Cycle-maximal triangle-free graphs

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Abstract

We conjecture that the balanced complete bipartite graph $K_{\lfloor n/2\rfloor,\lceil n/2\rceil}$ contains more cycles than any other n-vertex triangle-free graph, and we make some progress toward proving this. We give equivalent conditions for cycle-maximal triangle-free graphs; show bounds on the numbers of cycles in graphs depending on numbers of vertices and edges, girth, and homomorphisms to small fixed graphs; and use the bounds to show that among regular graphs, the conjecture holds. We also consider graphs that are close to being regular, with the minimum and maximum degrees differing by at most a positive integer k. For $k = 1$, we show that any such counterexamples have $n \leq 91$ and are not homomorphic to C_5; and for any fixed k there exists a finite upper bound on the number of vertices in a counterexample. Finally, we describe an algorithm for efficiently computing the matrix permanent (a $\#P$-complete problem in general) in a special case used by our bounds.

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1. Introduction

Many algorithmic problems that are computationally difficult on graphs can be solved easily in polynomial time when the graph is acyclic. Limiting input to trees (connected acyclic graphs) or forests (acyclic graphs), however, is often too restrictive; many of these problems remain efficiently solvable when the graph

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is "nearly" a tree [6, 7, 8, 21]. Various notions exist formalizing how close a given graph is to being a tree, including bounded treewidth (partial k-trees), k-connectivity, and number of cycles.

The problem of evaluating $c(G)$ for a given graph is $\#P$-complete, equivalent in difficulty to counting the certificates of an NP-complete decision problem, even though the problem of testing for the existence of a single cycle is trivially polynomial-time. Existence of a cycle is a graph property definable in monadic second-order logic. By the result known as Courcelle's Theorem [15], such properties can be decided in linear time for graphs of bounded treewidth, and as described by Arnborg, Lagergren, and Seese, the counting versions are also linear-time for fixed treewidth [6]. On the other hand, if we parameterize by length of the cycles instead of structure of the graph, Flum and Grohe [19] give evidence against fixed-parameter tractability: they show that counting cycles of length k is $\#W[1]$-complete, with no $(f(k) \cdot n^c)$-time algorithm unless the Exponential Time Hypothesis fails.

When no restrictions are imposed on the graph, the number of cycles in an n-vertex graph is maximized by the complete graph on n vertices, K_n. In this case the number of cycles is easily seen to be

$$\sum_{i=3}^{n} \left(\binom{n}{i} \frac{(i-1)!}{2} \right) = n! \sum_{i=3}^{n} \frac{1}{2i(n-i)!} \,. \tag{1}$$

The bound (1) can be refined by introducing additional parameters. Previous results include bounds on the number of cycles in terms of n, m, δ, and Δ (the number of vertices, number of edges, minimum degree, and maximum degree of G, respectively) [16, 20, 36], as well as bounds on the number of cycles for various classes of graphs, including k-connected graphs [25], Hamiltonian graphs [29, 33], planar graphs [1, 2], series-parallel graphs [27], and random graphs [34].

A graph's cycles can be classified by length. For each value of i, the summand in (1) corresponds to the number of cycles of length i in K_n. If short cycles are disallowed, the number of long cycles possible is also reduced. Every graph G of girth g that contains two or more cycles has $n \geq 3g/2 - 1$ vertices or, equivalently, if $g > 2(n+1)/3$, then G has at most one cycle [9]. The bound on the number of cycles increases as g decreases. As mentioned earlier, the case $g = 3$ is maximized by K_n for which the number of cycles is exactly (1). Can the maximum number of cycles be expressed exactly or bounded tightly as a function of arbitrary values for n and g? Even when $g = 4$ the maximum number of possible cycles is unknown. Graphs of girth four or greater are exactly the triangle-free graphs. One goal of this research program is to show that the number of cycles in a triangle-free n-vertex graph is maximized by the complete bipartite graph $K_{\lfloor n/2 \rfloor, \lceil n/2 \rceil}$, and the results in this paper represent significant progress toward that goal.

We first encountered the problem of bounding the number of cycles as a function of n and g when examining path-finding algorithms on graphs. A tree traversal can be achieved by applying a right-hand rule (e.g., after reaching a vertex v via its ith edge, depart along its $(i+1)$st edge). Traversing a graph using

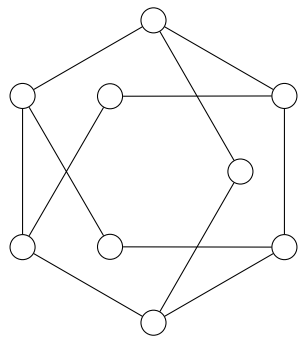

Figure 1: The Petersen graph minus one vertex, which contains a C_6 that cannot be bridged without creating a triangle.

only local information at each vertex is significantly more difficult in graphs with cycles. A successful traversal can be guaranteed, however, if the local neighbourhood of every vertex v is tree-like within some distance k from v (e.g., the graph has girth $g \geq 2k+1$) and that a fixed upper bound is known on the number of possible cycles along paths that join pairs of leaves outside each such local tree (Bose, Carmi, and Durocher [9] give a more formal discussion). Deriving a useful bound on this number of cycles led to the work presented in this paper.

In any graph, every chordless cycle of length seven or greater can be bridged by the addition of a chord without creating any triangles. Similarly, in any graph of girth six or greater, any given cycle can be bridged without creating any triangles. There exist graphs of girth four and five, however, that contain cycles of length six that cannot be bridged without creating a triangle. The Petersen graph minus one vertex, as shown in Figure 1, is such a graph of girth five; replacing one of its vertices with two sharing the same neighbourhood results in a graph of girth four with the same property. To increase the number of cycles in a graph, large chordless cycles can be bridged greedily until the graph is triangle-free but the addition of any edge would create a triangle. This suggests that a cycle-maximal triangle-free graph should contain many cycles of length four or five. Since bipartite graphs are triangle free, complete bipartite graphs and, more specifically, balanced bipartite graphs are natural candidates for maximizing the number of cycles. We verified the following conjecture to be true by exhaustive computer search for $n \leq 13$:

Conjecture 1.1. The cycle-maximal triangle-free graphs are exactly the bipartite Turán graphs, $K_{\lfloor n/2 \rfloor, \lceil n/2 \rceil}$ for all n.

1.1. Overview of results

Our main results, Theorems 4.2 and 5.2, show that Conjecture 1.1 holds for all regular cycle-maximal triangle-free graphs, and all near-regular cycle-maximal triangle-free graphs with greater than 91 vertices. In Section 2 we give some properties of cycle-maximal graphs. In Section 3 we establish bounds on the number of cycles in triangle-free graphs. In Section 4 we prove Theorem 4.2, and in Section 5 we prove Theorem 5.2. Section 6 describes an algorithm for computing the matrix permanent, which is used in our bounds.

1.2. Definitions and notation

Graphs are simple and undirected unless otherwise specified. A *block* in a graph G is a maximal 2-connected subgraph of G. Given a graph G, let $V(G)$, $E(G)$, $\delta(G)$, and $\Delta(G)$ denote, respectively, the vertex set of G, edge set of G, minimum degree of any vertex in G, and maximum degree of any vertex in G. Given a vertex $v \in V(G)$, let $N(v)$ denote the neighbourhood of v; that is, the set of all vertices adjacent to v in G. Given positive integers s and t, let K_s denote the complete graph on s vertices, $K_{s,t}$ denote the complete bipartite graph with part sizes s and t, C_s denote the cycle of s vertices, and P_s denote the path of s vertices. Given a positive integer n, let $T(n, 2)$ represent the bipartite Turán graph on n vertices, that is, $K_{\lfloor n/2\rfloor,\lceil n/2\rceil}$.

A graph is *triangle-free* if it does not contain C_3 (a *triangle*) as a subgraph. The *girth* of a graph is the size of the smallest cycle, by convention ∞ if there are no cycles. Triangle-free is equivalent to having girth at least 4. A graph G is *maximal triangle-free* if it is triangle-free, but adding any edge would create a triangle. Let $c(G)$ denote the number of labelled cycles in G. That is the number of distinct subsets of $E(G)$ that are cycles; note we are not only counting distinct cycle *lengths*, which may also be interesting but is a completely different problem. Then G is *cycle-maximal* for some class of graphs and number of vertices n if G maximizes $c(G)$ among n-vertex graphs in the class. Most often we are interested in cycle-maximal graphs for fixed minimum girth g, especially the case $g \geq 4$, *cycle-maximal triangle-free* graphs. It is easy to prove (see Lemma 2.4) that a cycle-maximal triangle-free graph, if large enough to have any cycles at all, is also maximal triangle-free.

A graph G is *homomorphic* to a graph H when there exists a function $f : V(G) \to V(H)$, called a *homomorphism*, such that if $(u, v) \in E(G)$ then $(f(u), f(v)) \in E(H)$. A graph is s-colorable if and only if it is homomorphic to K_s. Given a positive integer t and a graph H, let $H(t)$ represent the uniform *blowup* of H: that is the graph homomorphic to H formed by replacing the vertices in H with independent sets, each of size t, and adding edges between all vertices in two independent sets if the sets correspond to adjacent vertices in H. If H has p vertices, then $H(t)$ has pt vertices. When H is a labelled graph with p vertices $v_1, v_2, \dots, v_p$, let $H(n_1, n_2, \dots, n_p)$ represent the not necessarily uniform blowup of H in which v_1 is replaced by an independent set of size n_1, v_2 by an independent set of size n_2, and so on, with all edges added that are allowed by the homomorphism.

We define the family of *gamma graphs* as follows. For any positive integer i, Γ_i is a graph with $n = 3i-1$ vertices $v_1, v_2, \dots, v_n$. Each vertex v_j is adjacent to the i vertices $v_{j+i}, v_{j+i+1}, \dots, v_{j+2i-1}$, taking the indices modulo n. For $i \geq 2$, this is the complement of the $(i-1)$st power of the cycle graph C_{3i-1}. Then

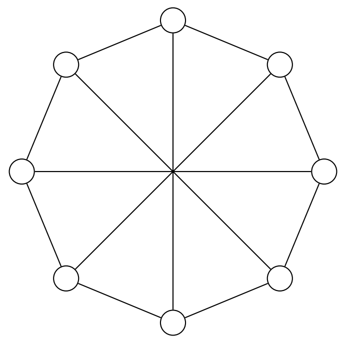

Figure 2: The Möbius ladder Γ_3.

