d-regular graph on n vertices with the most k-cycles

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Abstract

We construct the unique d-regular graph G with the maximum number of k-cycles for $k = 5, 6$ with a fixed number $n = c(d+1)$ of vertices for $k = 5$ and $n = 2cd$ vertices for even $k = 6$. Using a Möbius inversion relation between graph homomorphism numbers and injective homomorphism numbers, we reframe the problem as a continuous optimization problem on the eigenvalues of G by leveraging the fact that the number of closed walks of length k is $\mathrm{tr}(A^k)$. For $k = 5$ and $d > 3$, we show G is a collection of disjoint K_{d+1} graphs. For $d = 3$, disjoint Petersen graphs emerge. For $k = 6$ and d large enough, G consists of copies of $K_{d,d}$. We conjecture that for odd k and sufficiently large d, the optimal G is a collection of K_{d+1}, while for even k with sufficiently large d, the optimal G consists of $K_{d,d}$.

Additionally, we introduce and give formulas for non-backtracking homomorphism numbers and backtracking homomorphism numbers, respectively. Moreover, we find the unique d-regular graph on n vertices with the most non-backtracking closed walks of length k by considering an optimization problem on the non-backtracking spectrum of G. We also solve the same problem, but for backtracking closed walks. Lastly, a corollary gives formulas for the number of 4-cycles and 5-cycles of a graph with respect to its spectrum, regardless of regularity.

1 Introduction

For given positive integers d, n, k we consider the d-regular graph G on n vertices that maximizes the number of k-cycles. For convenience, throughout this paper, n will be a multiple of $c(d+1)$ or of $2cd$ as we are ultimately interested in asymptotic behavior similar to [5]. Note that uniqueness of an optimizer is not true for all n, d, k. However, if there are no 'remainder vertices,' then the optimizer is unique. Here are some preliminary and elementary results from [5].

1. For $k = 3$ and $n = c(d+1)$, c copies of K_{d+1} is optimal.
2. For $k = 4$ and $n = 2cd$, c copies of $K_{d,d}$ is optimal.
3. Let $n = c(d+1)$. The d-regular graph with the most K_k subgraphs is c copies of K_{d+1}.

First, we give a technical lemma that will be used for the continuous optimization problems that follow. Furthermore, every graph that we call "optimal" or "maximal" is the *unique* graph that maximizes the objective. Furthermore, all optimizers given are graphs that are determined by their spectra [7].

Lemma 1. *Let p be a degree k polynomial with a positive leading coefficient. For d large enough, the constrained optimization problem,*

$$\text{maximize} \sum_{i=1}^{n} p(\lambda_i), \quad \text{subject to} \sum_{i=1}^{n} \lambda_i = 0, \sum_{i=1}^{n} \lambda_i^2 = nd, \lambda_{\max} = d, |\lambda_i| \le d,$$

is uniquely solved by

$$\begin{cases} \lambda_1 = \ldots = \lambda_{n/c} = d, \quad \lambda_{n/c+1} = \ldots = \lambda_n = -1, \ \text{if } k \text{ odd, } n = c(d+1) \\ \lambda_1 = \ldots = \lambda_{n/c} = d, \quad \lambda_{n/c+1} = \ldots = \lambda_{2n/c} = -d, \quad \lambda_{2n/c+1} = \ldots = \lambda_n = 0, \ \text{if } k \text{ even, } n = 2cd \end{cases}.$$

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Proof for odd k. We will show this in two steps. First, that there must be exactly n/c variables with a value of d, and then that the rest of the variables must be equal to each other.
Step 1: Exactly n/c variables are equal to d.
Case 1: Suppose $\lambda_1, ..., \lambda_n$ satisfy the constraints and that $\ell < n/c$ of them are equal to d. Then, for large enough d, it suffices to consider $p(x) = x^k$. Then, since k is odd, $\lambda_i \leq d$, and the fact that $|\sum x_i|^k \geq |\sum x_i^k|$, we have

$$\ell d^k + \sum_{i=\ell+1}^{n} \lambda_i^k < (\ell+1)d^k + \sum_{i=\ell+2}^{n} \left(\lambda_i - \frac{d - \lambda_{\ell+1}}{n - \ell - 1}\right)^k .$$

