

Computing positive semidefinite minimum rank for small graphs

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The positive semidefinite minimum rank of a simple graph *G* is defined to be the smallest possible rank over all positive semidefinite real symmetric matrices whose *ij*-th entry (for $i \neq j$) is nonzero whenever $\{i, j\}$ is an edge in *G* and is zero otherwise. The computation of this parameter directly is difficult. However, there are a number of known bounding parameters and techniques which can be calculated and performed on a computer. We programmed an implementation of these bounds and techniques in the open-source mathematical software Sage. The program, in conjunction with the orthogonal representation method, establishes the positive semidefinite minimum rank for all graphs of order 7 or less.

1. Introduction

Define a graph G = (V, E) with vertex set V = V(G) and edge set E = E(G). The graphs discussed herein are simple (no loops or multiple edges) and undirected. The order of G, |G|, is the cardinality of V(G). Two vertices v and w of a graph G are neighbors if $\{v, w\} \in E(G)$. If H is a graph with $V(H) \subseteq V(G)$ and $E(H) \subseteq E(G)$ we call H a subgraph of G. H is an induced subgraph of G if H is a subgraph of G and if for all pairs $v, w \in V(H)$, $\{v, w\} \in E(H)$ if $\{v, w\} \in E(G)$. Given a set of vertices $S \subseteq V(G)$, G - S is the induced subgraph of G with vertices $V(G) \setminus S$.

A graph P = (V, E), where $V(P) = \{v_1, v_2, \dots, v_n\}$, is called a *path* if the edges of the graph are exactly $\{v_i, v_{i+1}\}$ for $i = 1, 2, \dots, n-1$. A *cycle* is a path that also has the edge $\{v_n, v_1\}$. A graph *G* is *chordal* if every induced cycle has length no greater than 3. A graph is *connected* if for any two vertices, v_1, v_2 , there exists a path with endpoints v_1 and v_2 . A connected graph with no cycles is a *tree*. An induced graph that is a tree is an *induced tree*. A graph with *n* vertices in which there is an edge between every vertex is called a *complete* graph and is denoted K_n . See Figure 1 for examples.

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Figure 1. Examples of graphs: (a) a path; (b) a cycle; (c) a tree; (d) the complete graph on 7 vertices.

Let $S_n(\mathbb{R})$ denote the set of real symmetric $n \times n$ matrices. For $A = [a_{ij}] \in S_n(\mathbb{R})$, the graph of A, denoted $\mathcal{G}(A)$, is the graph with vertices $\{1, 2, ..., n\}$ and edges $\{\{i, j\} : a_{ij} \neq 0 \text{ and } i \neq j\}$.

The positive semidefinite maximum nullity of G is

 $M_+(G) = \max\{ \text{null } A : A \in S_n(\mathbb{R}) \text{ is positive semidefinite and } \mathcal{G}(A) = G \}$

and the positive semidefinite minimum rank of G is

 $\operatorname{mr}_+(G) = \min\{\operatorname{rank} A : A \in S_n(\mathbb{R}) \text{ is positive semidefinite and } \mathscr{G}(A) = G\}.$

Clearly $mr_{+}(G) + M_{+}(G) = |G|$.

The following concept was introduced in [Barioli et al. 2010]: in a graph *G* where all vertices in some vertex set $S \subseteq V(G)$ are colored black and the remaining vertices are colored white, the *positive semidefinite color change rule* is: If W_1, W_2, \ldots, W_k are the sets of vertices of the *k* connected components of G-S (k = 1 is a possibility), $w \in W_i, u \in S$, and *w* is the only white neighbor of *u* in the subgraph of *G* induced by $V(W_i \cup S)$, then change the color of *w* to black, written as $u \to w$. Given an initial set *B* of black vertices, the *final coloring* of *B* is the set of vertices colored black as result of applying the positive semidefinite color change rule iteratively until no more vertices may be colored black. If the final coloring of *B* is V(G), *B* is called a *positive semidefinite zero forcing set* of *G*. The *positive semidefinite zero forcing number* of a graph *G*, denoted $Z_+(G)$, is the minimum of |B| for all *B* positive semidefinite zero forcing sets of *G*. In [Barioli et al. 2010] it was shown that if *G* is a graph then $M_+(G) \leq Z_+(G)$.