Γ_1 is K_2, Γ_2 is C_5, and Γ_3 is the eight-vertex Möbius ladder, or twisted cube, shown in Figure 2.

A few relevant pieces of notation from outside graph theory will be used. Let $\Gamma(z)$ represent the usual gamma function (generalized factorial); $n! = \Gamma(n+1)$ for integer n, but the gamma function is also well-defined for arbitrary complex arguments. We will use it only for nonnegative reals, but not only for integers. The similarity of notation between $\Gamma(n+1)$ and Γ_i is unfortunate, but these are widely-used standard symbols for these concepts. Some authors also use $\Gamma(v)$ for the neighbourhood of a vertex v; we avoid that here.

For positive integers n and m, let I_n denote the $n \times n$ identity matrix, and $J_{n,m}$ denote the $n \times m$ matrix with all entries equal to 1. Given an $n \times n$ square matrix A, let $\operatorname{perm} A$ denote the *permanent* of A. That is the sum, over all ways to choose n entries from A with one in each row and one in each column, of the product of the chosen entries. Note that the definition of the permanent is the same as the definition of the determinant without the alternating signs.

1.3. Related work

A number of previous results examine the problem of characterizing cycle-maximal graphs and bounding the number of cycles as a function of girth, degree, or the number of edges for various classes of graphs. Entringer and Slater [16] show that some n-vertex graph with m edges has at least 2^{m-n} cycles and every such graph has at most 2^{m-n+1} cycles. Aldred and Thomassen [1] improve the upper bound to $(15/16)2^{m-n+1}$. Guichard [20] examines bounds on the number of cycles to which any given edge can belong, including a discussion of cubic graphs and triangle-free graphs. Alt *et al.* [2] show that the maximum number of cycles in any n-vertex planar graph is at least 2.27^n and at most 3.37^n. Buchin *et al.* [13] improve these bounds to 2.4262^n and 2.8927^n, respectively. De Mier and Noy [27] examine the maximum number of cycles in outerplanar and series-parallel graphs. Knor [25] examines bounds on the maximum number of cycles in k-connected graphs, including bounds expressed in terms of the minimum and maximum degrees. Markström [26] presents results of a computer search examining the minimum and maximum numbers of cycles as a function of girth and the number of edges in small graphs.

Several results in extremal graph theory examine bounds on triangle-free graphs. Andrásfai *et al.* [4] show that every n-vertex graph that has chromatic number r but does not contain K_r as a subgraph has minimum degree at most $n(3r-7)/(3r-4)$. Brandt [10] examines the structure of triangle-free graphs with minimum degree at least $n/3$. Brandt and Thomassé [11] show that every triangle-free graph with minimum degree greater than $n/3$ has chromatic number at most four. Jin [24] gives an upper bound on the minimum degree of triangle-free graphs with chromatic number four or greater. Pach [28] characterizes triangle-free graphs in which every independent set has a common neighbour: a triangle-free graph has that property if and only if it is a maximal triangle-free graph homomorphic to some Γ_i. Brouwer [12] provides a simpler proof of Pach's result.

2. Properties of triangle-free and cycle-maximal graphs

This section lists some properties of graphs that we will use in subsequent sections. Most of the proofs are simple, or already given by others, but we describe them for completeness.

First, consider the gamma graphs defined in Subsection 1.2. This family of graphs recurs throughout the literature on maximal triangle-free graphs. They seem to have been first introduced in 1964 by Andrsfai [3]. Notation and the order of labelling the vertices varies among authors; we follow Brandt and Thomassé [11] here. All the Γ_i graphs are i-regular, circulant, and three-colorable. As the following lemma describes, the Γ_i graphs form a hierarchy in which each one is homomorphic to the next one, and deleting a vertex renders it homomorphic to the previous one.

Lemma 2.1. *For all $i > 1$, Γ_i with one vertex deleted is homomorphic to Γ_{i-1}, and Γ_{i-1} is homomorphic to Γ_i.*

Proof. Let $v_1, v_2, \ldots, v_{3i-1}$ denote the vertices of Γ_i and $w_1, w_2, \ldots, w_{3i-4}$ denote the vertices of Γ_{i-1}. Assume without loss of generality that v_{3i-1} is the vertex deleted from Γ_i. Then define f and F as follows.

$$f(v_j) = \begin{cases} w_j & \text{if } j < i, \\ w_{j-1} & \text{if } i \leq j < 2i, \\ w_{j-2} & \text{if } j \geq 2i; \end{cases}$$

$$F(w_j) = \begin{cases} v_j & \text{if } j < i, \\ v_{j+1} & \text{if } i \leq j < 2i-2, \\ v_{j+2} & \text{if } j \geq 2i-2. \end{cases}$$

By checking their effects on the vertex neighbourhoods, f and F are homomorphisms in both directions between Γ_i with the vertex v_{3i-1} deleted, and Γ_{i-1}. Reinserting the deleted vertex, Γ_{i-1} is also homomorphic to Γ_i. □

Several known results classify triangle-free graphs according to minimum degree. In particular, if a triangle-free graph G has n vertices and minimum degree $\delta(G)$, then

- for every $i \in \{2, 3, \ldots, 10\}$, if $\delta(G) > in/(3i-1)$ then G is homomorphic to Γ_{i-1};
- if $\delta(G) > 2n/5$ then G is bipartite;
- if $\delta(G) > 10n/29$ then G is three-colorable; and
- if $\delta(G) > n/3$ then G is four-colorable.

Jin [23] proves that $\delta(G) > in/(3i-1)$ implies G homomorphic to Γ_{i-1} for all i up to 10. The case $i = 2$, which also implies G is bipartite because $\Gamma_1 = K_2$, was first proved by Andrásfai [3]; a later paper, in English, by Andrásfai, Erdős, and Sós, is often cited for this result [4]. Häggkvist proved the case $i = 3$ [22]. Three-colorability when $\delta(G) > 10n/29$ follows from the three-colorability of Γ_9. Four-colorability when $\delta(G) > n/3$ is due to Brandt and Thomassé [11].

The following property of cycle-maximal graphs applies to graphs of general girth, not only triangle-free graphs: we can limit consideration to 2-connected graphs.

Lemma 2.2. *Let $3 \le g \le n$. Among all n-vertex cycle-maximal graphs for girth at least g, there is one that is 2-connected.*

Proof. Because $g \le n$, there exists a graph with one cycle and these parameters. That graph consists of a cycle of length g and $n - g$ degree-zero vertices. Therefore any cycle-maximal graph for girth at least g contains at least one cycle.

Given a disconnected graph with maximal cycle count, choose a vertex v; then choose one vertex in each connected component other than the one containing v, and add an edge from each of those vertices to v. The resulting connected graph contains all and only the cycles from the original, so it has the same girth and cycle count. Therefore we need only consider connected graphs.

Any block either is a single edge, or contains a cycle; if it is a single edge, it cannot be part of any cycle. We can contract it without removing any cycles nor decreasing the girth, and then insert one new vertex to replace the one we eliminated, in the middle of some edge that is part of a cycle. Therefore we need only consider blocks that contain cycles, necessarily of at least g vertices.

Suppose there is a cut-vertex u. Removing it would disconnect at least two blocks; let v and w be two vertices maximally distant from u that would be disconnected from each other by the removal of u. Each of v and w is at least distance $\lfloor g/2 \rfloor$ from u. Then by adding an edge (v, w), we create at least one new cycle, but none of length less than g. □

In the case of triangle-free graphs, Lemma 2.2 can be strengthened to require 2-connectedness in all cycle-maximal graphs.

Corollary 2.3. *All cycle-maximal triangle-free graphs with at least four vertices are 2-connected.*

Proof. Suppose G is a cycle-maximal triangle-free graph with at least four vertices. Because C_4 contains a cycle, G contains at least one cycle and therefore at least one vertex of degree at least two. If G is disconnected, let u and v be two vertices in distinct components and with the degree of u at least two. Then add edges from v to all neighbours of u. These edges do not create any triangles, but create at least one new cycle through u, v, and two neighbours of u, contradicting the cycle-maximality of G. Therefore G is connected.

Suppose G contains a block that is a single edge. Then as in the proof of Lemma 2.2 we can contract it, removing a vertex while keeping all cycles and not creating any triangles; and then we can add a new vertex v sharing all the neighbours of some vertex u with degree at least two. By doing so we create at least one new cycle through u, v, and two neighbours of u, contradicting the cycle-maximality of G. Therefore G contains no blocks that are single edges. All remaining cases are covered by the last paragraph of the proof of Lemma 2.2. □

The next property is also specific to the triangle-free case: every edge in a cycle-maximal graph is part of some minimum-length cycle.

Lemma 2.4. *If G is a cycle-maximal triangle-free graph with at least four vertices, then G is maximal triangle-free and every edge in G is in some 4-cycle.*

Proof. Suppose u and v are non-adjacent vertices in G and adding the edge (u, v) would not create a triangle. By 2-connectedness (Corollary 2.3) there exist two edge-disjoint paths from u to v in G, and then adding the edge (u, v) creates at least two new cycles, contradicting cycle-maximality; therefore G is maximal triangle-free.

Suppose (u, v) is an edge in G that is not part of any 4-cycle. Let G' be the graph formed from G by contracting (u, v). This operation cannot create any triangles; and G' contains one less vertex than G and all the cycles of G except any that included both u and v without including the edge (u, v). Let w be the vertex created by the edge contraction; and add a new vertex w' to G' with the same neighbourhood as w. For each cycle in G that used u and v without the edge between them, the new graph contains at least one cycle using w and w' instead; and there is also at least one new 4-cycle through w, w', and two of their neighbours. (They have at least two neighbours because G was 2-connected.) Therefore we have increased the number of cycles for an n-vertex triangle-free graph, contradicting cycle-maximality. Therefore every edge in G is part of some 4-cycle. □

Also note that by a result of Erdős *et al.* [18, Lemma 2.4(ii)], any triangle-free graph (not only maximal or cycle-maximal) with n vertices and m edges has at least one edge contained in at least $4m(2m^2 - n^3)/n^2(n^2 - 2m)$ cycles of length four.