Case 2: Suppose there are $m > n/c$ variables that are equal to d. Then, for some $\epsilon > 0$,

$$md^k + \sum_{i=m+1}^{n} \lambda_i^k < (m-1)d^k + (d-\epsilon)^k + \sum_{i=m+1}^{n} \left(\lambda_i + \frac{\epsilon}{n-m}\right)^k$$
$$= md^k + \sum_{i=m+1}^{n} \lambda_i^k + \sum_{i=m+1}^{n} \left[\sum_{j=1}^{k} \binom{k}{j} d^{k-j}(-\epsilon)^j + \sum_{j=1}^{k} \binom{k}{j} \lambda_i^{k-j} \left(\frac{\epsilon}{n-m}\right)^j\right].$$

Thus, the optimizer has $\lambda_1, ..., \lambda_{n/c} = d$. **Step 2: The rest of the variables are equal.**
Suppose that they are not equal. Then, without loss of generality, by the constraints, we can assume that $\lambda_{n/c+1} > -1 > \lambda_{n-s} \geq ... \geq \lambda_n$ so that $|\lambda_{c/n+1} + 1| \leq |\lambda_{n-s} + 1|$. Note that if this is not true then the same holds in the reverse direction. Then,

$$\sum_{i=m+1}^{n} \lambda_i^k = \lambda_{n/c+1}^k + \left(\frac{n(c-1)}{c} - 1 - s\right)(-1)^k + \sum_{i=n-s}^{n} \lambda_i^k < \left(\frac{n(c-1)}{c} - s\right)(-1)^k + \sum_{i=n-s}^{n} (\lambda_i^k + g(\lambda_i))^k,$$

for some function g such that the constraints are still satisfied. Thus, $\lambda_1 = ... = \lambda_{n/c} = d$, $\lambda_{n/c+1} = ... = \lambda_n = -1$ is a maximizer. ☐

Proof for even k. A similar argument is used to find the solutions. For sufficiently large d, it suffices to consider $p(x) = x^k$. Suppose there are $\ell < 2n/c$ variables that have magnitude d, that $|\lambda_{\ell+1}| \geq ... \geq |\lambda_n|$, and that the constraints are satisfied. Without loss of generality, let $\lambda_{\ell+1} > 0$. Then, for $\epsilon > 0$,

$$\ell d^k + \sum_{i=\ell+1}^{n} \lambda_i^k < \ell d^k + (\lambda_{\ell+1} + \epsilon)^k + \sum_{i=\ell+2} \left(\lambda_i^k - \frac{\epsilon}{n-m}\right)^k .$$

Thus, exactly $2n/c$ variables have magnitude d. The constraints force the optimizer to be what is claimed in the statement. ☐

Lemma 2. *For odd k and $n = c(d+1)$, the graph with the maximal number of closed walks of length k is the graph consisting of c copies of K_{d+1}.*

Proof. If there is a graph with adjacency matrix A with eigenvalues λ_i that solve the optimization problem,

$$\text{maximize} \sum_{i=1}^{n} \lambda_i^k, \quad \text{subject to} \sum_{i=1}^{n} \lambda_i = 0, \sum_{i=1}^{n} \lambda_i^2 = nd, \lambda_{\max} = d, |\lambda_i| \leq d,$$

then it is an optimizer. By Lemma 1, $\lambda_1 = ... = \lambda_{n/c} = d$, $\lambda_{n/c+1} = .. = \lambda_n = -1$ is optimal. The graph consisting of c copies of K_{d+1} uniquely has this spectrum and is thus optimal. ☐

Lemma 3. *For even k and $n = 2cd$ the graph with the maximal number of closed walks of length k is the graph consisting of c copies of $K_{d,d}$.*

Proof. The problem is equivalent to the optimization problem in the previous lemma. By Lemma 1, $\lambda_1 = ... = \lambda_{n/c} = d, \lambda_{n/c+1} = ... = \lambda_{2n/c} = -d, \lambda_{2n/c+1} = ... = \lambda_n = 0$ is a maximizer. The graph with c copies of $K_{d,d}$ uniquely has this spectrum. □

It is remarkable that there exist graphs whose spectra are the solutions to these optimization problems, which is not *a priori* the case. This happens for every optimization problem we consider. In the language of graph homomorphisms we just found $\max \hom(C_k, G)$ over all $d-$regular G with n vertices. For k-cycles instead of closed walks, the problem becomes $\max \operatorname{inj}(C_k, G)$. The following equations relate these quantities using the Möbius inverse of the partition lattice.

