

Algorithmic Search for Extremal Graphs of Girth At Least Five

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Abstract

Let $f(v)$ denote the maximum number of edges in a graph of order v and of girth at least 5. In this paper, we discuss algorithms for constructing such extremal graphs. This gives constructive lower bounds of $f(v)$ for $v \leq 200$. We also provide the exact values of $f(v)$ for $v \leq 24$, and enumerate the extremal graphs for $v \leq 10$.

1 Introduction

All graphs considered in this paper are simple graphs. By $V(G)$, $E(G)$, v and e , we mean the vertex-set, edge-set, order and size of a graph

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G , respectively. Other undefined terms can be found in any standard textbook in graph theory.

Given graphs G_1, \dots, G_k , $ex(v; G_1, \dots, G_k)$ denotes the maximum size of a graph of order v containing no subgraph isomorphic to any G_i , $1 \leq i \leq k$. Consult [22] for a brief survey of the subject. It is well known that $ex(v; C_3) = \lfloor v^2/4 \rfloor$, and the extremal graph is $K_{\lfloor v/2 \rfloor, \lceil v/2 \rceil}$. The exact value of $ex(v; C_4)$ is known for some specific v [3, 9, 10]. Also, see [2, 8], $ex(v; C_4) = (1/2 + o(1))v^{3/2}$.

The *girth* of a graph is the size of its smallest cycle. In this paper, we study the value of $f(v)$, the maximum size of a graph of order v and girth at least 5; that is, $f(v) = ex\{v; C_3, C_4\}$. An old conjecture of Erdős, see for instance [7], states that $f(v) = (1/2 + o(1))^{3/2}v^{3/2}$. Attempts to construct extremal graphs by destroying all 4-cycles (resp. 3-cycles) in the extremal graphs for $ex(v; C_3)$ (resp. $ex(v; C_4)$) fail. Using computer search techniques such as hill-climbing and hill-tracking (see Section 4), we find graphs without C_3 or C_4 , thus giving lower bounds on $f(v)$ for $v \leq 200$. Together with theoretical bounds (see Section 2) from [13], we obtain in Section 3 exact values of $f(v)$ for $1 \leq v \leq 24$. We also enumerate all extremal graphs of order at most 10 in Section 3.

2 Preliminaries and Notations

In this section we summarize the results we derived in [13]. A graph G of order v is said to be *extremal* if its size is $f(v)$ and has girth 5.

It is clear that the diameter of an extremal graph is at most 3. It was shown in [1] that graphs of order v with no 4-cycles and of diameter 2 are very rare. Among them, only Moore graphs contain no C_3 . These Moore graphs are C_5 , Petersen graph, Hoffman-Singleton graph [15], and a 57-regular graph of order 3250 and girth 5 if it exists (its existence is still an open problem [15]).

Theorem 2.1 *For $v \geq 1$, $f(v) \leq v\sqrt{v-1}/2$. Equality holds if and only if $G = K_1$, or G is a Moore graph of diameter 2.*

Theorem 2.2 *Let G be an extremal graph of order v and size e , and let q be the largest prime power such that $2(q^2 + q + 1) \leq v$. Then $f(v) \geq 2v + (q - 3)(q^2 + q + 1)$.*

Corollary 2.3 $\frac{1}{2\sqrt{2}} \leq \liminf_{v \rightarrow \infty} \frac{f(v)}{v^{3/2}} \leq \limsup_{v \rightarrow \infty} \frac{f(v)}{v^{3/2}} \leq \frac{1}{2}$.

Remarks. The inequality in Theorem 2.1 was also found independently in [5, 6]. Murty [19] obtained the same asymptotic lower bound in Corollary 2.3 by showing that $f(2q^2) \geq q^2(q+2)$ for primes $q \geq 5$.

Let G be a $\{C_3, C_4\}$ -free graph, we next define a class of trees to be used in Section 3. Given any vertex r in G , it is clear that its neighborhood $N(r) = \{r_1, r_2, \dots\}$ is an independent set. Define $R_i = N(r_i) - \{r\}$. Since G is $\{C_3, C_4\}$ -free, $r_i r_j \notin E(G)$ and $R_i \cap R_j = \emptyset$ for $i \neq j$. For any set A of vertices of G , let $\langle A \rangle$ denote the subgraph of G induced by A . Then $\bigcup_i \langle N(r_i) \rangle$ forms a tree, which we call a (m, n) -star, denoted $S_{m,n}$, where $m = d(r)$, the degree of r , and $n = \min\{|R_i| : 1 \leq i \leq m\}$. In other words, $S_{m,n}$ is a tree in which the root has m children, and every child has *at least* n children of its own. Note, however, leaves from different branches of $S_{m,n}$ may be adjacent in G . Clearly, if G has at least 5 vertices, it contains $S_{\Delta, \delta-1}$, where Δ and δ are the maximum and minimum degree of G , respectively. Proof of the following proposition is immediate.