Example 1.1. Consider the graph *G* in Figure 2(a) with the set $B = \{v_4\}$ initially colored black. When the positive semidefinite color change rule is applied, the connected component W_1 of G - B is the induced subgraph of *G* on the vertices $\{v_1, v_2, v_3\}$. Since v_3 is the only white neighbor of v_4 in the subgraph of *G* induced by $W_1 \cup B$ (this is actually all of G), $v_4 \rightarrow v_3$ as demonstrated in Figure 2(b). For the



Figure 2. Illustrating Example 1.1.

next iteration, the set of black vertices is $B' = \{v_3, v_4\}$. The connected components of G - B' are W'_1 , induced by $\{v_1\}$, and W'_2 , induced by $\{v_2\}$. Vertex v_1 is the only white neighbor of vertex v_3 in the subgraph of G induced by $W'_1 \cup B'$ and v_2 is the only white neighbor of vertex v_3 in the subgraph of G induced by $W'_2 \cup B'$. Therefore, $v_3 \rightarrow v_1$ and $v_3 \rightarrow v_2$; see Figure 2(c). Now, the entire graph has been forced black, as shown in Figure 2(d), and since the process was started by a single black vertex, $Z_+(G) \leq 1$. However, at least one vertex must be colored to begin the zero forcing process. Therefore, $Z_+(G) = 1$.

Let *G* be a graph and *S* the smallest subset of V(G) such that G - S is disconnected. Then $|S| = \kappa(G)$ is called the *vertex connectivity* of *G*. A *clique covering* of *G* is a set of induced subgraphs $\{S_i\}$ of *G* such that each S_i is complete and $E(G) = \bigcup E(S_i)$. The *clique cover number* of a graph *G*, denoted cc(*G*), is the minimum of $|\{S_i\}|$ over all $\{S_i\}$ clique coverings of *G*.

In [Booth et al. 2008] $M_+(G)$ was determined for every graph G of order at most 6. Use of published software (Zq.py; see [Butler and Grout 2011]) for computing $Z_+(G)$ establishes $M_+(G) = Z_+(G)$ for $|G| \le 6$. We developed a program (see [Osborne and Warnberg 2011a]) in the open-source computer mathematics software system Sage (sagemath.org) to compute bounds for positive semidefinite maximum nullity. The program uses Zq.py [Butler and Grout 2011] and known results for computing positive semidefinite maximum nullity. These results are summarized in Section 2. A detailed description of the program may be found in Appendix A. Sections 2 and 3 provide a survey of techniques for computing positive semidefinite minimum rank.

In Section 3 we determine $M_+(G)$ for $|G| \le 7$ and show $M_+(G) = Z_+(G)$ for all such graphs. For all but 13 graphs of order 7, $M_+(G)$ can be computed by the program. We then established $M_+(G)$ for the remaining 13 graphs by utilizing orthogonal representation to find a positive semidefinite matrix A with $\mathscr{G}(A) = G$ and nullity of $A = Z_+(G)$. This establishes that $M_+(G) = Z_+(G)$ for each graph G of order at most 7. These matrices are listed in Appendix B.

2. Known results used by the program to establish positive semidefinite minimum rank/maximum nullity

Note that all of our parameters sum over the connected components of a disconnected graph. Given its relation to the positive semidefinite zero forcing number, the following results are given in terms of positive semidefinite maximum nullity. However, given a graph G, $M_+(G) + mr_+(G) = |G|$, so all of the following results may easily be translated to positive semidefinite minimum rank.

Theorem 2.1 [Ekstrand et al. 2013]. Let G be a graph.

- (i) $Z_+(G) = 1$ if and only if $M_+(G) = 1$.
- (ii) $Z_+(G) = 2$ if and only if $M_+(G) = 2$.
- (iii) $Z_+(G) = 3$ implies $M_+(G) = 3$.

