B, J); k) = \sum_{r=1}^{s} m_r(k)\, \lambda_r(k)^n.$$

Proof. This is a consequence of the fact that the trace of a matrix is the sum of its eigenvalues with appropriate multiplicities. ∎

Since $T(k)$ is a non-negative matrix, the well-known Perron–Frobenius theory asserts that in certain circumstances it will have a unique eigenvalue of largest modulus. For examples, in the case of the cyclic ladder L_n, $T(k)$ has $k(k-1)$ rows and columns, and each row and column contains k^2-3k+3 1's and $2k-3$ 0's. This means that k^2-3k+3 is the unique eigenvalue of largest modulus, and it has multiplicity 1.

In the next section we shall calculate all the eigenvalues of $T(k)$ and their multiplicities, for $B=K_2$ and various choices of J. In fact, it is simpler to work with $S=U-T$, where U is the matrix each of whose entries is 1. Thus S corresponds to the *incompatibility* of colourings of K_2, with respect to J. Since $k(k-1)$ is an eigenvalue of U with multiplicity 1, the unique eigenvalue λ_T of T with largest modulus corresponds to an eigenvalue $\lambda_S=k(k-1)-\lambda_T$ of S. The remaining eigenvalues of U are all zero, and so the other eigenvalues μ_T of T correspond to eigenvalues $-\mu_T$ of S.

The following table summarises the results about the incompatibility matrix, for various choices of J (for convenience we write *aa* instead of (a, a), and so on). It shows that the existence of eigenspaces U, W_1, W_2, X_1, X_2, having dimensions 1, $k-1$, $k-1$, m_k and m_k-1 respectively, where $m_k=(k-1)(k-2)/2$, is a common feature of this situation. The eigenvalues $\mu_1(k)$, $\mu_2(k)$ will be given explicitly in Section 3.

Eigenvalues and multiplicities for the incompatibility matrix

	Eigenspace:	U	W_1	W_2	X_1	X_2
	Dimension:	1	$k-1$	$k-1$	m_k	m_k-1
J						
aa, *ab*, *ba*, *bb*		$4k-6$	0	$2k-6$	0	-2
aa, *ba*, *bb*		$3k-4$	$\mu_1(k)$	$\mu_2(k)$	-1	-1
ab, *ba*		$2k-3$	$1-k$	$k-3$	1	-1
aa, *bb*		$2k-3$	$k-1$	$k-3$	-1	-1
aa, *ba*		$2k-2$	$k-2$	0	0	0

3. CALCULATION OF THE EIGENFUNCTIONS

Throughout this section we deal with a fixed integer $k \geqslant 3$. Denote a proper colouring of K_2, with k colours available, by (i, j), where $1 \leqslant i, j \leqslant k$ and $i \neq j$, and let V denote the vector space of real-valued functions defined on the set of such colourings. The *standard basis* for V consists of the functions e_{ij} which are defined, for i and j in the given range, by

$$e_{ij}(r, s) = \begin{cases} 1 & \text{if} \quad (r, s) = (i, j); \\ 0 & \text{otherwise.} \end{cases}$$

Let u be the function that takes the value 1 on every colouring, and let

$$a_i = \sum_{j \neq i} e_{ij}, \qquad b_j = \sum_{i \neq j} e_{ij}, \qquad d_i = k(a_i - b_i), \qquad s_i = k(a_i + b_i) - 2u,$$

$$p_{ij} = k^2(e_{ij} - e_{ji}) - (d_i - d_j),$$

$$q_{ij} = k(k-1)(k-2)(e_{ij} + e_{ji}) - (k-1)(s_i + s_j) - 2(k-2)\, u.$$

LEMMA. *If S is the incompatibility matrix for the scheme (K_2, J) with $J = \{aa, bb\}$, the functions u, d_i, s_i, p_{ij}, q_{ij} are eigenfunctions of S. The corresponding eigenvalues are* $2k-3$, $k-1$, $k-3$, -1, -1. *The total multiplicities of the eigenvalues* $2k-3$, $k-1$, $k-3$, -1 *are* 1, $k-1$, $k-1$, k^2-3k+1, *respectively.*

Proof. We have $S(e_{ij}) = a_i + b_j - e_{ij}$, from which the eigenvalues can be deduced. The fact that u has multiplicity 1 follows from the remarks at the end of the previous section. There are k eigenfunctions d_i with eigenvalue $k-1$, and k eigenfunctions s_i with eigenvalue $k-3$, but in each case the dimension of the eigenspace is $k-1$, because the sum of all k eigenfunctions is identically zero. Similarly, the dimensions of the spaces spanned the p_{ij} and the q_{ij} are m_k and $m_k - 1$ respectively, where $m_k = (k-1)(k-2)/2$. This gives the stated multiplicity of the eigenvalue -1. ∎