Lemma 2.2 and Corollary 2.3 do not generalize to higher girth. A graph consisting of the Petersen graph plus one vertex added with degree one is cycle-maximal for 11 vertices and girth at least five, but the edge to the added vertex is not in any 5-cycle, nor any cycle at all, and the graph is not 2-connected.

Finally, we list some simple equivalent conditions for cycle-maximal triangle-free graphs to be the Turán graph. Any counterexample to Conjecture 1.1 would have to lack all these properties.

Lemma 2.5. *If G is a cycle-maximal triangle-free graph with $n \geq 4$ vertices, then these statements are equivalent:*

1. *G is the bipartite Turán graph $T(n, 2)$;*
2. *G is complete bipartite;*
3. *G is bipartite;*
4. *G is perfect;*
5. *G contains no induced P_4; and*
6. *for $n \neq 5$, G has minimum degree greater than $2n/5$.*

Proof. The bipartite Turán graph has all the listed properties ($1 \Rightarrow \{2, 3, 4, 5, 6\}$), so it remains to prove the implications in the other direction. By exact cycle count, $T(n, 2)$ maximizes cycles among complete bipartite graphs (see Corollary 3.2; $2 \Rightarrow 1$). If G is bipartite, it is necessarily complete bipartite in order to be maximal triangle-free ($3 \Rightarrow 2$). Triangle-free perfect graphs are bipartite as a trivial consequence of the definition ($4 \Rightarrow 3$). Any graph without an induced P_4 is perfect by a result of Seinsche [32], with a simpler proof given by Arditti and de Werra [5] ($5 \Rightarrow 4$). Any triangle-free graph with minimum degree greater than $2n/5$ is bipartite ($6 \Rightarrow 3$) [3, 4]. □

Our Theorems 4.2 and 5.2 have the effect of adding "G is regular" to the list of equivalent conditions for all even n, and "G is near-regular" for odd $n > 91$.

3. Bounds on cycle counts

In this section we prove bounds on the numbers of cycles in certain kinds of graphs. We have three basic kinds of bounds, each of which admits some variations. First, for the bipartite Turán graph $T(n, 2)$ it is possible to compute the number of cycles exactly for any given n, but the resulting expression is a summation; we also find a reasonably tight closed-form lower bound. We can then rule out potential counterexamples to Conjecture 1.1 by showing upper bounds on the number of cycles in other kinds of graphs. The remaining two kinds of bounds are based on the number of edges, and on homomorphism.

The asymptotic results come from applying Stirling's approximation for the factorial in the following form, which gives precise upper and lower bounds. Note that the approximation is actually an approximation for the gamma function, so we can apply it to non-integer arguments. The approximation is:

$$n \ln n - n + \frac{1}{2} \ln n + \frac{1}{2} \ln 2\pi \leq \ln \Gamma(n+1)\,, \text{ and} \tag{2}$$

$$\ln \Gamma(n+1) \leq n \ln n - n + \frac{1}{2} \ln n + \frac{1}{2} \ln 2\pi + \frac{1}{12} \cdot \frac{1}{n}\,. \tag{3}$$

Our general approach will be to prove bounds on $\ln c(G)$ as a function of n for G in various classes of graphs. The bounds typically take the form $n \ln n - cn + O(\ln n)$ for some constant coefficient $c \geq 1$. These amount to proofs that the number of cycles is on the order of $n!$ divided by some exponential function, with the coefficient of n in $\ln c(G)$ describing the size of the exponential function. Comparing the coefficients suffices to show that one class of graphs has more cycles than another for sufficiently large n; and with more careful attention to the lower-order terms we can bound the values of n that are "sufficiently large," leaving a known finite number of smaller cases to address with other techniques.

3.1. Cycles in $T(n,2)$

It is relatively easy to count cycles in the bipartite Turán graph $T(n,2)$. The following result gives the exact count as a summation, and an asymptotic approximation.

Lemma 3.1. *The number of cycles in $T(n,2)$ is given exactly by*

$$c(T(n,2)) = \sum_{k=2}^{\lfloor n/2 \rfloor} \frac{\lfloor n/2 \rfloor! \lceil n/2 \rceil!}{2k(\lfloor n/2 \rfloor - k)!(\lceil n/2 \rceil - k)!}\,, \tag{4}$$

and satisfies the bound

$$\begin{aligned} \ln c(T(n,2)) &\geq n \ln n - (1 + \ln 2)n + \ln \pi \\ &\approx n \ln n - 1.693147n + 1.44730\,. \end{aligned} \tag{5}$$

Proof. To describe a cycle in the bipartite Turán graph $T(n,2)$, we can start by choosing a value k to be the number of vertices the cycle includes on each side of the bipartite graph. The length of the cycle will be $2k$, and necessarily $2 \leq k \leq \lfloor n/2 \rfloor$. Then we choose a permutation for k of the $\lfloor n/2 \rfloor$ vertices in the smaller part, and a permutation for k of the $\lceil n/2 \rceil$ vertices in the larger part. These choices will describe each possible cycle $2k$ times, because there are k equivalent starting points and two equivalent directions. Therefore we divide by $2k$ to avoid overcounting, and the overall total number of cycles is given by (4).

The term for $k = \lfloor n/2 \rfloor$ is by far the largest, so we can use it alone as a reasonably tight lower bound. The factorials in the denominator become one and drop out. By the properties of the gamma function, $\lfloor n/2 \rfloor! \lceil n/2 \rceil! \geq \Gamma((n/2)+1)^2$, so we can drop the floors and ceilings in the numerator, use gamma instead of factorial, and have a valid lower bound for both even and odd

n. Similarly, replacing $2\lfloor n/2 \rfloor$ by n in the denominator does not increase the bound. We have:

$$c(T(n,2)) \geq \frac{\Gamma((n/2)+1)^2}{n} \,.$$

Applying Stirling's approximation (2) gives (5). ☐

The following corollary confirms the intuition that $T(n,2)$ should have more cycles than a less-balanced complete bipartite graph.

Corollary 3.2. *The graph $T(n,2)$ for $n \geq 4$ is uniquely cycle-maximal among complete bipartite graphs on n vertices.*

Proof. The requirement $n \geq 4$ is to rule out pathological cases in which no cycles are possible at all. Let a and b represent the sizes of the two parts, with $n = a + b$ and assume without loss of generality $a \leq b$. The number of cycles in $K_{a,b}$ is a suitably modified version of (4):

$$\begin{aligned} c(K_{a,b}) &= \sum_{k=2}^{a} \frac{a!b!}{2k(a-k)!(b-k)!} \\ &= \sum_{k=2}^{a} \frac{1}{2k} \cdot (ab) \cdot ((a-1)\cdot(b-1)) \cdots ((a-k+1)\cdot(b-k+1)) \,. \end{aligned}$$

If $b > a + 1$, then subtracting one from b and adding one to a will strictly increase all the factors (ab), $((a-1)\cdot(b-1))$, and so on. Making this change will also add an additional positive term to the sum. Therefore the sum is uniquely maximized when $b \leq a + 1$, which means the graph is $T(n,2)$. ☐

3.2. Cycles as a function of number of edges

It seems intuitively reasonable that more edges should mean more cycles. We can make that more precise by giving an upper bound on number of cycles as a function of number of edges, and therefore (by comparison with the previous bound) a lower bound on number of edges necessary for a graph to potentially exceed the number of cycles in the bipartite Turán graph. First, we define notation for the maximal product of a constrained sequence of integers, which will be used in bounding the cycle count.

Definition 3.3. Let $\Pi(n,m)$, with $2 \leq m \leq \binom{n}{2}$, denote the greatest possible product for any $k < n$ of a sequence of positive integers $c_1, c_2, \ldots, c_k$ with $c_i \leq n - i$ for all $1 \leq i \leq k$ and $\sum_{i=1}^{k} c_i = m$.

The following lemma describes the value of $\Pi(n,m)$.

Lemma 3.4. *If $m = \binom{n}{2}$, then*

$$\Pi(n,m) = (n-1)! \,. \tag{6}$$

If $2 \le m \le 3n-7$*, then*

$$\Pi(n,m) = \begin{cases} 3^{m/3} & \text{for } m \equiv 0 \pmod 3; \\ 4 \cdot 3^{(m-4)/3} & \text{for } m \equiv 1 \pmod 3; \text{ and} \\ 2 \cdot 3^{(m-2)/3} & \text{for } m \equiv 2 \pmod 3\,. \end{cases} \tag{7}$$

If $3n-7 < m < \binom{n}{2}$*, then* $k = n-2$ *and there exist integers* $s \ge 3$ *and* $t \ge 0$ *such that*

$$\Pi(n,m) = (s+1)^t s^{n-s-t}(s-1)!\,. \tag{8}$$

Proof. In the case $m = \binom{n}{2}$, the only sequence satisfying the constraints is $n-1, n-2, \ldots, 1$ and Π is the product of that sequence, giving (6).

Sorting the c_i into nonincreasing order cannot cause them to violate the constraints, so we assume it. Removing a c_i term greater than 3 and replacing it with two terms $c_i - 2$ and 2 will never decrease the product. Removing a term equal to 1 and adding 1 to some other term will always increase the product, as will removing three terms equal to 2 and replacing them with two terms equal to 3. Repeated application of these rules uniquely determines a sequence ending with at most two terms equal to 2, all other terms equal to 3, and if the constraints allow this sequence, then it determines Π, giving (7).

Subtracting 1 from a term $c_i > 3$ and adding 1 to some other term less than $c_i - 1$ will always increase the product. Repeated application of that operation and the operations used for (7), wherever permitted by the constraints, uniquely determines a sequence in the form given by (8). □

Now the Π function is applied to bound the number of cycles.