Corollary 2.2. *If* $Z_+(G) \ge 3$ *, then* $M_+(G) \ge 3$ *.*

Observation 2.3 [Ekstrand et al. 2013]. $Z_+(G) = |G| - 1$ *if and only if* $M_+(G) = |G| - 1$.

Note that the only graph *G* having $Z_+(G) = |G| - 1$ is K_n , the complete graph on *n* vertices.

For a chordal graph G, it was shown in [Booth et al. 2008] that $cc(G) = mr_+(G)$, in [Hackney et al. 2009] it was shown that OS(G) = cc(G), and in [Barioli et al. 2010] it was shown that $Z_+(G) + OS(G) = |G|$, where OS(G) is the ordered subgraph number of G (see [Mitchell et al. 2010] for the definition of OS(G)). Thus $Z_+(G) = M_+(G)$, which gives the next theorem.

Theorem 2.4 [Barioli et al. 2010; Booth et al. 2008; Hackney et al. 2009]. *If G is chordal, then* $M_+(G) = Z_+(G)$.

Example 2.5. Consider graph *G*551 in Figure 3, left. Sets of vertices of size 1 or 2 are clearly not positive semidefinite zero forcing sets, so $Z_+(G551) \ge 3$. Notice that choosing an initial set of 3 black vertices that are all nonadjacent does not force anything. By symmetry this reduces to two cases. In the first case we choose $\{1, 2\}$ as our adjacent black vertices and as our third we choose any of the remaining vertices and notice that the graph will not be forced. Similarly, choosing $\{1, 3\}$ as our adjacent black vertices and any of the remaining vertices as our third also fails to force the graph. Thus, $Z_+(G551) \ge 4$. Observe that $\{1, 3, 4, 5\}$ forms a positive semidefinite zero forcing set meaning $Z_+(G551) \le 4$, hence $Z_+(G551) = 4$. However, *G*551 is chordal as its largest cycle is size 3. Therefore, by Theorem 2.4 $M_+(G551) = 4$.

Theorem 2.6 [Lovász et al. 1989; 2000]. For every graph G, $\kappa(G) \leq M_+(G)$.



Figure 3. Graphs G551 (left) and G128 (right).

Example 2.7. By inspection, removing any one vertex from graph *G*128 (see Figure 3, right) will not result in a disconnected graph. Therefore, $\kappa(G) \ge 2$. Further, {3, 4} forms a positive semidefinite zero forcing set for *G*128. Thus, $Z_+(G) \le 2$. This gives $2 \le \kappa(G) \le M_+(G) \le Z_+(G) \le 2$.

For a graph G the *neighborhood* of $v \in V(G)$ is

 $N_G(v) = \{ w \in V(G) \mid v \text{ is adjacent to } w \}.$

Vertices v and w are called *duplicate vertices* if $N_G(v) \cup \{v\} = N_G(w) \cup \{w\}$.

Proposition 2.8 [Ekstrand et al. 2013]. *If* v and w are duplicate vertices in a connected graph G with $|G| \ge 3$, then $Z_+(G - v) = Z_+(G) - 1$.

Proposition 2.9 [Booth et al. 2008]. *If* v and w are duplicate vertices in a connected graph G with $|G| \ge 3$, then $mr_+(G-v) = mr_+(G)$.

Recall that for any graph G, $mr_+(G) + M_+(G) = |G|$, which gives the following corollary.

Corollary 2.10. If v and w are duplicate vertices in a connected graph G with $|G| \ge 3$, then $M_+(G-v) = M_+(G) - 1$.

Example 2.11. In graph *G*1196 (see Figure 4, left) notice that 2 and 4 are duplicate vertices, as are vertices 3 and 5. Removal of vertices 2 and 3 results in a graph that is isomorphic to graph *G*43 (see Figure 4, right). $Z_+(G43) = 2$ thus $M_+(G43) = 2$ by Theorem 2.1. Therefore, $M_+(G1196) = 4$ by Corollary 2.10.