Now consider the graph $L_n^\times$ obtained by taking $J^\times = \{ab, ba\}$. Here the action of $S^\times$ on the standard basis is given by $S^\times(e_{ij}) = a_j + b_i - e_{ji}$ and it follows that

$$S^\times(u) = (2k-3)\, u, \qquad S^\times(d_i) = (1-k)\, d_i, \qquad S^\times(s_i) = (k-3)\, s_i.$$

$$S^\times(p_{ij}) = p_{ij}, \qquad S^\times(q_{ij}) = -q_{ij}.$$

Note that the eigenvalues are slightly different from those of S, although the dimensions of the various spaces are the same. When n is even the resulting formula for the chromatic polynomial of $L_n^\times$ is the same as that for L_n (indeed the graphs are isomorphic). But when n is odd we get the well-known formula [6] for chromatic polynomial of the Moebius ladder.

Now let $J^+ = \{aa, ba, bb\}$, $J^{++} = \{aa, ab, ba, bb\}$. The corresponding graphs L_n^+ and L_n^{++} are modifications of the ladder L_n with additional "rungs", one and two (respectively) in each section. For L_n^{++} we do not need any new calculations. This is because J^{++} is the disjoint union of J and $J^{\times}$, and $S^{++}=S+S^{\times}$. Since the eigenspaces of S and $S^{\times}$ are identical, the eigenvalues of S^{++} are the sums of the corresponding eigenvalues of S and $S^{\times}$.

For L_n^{+} the calculations are similar but not identical. The basic equation is

$$S^{+}(e_{ij})=a_i+a_j+b_j-e_{ij}.$$

For each i the subspace spanned by u, a_i, b_i is invariant under S^{+}, and the action of S^{+} is represented by the matrix

$$\begin{pmatrix} 3k-4 & 0 & 0 \\ 2 & k-3 & -1 \\ 1 & k-2 & k-2 \end{pmatrix}.$$

So we have eigenvalues $3k-4$ and the roots $\mu_1(k)$, $\mu_2(k)$ of the equation

$$\mu^2-(2k-5)\,\mu+(k-2)^2=0.$$

The eigenvalue $3k-4$ has multiplicity 1. The eigenvalues $\mu_1(k)$, $\mu_2(k)$ are irrational, but it is easy to check that when $\mu=\mu_1(k)$ or $\mu=\mu_2(k)$, and $1\leqslant i\leqslant k$, the function

$$k(k-2-\mu)\,a_i+kb_i-(k-1-\mu)\,u$$

is an eigenfunction with the appropriate eigenvalue. As before, the sum of all k eigenfunctions is zero in each case, so the eigenspaces have dimension $k-1$.

For the remaining eigenvalues define

$$f_{ij}=e_{ij}-e_{i+1,\,j}-e_{i,\,j+1}+e_{i+1,\,j+1},$$

provided all the terms exist (and with the convention that $k+1=1$). Then it follows immediately from the formula for $S^{+}(e_{ij})$ that $S^{+}(f_{ij})=-f_{ij}$, so each f_{ij} is an eigenfunction with eigenvalue -1. Similarly, if we define

$$c_l=e_{1,\,1+l}+e_{2,\,2+l}+\cdots+e_{k,\,k+l},$$

then we have $S^{+}(c_l)=3u-c_l$, so $c'_l=(k-1)\,c_l-u$ is also an eigenfunction with eigenvalue -1. Working out the linear relationships among the various f_{ij} and c'_l leads to the conclusion that the total multiplicity of the eigenvalue -1 is k^2-3k+1. Translating them into eigenvalues of T^{+}

we obtain a formula for the chromatic polynomial of L_n^+, as given in Section 4.

The table in Section 2 summarises all these results.

4. LOCATION OF ZEROS

The general formula for $P(\mathscr{C}_n(B, J); k)$, in the form stated in Section 2, invites us to extend the result to a complex variable z:

$$P(\mathscr{C}_n(B, J); z) = \sum_{r=1}^{s} m_r(z)\, \lambda_r(z)^n.$$

This extension requires some care. The left-hand side is certainly a polynomial function, defined in the entire complex plane, but the individual terms on the right-hand side may not be so well-behaved. However, in the case of the graphs discussed here, it is easy to ensure that everything is in order. The only problem is that in the case of L_n^+ two of the eigenvalues of the compatibility matrix are irrational. However, their contribution to the sum can be written as the trace of a 2×2 matrix with polynomial terms, so we have:

$$P(L_n^+; z) = (z-2)^{2n} + (z-1)\,\text{trace}\begin{pmatrix} 3-z & 1 \\ 2-z & 2-z \end{pmatrix}^n + (z^2 - 3z + 1).$$

In this form, it is clear that all terms are polynomial functions.

