

Maximal Number of k -cycles in a d -regular Graph

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Abstract

We construct the d -regular graph with the maximum number of k -cycles for $k = 5, 6$.

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 $\text{tr}(A^k)$.

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 $K_{d,d}$.

Additionally, we introduce and give formulas for non-backtracking homomorphism numbers and backtracking homomorphism numbers, respectively. Moreover, we find the 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.

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 $K_{d,d}$.

1 Introduction

Let $G = (V, E)$ be a simple d -regular graph on n vertices. For convenience, we will assume that n is nice. For example, always a multiple of $d + 1$. This is not a big assumption as for large n , we will get many copies of the optimal graph and a vanishingly small remainder component.

The main problem that is tackled in this paper is that of finding the d -regular graph on n vertices with the most k -cycles for any $d, n, k \in \mathbb{N}$.

The rest of this paper is structured as follows: the rest of Section 1 presents our main results, gives a proof overview, and discusses recent and relevant research developments. Section 2 gives proof of the main problem for $k = 5$ and $k = 6$. Then, Section 3, introduces non-backtracking and backtracking homomorphism numbers and relates them to homomorphism numbers and injective homomorphism numbers. We also find the graph with the most closed non-backtracking (and backtracking) walks of length k .

1.1 Results

Theorems 1.1.1 and 1.1.2 solve our main problem for the cases of 5-cycles and 6-cycles.

Theorem 1.1.1. *Let $d > 3$ and $n = c(d + 1)$, the d -regular graph on n vertices with the most 5-cycles is c copies of K_{d+1} .*

Theorem 1.1.2. *Let $d > 5$ and $n = 2cd$, the d -regular graph on n vertices with the most 5-cycles is c copies of $K_{d,d}$.*

To attempt solving for the general case, we introduce the notion of a non-backtracking homomorphism in Section 3. In [6], $\text{hom}(H, G)$ and $\text{inj}(H, G)$ are introduced to denote the number of (injective) homomorphisms between H and G . We denote the number of non-backtracking homomorphisms, respectively backtracking homomorphisms, from H to G as $\text{nob}(H, G)$ and $\text{bac}(H, G)$, respectively. We show the following relations.

Theorem 1.1.3.

$$\text{nob}(H, G) = \sum_Q \text{inj}(H/Q, G),$$

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

We use this to show general theorems for closed non-backtracking walks and closed backtracking walks.

Theorem 1.1.4. *Let k be odd and $n = c(d + 1)$. Then, the d -regular graph on n vertices with the most non-backtracking closed walks of length k is c copies of K_{d+1} .*

If k is even and $n = 2cd$, then the d -regular graph on n vertices is c copies of $K_{d,d}$.

Lemma 1.1.5. *Let $n = c(d + 1)$ and k be odd. Then, the d -regular graph on n vertices with the most closed backtracking walks of length k is c copies of K_{d+1} .*

Similarly, if $n = 2cd$ and k is even, then the optimal graph is c copies of $K_{d,d}$.

1.2 Proof Overview

Let $\text{hom}(H, G)$ denote the number of homomorphisms from H to G . Similarly, let $\text{inj}(H, G)$ be the number of injective homomorphisms from H to G . In the language of homomorphism numbers, our task is to find the maximizer of $\max_G \text{inj}(C_k, G)$. In [6], Lovasz showed the following relation between these two numbers.

Proposition 1.2.1.

$$\text{inj}(H, G) = \sum_P \mu_P \text{hom}(H/P, G),$$

where P ranges over all partitions of $V(H)$ and

$$\mu_P = (-1)^{v(G)-|P|} \prod_{S \in P} (|S| - 1)!,$$

where $|P|$ is the number of classes in P and S are the classes in P . [6]

We use this and the fact that

$$\text{hom}(C_k, G) = k! \text{tr}(A^k) = k! \sum_{i=1}^n \lambda_i^k$$

to get a continuous optimization problem on the spectrum of the graph. This method is used in 1.1.1, 1.1.2, 1.1.4, and 1.1.5. it is remarkable that the solutions to these optimization problems give eigenvalues of graphs, which is not a priori the case.

For 1.1.4, we use the non-backtracking spectrum, which is introduced in [3]. We use an analogous version of the fact that the number of closed walks of length k is $\text{tr}(A^k)$.