Cut-vertex reduction is a standard technique in the study of minimum rank. A vertex v of a connected graph G is a *cut-vertex* if G - v is disconnected. Suppose $G_i, i = 1, ..., h$, are graphs of order at least two, there is a vertex v such that for all $i \neq j$, $G_i \cap G_j = \{v\}$, and $G = \bigcup_{i=1}^h G_i$ (if $h \ge 2$, then clearly v is a cut-vertex of G). Then it is observed in [van der Holst 2009] that

$$\operatorname{mr}_{+}(G) = \sum_{i=1}^{h} \operatorname{mr}_{+}(G_{i}).$$



Figure 4. Graphs G1196 (left) and G43 (right).



Figure 5. Graph G419.

Because $mr_+(G) + M_+(G) = |G|$, this is equivalent to

$$\mathbf{M}_{+}(G) = \left(\sum_{i=1}^{h} \mathbf{M}_{+}(G_{i})\right) - h + 1.$$
(1)

It is shown in [Mitchell et al. 2010] that

$$OS(G) = \sum_{i=1}^{h} OS(G_i).$$

Since $OS(G) + Z_+(G) = |G|$ (shown in [Barioli et al. 2010]), this is equivalent to

$$Z_{+}(G) = \left(\sum_{i=1}^{h} Z_{+}(G_{i})\right) - h + 1.$$
 (2)

Example 2.12. Equation (2) can be used to compute $Z_+(G419)$ and $M_+(G419)$ (see Figure 5(a)). Notice that vertex 5 is a cut vertex of the graph since removing it results in a disconnected graph with 3 components, namely H_1 , H_2 and H_3 . When vertex 5 is reconnected to each of our components it is easy to see that $G_i \cap G_j = \{5\}$ for $i, j \in \{1, 2, 3\}$ with $i \neq j$, as illustrated by Figures 5(c)–(e). It is also clear that $\bigcup_{i=1}^{3} G_i = G419$, $Z_+(G_1) = 2$, $Z_+(G_2) = 1$, and $Z_+(G_3) = 2$. Thus, by



Figure 6. Graphs G200 (left) and G1090 (right).

Equation (2), $Z_+(G419) = 2 + 1 + 2 - 3 + 1 = 3$. A similar argument shows that $M_+(G419) = 3$.

Observe that if $\kappa(G) = 1$, there exists a cut vertex. The next result is an immediate consequence of the cut-vertex reduction Equations (1) and (2).

Observation 2.13 [Ekstrand et al. 2013]. Suppose G_i , i = 1, ..., h are graphs, there is a vertex v such that for all $i \neq j$, $G_i \cap G_j = \{v\}$, and $G = \bigcup_{i=1}^h G_i$. If $M_+(G_i) = Z_+(G_i)$ for all i = 1, ..., h, then $M_+(G) = Z_+(G)$.

Observation 2.14 [Hackney et al. 2009]. *If G is a graph then* $cc(G) \ge mr_+(G)$.

Corollary 2.15. $|G| - cc(G) \le M_+(G)$.

Example 2.16. In Figure 6, left, notice that graph G200 is not complete so

$$\mathrm{mr}_+(G200) \ge 2.$$

Also, note that the subgraphs induced by $S_1 = \{1, 2, 3, 4, 5\}$ and $S_2 = \{4, 5, 6\}$ are complete and $E(G200) = E(S_1) \cup E(S_2)$ so $cc(G200) \le 2$, hence $mr_+(G200) = 2$.

In [Booth et al. 2008] the *tree size* of a graph G, denoted ts(G), is defined to be the number of vertices in a maximum induced tree of G. Also from [Booth et al. 2008], if T is a maximum induced tree and w is a vertex not belonging to T, denote by $\mathscr{E}(w)$ the set of all edges of all paths in T between every pair of vertices of T that are adjacent to w. The following theorem was established by Booth et al. [2008].

Theorem 2.17 [Booth et al. 2008]. For a connected graph G,

$$mr_+(G) = ts(G) - 1 \tag{3}$$

if the following condition holds: there exists a maximum induced tree T such that for u and w not on T, $\mathscr{C}(u) \cap \mathscr{C}(w) \neq \emptyset$ if and only if u and w are adjacent in G.