We shall focus on the problem of locating the zeros of chromatic polynomials within a suitable disc. It is well-known [4, p. 76] that if G has N vertices and M edges then the coefficient of z^{N-1} in $P(G; z)$ is equal to $-M$. Equivalently, the centroid of the zeros of $P(G; z)$ is the point $\delta/2$, where δ is the average degree of G. It is therefore reasonable to consider the location of the zeros with respect to a disc of the form

$$D_R = \{z\colon |z - \delta/2| \leqslant R\}.$$

In the case $G = \mathscr{C}_n(B, J)$, the key idea is to write the chromatic polynomial in the form

$$P_n(z) = P(\mathscr{C}_n(B, J); z) = F(z)^n + G_n(z),$$

where $F(z)$ represents the dominant eigenvalue, which has unit multiplicity, and $G_n(z)$ represents the sum of the remaining eigenvalues according to their multiplicities. Suppose we can show that, for some R and all sufficiently large n,

$$|F(z)|^n > |G_n(z)| \qquad \text{whenever} \quad |z-\delta/2| = R.$$

When this condition is satisfied, Rouché's Theorem tells us that if all zeros of $F(z)$ are inside D_R, then so are all zeros of $P_n(z)$. It remains to choose the smallest value of R for which the condition holds.

The strategy outlined in the previous paragraph works well in the case of the graphs $\mathscr{C}_n(B, J)$ with $B = K_2$. For L_n we have $\delta = 3$ and

$$|F(z)| = |z^2 - 3z + 3| = |(z - \tfrac{3}{2})^2 + \tfrac{3}{4}| \geqslant R^2 - \tfrac{3}{4},$$

on the circle $|z - \frac{3}{2}| = R$.

For $G_n(z)$ we have

$$\begin{aligned}|G_n(z)| &= |(z-1)[(3-z)^n + (1-z)^n] + (z^2 - 3z + 1)| \\ &\leqslant |z-1|\,[\,|z-3|^n + |z-1|^n] + |z^2 - 3z + 1|,\end{aligned}$$

and on the circle $|z - \frac{3}{2}| = R$,

$$|z-1| \leqslant R + 1/2, \qquad |z-3| \leqslant R + 3/2, \qquad |z^2 - 3z + 1| \leqslant R^2 + 5/4.$$

The "largest" term in $|G_n(z)|$ is the one involving $|z-3|^n$, and so we have an estimate of the form

$$|G_n(z)| < c_R(R + \tfrac{3}{2})^n \qquad \text{on} \quad |z - \tfrac{3}{2}| = R.$$

Choose R to be any fixed real number such that

$$R^2 - \tfrac{3}{4} > R + \tfrac{3}{2}.$$

Then there is a positive integer $n_0(R)$ such that, for all $n \geqslant n_0(R)$,

$$(R^2 - \tfrac{3}{4})^n > c_R(R + \tfrac{3}{2})^n.$$

It follows that the condition $|F(z)|^n > |G_n(z)|$ holds on $|z - \frac{3}{2}| = R$ for all sufficiently large n. We have established the desired result under the condition that $R > R_0$, where R_0 is the positive root of the equation

$$R^2 - \tfrac{3}{4} = R + \tfrac{3}{2}.$$

Explicitly, $R_0 = \frac{1}{2}(1 + \sqrt{10}) = 2.081\ldots$. The function $F(z)$ has zeros at the points $(3 \pm i\sqrt{3})/2$, and so all zeros of $F(z)^n$ are in D_R whenever $R > R_0$. It follows from Rouché's Theorem that, for all sufficiently large n, all zeros of $P_n(z)$ also lie in D_R whenever $R > R_0$.

This is a minor improvement on the old result [6] that the zeros lie in the disc $|z| \leqslant 3$. It suggests that similar results may hold more generally, and in fact the generalisation to L_n^+ and L_n^{++} is almost automatic.

For L_n^+ we have $\delta = 4$, so we need to consider the circle $|z-2| = R$, where clearly $|F(z)| = |z-2|^2 = R^2$. In this case

$$\begin{aligned} |G_n(z)| &= |(z-1)[(-\mu_1(z))^n + (-\mu_2(z))^n] + (z^2 - 3z + 1)| \\ &\leqslant |z-1| \, [|\mu_1(z)|^n + |\mu_2(z)|^n] + |z^2 - 3z + 1|. \end{aligned}$$