Lemma 3.5. *If a graph* G *has* n *vertices,* m *edges, and girth at least* g*, then*

$$c(G) \le \Pi(n-1,m)\frac{n^2}{2g}\,, \tag{9}$$

and if $3n-7 < m < \binom{n}{2}$*,*

$$\ln c(G) \le n \ln n - (\alpha - \ln \alpha)n + \frac{5}{2}\ln n + \frac{1}{2}\ln \alpha + \frac{1}{2}\ln\frac{\pi}{2} - \ln g + \frac{1}{12\alpha n}\,, \tag{10}$$

where $\alpha = 1 - \sqrt{1 - 1/n - 2(m+1)/n^2}$*.*

Proof. Suppose we are counting Hamiltonian cycles in a complete graph. We might start at the first vertex, leave via one of its $n-1$ edges, then from the next vertex, choose one of the $n-2$ edges remaining (excluding the one from the first vertex), and so on. At the last vertex, there are no remaining edges to previously unvisited vertices, and we return to the starting point. Overall there are $(n-1)!$ choices of successor vertices, which suffices as an upper bound. Note that $(n-1)!$ is the product of $n-1$ positive integer factors whose sum is exactly the number of edges in the complete graph. Every time we consider an edge as a choice for leaving a vertex, that edge is eliminated from consideration

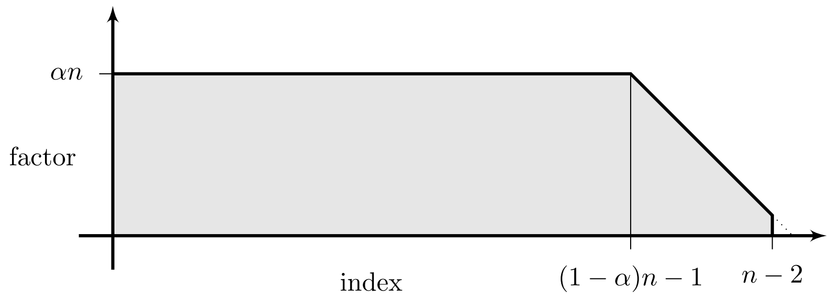

Figure 3: Factors in the upper bound on $\Pi(n,m)$.

for all future vertices, hence the bound on the sum. The last few factors in the sequence are $3, 2, 1$ because we can only visit a previously unvisited vertex and no term can be greater than the number of previously unvisited vertices that remain.

For a more general graph G with n vertices, m edges, girth at least g, and cycles that might not be maximal length, we can follow a similar procedure. There are at most $n-1$ positive integers representing choices of successors of all but the last vertex; their sum is at most m; and if the factors are $c_1, c_2, \ldots, c_k$, the remaining vertex constraint is $c_i \leq n-i$ for all $1 \leq i \leq k$. By definition, $\Pi(n,m)$ is an upper bound on the product of such a sequence.

Since we are not requiring cycles to be Hamiltonian, we cannot assume that any single vertex is the first one in the cycle or is in the cycle at all, so we multiply the bound by n to account for choosing any starting vertex. To account for choosing the length, we multiply by n for choosing which vertex is the last vertex, assume that the cycle closes as soon as it reaches that vertex, and then any remaining choices we may have counted for vertices not in the cycle will only go to make the upper bound a little less tight. Finally, we can remove a small amount of overcounting. With a girth of g (necessarily at least 3) there will be g distinct choices of starting vertex that actually generate the same cycle; and we can always generate each cycle in two equivalent directions. So we can divide by $2g$ and still have a valid upper bound. Multiplying $\Pi(n,m)$ for choices of successors with n^2 for choices of starting and ending vertices, and dividing by $2g$, gives exactly the bound (9).

The form of the sequence c_i that achieves $\Pi(n,m)$ is described in Lemma 3.4. In the case $3n-7 < m < \binom{n}{2}$ (dense but not complete graphs), this sequence is of length $n-2$ and in general is of the form $\lceil \alpha n \rceil, \ldots, \lceil \alpha n \rceil, \lfloor \alpha n \rfloor, \ldots, \lfloor \alpha n \rfloor, \lfloor \alpha n \rfloor - 1, \lfloor \alpha n \rfloor - 2, \ldots, 4, 3, 2$, for some α chosen so that the sum of the sequence is m. Note there is no final factor of 1 counted in the sequence, because adding it to an earlier term gives a greater product. These factors are shown schematically in Figure 3.

If αn is an integer, then this product is $(\alpha n)^{(1-\alpha)n}(\alpha n - 1)!$. The sum is $(\alpha n)(1-\alpha n)n + (\alpha n - 1 + \alpha n - 2 + \cdots + 3 + 2)$. Setting that to m and applying the usual formula for the sum of consecutive integers, we have $(-n^2/2)\alpha^2 +$

$(n^2 - n/2)\alpha - m - 1 = 0$. Solving the quadratic, choosing the solution between 0 and 1, and removing some terms for an upper bound, gives

$$\begin{aligned}\alpha &= 1 - \frac{1}{2n} - \sqrt{1 - \frac{1}{n} + \frac{1}{4n^2} - \frac{2(m+1)}{n^2}} \\ &\leq 1 - \sqrt{1 - \frac{1}{n} - \frac{2(m+1)}{n^2}}\,.\end{aligned}$$

For αn not an integer, removing the floors and ceilings outside the factorial can only increase the product, because making those terms equal maximizes their product given that their sum is fixed. The factorial is at most $\lceil \alpha n - 1 \rceil!$, and changing it to $\Gamma(\lceil \alpha n - 1 \rceil + 1) \leq \Gamma(\alpha n + 1)$ similarly cannot decrease the product. Where $\alpha = 1 - \sqrt{1 - 1/n - 2(m+1)/n^2}$, we have

$$\Pi(n, m) \leq (\alpha n)^{(1-\alpha)n} \Gamma(\alpha n + 1)\,.$$

The result (10) follows by Stirling's approximation (3):

$$\begin{aligned}\ln c(G) &\leq (1-\alpha)n \ln \alpha n + \ln \Gamma(\alpha n + 1) + \ln \frac{n^2}{2g} \\ &\leq n \ln n - (\alpha - \ln \alpha)n + \frac{5}{2} \ln n + \frac{1}{2} \ln \alpha + \frac{1}{2} \ln \frac{\pi}{2} - \ln g + \frac{1}{12\alpha n}\,. \quad \square\end{aligned}$$

A cycle-maximal triangle-free graph G necessarily contains enough edges for (10) to exceed (5). For sufficiently large n, the coefficients of n in the bounds on $\ln c(G)$ will determine which bound is greater; for (10) to exceed (5) requires that $\alpha - \ln \alpha \leq 1 + \ln 2$. Then $\alpha \geq 0.231961\ldots$ and $2m/n$ (the average degree of G) is at least $n(0.410116\ldots)$. Critically, that is greater than $2n/5$. In a graph that is regular, or close to regular in the sense that the difference between minimum and maximum degrees is bounded by some constant, the minimum degree approaches the average and so is also greater than $2n/5$ for sufficiently large n. But any triangle-free graph with minimum degree greater than $2n/5$ is bipartite [3, 4], giving the following corollary.

Corollary 3.6. *Let k be any fixed nonnegative integer and let G be any cycle-maximal triangle-free graph with n vertices and $\Delta(G) - \delta(G) \leq k$. Then for sufficiently large n, G is the bipartite Turán graph.*

In particular, note that $C_5(t)$, which is an important case for many previous results on maximal triangle-free graphs including that of Andrásfai used above [3, 4], is regular with degree exactly $2n/5$ and so is *not* cycle-maximal triangle-free once n is sufficiently large. It does not have enough edges to be cycle-maximal triangle-free. Neither does any other non-bipartite regular graph for sufficiently large n. Later in the present work, when we show that no regular graph is a counterexample to Conjecture 1.1, we need only consider the finite number of cases in which n is not "sufficiently large."

However, this result concerns average degree, not minimum degree. A graph could have a large gap between average and minimum degree. For instance, the graph formed by inserting a degree-two vertex in one edge of $T(n-1,2)$ has average degree approaching $n/2$ despite its minimum degree being fixed at 2; and although it clearly has fewer cycles than $T(n,2)$, Lemma 3.5 is not strong enough to prove that. Note that by a result of Erdős [17, Lemma 1], this graph also contains the maximum possible number of edges for a non-bipartite triangle-free graph on n vertices.

3.3. Cycle bounds from homomorphisms

Several important results on maximal triangle-free graphs amount to proving that a graph G with certain properties is necessarily homomorphic to some fixed, usually small, graph H. The following lemmas provide bounds on the number of cycles in a graph with that kind of homomorphism; first for G a uniform blowup of H, and then more generally where the sizes of the sets mapping onto each vertex of H are known but not necessarily all the same.

Lemma 3.7. *If G and H are graphs with n and p vertices respectively, n an integer multiple of p, G is a subgraph of $H(n/p)$, g is the girth of G, and $q = \Delta(H)$, then*

$$c(G) \leq q^n \left[\left(\frac{n}{p}\right)!\right]^p \frac{n}{2g}\,, \ \text{and} \tag{11}$$

$$\ln c(G) \leq n \ln n - \left(1 + \ln \frac{p}{q}\right) n + \left(1 + \frac{p}{2}\right) \ln n + \frac{p}{2} \ln \frac{2\pi}{p} - \ln 2g + \frac{p^2}{12n}\,. \tag{12}$$

Proof. For each vertex in G, we will choose a successor in H. There are at most q^n ways to do that. By also choosing a permutation for the n/p vertices in G corresponding to each of the p vertices of H (overall $(n/p)!^p$ choices), we can uniquely determine a successor for each vertex in the cycle. Note that we can choose any arbitrary successors for vertices not in the cycle, since we have not limited the total number of times we might choose a vertex of H; special handling of non-cycle vertices as in Lemma 3.8 is not necessary here.

The starting vertex is determined by choosing one of the p partitions. To determine the length of the cycle, bearing in mind that the cycle can only end when it returns to its initial partition, we can choose how many of the n/p vertices in the initial partition to include in the cycle. Multiplying those factors, the p cancels out, leaving a factor of n for the choice of both starting vertex and cycle length. Alternately, this choice can be viewed as selecting from among n vertices one to be the *last* vertex in the cycle, with the starting partition implicitly the partition containing that vertex, and the starting vertex implicitly the first one in the starting partition according to the earlier-counted vertex permutations. We can also remove a factor of $2g$ because any cycle (necessarily of length at least g) can be described using any of 2 directions and at least g starting vertices. Multiplying all these factors gives (11).