Proposition 2.4 *For all $\{C_3, C_4\}$ -free graphs G , we have*

1. $v \geq 1 + \Delta\delta \geq 1 + \delta^2$.
2. $\delta \geq e - f(v-1)$ and $\Delta \geq \lceil 2e/v \rceil$.
3. $v \geq 1 + \lceil 2f(v)/v \rceil (f(v) - f(v-1))$.

Several more notations. Denote the set of $\{C_3, C_4\}$ -free graphs of order v and the corresponding set of extremal graphs by \mathcal{F}_v and \mathcal{F}_v^* , respectively. Let $F(v) = |\mathcal{F}_v^*|$. For any graph G , define $Q_i = Q_i(G) = \{x \in V(G) : d(x) = i\}$.

3 Values of $f(v)$ for $v \leq 24$

For $1 \leq v \leq 10$, we have $f(v) = \lfloor v\sqrt{v-1}/2 \rfloor$.

Theorem 3.1 *For $1 \leq v \leq 10$, the values of $f(v)$ and $F(v)$ are:*

v	1	2	3	4	5	6	7	8	9	10
$f(v)$	0	1	2	3	5	6	8	10	12	15
$F(v)$	1	1	1	2	1	2	1	1	1	1

Proof: Figure 1 shows \mathcal{F}_v^* for $1 \leq v \leq 10$. Thus $f(v) \geq \lfloor v\sqrt{v-1}/2 \rfloor$ for $v \leq 10$, and the equality follows from Theorem 2.1.

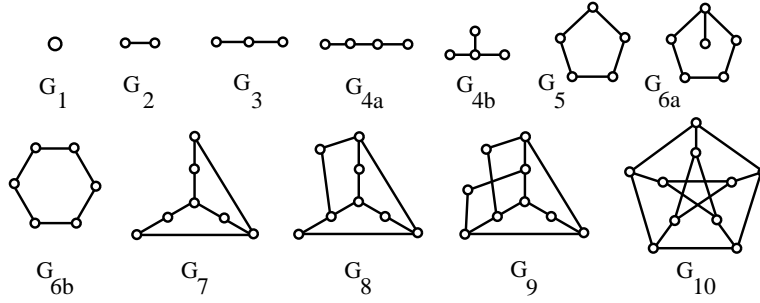


Figure 1: Extremal graphs with $v \leq 10$

The value of $F(v)$ is trivial when $v \leq 5$. For $v \geq 6$, Proposition 2.4 leads to the following possible values of δ and Δ :

v	6	7	8	9	10
(δ, Δ)	(1,2), (1,3), (1,4) (1,5), (2,2)	(2,3)	(2,3)	(2,3) (2,4)	(3,3)

Let $G \in \mathcal{F}_6^*$. If G is 2-regular, then it must be C_6 . Otherwise, let x be a pendant vertex of G . Since $f(5) = 5$ and $F(5) = 1$, we have $G - x \cong C_5$, so $G \cong G_{6a}$ in Figure 1. For the rest of the proof, the graphs G_i would be those depicted in Figure 1.

Every $G \in \mathcal{F}_7^*$ contains $S_{3,1}$, which has 7 vertices and 6 edges. The remaining two edges must connect the leaves, thus yielding G_7 . Assume $r_{2,1}$ is adjacent to $r_{1,1}$ and $r_{3,1}$.

Let $z_1 \in Q_2(G)$, where $G \in \mathcal{F}_8^*$. Then $G - z_1 \cong G_7$ since $|E(G)| = 10$, $f(7) = 8$ and $F(7) = 1$. So $N(z_1) = \{r_3, r_{1,1}\}$; thus $G \cong G_8$.

Let $z_2 \in Q_2(G)$, where $G \in \mathcal{F}_9^*$; then $G - z_2 \cong G_8$. If $z_1 z_2 \notin E(G)$, then $N(z_2) = \{r_1, r_{3,1}\}$, yielding G_9 . If $z_1 z_2 \in E(G)$, then $N(z_2) = \{z_1, r_2\}$, yielding G'_9 . It is easily seen that $G_9 \cong G'_9$, so $F(9) = 1$.

