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Ordering graphs in a normalized singular value measure

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A proposed measure of network cohesion for graphs arising from interrelated economic activity is studied. The measure is the largest singular value of a row-stochastic matrix derived from the adjacency matrix. It is shown here that among graphs on n vertices, the star universally gives the (strictly) largest measure. Other universal comparisons among graphs with larger measures are difficult to make, but one is conjectured, and a selection of empirical evidence is given.

1. Introduction

In [Cavalcanti et al. 2012; 2013] the authors studied the role of network "cohesion" in the equilibration of economic or other activity among agents whose interaction is governed by a particular graph. An example is the one in which adjacency is the bordering relationship among countries. Giannitsarou and Johnson (personal communication, 2011) proposed a particular numerical measure of network cohesion and raised the question of which graph on n vertices resulted in the highest measure. That measure may be described as follows. Let A be the adjacency matrix of a graph G, define $B = A + I$, and let D be the positive diagonal matrix whose diagonal entries are the row sums of B. If $R = D^{-1}B$, then R is row-stochastic, and $\sigma(G)$, the measure of cohesion, is the largest singular value of R. Recall that the singular values of R are the square roots of the eigenvalues of RR^T. Another application where the matrix R has appeared is in [Echenique and Fryer 2007], where it is referred to as the matrix of social interactions.

Here, we show that, for any n, $\sigma(G)$ is maximized by the star S_n. The measure $\sigma(G)$ is 1 if and only if G is regular, and 1 is the smallest possible value (Section 2, Proposition 1). Using our methods, it is difficult to determine, in advance, the relative position in this order of other graphs. Indeed, for graphs naturally defined on any number of vertices, the position often changes with n. However, we do

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conjecture that the star plus an edge that connects two of the pendant vertices is next after the star, based, in part, on empirical evidence. After that, however, there may be no universal third place independent of n.

In the next section we mention known results that we use, and develop some new ideas that are important for our observations. In particular, the entries of RR^T have a nice and useful interpretation. Then, we show the star yields the highest measure by showing that a lower bound for the square of its largest singular value beats an upper bound for that of any other graph. Finally, in an Appendix, we give a selection of empirical information of interest (Table 1 and Figures 2, 3, 4, 5).

2. Background and tools

Given a graph G on n vertices, let A be the adjacency matrix of G. Unless otherwise noted, our notation follows [West 1996]. Let $R = D^{-1}(A + I)$, where D is the unique positive diagonal matrix such that R is row-stochastic. Let $\lambda(G)$ denote the maximum eigenvalue of RR^T, and note that $\sigma(G) = \sqrt{\lambda(G)}$.

Proposition 1. *For any connected graph G on n vertices, $\sigma(G) \geq 1$, and $\sigma(G) = 1$ if and only if G is regular.*

Proof. Note that G is regular if and only if R is doubly stochastic. If R is doubly stochastic, then it is a convex combination of permutation matrices by Birkhoff's theorem [Horn and Johnson 1990, Theorem 8.1.7], and therefore the operator norm of R, which equals the maximum singular value, is 1. Let $e \in \mathbb{R}^n$ denote the vector with 1 in every entry. By the Cauchy–Schwarz inequality, $\|e^T R\|_2 \geq \langle e^T R, e/\sqrt{n}\rangle = \sqrt{n} = \|e^T\|_2$, with equality if and only if $e^T R$ is a multiple of e^T. Therefore, when R is row-stochastic but not doubly stochastic, the operator norm of R is strictly greater than one. It follows that $\sigma(G) > 1$ when G is not regular. ☐

Note that $D = \operatorname{diag}(\{d_i + 1\}_{i \in 1,\dots,n})$, where d_i is the degree of vertex i in G. Let $C = (A + I)(A + I)^T$. The (i, j) entry of C, which we denote by c_{ij}, is the number of vertices that are adjacent to both vertex i and vertex j, with the convention that two adjacent vertices are common neighbors of each other, that is, $c_{ij} = |N[i] \cap N[j]|$. In particular $c_{ii} = d_i + 1$. Thus the entries of RR^T are

$$r_{ij} = \frac{c_{ij}}{(d_i + 1)(d_j + 1)}. \tag{1}$$

Lemma 1. *Let RR^T be defined as above and assume that $n > 2$. When $i \neq j$, the largest possible values of r_{ij} are $\frac{1}{3}$ and $\frac{1}{4}$. If $r_{ij} = \frac{1}{3}$ for some $i \neq j$, then $d_i = d_j = 2$ with $c_{ij} = 3$ or $\{d_i, d_j\} = \{1, 2\}$ with $c_{ij} = 2$ (see* Figure 1).