Note that Equation (3) may be rewritten as $M_+(G) = |G| - ts(G) + 1$.

Example 2.18. To illustrate the previous theorem we consider graph *G*1090 (see Figure 6, right). To find ts(*G*1090) notice that *G*1090 has two disjoint, induced *K*₃'s, namely the graphs induced by vertex sets {1, 2, 3} and {5, 6, 7}. This means in order to find an induced tree, removal of one vertex from each *K*₃ is required. By inspection, removal of any of the nine pairs {{1, 5}, {1, 6}, {1, 7}, {2, 5}, ..., {3, 7}} results in a graph with a cycle, thus ts(*G*1090) \leq 4. However, the subgraph induced by {1, 4, 5, 6} is a tree (call it *T*), hence ts(*G*1090) = 4. We show *T* satisfies the condition of Theorem 2.17. The vertices not in *G*1090 – *T* are 2, 3, and 7, which are all adjacent in *G*1090.

$$\mathscr{E}(2) = \{(1, 6), (5, 6), (4, 5)\} = \mathscr{E}(3) \text{ and } \mathscr{E}(7) = \{(5, 6)\}$$

Therefore, $\mathscr{E}(2) \cap \mathscr{E}(3) \cap \mathscr{E}(7) \neq \emptyset$ and the condition holds because $\{2, 3, 7\}$ are pairwise adjacent. Thus $M_+(G1090) = 4$.

3. Computation of positive semidefinite maximum nullity of graphs of order 7 or less

The program developed by Osborne and Warnberg [2011a] implements the results from Section 2. Running the program on all graphs of order 7 or less yielded positive semidefinite maximum nullity for 1239 of 1252 graphs. It may be noted that the positive semidefinite maximum nullity was already known for the 208 graphs of order 6 or less (see [Booth et al. 2008]). However, the program was able to successfully compute the positive semidefinite maximum nullity for these graphs without referencing this information. For the remaining 13 graphs, the method of orthogonal representations was used to construct a matrix representation exhibiting nullity equal to the positive semidefinite zero forcing number. These matrices are shown in Appendix B.

A set $\vec{V} = {\vec{v_1}, ..., \vec{v_n}}$ in \mathbb{R}^d is an *orthogonal representation* of the graph *G* if for $i \neq j$, the dot product of $\vec{v_i}$ with $\vec{v_j}$ is nonzero if the vertices *i* and *j* are adjacent, and zero otherwise. If $\vec{V} = {\vec{v_1}, ..., \vec{v_n}}$ is an orthogonal representation of the graph *G* in \mathbb{R}^d and $B = [\vec{v_1} ... \vec{v_n}]$, then $B^T B \in \mathcal{G}_+(G)$ and rank $B^T B \leq d$. Thus, if a representation is found in \mathbb{R}^d then $mr_+(G) \leq d$ and $M_+(G) \geq |G| - d$.

Example 3.1. Consider graph *G*17 in Figure 7, left. Note that when we refer to a graph in the form *G*17 we are using notation from [Read and Wilson 1998]. To start constructing an orthogonal representation for *G*17 let v_1 , v_2 , v_3 , $v_4 \in \mathbb{R}^2$ correspond to vertices 1, 2, 3 and 4 respectively. Choose as many disjoint vertices as possible, say 1 and 4. By definition $v_1 \cdot v_4 = 0$ so let $v_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$ and $v_4 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$. To find v_2 and v_3 , set

$$v_2 = \begin{bmatrix} ca_2 \\ b_2 \end{bmatrix}$$
 and $v_3 = \begin{bmatrix} a_3 \\ b_3 \end{bmatrix}$.



Figure 7. Graph G17 (left); A, a matrix representation of G17 (right).



Figure 8. Möbius ladder on 8 vertices.