Then (12) follows by Stirling's approximation as follows:

$$\begin{aligned}
\ln c(G) &\leq n \ln q + p \left[\frac{n}{p} \ln \frac{n}{p} - \frac{n}{p} + \frac{1}{2} \ln \frac{n}{p} + \frac{1}{2} \ln 2\pi + \frac{p}{12n} \right] + \ln \frac{n}{2g} \\
&= n \ln q + n \ln \frac{n}{p} - n + \frac{p}{2} \ln \frac{n}{p} + \frac{p}{2} \ln 2\pi + \frac{p^2}{12n} + \ln \frac{n}{2g} \\
&= n \ln n - \left(1 + \ln \frac{p}{q} \right) n + \left(1 + \frac{p}{2} \right) \ln n + \frac{p}{2} \ln \frac{2\pi}{p} - \ln 2g + \frac{p^2}{12n} \, . \, \square
\end{aligned}$$

Lemma 3.7 can potentially overcount by a significant margin because of the q^n term, which allows each vertex of G to choose a successor in H without restriction. A Hamiltonian cycle in G would necessarily visit each vertex of H exactly n/p times, not any arbitrary number of times; many of the q^n successor-in-H choices involve choosing a vertex of H more than n/p times and so cannot actually correspond to feasible full-length cycles in G. There are many fewer than q^n ways to choose each vertex of H exactly n/p times while obeying the other applicable constraints. The situation is complicated somewhat by the possibility of non-Hamiltonian cycles, but it remains that the bound (11) is quite loose for many graphs of interest.

The matrix permanent offers a way to prove a tighter upper bound on cycles given a homomorphism. The following result replaces the successor choice in Lemma 3.7 with a computation of the permanent of the adjacency matrix of the graph. Choosing a permutation of the rows and columns for which all the chosen entries of the adjacency matrix are nonzero corresponds to choosing a neighbour as successor for each vertex in the graph such that each vertex is chosen exactly once, and the permanent counts such choices, including all Hamiltonian cycles. To allow for non-Hamiltonian cycles, which might not involve all vertices, we add loops to all the vertices, corresponding to ones along the diagonal of the matrix, allowing any vertex to choose itself as successor and therefore not need to be chosen by any other vertex. The result is a simple upper bound on number of cycles. This approach is also more easily applicable to non-uniform blowups; that is, where different vertices in H do not all correspond to the same size of independent sets in G. We will discuss later how to compute the permanent efficiently for the cases of interest here.

Lemma 3.8. *In a graph G with n vertices whose adjacency matrix is (g_{ij}),*

$$c(G) \leq \frac{1}{2} \operatorname{perm} \left((g_{ij}) + I_n \right) \, . \tag{13}$$

Furthermore, if G is homomorphic to a graph H with p vertices labelled $1 \ldots p$ and adjacency matrix (h_{ij}), via a homomorphism $f : V(G) \to V(H)$ that maps $n_i = |f^{-1}(i)|$ vertices of G to each vertex i of H, then

$$c(G) \leq \frac{1}{2} \operatorname{perm} \begin{pmatrix} I_{n_1} & h_{12} J_{n_1 n_2} & \ldots & h_{1p} J_{n_1 n_p} \\ h_{21} J_{n_2 n_1} & I_{n_2} & \ldots & h_{2p} J_{n_2 n_p} \\ \vdots & \vdots & \ddots & \vdots \\ h_{p1} J_{n_p n_1} & h_{p2} J_{n_p n_2} & \ldots & I_{n_p} \end{pmatrix} . \tag{14}$$

Proof. A directed cycle cover, or oriented 2-factor, of G is a choice, for each vertex v in G, of a successor vertex adjacent to v such that each vertex is chosen exactly once. If we add a loop to every vertex of G (making each vertex adjacent to itself), then every cycle in G is uniquely determined by at least two directed cycle covers of the resulting graph: namely those in which the cycle vertices choose their successors in the cycle, going around the cycle in either direction, and any other vertices choose themselves. The permanent of $((g_{ij}) + I_n)$ counts exactly those directed cycle covers, and dividing it by two for the two directions gives (13).

When G is homomorphic to H, we can assume for an upper bound that G contains all edges allowed by the homomorphism; adding edges does not decrease the number of cycles. Then (14) is just (13) applied to the maximal graph. □

4. Cycles in regular triangle-free graphs

By Corollary 3.6, no regular graph with n vertices except $T(n, 2)$ can be cycle-maximal triangle-free for n sufficiently large. In this section we show that in fact that statement applies to all n.

Recall that a maximal triangle-free graph with n vertices and minimum degree greater than $10n/29$ is homomorphic to some Γ_i with $i \leq 9$. If the graph is also regular, the following lemma narrows the possibilities further.

Lemma 4.1. *An n-vertex regular maximal triangle-free graph G homomorphic to some Γ_i is exactly $\Gamma_j(n/(3j-1))$ for some $j \leq i$.*

Proof. Edge-maximality implies G is exactly Γ_i with all vertices replaced by independent sets and all the edges that are allowed by the homomorphism; that is, $\Gamma_i(n_1, n_2, \ldots, n_p)$ with $p = 3i - 1$. Suppose one of those independent sets is empty; then some $n_k = 0$ and G is homomorphic to Γ_i minus one vertex. But by Lemma 2.1, deleting a vertex from Γ_i leaves a graph homomorphic to Γ_{i-1}. By transitivity G is homomorphic to Γ_{i-1}, and by induction there exists $j \leq i$ such that $G = \Gamma_j(n_1, n_2, \ldots, n_{3j-1})$ with all the $n_k > 0$.

The neighbourhoods of v_{2j} and v_{2j+1} in Γ_j are $\{v_1, v_2, \ldots, v_j\}$ and $\{v_2, v_3, \ldots, v_{j+1}\}$ respectively; these differ only by the substitution of v_{j+1} for v_1. If G is regular, we have

$$\sum_{k=1}^{j} n_k = \sum_{k=2}^{j+1} n_k \quad \text{and} \quad n_1 = n_{j+1}\,.$$

Symmetrically around the cycle, $n_k = n_{j+k}$ for all k, taking the subscripts modulo $3j - 1$. Because j does not divide $3j - 1$, these equalities form a Hamiltonian cycle covering all the vertices of Γ_j. Then all the n_k are equal, and $G = \Gamma_j(n/(3j-1))$. □

Figure 4 summarizes the regular graphs of interest according to number of vertices and regular degree. The horizontal line at $2m/n^2 = 2/5$ represents the known result that minimum degree greater than $2n/5$ in a triangle-free graph implies the graph is bipartite; anything strictly above that line is bipartite. On or below that line, but above the horizontal line at $2m/n^2 = 10/29$, Lemma 4.1 implies only symmetric blowups of Γ_i graphs (denoted by circles in the figure) could be regular counterexamples to Conjecture 1.1. And Corollary 3.6 implies that the curve labelled "(5) and (10)" eventually crosses (and then permanently remains above) the line at $2m/n^2 = 2/5$, somewhere to the right of the region shown; it is approaching an asymptote at $2m/n^2 \approx 0.41 > 2/5$, and therefore the number of $\Gamma_i(t)$ to consider is finite.

The bounds (10) and (12) complement each other, as shown in Figure 4; the first works well for Γ_i with relatively large i and the second works well with relatively small i. Applying both, we can exclude all blowups of Γ_i for $2 \le i \le 9$ except these: $\Gamma_2(t)$ for $t \le 9$; $\Gamma_3(t)$ for $t \le 6$; $\Gamma_4(t)$ for $t \le 5$; $\Gamma_5(t)$ for $t \le 5$; $\Gamma_6(t)$ for $t \le 4$; $\Gamma_7(t)$ for $t \le 3$; $\Gamma_8(t)$ for $t \le 2$; $\Gamma_9(t)$ for $t \le 2$.

By comparing (4) and (9), which are tighter but not closed-form versions of (10) and (12), we can exclude a few more. This comparison is shown by the zigzag dotted line in the figure; it assumes roughly the same shape and is tending to the same asymptote as the curve for (10) and (12), because it comes from the same calculation. The zigzag pattern seems to result from parity effects in (4). Although we conjecture that $T(n, 2)$ is cycle-maximal for both even and odd n, $T(n, 2)$ is Hamiltonian only for even n. With odd n, there is always at least one vertex not included in each cycle. The fact that maximal-length cycles are a little shorter, and therefore less numerous, when n is odd makes $T(n, 2)$ relatively poor in cycles for odd n overall, because almost all cycles are maximal-length or very close. The bound (9) has no special dependence on parity, and so the gap between it and (4) tends to be narrower for odd n, creating the zigzag pattern. Using this bound allows us to eliminate as possibilities $\Gamma_4(4)$, $\Gamma_4(5)$, all $\Gamma_5(t)$ except Γ_5 itself, all $\Gamma_6(t)$ except Γ_6 itself, and all $\Gamma_7(t)$, $\Gamma_8(t)$, and $\Gamma_9(t)$. These computations, and the integer programming below, were performed in the ECL^{i}PS^e constraint logic programming environment, which provides easy access to backtracking search and large integer arithmetic [31].

Only 20 cases remain for maximal triangle-free graphs that are regular with degree $> 10n/29$. All are eliminated by comparing (4) with (14) except $\Gamma_2(1) = C_5$, which has one cycle and therefore is not cycle-maximal by comparison with $T(5, 2) = K_{2,3}$, which has three cycles. The numerical values for these cases are included in Appendix B.