Lemma 4.

$$\hom(H,G) = \sum_P \operatorname{inj}(H/P, G).$$

$$\operatorname{inj}(H,G) = \sum_P \mu_p \cdot \hom(H/P, G), \ \textit{with } \mu_p = (-1)^{v(G)-|P|} \prod_{S \in P} (|S|-1)!$$

where P ranges over all partitions of $V(H)$ and where $|P|$ is the number of classes in the partition and S are the classes of P. [6]

It is important to note that some of the resulting quotient graphs will have self-loops. Since G is simple, these terms vanish. We will use these formulas to find an eigenvalue optimization problem corresponding to finding the d-regular graph with the most k-cycles. When the context is clear we will write $\hom(H) = \hom(H, G)$. We will now display the type of results that can be achieved by using spectral theory and Lemma 4 by giving a formula for the number of 4-cycles of a graph.

Proposition 5. *Given a graph G, with adjacency matrix A and eigenvalues $\lambda_1, ..., \lambda_n$, the number of 4-cycles in G is*

$$\frac{1}{8}\left(\left[\sum_{i=1}^{n} \lambda_i^4\right] - 2 \cdot \mathbf{1}^T A^2 \mathbf{1} + \mathbf{1}^T A \mathbf{1}\right),$$

where $\mathbf{1}$ is the all ones vector. In particular, if G is d-regular, then the number of 4-cycles is

$$\frac{1}{8}\left(\sum_{i=1}^{n} \lambda_i^4 - nd^2 + nd\right).$$

Proof. Notice that the number of 4-cycles is exactly $\frac{1}{8}\operatorname{inj}(C_4, G)$. Then, by Lemma 4,

$$\operatorname{inj}(C_4, G) = \hom(C_4, G) - 2 \cdot \hom(P_3, G) + \hom(K_2, G).$$

The first term is the number of closed walks of length 4, the second the number of walks of length 2, and the last being the number of walks of length 1. □

Theorem 6. *For $d > 3$ and $n = c(d+1)$, the d-regular graph on n vertices with the most 5-cycles is c copies of K_{d+1}. For $d = 3$ and $n = 10c$, then the optimal graph is c copies of the Petersen graph.*

Proof. By Lemma 4, we calculate: $\operatorname{inj}(C_5, G) = \hom(C_5) - 5 \cdot \hom(K_3 + e) + 5 \cdot \hom(K_3)$, where the "$+e$" means with an antenna. Then, since G is d-regular, we have $\hom(K_3 + e) = d \cdot \hom(K_3)$. Thus, we consider the optimization problem,

$$\text{maximize} \sum_{i=1}^{n} \lambda_i^5 + (5-5d)\lambda_i^3, \quad \text{subject to } \sum_{i=1}^{n} \lambda_i = 0, \sum_{i=1}^{n} \lambda_i^2 = nd, \lambda_{\max} = d, |\lambda_i| \leq d.$$

By Lemma 1, for $d > 3$, this is solved when $\lambda_i = ... = \lambda_c = d$ and $\lambda_{c+1}, ..., \lambda_n = -1$. The graph consisting of c copies of K_{d+1} has this spectrum. For $d = 3$, the solution is the spectrum of the Petersen graph. □

Alternate proof for Petersen graphs. Consider a 3-regular graph with an edge containing the maximal number of 5-cycles going through it, which is 11. Then, there is an edge with no 5-cycles going through it. Thus, the Petersen graph, with 10 5-cycles going through every edge, is optimal. □

This alternate method, which was originally used to find maximal graphs in [5], becomes impractical for large d and k. The new spectral method works for all d and can be used to obtain formulas for the number of 4-cycles and 5-cycles of a graph, regardless of regularity.

Corollary 7. *Given a graph G with adjacency matrix A with eigenvalues $\lambda_1, ..., \lambda_n$, the number of 5-cycles in G is*

$$\frac{1}{10}\left(\left[\sum_{i=1}^{n} \lambda_i^5 + 5\lambda_i^3\right] - 5 \cdot \mathrm{tr}(\mathrm{diag}(A^3)D)\right),$$

where D is the diagonal degree matrix and the diag *operator sets the non-diagonal entries to zero. In particular, if G is d-regular then, the number of 5-cycles is*

$$\frac{1}{10}\left(\sum_{i=1}^{n} \lambda_i^5 + (5-5d)\lambda_i^3\right).$$

Proof. The only term that is not immediately clear is $-5 \cdot \mathrm{tr}(\mathrm{diag}(A^3)D)$. This is the number of homomorphisms $\phi : K_3 + e \to G$. Without loss of generality, this equals the number of homomorphisms $\psi : K_3 \to G$ with $\psi(1) = v$ times the degree of v summed over all $v \in G$ as the antenna may map to any of the neighbors of v. □

Furthermore, the new method also works for $k = 6$. When using Lemma 4, we notice that the terms where H/P is a tree are constant for d-regular G. So, we can omit them. We get

$$\mathrm{inj}(C_6, G) = \left[\sum_{i=1}^{n} \lambda_i^6 + (6-6d)\lambda_i^4 - 6\lambda_i^3\right] - 3 \cdot \hom(B, G) + 9 \cdot \hom(K_4 \setminus e, G) + C, \qquad (*)$$

for some $C \in \mathbb{Z}$ where B is the 'bowtie' graph. We note that $\hom(B)$ and $\hom(K_4 \setminus e)$ cannot be expressed using eigenvalues. Thus, we need the following.