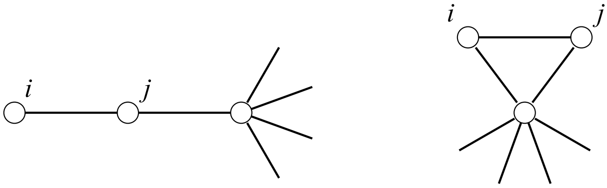


Figure 1. Possible adjacency graphs when $r_{ij} = \frac{1}{3}$.

Proof. We may assume that $d_j \geq d_i$. Note that $c_{ij} \leq d_i + 1$; thus $r_{ij} \leq 1/(d_j + 1)$. If $r_{ij} > \frac{1}{4}$, then $d_j = 1$ or $d_j = 2$. In the former case, $d_i = d_j = 1$, which can only happen if $n = 2$, since G is assumed to be connected. In the latter case, $d_i = 1$ or $d_i = 2$ while $d_j = 2$. If $d_i = 1$ and $d_j = 2$, then $r_{ij} = c_{ij}/6 \in \{0, \frac{1}{6}, \frac{1}{3}\}$, depending on the value of c_{ij}. If $d_i = d_j = 2$, then $r_{ij} = c_{ij}/9 \in \{0, \frac{1}{9}, \frac{2}{9}, \frac{1}{3}\}$. ☐

Suppose that G is a connected graph with n vertices such that every vertex has degree 1 (is pendant) except for a single central vertex with degree $n - 1$. We refer to any such graph as a *star* on n vertices, denoted by S_n. We may assume without loss of generality that vertex 1 is the central vertex of the star. Using (1), we see that, for the star,

$$RR^T = \begin{bmatrix} \frac{g}{n} & \frac{1}{n} & \cdots & \cdots & \frac{1}{n} \\ \frac{g}{n} & \frac{1}{2} & \frac{1}{4} & \cdots & \frac{1}{4} \\ \vdots & \frac{1}{4} & \frac{1}{2} & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & \frac{1}{4} \\ \frac{g}{n} & \frac{1}{4} & \cdots & \frac{1}{4} & \frac{1}{2} \end{bmatrix}.$$

Note that $RR^T - \frac{1}{4}I$ is of rank 2, and therefore it is possible to explicitly calculate the characteristic polynomial of this matrix. Recall [Horn and Johnson 1990, Theorem 1.2.12] that the characteristic polynomial of a matrix is given by

$$p(t) = t^n - E_1 t^{n-1} + E_2 t^{n-2} + \cdots + (-1)^n E_n,$$

where each E_k is the sum of the k-by-k principal minors of the matrix. For $RR^T - \frac{1}{4}I$, only the 1-by-1 and 2-by-2 principal minors can be nonzero. Thus the characteristic equation for $RR^T - \frac{1}{4}I$ is

$$p(t) = t^n - \left(\frac{1}{n} + \frac{1}{4}(n-1)\right)t^{n-1} + \left(\frac{n-4}{4n^2}\right)(n-1)t^{n-2}.$$

The nonzero roots of this polynomial are

$$\frac{\frac{1}{4}(n-1)+\frac{1}{n}\pm\sqrt{\left(\frac{1}{4}(n-1)+\frac{1}{n}\right)^2-\frac{n-4}{n^2}}}{2},$$

and therefore the maximum eigenvalue of RR^T for the star on n vertices is

$$\lambda(S_n)=\frac{1}{4}+\frac{\frac{1}{4}(n-1)+\frac{1}{n}+\sqrt{\left(\frac{1}{4}(n-1)+\frac{1}{n}\right)^2-\frac{n-4}{n^2}}}{2}.$$

3. The star is a maximum

We seek to estimate the maximum eigenvalue $\lambda(G)$ of RR^T. The row sums of RR^T place constraints on $\lambda(G)$. By [Horn and Johnson 1990, Theorem 8.1.22],

$$\min_i\left\{\sum_j r_{ij}\right\}\le\lambda(G)\le\max_i\left\{\sum_j r_{ij}\right\}. \tag{2}$$

For the star on n vertices, $RR^T-\frac{1}{4}I$ contains an $(n-1)$-by-$(n-1)$ submatrix with all entries equal to $\frac{1}{4}$. It follows from the inclusion principle [Horn and Johnson 1990, Theorem 4.3.15] that $\lambda(S_n)\ge\frac{1}{4}n$. Combining this with the maximum row sum, we see that $\frac{1}{4}n\le\lambda(S_n)\le\frac{1}{4}n+\frac{1}{n}$.