Finally, every $G \in \mathcal{F}_{10}^*$ is 3-regular, and $G - x \cong G_9$ for every vertex $x \in V(G)$. Since $|Q_2(G_9)| = 3$, we have $N(x) = Q_2(G_9)$. Thus G is the Petersen graph G_{10} . ■

Theorem 3.2 *The values of $f(v)$ for $11 \leq v \leq 24$ are as follows:*

v	11	12	13	14	15	16	17	18	19	20	21	22	23	24
$f(v)$	16	18	21	23	26	28	31	34	38	41	44	47	50	54

The strategy we use to prove $f(v) = N$ is similar to that typically used in Ramsey theory. First, we generate (with computer search, see Section 4) a graph $G_v \in \mathcal{F}_v$ with N edges, this shows that $f(v) \geq N$. Figure 2 displays G_{18} , G_{19} and G_{24} . Note that $G_{17}, G_{16}, \dots, G_{11}$

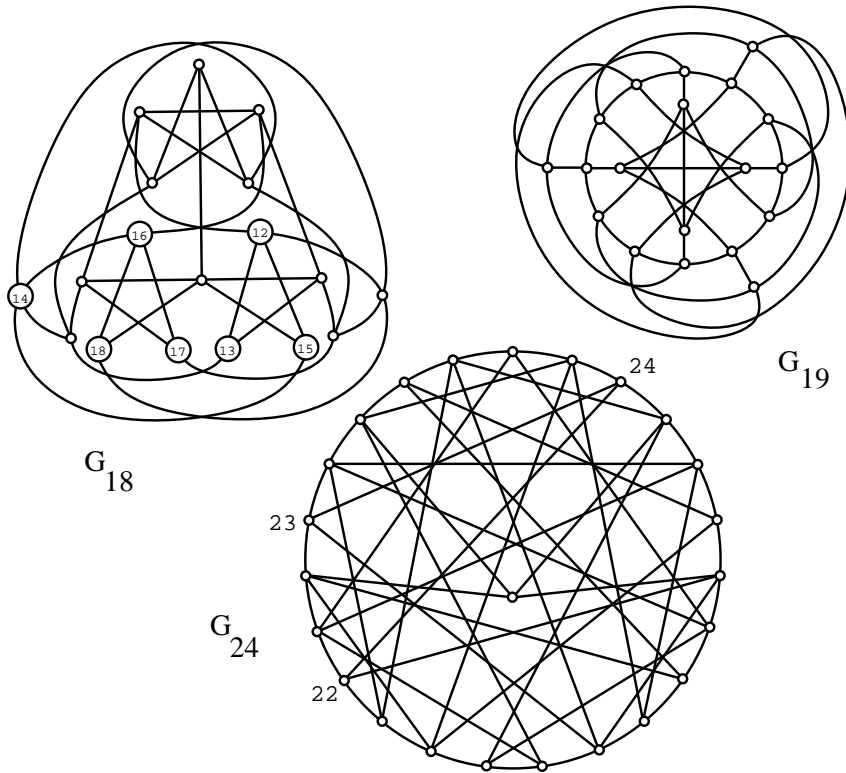


Figure 2: Extremal graphs with 18, 19 and 24 vertices

can be obtained from G_{18} by deleting vertices labeled 18, 17, \dots , 12 in succession; G_{21} , G_{22} and G_{23} can be similarly constructed from G_{24} . G_{19} is the Robertson graph [21], which is the unique 4-regular graph of girth 5, which in turn implies that $F(19) = 1$. G_{20} can be formed from G_{19} by adding a vertex that is adjacent to the three outer vertices.

Next, we prove that $f(v) < N + 1$. Suppose there exists $G \in \mathcal{F}_v$ with more than N edges. Deduce possible values of δ and Δ from Proposition 2.4. Complete the proof by showing that $G - N[r]$ always contains C_3 or C_4 for any $r \in Q_\Delta$.

Typical examples can be found in [13]. The proofs of $f(16) = 28$ and $f(23) = 50$ are the most complicated. We only show the proof of $f(23) = 50$ here.