Now, v_2 is adjacent to v_1 and v_4 so $v_1 \cdot v_2 \neq 0$ and $v_2 \cdot v_4 \neq 0$. Thus $a_2 \neq 0 \neq b_2$. Similarly, $a_3 \neq 0 \neq b_3$. Since v_2 and v_3 are not adjacent, we know $v_2 \cdot v_3 =$ $a_2a_3+b_2b_3=0$. With these restrictions it is clear that $a_2=a_3=b_2=1$ and $b_3=-1$ is a solution and an orthogonal representation construction is complete. This gives

$$B = \begin{bmatrix} 1 & 1 & 1 & 0 \\ 0 & 1 & -1 & 1 \end{bmatrix} \text{ and } B^T B = A$$

(see Figure 7, right). By construction, rank(A) = 2. Thus mr₊ $(G17) \le 2$ and $M_+(G17) \ge |G| - 2 = 2$. Observe that $\{1, 2\}$ forms a positive semidefinite zero forcing set for graph G17 hence $Z_+(G17) \le 2$. Finally, $2 \le M_+(G17) \le Z_+(G17) \le 2$.

In every case, positive semidefinite maximum nullity was found to equal the positive semidefinite zero forcing number. This has established the next result.

Theorem 3.2. If G is a graph with 7 or fewer vertices, then $M_+(G) = Z_+(G)$.

See [Osborne and Warnberg 2011b] for a complete spreadsheet containing positive semidefinite maximum nullity and zero forcing number for all graphs with 7 or fewer vertices.

Corollary 3.3. Suppose G_i , i = 1, ..., h, are graphs with $|G_i| \le 7$, there is a vertex v such that for all $i \neq j$, $G_i \cap G_j = \{v\}$, and $G = \bigcup_{i=1}^h G_i$. Then $M_+(G) = Z_+(G)$.

Proof. Apply Theorem 3.2 to Observation 2.13.

Note that Theorem 3.2 cannot be extended to graphs with more than 7 vertices as $Z_+(V_8) = 4$ and $M_+(V_8) = 3$ (shown in [Mitchell et al. 2010]), where V_8 is the Möbius ladder on 8 vertices (see Figure 8).

Appendix A: Method used by the program

The program uses the following general method:

(1) Separate the graph into its connected components and work on each component separately. Results will be summed before reporting.

(2) Compute $Z_+(G)$.

(a) If $Z_+(G) \le 3$, apply the results of Theorem 2.1.

(b) Else, use Corollary 2.2 to establish a lower bound for $M_+(G)$.

(3) If $Z_+(G) = |G| - 1$, apply the results of Observation 2.3.

(4) If G is chordal, apply Theorem 2.4.

(5) Compute the vertex connectivity of $G(\kappa(G))$.

(a) If $\kappa(G) = \mathbb{Z}_+(G)$, apply Theorem 2.6.

(b) Else, if $\kappa(G)$ is a tighter bound for $M_+(G)$, improve the lower bound.

(6) If there are duplicate vertices in the graph, discard all but one copy by applying Corollary 2.10 and returning to step 2.

(7) Apply the cut-vertex formula iteratively by applying Equation (1) and returning to step 2 for each component.

- (8) Compute the clique cover number of G.
- (a) If $|G| cc(G) = Z_+(G)$, apply Corollary 2.15.
- (b) Else, if cc(G) is a tighter bound for $M_+(G)$, improve the lower bound.
- (9) Apply Theorem 2.17 to determine if $M_+(G) = |G| ts(G) + 1$.

Appendix B: Matrix representations

Each of the following thirteen matrices satisfies $null(A) = 4 = Z_+(G)$.