The following observation is an immediate consequence of Lemma 1:

Lemma 2. *Suppose that $n>2$, and consider the rows of RR^T. If row i has diagonal entry $r_{ii}=\frac{1}{k}$ with $k\ge 4$ and no off-diagonal entry equals $\frac{1}{3}$, then the sum of the entries in row i is at most $\frac{1}{k}+\frac{1}{4}(n-1)$.*

Let us make a basic observation which we will use in the proofs of several subsequent propositions.

Lemma 3. *Let $c>0$. The function $x\mapsto 1/(x+1)+cx$ is concave up for all $x>0$, and therefore its maximum on any interval $[a,b]\subset(0,\infty)$ is attained at one of the endpoints.*

The following observations about the row sums of RR^T cover the cases when Lemma 2 does not apply:

Lemma 4. *Suppose that $n>3$. If row i has diagonal entry $r_{ii}=\frac{1}{2}$ and G is not the star, then the sum of the entries in row i is at most $-\frac{1}{6}+\frac{1}{n}+\frac{1}{4}n$.*

Proof. Since $r_{ii}=\frac{1}{2}$, $d_i=1$. Let j denote the vertex adjacent to i. The sum of the entries in row i is then

$$r_{ii}+r_{ij}+\sum_{m\neq i,j}r_{im}=\frac{1}{2}+\frac{1}{d_j+1}+\sum_{m\neq i,j}\frac{c_{im}}{d_m+1}.$$

Note that $c_{im}=1$ if there is an edge connecting vertex j to vertex m and $c_{im}=0$ otherwise. Therefore we have the following upper bound for the sum of entries in row i:

$$r_{ii}+r_{ij}+\sum_{m\neq i,j} r_{im} \leq \frac{1}{2}+\frac{1}{d_j+1}+\sum_{m\in N(j)} \frac{1}{2(d_m+1)}.$$

If $d_j=n-1$, and the graph is not the star, then there must be at least two vertices m_1 and m_2 such that $d_{m_1}>1$ and $d_{m_2}>1$. In this case an upper bound for the sum of the entries in row i is

$$\frac{1}{2}+\frac{1}{n}+\frac{1}{4}(d_j-3)+2\,\frac{1}{6}=-\frac{1}{6}+\frac{1}{n}+\frac{1}{4}n.$$

If $d_j<n-1$, then

$$\begin{aligned} r_{ii}+r_{ij}+\sum_{m\neq i,j} r_{im} &\leq \frac{1}{2}+\frac{1}{d_j+1}+\sum_{m\in N(j)} \frac{1}{2(d_m+1)} \\ &\leq \frac{1}{2}+\frac{1}{d_j+1}+\frac{1}{4}(d_j-1). \end{aligned}$$

Since $2\leq d_j<n-1$, we use Lemma 3 to see that an upper bound for this expression is

$$\max\left\{\frac{13}{12},-\frac{1}{4}+\frac{1}{n-1}+\frac{1}{4}n\right\}.$$

For $n>3$,

$$\max\left\{\frac{13}{12},-\frac{1}{4}+\frac{1}{n-1}+\frac{1}{4}n\right\} \leq -\frac{1}{6}+\frac{1}{n}+\frac{1}{4}n. \qquad \square$$

Lemma 5. *Suppose $n>3$. If row i has diagonal entry $r_{ii}=\frac{1}{3}$, then the sum of the entries in row i is less than $-\frac{1}{6}+\frac{1}{n}+\frac{1}{4}n$.*

Proof. Since $r_{ii}=\frac{1}{3}$, $d_i=2$. Let j and k denote the two vertices adjacent to i.