Proof of $f(23) = 50$. By construction, $f(23) \geq 50$. Suppose there exists $G \in \mathcal{F}_{23}$ with 51 edges, then $\delta = 4$, $\Delta = 5$, $|Q_4| = 13$ and $|Q_5| = 10$. First note that G does not contain a subgraph $G' \in \{P_4, K_{1,3}\}$ with $V(G') \subset Q_4$. For if it does, then $G - V(G') \cong G_{19}$ (because $f(19) = 38$ and $F(19) = 1$), G' has at least two pendant vertices, each has 3 neighbors in $G - V(G')$ that are mutually distance 3 apart, but G_{19} has only one such set of 3 vertices.

Consider the (5,3)-star S rooted at any $r \in Q_5$. Let $W = V - N[r]$ and $H = \langle W \rangle$. There are at most 2 vertices not in S , so $|Q_5 \cap N(r)| \leq 2$. We may assume $d(r_i) = 4$ for $1 \leq i \leq 3$. Note that if $d(r_i) = 4$ then $|Q_5 \cap R_i| \geq 1$, since otherwise $R_i \subseteq Q_4$ implies that $K_{1,3} \subseteq Q_4$, a contradiction.

Suppose $|Q_5 \cap N(r)| = 2$ for some $r \in Q_5$. Then for $i = 4, 5$, $d(r_i) = 5$ and $|Q_4 \cap R_i| \geq 3$; also, $|Q_4 \cap (R_1 \cup R_2 \cup R_3)| \geq 2$. Since $\sum_{x \in R_i} d_H(x) \geq 12$ for $i = 4, 5$, there exists a path P_4 of the form $r_{5,a}r_{4,b}r_{c,d}r_c$ or $r_{4,a}r_{5,b}r_{c,d}r_c$ for some $1 \leq c \leq 3$ such that $V(P_4) \subset Q_4$. But such path cannot exist, so $|Q_5 \cap N(r)| \leq 1$ for all $r \in Q_5$.

If $\langle Q_5 \rangle$, the graph induced by Q_5 , has t edges, then counting degrees shows that Q_5 is joined by $5 \cdot 10 - 2t$ edges, and consequently $\langle Q_4 \rangle$ must have $t + 1$ edges. Now if $t \geq 6$, it forces some $r \in Q_5$ to have $|N(r) \cap Q_5| \geq 2$, which we have just shown to be impossible. Therefore, $t \leq 5$. But now consider the 45 pairs of vertices in Q_5 . Each of the t edges covers one of these pairs. But we shall also consider a pair covered if both of its vertices have a common neighbor in Q_4 . Now the 13 vertices of Q_4 have $50 - 2t$ edges joining them to Q_5 . These cover the minimum number of pairs when they are distributed evenly, that is,

$2t+2$ vertices joined to 3 vertices and $11-2t$ joined to 4. Since 3 and 4 vertices comprise 3 and 6 pairs, respectively, we may total the number of pairs covered to obtain $t+3(2t+2)+6(11-2t) = 72-5t \geq 47$. But since Q_5 only has 45 pairs, the pigeonhole principle forces some pair to be covered twice, contradicting the girth being 5. This contradiction shows that t cannot be less than 6. Since we have considered every possible value for t , it must be that $f(23) < 51$. ■

Values of $F(v)$, for $11 \leq v \leq 28$, can be found in [14].

4 Algorithmic lower bound construction for $f(v)$

By combining hill-climbing and backtracking techniques, we have developed and implemented algorithms that attempt to find maximal graphs without C_3 or C_4 . We have succeeded in generating graphs, for $25 \leq v \leq 200$, with sizes exceeding the lower bounds given in Section 2. Adjacency lists for the graphs appear in [12]. The constructive lower bounds thus obtained are listed in Table 1; the value of $f(v)$ for $0 \leq v \leq 30$, and $v = 50$, are exact. Values of $f(v)$ for $25 \leq v \leq 30$ are determined in [14]; $f(50) = 175$ because the size of the Hoffman-Singleton graph attains the upper bound in Theorem 2.1.

The algorithmic techniques we used to generate the graphs are based on heuristic local search algorithms. These are algorithms that propose random changes to partial solutions, and then accept those changes which do not move the solution further away from the goal. We also used standard backtracking techniques for parts of the solutions. Before describing the techniques, and how they were combined, we first present some terminology.

In general, the class of techniques that we employ is known as *hill-climbing*. One climbs a hill by looking for a step that increases the climber's altitude. When it is not possible to efficiently identify a nearby point with a greater altitude, then it is acceptable to take a *sideways* step which maintains the current altitude, but with luck brings the climber nearer to a point with a higher altitude. At times it is prudent to even step downhill to get away from a local peak which does not have satisfactory altitude.