At this point we have eliminated as possible counterexamples to Conjecture 1.1 all regular graphs above the $2m/n^2 = 10/29$ line on Figure 4. Then the comparison of (5) with (10) eliminates all regular graphs with $n > 61$. Any remaining regular counterexamples are described by integers n (number of vertices) and δ (regular degree) satisfying these constraints:

$$\begin{gathered} 3 \le n \le 61\,, \\ 2 \le \delta \le 10n/29\,, \text{ and} \\ m = n\delta/2 \text{ is an integer.} \end{gathered} \tag{15}$$

There are 428 pairs of (n, δ) satisfying (15). All are excluded by comparing

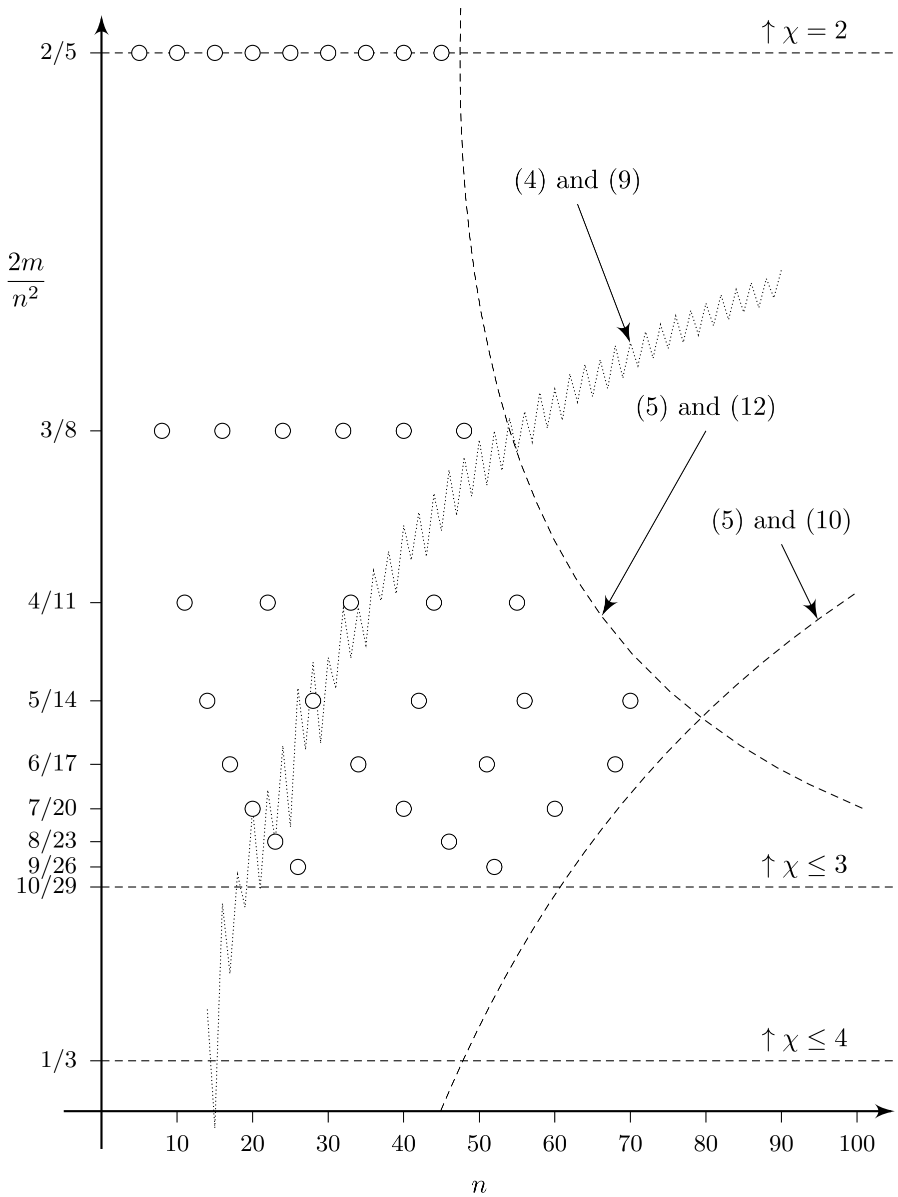

Figure 4: Cases and bounds.

(4) with (9). No more cases remain, so the only regular graphs that can be cycle-maximal triangle-free are of the form $T(n,2)$. Finally, note that $T(n,2)$ is a regular graph only when n is even, so we have the following result.

Theorem 4.2. *If G is a regular cycle-maximal triangle-free graph with n vertices, then n is even and G is $K_{n/2,n/2}$.*

5. Cycles in near-regular triangle-free graphs

If the minimum and maximum degrees in a graph differ by one, we will call the graph *near-regular*. Note this definition is strict: regular graphs are not near-regular. When the minimum degree in a near-regular graph is at most $2n/5$, then by counting $n-1$ vertices of degree $(2n/5)+1$ and one vertex of degree $2n/5$, the maximum possible number of edges is

$$\frac{n^2}{5} + \frac{n-1}{2} .$$

By substituting that into (10) and comparing with (5), any near-regular cycle-maximal triangle-free graph that is not $T(n,2)$ can have at most 804 vertices.

To any near-regular graph G we can assign the integer variables n (number of vertices); m (number of edges); δ and Δ (the lower and higher degrees respectively); and n_δ and n_Δ (number of low and high-degree vertices respectively). This collection of variables is redundant, but naming them all explicitly makes the constraints simpler. With the upper bound of 804 vertices, and comparing (4) with (9), the following constraints apply to any near-regular triangle-free graph that could be a counterexample to Conjecture 1.1.

$$\begin{gathered} 4 \le n \le 804, \\ n = n_\delta + n_\Delta,\ n_\delta > 0,\ n_\Delta > 0, \\ 2 \le \delta \le \frac{2n}{5},\ \Delta = \delta + 1, \\ m = \frac{1}{2} n_\delta \delta + \frac{1}{2} n_\Delta \Delta, \text{ and} \\ \Pi(n,m)\frac{n^2}{8} \ge \sum_{k=2}^{\lfloor n/2 \rfloor} \frac{\lfloor n/2\rfloor! \lceil n/2 \rceil!}{2k(\lfloor n/2 \rfloor - k)!(\lceil n/2 \rceil - k)!} . \end{gathered} \tag{16}$$

By computer search with ECL^{i}PS^e [31], $n \le 435$; and we can obtain tighter bounds on n for specific classes of graphs by further constraining the minimum degree.

- If G is not homomorphic to Γ_2, $\delta \le 3n/8$ and then $n \le 91$.
- If G is not homomorphic to Γ_3, $\delta \le 4n/11$ and then $n \le 61$
- If G is not homomorphic to Γ_4, $\delta \le 5n/14$ and then $n \le 51$.

- If G is not homomorphic to Γ_5, $\delta \leq 6n/17$ and then $n \leq 51$.
- If G is not homomorphic to Γ_6, $\delta \leq 7n/20$ and then $n \leq 43$.
- If G is not homomorphic to Γ_7, $\delta \leq 8n/23$ and then $n \leq 35$.
- If G is not 3-colorable, $\delta \leq 10n/29$ and then $n \leq 35$.
- If G is not 4-colorable, $\delta \leq n/3$ and then $n \leq 33$.

The same kind of argument used in Lemma 4.1 can be used to show that a not necessarily uniform blowup of a Γ_i graph which is near-regular obeys narrow bounds on its partition sizes. The following lemma gives the details for the case of $\Gamma_2 = C_5$.

Lemma 5.1. *If a near-regular graph G is maximal triangle-free, homomorphic to Γ_2, and not bipartite, then $G = \Gamma_2(n_1, n_2, n_3, n_4, n_5)$ with $n_2 \leq n_1 + 2$, $n_3 \leq n_1 + 1$, $n_4 \leq n_1 + 1$, and $n_5 \leq n_1 + 2$; and therefore it is a subgraph of $\Gamma_2(\lfloor (n+6)/5 \rfloor)$.*

Proof. If G is maximal triangle-free and homomorphic to Γ_2, then there exist nonnegative integers $n_1, \ldots, n_5$, summing to n, so that $G = \Gamma_2(n_1, \ldots, n_5)$. If G is not bipartite, then these are all positive; and they cannot all be the same for the graph to be strictly near-regular. Therefore n is at least 6.

Let v_1, v_2, v_3, v_4, and v_5 be the vertices of Γ_2. Their neighbourhoods are respectively $\{v_3, v_4\}$, $\{v_4, v_5\}$, $\{v_1, v_5\}$, $\{v_1, v_2\}$, and $\{v_2, v_3\}$. The degree of vertices in G mapped by the homomorphism to any given vertex in Γ_2 is equal to the sum of the sizes of sets of vertices in G mapped to that vertex's neighbours. Therefore the following constraints hold:

$$\begin{aligned}
|(n_3 + n_4) - (n_4 + n_5)| &= |n_3 - n_5| \leq 1, \\
|(n_4 + n_5) - (n_1 + n_5)| &= |n_4 - n_1| \leq 1, \\
|(n_1 + n_5) - (n_1 + n_2)| &= |n_5 - n_2| \leq 1, \\
|(n_1 + n_2) - (n_2 + n_3)| &= |n_1 - n_3| \leq 1, \\
|(n_2 + n_3) - (n_3 + n_4)| &= |n_2 - n_4| \leq 1.
\end{aligned}$$

Let n_1 be the least of the n_k; then $n_2 \leq n_1 + 2$, $n_3 \leq n_1 + 1$, $n_4 \leq n_1 + 1$, and $n_5 \leq n_1 + 2$.

Up to symmetry, there are nine cases for near-regular $\Gamma_2(n_1, n_2, n_3, n_4, n_5)$ obeying the above constraints:

- $G = \Gamma_2(n_1, n_1, n_1, n_1, n_1 + 1)$; then $n \equiv 1 \pmod 5$ and G is a subgraph of $\Gamma_2(n + 4)$.
- $G = \Gamma_2(n_1, n_1, n_1, n_1 + 1, n_1 + 1)$; then $n \equiv 2 \pmod 5$ and G is a subgraph of $\Gamma_2(n + 3)$.