Case I. If there is an edge connecting j and k, then $c_{ij}=c_{ik}=3$. If $m\neq i$ is a vertex adjacent to both j and k, then

$$r_{im}=\frac{2}{3(d_m+1)}\leq\frac{2}{9}.$$

If m is only adjacent to one of j or k, then

$$r_{im}=\frac{1}{3(d_m+1)}\leq\frac{1}{6}.$$

Let $d = \max\{d_j, d_k\}$ and $D = \max\{d_j, d_k\}$. There are at most $d-2$ vertices other than i that are common neighbors of both j and k, and there are at most $D-d$ remaining vertices other than i that could be adjacent to exactly one of j or k. Therefore the sum of the entries in row i is at most

$$r_{ii} + r_{ij} + r_{ik} + \frac{2}{9}(d-2) + \frac{1}{6}(D-d) \leq -\frac{1}{9} + \frac{1}{(d+1)} + \frac{1}{(D+1)} + \frac{1}{18}d + \frac{1}{6}D.$$

In this case, $2 \leq d \leq D \leq n-1$. By Lemma 3, it follows that the possible maximum values in the expression above occur when either $d = D = 2$, or $d = 2$, $D = n-1$, or $d = D = n-1$. The corresponding upper bounds on the row sum are

$$1, \quad \frac{1}{6} + \frac{1}{n} + \frac{1}{6}n, \quad -\frac{1}{3} + \frac{2}{n} + \frac{2}{9}n.$$

Each of these bounds is less than $-\frac{1}{6} + \frac{1}{n} + \frac{1}{4}n$ for all $n > 3$.

Case II. If there is no edge connecting j with k, then $c_{ij} = c_{ik} = 2$. If $m \neq i$ is a vertex adjacent to both j and k, then

$$r_{im} = \frac{2}{3(d_m+1)} \leq \frac{2}{9}.$$

If m is only adjacent to one of j or k, then

$$r_{im} = \frac{1}{3(d_m+1)} \leq \frac{1}{6}.$$

Let $d = \max\{d_j, d_k\}$ and $D = \max\{d_j, d_k\}$. There are at most $d-1$ vertices other than i that are common neighbors of both j and k, and there are at most $D-d$ remaining vertices other than i that could be adjacent to exactly one of j or k. Therefore the sum of the entries in row i is at most

$$r_{ii} + r_{ij} + r_{ik} + \frac{2}{9}(d-1) + \frac{1}{6}(D-d) \leq \frac{1}{9} + \frac{2}{3(d+1)} + \frac{2}{3(D+1)} + \frac{1}{18}d + \frac{1}{6}D.$$

We know that $1 \leq d \leq D \leq n-2$. By Lemma 3, it follows that the possible maximum values in the expression above occur when either $d = D = 1$, or $d = 1$, $D = n-2$, or $d = D = n-2$. The corresponding upper bounds on the row sum are

$$1, \quad \frac{1}{6} + \frac{2}{3(n-1)} + \frac{1}{6}n, \quad \frac{-1}{3} + \frac{4}{3(n-1)} + \frac{2}{9}n.$$

Once again, each of these bounds is less than $-\frac{1}{6} + \frac{1}{n} + \frac{1}{4}n$ for all $n > 3$. □

Lemma 6. *Suppose $n > 3$. If row i contains an off-diagonal entry $r_{ij} = \frac{1}{3}$, then the sum of the entries in row i is at most $-\frac{1}{6} + \frac{1}{n} + \frac{1}{4}n$.*

Proof. There are three possible cases, depending on the possible degrees of i and j given by Lemma 1.

Case I. If $d_i = 1$ and $d_j = 2$, then there is only one other vertex, aside from i and j, that can share a common neighbor with i. Call that vertex k. The sum of entries in row i is

$$r_{ii} + r_{ij} + r_{ik} = \frac{1}{2} + \frac{1}{3} + \frac{1}{2(d_k+1)} \leq \frac{1}{2} + \frac{1}{3} + \frac{1}{4} = \frac{13}{12},$$

which is less than or equal to $-\frac{1}{6} + \frac{1}{n} + \frac{1}{4}n$ for all $n > 3$ (equality occurs only when $n = 4$).

Case II. If $d_i = 2$ and $d_j = 1$, then Lemma 5 implies that the sum of the entries in row i is less than $-\frac{1}{6} + \frac{1}{n} + \frac{1}{4}n$.