Thus, we have the notion of an algorithm which wanders from one *partial solution* to another; in our problem, a *partial solution* on v ver-

$f(v)$	0	1	2	3	4	5	6	7	8	9
0	0	0	1	2	3	5	6	8	10	12
10	15	16	18	21	23	26	28	31	34	38
20	41	44	47	50	54	57	61	65	68	72
30	76	80	85	87	90	94	99	104	109	114
40	120	124	129	134	139	144	150	156	162	168
50	175	176	178	181	185	188	192	195	199	203
60	207	212	216	221	226	231	235	240	245	250
70	255	260	265	270	275	280	285	291	296	301
80	306	311	317	323	329	334	340	346	352	357
90	363	368	374	379	385	391	398	404	410	416
100	422	428	434	440	446	452	458	464	470	476
110	483	489	495	501	508	514	520	526	532	538
120	544	551	558	565	571	578	584	590	596	603
130	610	617	623	630	637	644	651	658	665	672
140	679	686	693	700	707	714	721	728	735	742
150	749	756	763	770	777	784	791	798	805	812
160	819	826	834	841	849	856	863	871	878	886
170	893	901	909	917	925	933	941	948	956	963
180	971	979	986	994	1001	1009	1017	1025	1033	1041
190	1049	1057	1065	1073	1081	1089	1097	1105	1113	1121
200	1129									

Table 1: Constructive lower bounds on $f(v)$

tices is any graph with v vertices. We distinguish between *valid partial solutions* which, in our case, are graphs on v vertices that contain neither a C_3 nor a C_4 , and partial solutions in general. The *search space* for a problem is the set of all partial solutions. A *neighbor* of a valid partial solution, G , is any point adjacent to G as defined by some perturbation function. (Since, in practice, a good perturbation function does not always return the same value when given the same valid partial solution, strictly speaking these are perturbation relations.)

The *cost* of a valid partial solution, G , is the distance from G to an optimal (or acceptable) solution. Thus, we define the cost of a valid partial solution, G , in the problem of finding an extremal graph on v vertices, to be $f(v) - |E(G)|$. When we are attempting to find a lowest cost valid partial solution on v vertices when $f(v)$ is not known, then we can think of the cost as being $1/|E(G)|$.

Given a point G in the search space, a *hill-climbing heuristic*, $h(G)$, attempts to return a neighbor of G that has lesser or equal cost. A *hill-climbing algorithm* begins with an initial valid partial solution (which is either a graph with no edges, or one where some edges have been ran-

domly included, but such that validity is maintained), and repeatedly applies hill-climbing heuristics to locate a point in the search space with sufficiently low cost. Hill-climbing algorithms have been used successfully in a number of combinatorial problems to quickly find approximate solutions (i.e. [17]). More recently, such algorithms have proven effective in finding optimal solutions to a variety of combinatorial problems ([4, 11, 23]). Classic references on this type of algorithm are [16] and [20] (pp. 454–481).

To see how hill-climbing can be applied to the problem of finding extremal graphs, we first define the notion of a *k-candidate*. A *k-candidate*, x , is a non-edge in a valid partial solution G where $E(G) \cup \{x\}$ contains at most k triangles and quadrilaterals combined. We now define a hill-climbing heuristic, **Climb**, which receives a valid partial solution, G , and a list of all 1-candidates (denoted *Candidates*).

procedure **Climb** (G , *Candidates*)

- remove a randomly chosen edge x from *Candidates*
- (a) if $\langle E(G) \cup \{x\} \rangle$ contains neither C_3 nor C_4 then
 - add x to $E(G)$
- (b) else if $\langle E(G) \cup \{x\} \rangle$ contains a single cycle $C \in \{C_3, C_4\}$, then
 - add x to $E(G)$
 - move from $E(G)$ to *Candidates* a random edge y in $E(C) - \{x\}$
 - add to *Candidates* non-edges that would complete C_3 or C_4 with y
- (c) else if x completes more than one cycle isomorphic to C_3 or C_4 then
 - do nothing

When the condition in clause (a) is true, the algorithm takes an uphill step. When the condition in clause (b) is met, the resulting graph represents a sideways step; though the procedure returns a different point in the search space, the cost is unchanged. When condition (c) is met, acceptance of the candidate would require a downhill step by removing several edges in order to maintain the validity of the partial solution; therefore the proposed candidate is rejected.