Proposition 1.2.2. *Let G be a d -regular graph. Then, the number of closed non-backtracking walks of length k is equal to*

$$\sum_{i=1}^n \left(\frac{\lambda_i + \sqrt{\lambda_i^2 - 4(d-1)}}{2} \right)^k + \left(\frac{\lambda_i - \sqrt{\lambda_i^2 - 4(d-1)}}{2} \right)^k. [3]$$

We use this to solve a similar type of constrained optimization problem to get 1.1.4. For backtracking homomorphisms, we notice that backtracking homomorphisms on a cycle are homomorphisms on smaller cycles with antennas. The size and number of antennas of this graph depends on the number of backtrackings and how many of them are consecutive.

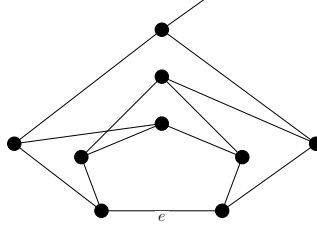
1.3 Discussion

It was showed in [5] that copies of K_{d+1} gives the optimal amount of triangles. They additionally proved that as $n \rightarrow \infty$, for any $\epsilon > 0$, any graph with an ϵ fraction of the maximum possible number of triangles, looks like disjoint copies of K_{d+1} and one small component almost surely.

They show the first of these results by maximizing the number of triangles going through one edge and showing that K_{d+1} gives every edge the maximum amount of triangles. This same method works for $k = 4$ and copies of $K_{d,d}$. We now use this method for $k = 5$ and $d = 3$.

Proposition 1.3.1. *Let $n = 10c$. Then, the 3-regular graph on n vertices with the most 5-cycles is c copies of the Petersen graph.*

Proof. Consider a 3-regular graph with an edge e 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, a 3-regular graph with 10 5-cycles going through every edge would be optimal. The Petersen graph achieves this. $\square$



This method becomes impractical for larger d and k . Thus, we turn to homomorphism numbers and injective homomorphism numbers. This allows us to solve the problem for $k = 5$. However, for $k \geq 6$, after applying 2.0.3 we get terms that are not expressible using the spectrum of the graph. For $k = 6$, we are able to show an inequality between these non-spectral terms. However, as k grows, more non-spectral terms appear and more inequalities between homomorphism 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 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] to show 1.1.4.

Proposition 1.3.2. *Let $A^{(k)}$ be a sequence of matrices such that*

$$\begin{cases} A^{(1)} = A \\ A^{(2)} = A^2 - dI \\ A^{(k+1)} = AA^{(k)} - (d-1)A^{(k-1)}, \quad k = 2, 3, \dots \end{cases}$$

Then, the number of non-backtracking walks of length k from i to j is $A_{ij}^{(k)}$. Moreover, the number of non-backtracking closed walks of length k of G is $\text{tr}(A^{(k)})$. [1]

In [3], 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 $\text{tr}(B^k)$. Furthermore, we have the following result.

Proposition 1.3.3. *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 .

1.2.2 follows from this.

2 Proof for 5-cycles and 6-cycles

In this section, we find $\max_G \text{inj}(C_k, G)$. To do this, we first consider $\max_G (C_k, G)$.

Lemma 2.0.1. *For odd k and $n = (c+1)$, 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,

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

$\lambda_1 = \dots = \lambda_{n/c} = d$, $\lambda_{n/c+1} = \dots = \lambda_n = -1$ is a maximizer. 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. If there are less than n/c variables with $\lambda_i = d$, then increasing one of the other variables to d while decreasing the others equally would result in a greater value. If there are more than n/c variables equal to d , then we can decrease one of them and increase the rest of the variables equally and obtain a more optimal output. Thus, there must be exactly n/c variables equal to d . The rest must sum to $-dn/c$. If they are not equal, we can always find some $\lambda_i > -1$ and $\lambda_j < -1$. Without loss of generality, $|\lambda_i| \leq |\lambda_j|$. We can decrease $\lambda_i \rightarrow -1$ and increase λ_j equally. This will be more optimal. Thus, $\lambda_1 = \dots = \lambda_{n/c} = d$, $\lambda_{n/c+1} = \dots = \lambda_n = -1$ is a maximizer. The graph consisting of c copies of K_{d+1} has this spectrum and is thus optimal. $\square$

For the other optimization problems, a similar argument can be used to find the solutions. For even k we consider the same optimization problem. However, in this case, we want to make negative eigenvalues large. So, we get a different optimal graph.