Lemma 8. *For any G, $\hom(B) \geq 4 \cdot \hom(K_4 \setminus e)$.*

Proof. $\hom(B) = \mathrm{inj}(B) + 4 \cdot \hom(K_4 \setminus e) + 2 \cdot \hom(K_3)$. □

Theorem 9. *For $n = 2cd$ and d large enough, the d-regular graph on n vertices with the most 6-cycles is c copies of $K_{d,d}$.*

Proof. Since $\hom(B, G) \geq 4 \cdot \hom(K_4 \setminus e, G)$, we have that the non-constant terms outside of the sum in $(*)$ are non-positive and thus maximized when they are zero. Note that if G is bipartite, then these terms are zero. By Lemma 1, the spectral part of $(*)$ is maximized when $\lambda_1 = ... = \lambda_c = d, \lambda_{c+1} = ... = \lambda_{2c} = -d, \lambda_{2c+1} = ... = \lambda_n = 0$. Thus the upper bound given by,

$$\mathrm{maxinj}(C_6, G) \leq \max\left(f(\lambda)\right) + \max\left(-3 \cdot \hom(B, G) + 9 \cdot \hom(K_4 \setminus e, G)\right),$$

where $f(\lambda)$ is the spectral term in $(*)$ is attained. □

As k grows, more non-spectral terms appear and more inequalities between homomorphsim numbers are needed. As a result, it is hard to come up with a scheme that does this for all k. In fact, in [4], it was shown that any linear inequality between homomorphism densities, which are defined using homomorphism numbers, can be shown using a (possibly infinite) number of Cauchy-Schwarz inequalities. However, deciding whether such an inequality is true is indeterminable. Thus, we introduce the notion of a non-backtracking, respectively backtracking, homomorphism number and use non-backtracking spectral theory developed in [1, 2, 3].

2 Non-backtracking Homomorphisms

A homomorphism $\phi : V(H) \to V(G)$ is a non-backtracking homomorphism if for each vertex $u \in G$, each neighbor of u has distinct images. That is, ϕ is a non-backtracking homomorphism if

$$\forall u \in V(H), \forall v, w \in N(u), \phi(v) \neq \phi(w).$$

Denote the number of non-backtracking homomorphisms from H to G as $\mathrm{nob}(H, G)$. We see that, $\hom(H, G) \geq \mathrm{nob}(H, G) \geq \mathrm{inj}(H, G)$. We give a relation between these quantities.

Proposition 10. *For graphs H, G, we have*

$$\mathrm{nob}(H, G) = \sum_{Q} \mathrm{inj}(H/Q, G),$$

where Q ranges over all partitions of G where each part is an independent set with no common neighbors.

Proof. For any partition Q and any injective homomorphism of H/Q, we get exactly one non-backtracking homomorphism of H. It is exactly the one where the vertices $v_i \in H$ that are in the part of Q represented by $v \in H/Q$ are mapped to the same vertex that v is mapped to in the injective homomorphism. There are no other non-backtraccking homomorphisms because any partition where some part has a common neighbor, the resulting homomorphism from $H \to G$ will be backtracking. □

Similarly, we can denote $\mathrm{bac}(H, G)$ as the number of backtracking homomorphisms from H to G. A backtracking homomorphsism is a homomorphsism that is not non-backtracking. Clearly, we have,

$$\hom(H, G) = \mathrm{nob}(H, G) + \mathrm{bac}(H, G) = \sum_{P} \mathrm{inj}(H/P, G) \implies \mathrm{bac}(H, G) = \sum_{S} \mathrm{inj}(H/S, G),$$

where S ranges over partitions of $V(H)$ with common neighbors in some part. Note that a Möbius inversion relation like in Lemma 4 does not hold. However, if we label the vertices and edges of the quotients and define neighbors in a way that considers the labeling, then such an inversion holds.