The efficiency of the procedure is not difficult to implement with a time complexity of $O(v^2)$. However, from invocation to invocation, **Climb** would redundantly check the candidacy of non-edges that are not 1-candidates. Thus, whenever an edge st is removed from the graph during a sideways step, all non-edges uv are added to *Candidates* whenever u or v is at most distance 2 from s or t . Step (c) in the procedure effectively removes any k -candidates (where $k > 1$) from

the list of candidates. This amounts to a lazy evaluation of the line under clause (b) that adds 1-candidates to *Candidates*.

In addition to hill-climbing, we make judicious use of exhaustive search. We use backtracking when the number of 0-candidates is not large, and we are trying to add few edges. This situation occurs when the cost of a valid partial solution is fairly low. The time complexity of backtracking for x edges from amongst c 0-candidates is $O(v_x^c)$. It is possible to search for 12 edges from amongst 75 0-candidates in about one minute on a machine rated at 24 mips. Sometimes it is possible to explore a much larger set of 0-candidates depending on the structure of the graph.

Multiple attempts at maximal solutions based solely on hill-climbing is analogous to making many narrow but deep probes for the ceiling of the search space. The use of backtracking near the end of a hill-climbing probe broadens the search in the neighborhood of a low cost valid partial solution. Since this second approach follows hill-climbing with backtracking, we call the technique *hill-tracking*.

We have been able to achieve better results with hill-tracking than with hill-climbing alone. (Our searches are of a magnitude that rule out backtracking alone.) As an example of the techniques, we describe now how we obtained a graph with $v = 97$, $e = 404$, and free of any C_3 or C_4 .

1. We began with G , a C_3 and C_4 free graph with $v = 96$ and $e = 397$ which was obtained through hill-tracking;
2. Adding an isolated vertex to G created 96 0-candidates;
3. Backtracking on the 0-candidates added 6 edges;
4. Hill-climbing from that point added one more edge to G , thus yielding the graph with $v = 97$ and $e = 404$;
5. Further hill-climbing re-arranged the edges in G such that a vertex, x , had degree 6. By removing x from G we improved our result on 96 vertices to 398 edges.

To illustrate the effectiveness of this technique we repeatedly applied hill-climbing to maximize the number of edges on 160 vertices; we never succeeded in placing more than 786 edges on the vertices. However, by hill-tracking from smaller graphs, we were able to place 819 edges on 160 vertices.

Without further theoretical insights on the values of $f(v)$ we cannot fully evaluate the effectiveness of our algorithm. However, it is worth noting that the algorithm repeatedly finds the unique extremal graph on 50 vertices (Hoffman-Singleton graph) in several seconds on a DECstation 5000 rated at 24 mips.

5 Closing Remarks

Figure 3 compares the computational and theoretical bounds. It is

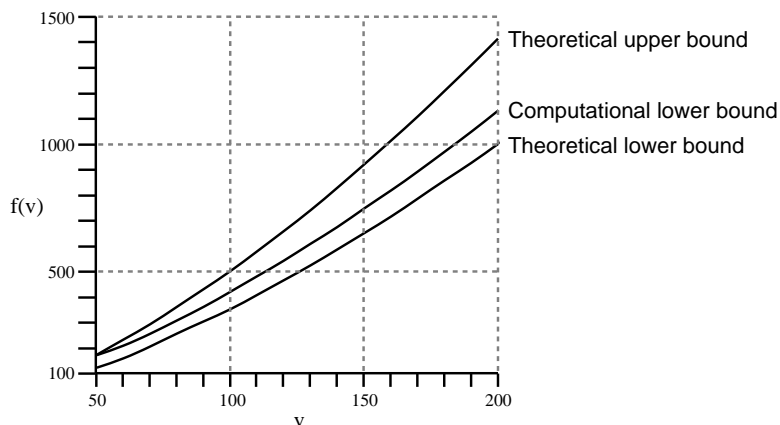


Figure 3: Computational and theoretical bounds on $f(v)$

not clear which theoretical bound seems to be closer to the asymptotic value of $f(v)$. The upper bound might be attained on 3250 vertices. To improve the theoretical bounds of $f(v)$, we need to derive more properties of the extremal graphs. The extremal graphs we obtained seem to have a highly symmetric structure, which suggests that it may be worthwhile to study the groups associated with them. Another interesting question: what are the necessary and sufficient conditions for $F(v) = 1$?

During the Kalamazoo conference in which this paper was presented, Professor McKay informed us via email (thanks to the conference organizers for providing a NeXT workstation for the conference attendants!) that he had computed $f(v)$ for $1 \leq v \leq 28$. His results

[18] agree with ours.

Acknowledgments

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