- $G = \Gamma_2(n_1, n_1, n_1+1, n_1, n_1+1)$; then $n \equiv 2 \pmod 5$ and G is a subgraph of $\Gamma_2(n+3)$.
- $G = \Gamma_2(n_1, n_1, n_1+1, n_1+1, n_1+1)$; then $n \equiv 3 \pmod 5$ and G is a subgraph of $\Gamma_2(n+2)$.
- $G = \Gamma_2(n_1, n_1+1, n_1+1, n_1, n_1+1)$; then $n \equiv 3 \pmod 5$ and G is a subgraph of $\Gamma_2(n+2)$.
- $G = \Gamma_2(n_1, n_1+1, n_1+1, n_1+1, n_1+1)$; then $n \equiv 4 \pmod 5$ and G is a subgraph of $\Gamma_2(n+1)$.
- $G = \Gamma_2(n_1, n_1+1, n_1+1, n_1, n_1+2)$; then $n \equiv 4 \pmod 5$ and G is a subgraph of $\Gamma_2(n+6)$.
- $G = \Gamma_2(n_1, n_1+1, n_1+1, n_1+1, n_1+2)$; then $n \equiv 0 \pmod 5$ and G is a subgraph of $\Gamma_2(n+5)$.
- $G = \Gamma_2(n_1, n_1+2, n_1+1, n_1+1, n_1+2)$; then $n \equiv 1 \pmod 5$ and G is a subgraph of $\Gamma_2(n+4)$.

In all these cases, G is a subgraph of $\Gamma_2(\lfloor (n+6)/5 \rfloor)$. □

Lemma 5.1 brings down the upper bound on n a little for the case of graphs homomorphic to Γ_2: because G homomorphic to Γ_2 can have no more cycles than its supergraph $\Gamma_2(\lfloor (n+6)/5 \rfloor)$, we can compare (4) for n vertices with (11) for $5\lfloor (n+6)/5 \rfloor$ vertices, and find that for G near-regular, cycle-maximal triangle-free, and homomorphic to Γ_2 but not bipartite, $n \leq 184$.

If we extend the constraint program (16) to include separate variables for n_1, n_2, n_3, n_4, and n_5, with the constraints on them given by Lemma 5.1 and the new bound $n \leq 184$, we can generate an exhaustive list of the Γ_2 blowups that remain as possible counterexamples to Conjecture 1.1. Comparing (4) with (14) for these cases eliminates all of them except the three graphs shown in Figure 5: $\Gamma_2(1, 2, 1, 1, 2)$, $\Gamma_2(1, 2, 2, 1, 3)$, and $\Gamma_2(1, 3, 2, 2, 3)$. Note that the order of indices in Γ_2 and thus the order of indices in the blowup notation is not consecutive around the five-cycle: v_1 in Γ_2, under the definition, is adjacent to v_3 and v_4. These graphs are small enough that we can count the cycles exactly; none have as many cycles as the bipartite Turán graph with the same number of vertices.

$$
\begin{aligned}
c(\Gamma_2(1,1,2,1,2)) &= 15\,, & c(\Gamma_2(1,2,2,1,3)) &= 216\,, & c(\Gamma_2(1,3,2,2,3)) &= 3051\,,\\
c(T(7,2)) &= 42\,, & c(T(9,2)) &= 660\,, & c(T(11,2)) &= 15390\,.
\end{aligned}
\tag{17}
$$

These results suffice to establish the following theorem, which limits the remaining possibilities for near-regular graphs that could be cycle-maximal triangle-free.

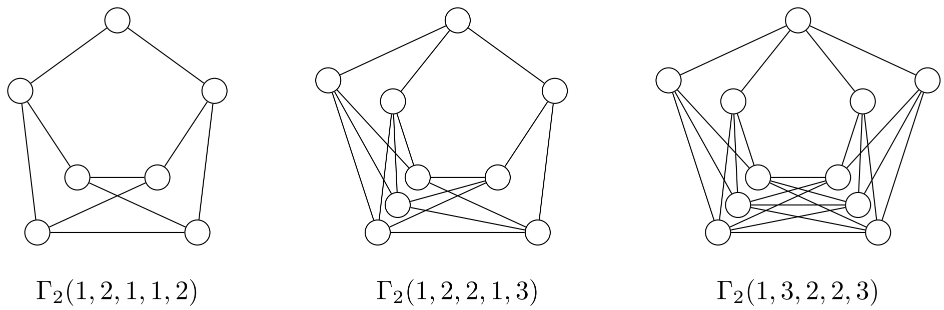

Figure 5: Near-regular graphs homomorphic to Γ_2 and not ruled out by comparing (4) with (14).

Theorem 5.2. *If a graph G with n vertices and m edges is cycle-maximal triangle-free, its minimum and maximum degrees differ by exactly one, and G is not $T(n,2)$ with n odd, then $n \leq 91$, the minimum degree in G is at most $3n/8$, and G is not homomorphic to C_5.*

Proof. Suppose G is a counterexample. By comparing (10) with (5), $n \leq 804$. By solving the constraints (16), $n \leq 435$.

For graphs homomorphic to C_5, by applying Lemma 5.1, $n \leq 184$. Then by examining specific graphs and comparing (4) with (14), the three graphs shown in Figure 5 are the last remaining graphs homomorphic to C_5, and (17) eliminates them. For graphs not homomorphic to C_5: the minimum degree is at most $3n/8$ because G is maximal triangle-free. Then by adding that constraint to (16) and solving, $n \leq 91$. □

6. Algorithmic aspects of the upper bound calculation

Lemma 3.8 gives a bound (14) on number of cycles in a graph in terms of the permanent of a matrix; that is the sum, over all ways to choose one entry from each row and column, of the product of the chosen entries. Note that the matrix permanent is identical to the matrix determinant except that in the determinant, each product is given a sign depending on the parity of the permutation. For the permanent, the products are simply added. Removing the signs has significant consequences for the difficulty of computing the permanent: whereas computing the determinant of an $n \times n$ matrix has the same asymptotic time complexity as matrix multiplication (Cormen *et al.* give this as an exercise [14, Exercise 28.2–3]), permanent, like cycle counting, is in general a $\#P$-complete problem, even when limited to 0-1 matrices [35].

Solving one $\#P$-complete problem just to bound another is not obviously useful. However, the matrices for which we compute the permanent to evaluate (14) are of a special form which makes the computation much easier. In this section we describe an algorithm to compute such permanents with time complexity having exponential dependence on p (the number of vertices in H) but not on n (the number of vertices in G, and size of the matrix).

Ryser's formula [30] for the permanent of an $n \times n$ matrix with entries (a_{ij}) is

$$\operatorname{perm}(a_{ij}) = \sum_{S \subseteq \{1,2,\ldots,n\}} (-1)^{n-|S|} \prod_{i=1}^{n} \sum_{j \in S} a_{ij} \,. \tag{18}$$

Ryser's formula is a standard method for computing the permanent. To summarize it in words, the permanent is the sum over all subsets of the columns of the matrix, of the product over all rows, of the sums of entries in the chosen columns, with signs according to the parity of the size of the subset. The formula follows from applying the principle of inclusion and exclusion to the permutation-based definition of permanent; and although evaluating it has exponential time complexity because of the 2^n distinct subsets of the columns, that is better than the factorial time complexity of examining each permutation separately.

Suppose A is an $n \times n$ binary matrix of the following form:

$$\begin{pmatrix} I_{n_1} & h_{12}J_{n_1n_2} & \ldots & h_{1p}J_{n_1n_p} \\ h_{21}J_{n_2n_1} & I_{n_2} & \ldots & h_{2p}J_{n_2n_p} \\ \vdots & \vdots & \ddots & \vdots \\ h_{p1}J_{n_pn_1} & h_{p2}J_{n_pn_2} & \ldots & I_{n_p} \end{pmatrix} .$$

The rows are divided into p blocks with sizes n_1, n_2, …, n_p, with $n = n_1 + n_2 + \cdots + n_p$. The columns are divided into the same pattern of blocks, giving the matrix an overall structure of p blocks by p blocks, with square blocks along the main diagonal but the other blocks not necessarily square. Furthermore, the blocks along the diagonal of A are identity matrices I_{n_i} and the other blocks are of the form $h_{ij}J_{n_in_j}$ with $h_{ij} \in \{0, 1\}$; that is, blocks of all zeroes or all ones. This is the form of the matrix for which we calculate the permanent to evaluate (14).

Observe that because of the block structure, many choices of the subset S in (18) will produce the same product of row sums. The inside of the first summation in (18), for matrices in the form we consider, depends on how many columns are chosen from each block, but not which ones. If we let k_i for $i \in \{1, 2, \ldots, p\}$ be the number of columns chosen in block i, then we can sum over the choices of all the k_i rather than the choices of S, using binomial coefficients to count the number of choices of S for each choice of all the k_i. Furthermore, the innermost sum need only contain p terms for the block columns rather than n for the matrix columns, because we can collapse the sum within a block of columns into 0 for a block of all zeroes; the number of columns selected from the block for a block of all ones; or either 0 or 1 for an identity-matrix block depending on whether we are in a row corresponding to a selected column. The product, similarly, only requires $2p$ factors, raised to the appropriate powers, for the block rows and the choice of "selected" or "not selected" matrix rows;

Algorithm 1

```
result ← 0
for all integer vectors ⟨k_1, k_2, ..., k_p⟩ such that 0 ≤ k_i ≤ n_i do
  cprod ← 1
  for row = 1 to p do
    rsum ← 0
    for col = 1 to p do
      if row ≠ col and h[row, col] = 1 then
        rsum ← rsum + k_col
      end if
    end for
    cprod ← cprod · (rsum + 1)^{k_row} · rsum^{n_row − k_row}
  end for
  result ← result + cprod · ∏_{i=1}^{p} (−1)^{n_i − k_i} (n_i choose k_i)
end for
return result
```

not n possibilities for all the matrix rows. Algorithm 1 gives pseudocode for the calculation.

There are $\prod_{i=1}^{p}(n_i+1)$ choices for the vector $\langle k_1, k_2, \ldots, k_p\rangle$; because equal division is the worst case, that is $O(((n/p)+1)^p)$. For each such vector, the inner loops do $O(p^2)$ operations, giving the following result.