Lemma 2.0.2. *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 Lemma 5. $\lambda_1 = \dots = \lambda_{n/c} = d, \lambda_{n/c+1} = \dots = \lambda_{2n/c} = -d, \lambda_{2n/c+1} = \dots = \lambda_n = 0$ is a maximizer since it is optimal to have as many $\pm d$ values as possible. The second constraint determines how many of these are possible. The graph with c copies of $K_{d,d}$ has this spectrum. $\square$

It is remarkable that there are 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.

The following equation relates $\text{hom}(H, G)$ and $\text{inj}(H, G)$ using the Möbius inverse of the partition lattice. The next lemma is equation 5.18 from [6].

Lemma 2.0.3.

$$\text{inj}(H, G) = \sum_P \mu_P \text{hom}(H/P, G),$$

where P ranges over all partitions of $V(F)$ and

$$\mu_P = (-1)^{v(G)-|P|} \prod_{S \in P} (|S| - 1)!$$

where $|P|$ is the number of classes in the partition and S are the classes in P .

We can also get homomorphism numbers from injective homomorphisms numbers.

Lemma 2.0.4.

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

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 that is equivalent to finding the d -regular graph with the most k -cycles.

For the rest of this paper, when the context is clear, we will write $\text{hom}(H) = \text{hom}(H, G)$.

2.1 Main result for 5-cycles

Proposition 2.1.1. *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 2.0.3, we calculate

$$\text{inj}(C_5, G) = \text{hom}(C_5) - 5\text{hom}(K_3 + e) + 5\text{hom}(K_3),$$

where the “ $+e$ ” means with an antenna.

Then, since G is d -regular, we have $\text{hom}(K_3 + e) = d\text{hom}(K_3)$. Thus, we consider the optimization problem,

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

For $d > 3$, this is solved when $\lambda_i = \dots = \lambda_c = d$ and $\lambda_{c+1}, \dots, \lambda_n = -1$. 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, which gives us 1.3.1. $\square$

2.2 Main result for 6-cycles

This method also works for $k = 6$. When using 2.0.3, we notice that quotients that are trees give constant terms for any d -regular G . Hence, we can omit them from any maximization problem. We compute

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

for some $C \in \mathbf{Z}$ where B is the ‘bowtie’ graph. We note that $\text{hom}(B)$ and $\text{hom}(K_4 \setminus e)$ cannot be expressed using eigenvalues. Thus, we make use of the following inequality.

Lemma 2.2.1. *For any G ,*

$$\text{hom}(B) \geq 4\text{hom}(K_4 \setminus e).$$

Proof.

$$\text{hom}(B) = \text{inj}(B) + 4\text{hom}(K_4 \setminus e) + 2\text{hom}(K_3).$$

$\square$

Proposition 2.2.2 (6-cycles). *Let $d > 5$ and $n = 2cd$. The d -regular graph on n vertices with the most 6-cycles is c copies of $K_{d,d}$.*

Proof. Since $\text{hom}(B, G) \geq 4\text{hom}(K_4 \setminus e, G)$, we have that the term outside of the sum in (1) is non-positive and thus maximized when it is zero. Note that if G is bipartite, then this value is zero. The spectral part of 1 is maximized when $\lambda_1 = \dots = \lambda_c = d, \lambda_{c+1} = \dots = \lambda_{2c} = -d, \lambda_{2c+1} = \dots = \lambda_n = 0$. Thus the upper bound given by

$$\max f(\lambda) - 3\text{hom}(B, G) + 9\text{hom}(K_4 \setminus e, G) \leq \max(f(\lambda)) + \max(-3\text{hom}(B, G) + 9\text{hom}(K_4 \setminus e, G)),$$

where $f(\lambda)$ is the spectral term, is attained. $\square$

3 Non-backtracking Homomorphisms

We can count the number of closed non-backtracking walks of length k of G with the following results from [1, 2, 3].