The "largest" term on the circle $|z-2| = R$ is $|\mu_1(z)|^n \leqslant (2R+1)^n$, with the appropriate choice of μ_1. Using the same argument as for L_n, we see that $|F(z)|^n > |G_n(z)|$ will hold for all sufficiently large n provided that $R > R_0$, where R_0 is the positive root of the equation

$$R^2 = 2R + 1.$$

In this case $R_0 = 1 + \sqrt{2} = 2.414....$

For L_n^{++} we have $\delta = 5$, and on the circle $|z - \frac{5}{2}| = R$, $|F(z)| = |z^2 - 5z + 6| \geqslant R^2 - \frac{1}{4}$. For $|G_n(z)|$ we have

$$\begin{aligned} |G_n(z)| &= |(z-1)(6-2z)^n + z(z-3)\, 2^{n-1}| \\ &\leqslant |z-1| \, |2z-6|^n + |z(z-3)| \, 2^{n-1}. \end{aligned}$$

So, on the circle $|z - \frac{5}{2}| = R$ the largest term is $|2z-6|^n \leqslant (2R+1)^n$ (provided $2R + 1 > 2$). In this case the critical value R_0 is the positive root of

$$R^2 - \tfrac{1}{4} = 2R + 1,$$

that is, $R_0 = 2.5$.

Some of the features observed in the preceding calculations can be generalised. Here we give a brief discussion, referring the reader elsewhere for more details [5].

If the base graph B has vertex-set V_B and edge-set E_B, the graph $\mathscr{C}_n(B, J)$ has $n\,|V_B|$ vertices and $n(|E_B| + |J|)$ edges. Hence the average degree of each graph in the family is given by

$$\delta = \frac{2(|E_B| + |J|)}{|V_B|}.$$

In particular, when $B = K_2$ we have $\delta = |J| + 1$.

Now, for a given J, the number of proper k-colourings of K_2 that are incompatible with a given one is of the form $\alpha k - \beta$, where α is the size of the set J, and β is a fixed positive integer. The number $\alpha k-\beta$ is the dominant eigenvalue of the incompatibility matrix, and hence the dominant eigenvalue of the compatibility matrix $T(k)$ is

$$\begin{aligned} k(k-1)-(\alpha k-\beta) &= k^2-(\alpha+1)\,k+\beta \\ &= k^2-\delta k+\beta \\ &= (k-\delta/2)^2+\gamma, \end{aligned}$$

for some real constant γ. Thus, on the circle $|z-\delta/2|=R$, the leading term $F(z)^n$ in the formula for the chromatic polynomial is such that

$$|F(z)|^n \geqslant (R^2-|\gamma|)^n.$$

We now discuss $G_n(z)$. Here too there is a simple observation based on the interpretation of $G_n(k)$ in terms of the eigenspaces of $T(k)$.

Suppose that π is any permutation of $\{1, 2, ..., k\}$. Then π induces a permutation of the set P_k of proper k-colourings of the base graph B. Clearly the property of compatibility is preserved under π, and so the compatibility matrix $T=T(k)$ commutes with the corresponding permutation matrix M_π. It follows that if $Tf=\lambda f$, then $TM_\pi f=M_\pi Tf=\lambda M_\pi f$. In other words, if f is an eigenfunction with eigenvalue λ, then so is $M_\pi f$.

If f is constant, then $M_\pi f=f$. But if f is not constant we can obtain new eigenfunctions by this method. For example, if π is a k-cycle, then we get k eigenfunctions

$$f_i=(M_\pi)^i f \qquad i=0, 1, ..., k-1.$$

Under quite general conditions the only linear relationship connecting the f_i is the fact that their sum is zero. It follows that the multiplicity of any eigenvalue that contributes to $G_n(k)$ is at least $k-1$. This explains why, in the case $B=K_2$, we obtain expressions of the form

$$G_n(k)=(k-1)\,g_n(k)+q(k)\,h_n.$$

Here the term g_n is a polynomial function of degree n, q is a quadratic polynomial, and h_n is independent of k.

The properties of $G_n(z)$ in the special cases considered above are necessary consequences of this general fact. Specifically, we have an estimate of the form

$$|G_n(z)| \leqslant c_R\theta_n(R) \qquad \text{on} \quad |z-\delta/2|=R,$$

where θ_n is a polynomial of degree n.

The method depends on the fact that we have a lower bound for $|F(z)|^n$ that is of order R^{2n}, and an upper bound for $|G_n(z)|$ that is of order R^n. This leads to the conclusion that there is a critical value R_0 such that, for sufficiently large n, we have $|F(z)|^n > |G_n(z)|$ whenever $|z - \delta/2| = R > R_0$. The values of R_0 obtained above do not provide a reliable guide to what may be true more generally. However, it is possible that there may exist a uniform estimate, of the form $R_0 \leqslant R_B$ for all families $\mathscr{C}_n(B, J)$ with a given base graph B.

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