Theorem 6.1. *There exists an algorithm to compute the permanent of a matrix A in $O(p^2((n/p)+1)^p)$ integer arithmetic operations if A is an $n \times n$ matrix divided into p blocks by p blocks, not necessarily all of the same size, in which the blocks along the main diagonal are identity matrices and the other blocks each consist of all zeroes or all ones.*

When $p = n$, the case of general unblocked $n \times n$ matrices, this time bound reduces to $O(n^2 2^n)$, which is the same as a straightforward implementation of Ryser's formula. Note that we describe the time complexity in terms of "integer arithmetic operations." The value of the permanent can be on the order of the factorial of the number of vertices n, in which case representing it takes $O(n)$ words of $O(\log n)$ bits each. We cannot do arithmetic on such large numbers in constant time in the standard RAM model of computation. However, including an extended analysis here of the cost of multiple-precision arithmetic would make the presentation more confusing without providing any deeper insight into how the algorithm works. Thus we do the analysis in the unit cost model, with the caution that the cost of arithmetic may be non-constant in practice and should be considered when implementing the algorithm. Even if our model does not include "binomial coefficient" as a primitive constant-time operation, we can first build a table of $k!$ for k from 1 to n with $O(n)$ multiplications, then calculate $\binom{n}{k}$ as $n!/k!(n-k)!$ with three table lookups; time and space to build the table are lower order than the overall cost of Algorithm 1.

For the proofs in the previous sections, we implemented this algorithm in the

ECL^{i}PS^e language [31] with no particular effort to optimize it, and found that the cost of calculating permanents to bound cycle counts was comparable to the cost of the integer programming to find the graphs in the first place, typically a few CPU seconds per graph for small cases, up to a few hours for the largest cases of interest.

7. Conclusions and future work

Conjecture 1.1 postulates that the bipartite Turán graphs achieve the maximum number of cycles among all triangle-free graphs. Depending on the parity of n, $T(n, 2)$ is either regular or near-regular; and we have ruled out all regular graphs and all but a finite number of near-regular graphs as potential counterexamples to Conjecture 1.1. It appears that our current techniques might be extended to cover a few more of the near-regular cases by proving results like Lemma 5.1 for Γ_3, Γ_4, and so on. Each one reduces the maximum value of $\delta(G)/n$, and therefore the maximum value of n, for which counterexamples could exist.

However, even if we could do this for all Γ_i, and extend the theory to cover 4-chromatic graphs too using the "Vega graph" classification results of Brandt and Thomassé [11], potential counterexamples with as many as 30 vertices would remain, and too many of them to exhaustively enumerate as we did in the case of regular graphs. Similar issues apply even more strongly to graphs with $\Delta(G) - \delta(g)$ a constant $k > 1$, even though by Corollary 3.6, the number of possible counterexamples is finite for any fixed k. It seems clear that to close these gaps will require a better theoretical understanding of graphs with $\delta(G)$ less than but close to $n/3$, and to finally prove Conjecture 1.1 we need better bounds for graphs that are far from being regular.

When the girth increases beyond four the structure of cycle-maximal graphs appears to change significantly. In particular, they are not just complete bipartite graphs with degree-two vertices inserted to increase the lengths of the cycles. For small values of n, our computer search showed that most vertices in cycle-maximal graphs of fixed minimum girth $g \geq 5$ have degree three, with a few vertices of degree two and four present in some cases. Our preliminary examination of cycle-maximal graphs of girth greater than four has yet to suggest any natural characterization of these graphs, even when graphs are restricted to having regular degree.

Acknowledgements

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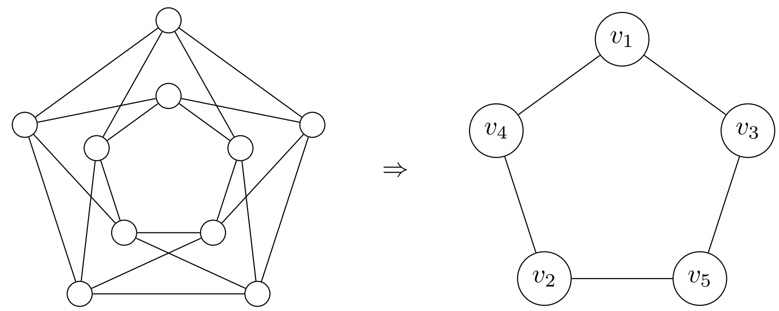

$G = C_5(2)$ $H = C_5$

Figure A.6: Graphs for the permanent bound example.

Appendix A. Example: the permanent bound for $C_5(2)$

This appendix demonstrates the permanent-based bound on number of cycles in the graph $C_5(2)$, shown at left in Figure A.6. This graph comes up when trying to think of counterexamples to Conjecture 1.1: there is no instantly obvious reason for it to have fewer cycles than $T(10, 2)$, but in fact, it does have fewer cycles.

Let G be the graph $C_5(2)$ and let H be the graph C_5, which is the same as Γ_2. Figure A.6 shows the vertices of H labelled as in the definition of Γ_2. The adjacency matrix of H is

$$\begin{pmatrix} 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 & 1 \\ 1 & 0 & 0 & 0 & 1 \\ 1 & 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 \end{pmatrix}.$$

The graph G is obtained by blowing up each vertex of H into a two-vertex independent set, and in the adjacency matrix that is equivalent to replacing each element with a 2×2 submatrix. To apply the bound of Lemma 3.8, we also add ones along the diagonal, giving this modified version of the adjacency matrix of G:

$$\left(\begin{array}{cc|cc|cc|cc|cc} 1 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 1 & 1 & 1 & 0 & 0 \\ \hline 0 & 0 & 1 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 & 1 & 1 & 1 & 1 \\ \hline 1 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 1 \\ \hline 1 & 1 & 1 & 1 & 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\ \hline 0 & 0 & 1 & 1 & 1 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 1 \end{array}\right).$$

Table B.1: Cycle counts and bounds for various graphs, $n \le 30$.

G	n	$c(G)$	from
$\Gamma_2 = C_5$	5	1	obvious
$K_{2,3}$	5	3	(4)
Γ_3	8	$\le$130	(14)
$K_{4,4}$	8	204	(4)
$\Gamma_2(2)$	10	$\le$2 876	(14)
$K_{5,5}$	10	3 940	(4)
Γ_4	11	$\le$6 151	(14)
$K_{5,6}$	11	15 390	(4)
Γ_5	14	$\le$602 261	(14)
$K_{7,7}$	14	4 662 231	(4)
$\Gamma_2(3)$	15	$\le$12 782 394	(14)
$K_{7,8}$	15	24 864 588	(4)
$\Gamma_3(2)$	16	$\le$36 552 880	(14)
$K_{8,8}$	16	256 485 040	(4)
Γ_6	17	$\le$104 770 595	(14)
$K_{8,9}$	17	1 549 436 112	(4)
Γ_7	20	$\le$29 685 072 610	(14)
$\Gamma_2(4)$	20	$\le$275 455 237 776	(14)
$K_{10,10}$	20	1 623 855 701 385	(4)
$\Gamma_4(2)$	22	$\le$3 544 330 396 616	(14)
$K_{11,11}$	22	177 195 820 499 335	(4)
$\Gamma_3(3)$	24	$\le$504 887 523 966 914	(14)
$K_{12,12}$	24	23 237 493 232 953 516	(4)
$\Gamma_2(5)$	25	$\le$19 610 234 100 506 750	(14)
$K_{12,13}$	25	205 717 367 581 496 628	(4)
$\Gamma_5(2)$	28	$\le$1 583 204 062 862 484 492	(14)
$K_{14,14}$	28	653 193 551 573 628 900 289	(4)
$\Gamma_2(6)$	30	$\le$3 664 979 770 718 930 748 156	(14)
$K_{15,15}$	30	136 634 950 180 317 224 866 335	(4)

The permanent of that 10×10 matrix is 5753, so by Lemma 3.8, taking the floor because the cycle count is an integer, $C_5(2)$ contains at most 2876 cycles. In fact, by exact count $C_5(2)$ contains 593 cycles. Both numbers are less than the 3940 cycles in $T(10, 2)$.

Appendix B. Numerical results

Tables B.1 and B.2 list exact counts and bounds on the number of cycles in various graphs, sorted by number of vertices for easier comparisons.

Table B.2: Cycle counts and bounds for various graphs, $n > 30$.

G	n	$c(G)$	from
$\Gamma_3(4)$	32	$\leq$93 314 267 145 221 727 988 928	(14)
$K_{16,16}$	32	32 681 589 590 709 963 123 092 160	(4)
$\Gamma_4(3)$	33	$\leq$472 536 908 624 040 051 159 801	(14)
$K_{16,17}$	33	380 842 679 006 967 756 257 282 880	(4)
$\Gamma_2(7)$	35	$\leq$1 538 132 015 230 964 742 594 686 226	(14)
$K_{17,18}$	35	109 481 704 025 024 759 751 150 754 248	(4)
$\Gamma_3(5)$	40	$\leq$121 876 741 093 584 265 201 282 594 275 138	(14)
$\Gamma_2(8)$	40	$\leq$1 295 546 973 219 341 717 643 333 826 977 344	(14)
$K_{20,20}$	40	350 014 073 794 168 154 275 473 348 323 458 540	(4)
$\Gamma_2(9)$	45	$\leq$2 011 552 320 593 475 430 049 513 125 845 530 235 126	(14)
$K_{22,23}$	45	1 072 464 279 544 434 376 131 539 091 650 605 148 971 323	(4)
$\Gamma_3(6)$	48	$\leq$765 658 164 243 897 411 689 143 843 074 192 950 614 512	(14)
$K_{24,24}$	48	18 847 819 366 080 117 996 802 964 862 587 612 140 097 642 544	(4)
$\Gamma_2(10)$	50	$\leq$5 387 065 180 713 482 750 668 088 096 305 965 320 151 649 500	(14)
$K_{25,25}$	50	11 294 267 336 237 005 395 453 340 472 970 226 376 143 920 186 000	(4)
$\Gamma_3(7)$	56	$\leq$17 877 864 251 518 595 245 276 779 749 582 885 338 633 210 045 796 098	(14)
$K_{28,28}$	56	3 883 426 377 993 747 808 177 077 817 275 217 253 080 577 404 858 001 996 940	(4)

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