Proposition 3.0.1. *Let $A^{(k)}$ be a sequence of matrices such that*

$$\begin{cases} A^{(1)} = A \\ A^{(2)} = A^2 - dI \\ A^{(k+1)} = AA^{(k)} - (d-1)A^{(k-1)}, \quad k = 2, 3, \dots \end{cases}$$

Then, the number of non-backtracking walks of length k from i to j is $A_{ij}^{(k)}$. Moreover, the number of non-backtracking closed walks of length k of G is $\text{tr}(A^{(k)})$. [1]

In [3], 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 $\text{tr}(B^k)$. Furthermore, we have the following result.

Proposition 3.0.2. *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 the problem becomes:

$$\begin{aligned} & \max_{\lambda} \sum_{i=1}^n \left(\frac{\lambda_i + \sqrt{\lambda_i^2 - 4(d-1)}}{2} \right)^k + \left(\frac{\lambda_i - \sqrt{\lambda_i^2 - 4(d-1)}}{2} \right)^k \\ & \text{subject to } \sum_{i=1}^n \lambda_i = 0, \sum_{i=1}^n \lambda_i^2 = nd, \lambda_{\max} = d, |\lambda_i| \leq d. \end{aligned}$$

Although the eigenvalues of B may be complex, the objective function above is always real as $z^k + \bar{z}^k = z^k + \overline{(z^k)} = 2\text{Re}(z^k)$.

Using the binomial theorem, we compute:

$$\begin{aligned} & \sum_{i=1}^n \left(\frac{\lambda_i + \sqrt{\lambda_i^2 - 4(d-1)}}{2} \right)^k + \left(\frac{\lambda_i - \sqrt{\lambda_i^2 - 4(d-1)}}{2} \right)^k \\ &= \sum_{j=1}^n \sum_{i=0}^k \binom{k}{i} 2 \left(\frac{\lambda_j}{2} \right)^{k-i} \left[\left(\frac{\sqrt{\lambda_j^2 - 4(d-1)}}{2} \right)^i + \left(-\frac{\sqrt{\lambda_j^2 - 4(d-1)}}{2} \right)^i \right] \\ &= \sum_{j=1}^n \sum_{i=1}^{\lfloor k/2 \rfloor} \binom{k}{2i} 4 \left(\frac{\lambda_j}{2} \right)^{k-2i} \frac{(\lambda_j^2 - 4(d-1))^i}{2^{2i}}. \end{aligned}$$

Similar to before, for odd k , we want small negative eigenvalues and large positive ones

Theorem 3.0.3. *For odd k 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} .*

Proof. The solution of the optimization problem is the spectrum for this graph as the derivative of the objective is much larger near d than it is near -1 or any other point. $\square$

Notice that if k is even, to maximize the objective, we need to make the $|\lambda_j|$ as large as possible. Thus,

Theorem 3.0.4. *For even k 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. $\lambda_1 = \dots = \lambda_c = d, \lambda_{c+1}, \dots = \lambda_{2c}, \lambda_{2c+1}, \dots, \lambda_n = 0$ is the solution to the optimization problem above by reasoning similar to Lemmas 5 and 6. We can see that the derivative of the objective is much larger near $-d$ and d than it is at any other point. $\square$

3.1 Maximizing Backtracking

We now find $\max_G \text{bac}(C_k, G)$. 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 $\text{bac}_{i_1, i_2, \dots, i_\ell}(C_k, G)$ as the number of backtracking homomorphisms that backtrack $i = \sum_{j=1}^{\ell} i_j$ times where i_j denotes the length of the j th backtracking streak.

In general we have to compute

$$\text{bac}(C_k) = \sum_{i=1}^n \sum_{i_1 + \dots + i_\ell = i} \text{bac}_{i_1, i_2, \dots, i_\ell}(C_k)$$

$$= \sum_{i=1}^n \sum_{i_1+\dots+i_\ell=i} \text{hom}(H_{i_1,\dots,i_\ell}) = \sum_{i=1}^n \sum_{i_1+\dots+i_\ell=i} d^a \sum_{j=1}^n \lambda_j^{k-i}$$

where $H_{i_1,\dots,i_\ell}$ is C_{k-i} with ($\#$ odd length streaks in $i_1, i_2, \dots, i_\ell$) = a antennas.

This is maximized at the desired spectrum because every coefficient is positive. Thus, we have the following result.

Proposition 3.1.1. *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, 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 gives the spectra of K_{d+1} , or $K_{d,d}$ respectively, as the optimizer. $\square$

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