2.1 Maximizing Non-backtracking and Backtracking

We can count the number of closed non-backtracking walks of length k of G with the following results from [1, 2, 3]. In the latter, it was shown that there is a closed form for the non-backtracking spectrum in terms of the ordinary spectrum of G. Consider the directed graph $\tilde{G} = (\tilde{V}, \tilde{E})$ where $|\tilde{V}| = 2|E|$, where each vertex is represented by $(u, v) \subset E$. Then, we have $\tilde{E} = \{(u, v), (x, y) : v = x, u \neq y\}$. The non-backtracking matrix of G, denoted B, is the adjacency matrix of $\tilde{G}$, which is given by,

$$B_{(u,v),(x,y)} = \begin{cases} 1, & \text{if } v = x, u \neq y \\ 0, & \text{otherwise} \end{cases}.$$

Note that each distinct directed closed walk of $\tilde{G}$ corresponds to a unique non-backtracking walk of G of the same length. Thus, the number of closed non-backtracking walks of length k of G is equal to $\mathrm{tr}(B^k)$. Furthermore, we have the following result.

Proposition 11. *Let G be a d-regular graph. Then, the eigenvalues of B are*

$$\pm 1, \frac{\lambda_i \pm \sqrt{\lambda_i^2 - 4(d-1)}}{2},$$

where λ_i are the eigenvalues of A and ± 1 each have multiplicity $m - n$, where m is the number of edges in G [3].

In general, by the binomial theorem, the problem of finding the graph with the most non-backtracking closed walks of length k becomes:

$$\max_{\lambda} \sum_{i=1}^{n} \left(\frac{\lambda_i + \sqrt{\lambda_i^2 - 4(d-1)}}{2} \right)^k + \left(\frac{\lambda_i - \sqrt{\lambda_i^2 - 4(d-1)}}{2} \right)^k$$

$$= \max_{\lambda} \sum_{j=1}^{n} \sum_{i=1}^{\lfloor k/2 \rfloor} \binom{k}{2i} 4 \left(\frac{\lambda_j}{2} \right)^{k-2i} \frac{(\lambda_j^2 - 4(d-1))^i}{2^{2i}}, \text{ s.t. } \sum_{i=1}^{n} \lambda_i = 0, \sum_{i=1}^{n} \lambda_i^2 = nd, \lambda_{\max} = d, |\lambda_i| \leq d.$$

Note that the objective function above is always real as $z^k + \overline{z}^k = z^k + \overline{(z^k)} = 2\mathrm{Re}(z^k)$. This is a sum of polynomials with positive leading coefficient and satisfies the assumptions of Lemma 1.

Theorem 12. *For odd k, sufficiently large d, and $n = c(d+1)$, the d-regular graph on n vertices with the most non-backtracking closed walks of length k is c copies of K_{d+1}.*

For even k, sufficiently large d and $n = 2cd$, the d-regular graph on n vertices with the most non-backtracking closed walks of length k is c copies of $K_{d,d}$.

Proof. By Lemma 1, the solution of the optimization problem is the spectrum for these graphs. □

We now find $\max_G \mathrm{bac}(C_k, G)$. The number of backtracking walks of length k is the sum of those that backtrack once, those that backtrack twice, thrice, and so on. Denote $\mathrm{bac}_{i_1,i_2,\ldots,i_\ell}(C_k, G)$ as the number of backtracking homomorphisms that backtrack $i = \sum_j^\ell i_j$ times where i_j denotes the length of the jth consecutive backtracking streak. We compute,

$$\mathrm{bac}(C_k) = \sum_{i=1}^{n} \sum_{i_1+\ldots i_\ell = i} \mathrm{bac}_{i_1,i_2,\ldots,i_\ell}(C_k) = \sum_{i=1}^{n} \sum_{i_1+\ldots+i_\ell = i} \hom(H_{i_1,\ldots,i_\ell}) = \sum_{i=1}^{n} \sum_{i_1+\ldots+i_\ell = i} d^a \sum_{j=1}^{n} \lambda_j^{k-i},$$

where $H_{i_1,\ldots,i_\ell}$ is C_{k-i} with a antennas with $a = (\#\text{ odd length streaks in } i_1, i_2, \ldots, i_\ell)$. This is maximized at the desired spectrum by Lemma 1 because every coefficient is positive. Thus, we have the following result.

Proposition 13. *For d sufficiently large, the d-regular graph on $n = c(d+1)$ vertices with the most closed backtracking walks of odd length k is c copies of K_{d+1}. Similarly, for sufficiently large d, if $n = 2cd$ and k is even, then the optimal graph is c copies of $K_{d,d}$.*

Proof. Using the above equation as the objective function with the same constraints as before, by Lemma 1, gives the spectra of K_{d+1}, or $K_{d,d}$ respectively, as the optimizer. □

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