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sosborne@iastate.edu	Department of Mathematics, Iowa State University, Ames, IA 50011, United States
warnberg@iastate.edu	Department of Mathematics, Iowa State University, Ames, IA 50011, United States



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Amarjit S. Budhiraja	U of North Carolina, Chapel Hill, USA budhiraj@email.unc.edu	Mary Meyer	Colorado State University, USA meyer@stat.colostate.edu
Pietro Cerone	La Trobe University, Australia P.Cerone@latrobe.edu.au	Emil Minchev	Ruse, Bulgaria eminchev@hotmail.com
Scott Chapman	Sam Houston State University, USA scott.chapman@shsu.edu	Frank Morgan	Williams College, USA frank.morgan@williams.edu
Joshua N. Cooper	University of South Carolina, USA cooper@math.sc.edu	Mohammad Sal Moslehian	Ferdowsi University of Mashhad, Iran moslehian@ferdowsi.um.ac.ir
Jem N. Corcoran	University of Colorado, USA corcoran@colorado.edu	Zuhair Nashed	University of Central Florida, USA znashed@mail.ucf.edu
Toka Diagana	Howard University, USA tdiagana@howard.edu	Ken Ono	Emory University, USA ono@mathcs.emory.edu
Michael Dorff	Brigham Young University, USA mdorff@math.byu.edu	Timothy E. O'Brien	Loyola University Chicago, USA tobrie1@luc.edu
Sever S. Dragomir	Victoria University, Australia sever@matilda.vu.edu.au	Joseph O'Rourke	Smith College, USA orourke@cs.smith.edu
Behrouz Emamizadeh	The Petroleum Institute, UAE bemamizadeh@pi.ac.ae	Yuval Peres	Microsoft Research, USA peres@microsoft.com
Joel Foisy	SUNY Potsdam foisyjs@potsdam.edu	YF. S. Pétermann	Université de Genève, Switzerland petermann@math.unige.ch
Errin W. Fulp	Wake Forest University, USA fulp@wfu.edu	Robert J. Plemmons	Wake Forest University, USA plemmons@wfu.edu
Joseph Gallian	University of Minnesota Duluth, USA jgallian@d.umn.edu	Carl B. Pomerance	Dartmouth College, USA carl.pomerance@dartmouth.edu
Stephan R. Garcia	Pomona College, USA stephan.garcia@pomona.edu	Vadim Ponomarenko	San Diego State University, USA vadim@sciences.sdsu.edu
Anant Godbole	East Tennessee State University, USA godbole@etsu.edu	Bjorn Poonen	UC Berkeley, USA poonen@math.berkeley.edu
Ron Gould	Emory University, USA rg@mathcs.emory.edu	James Propp	U Mass Lowell, USA jpropp@cs.uml.edu
Andrew Granville	Université Montréal, Canada andrew@dms.umontreal.ca	Józeph H. Przytycki	George Washington University, USA przytyck@gwu.edu
Jerrold Griggs	University of South Carolina, USA griggs@math.sc.edu	Richard Rebarber	University of Nebraska, USA rrebarbe@math.unl.edu
Sat Gupta	U of North Carolina, Greensboro, USA sngupta@uncg.edu	Robert W. Robinson	University of Georgia, USA rwr@cs.uga.edu
Jim Haglund	University of Pennsylvania, USA jhaglund@math.upenn.edu	Filip Saidak	U of North Carolina, Greensboro, USA f_saidak@uncg.edu
Johnny Henderson	Baylor University, USA johnny_henderson@baylor.edu	James A. Sellers	Penn State University, USA sellersj@math.psu.edu
Jim Hoste	Pitzer College jhoste@pitzer.edu	Andrew J. Sterge	Honorary Editor andy@ajsterge.com
Natalia Hritonenko	Prairie View A&M University, USA nahritonenko@pvamu.edu	Ann Trenk	Wellesley College, USA atrenk@wellesley.edu
Glenn H. Hurlbert	Arizona State University,USA hurlbert@asu.edu	Ravi Vakil	Stanford University, USA vakil@math.stanford.edu
Charles R. Johnson	College of William and Mary, USA crjohnso@math.wm.edu	Antonia Vecchio	Consiglio Nazionale delle Ricerche, Italy antonia.vecchio@cnr.it
K. B. Kulasekera	Clemson University, USA kk@ces.clemson.edu	Ram U. Verma	University of Toledo, USA verma99@msn.com
Gerry Ladas	University of Rhode Island, USA gladas@math.uri.edu	John C. Wierman	Johns Hopkins University, USA wierman@jhu.edu
		Michael E. Zieve	University of Michigan, USA zieve@umich.edu

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