Case III. If $d_i = d_j = 2$, then by Lemma 1, $c_{ij} = 3$. Let k denote the third common neighbor of i and j. The sum of the entries in row i is then

$$\begin{aligned} r_{ii} + r_{ij} + r_{ik} + \sum_{m \neq i,j,k} r_{im} &= \frac{1}{3} + \frac{1}{3} + \frac{1}{d_k+1} + \sum_{m \neq i,j,k} \frac{1}{3(d_m+1)} \\ &\leq \frac{2}{3} + \frac{1}{d_k+1} + \frac{1}{6}(d_k - 2) \\ &\leq \frac{2}{3} + \frac{1}{n-1} + \frac{1}{6}(n-4) \\ &= \frac{1}{6}n + \frac{1}{n-1}. \end{aligned}$$

This upper bound is less than $-\frac{1}{6} + \frac{1}{n} + \frac{1}{4}n$ for all $n > 3$. ☐

Theorem 1. *Of all connected graphs on n vertices, the star attains the maximum value of σ.*

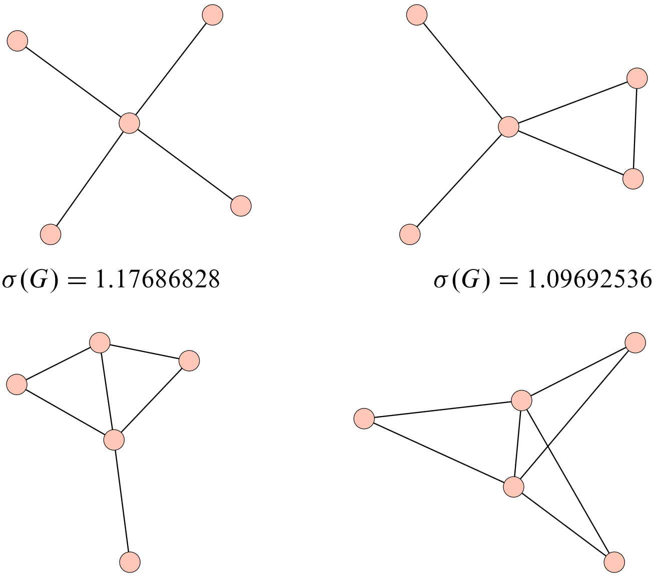
Proof. Suppose that G is not S_n. The contents of Lemmas 2, 4, 5, and 6 show that the maximum row sum of RR^T is less than or equal to $-\frac{1}{6} + \frac{1}{n} + \frac{1}{4}n$. If $n > 6$, then this upper bound is less than $\frac{1}{4}n$, and, by the comment after (2), we conclude that $\lambda(G) < \lambda(S_n)$ and therefore $\sigma(G) < \sigma(S_n)$. When $3 < n \leq 6$, we can verify by explicit computation that $-\frac{1}{6} + \frac{1}{n} + \frac{1}{4}n < \lambda(S_n)$. When $n = 3$, the theorem can be verified directly since there are only two connected graphs on 3 vertices. ☐

Appendix

Here we present the values of $\sigma(G)$ for every connected graph up to 6 vertices. The graphs are given in graph6 string format [McKay 1981; 2005], and the values of $\sigma(G)$ are given to 8 decimal places. The values for the stars are given in boldface.

Esa?	**1.26376262**
Eta?	1.17779971
Ds_	**1.17686828**
Epa?	1.12724256
Exg_	1.12719000
E|i_	1.11535507
E|g_	1.10702341
ExGg	1.10124485
Dt_	1.09692536
Cs	**1.09445053**
Exw_	1.09118881
Ehg_	1.08965849
Ex__	1.08492159
Eli_	1.08378641
E|__	1.08125829
Ep{G	1.07743057
Elg_	1.07386856
Et}G	1.06680419
E|w_	1.06420788
Etq_	1.06264937
Exo_	1.06170523
Ep__	1.06066017
EtuG	1.05968917
ExGG	1.05861770
D|_	1.05825411
D|g	1.05543372
Dp_	1.05417745
Eh__	1.05150374
El__	1.04879365
Er{G	1.04866795
EpsG	1.04851433
E|o_	1.04562708
ExWG	1.04512215
ExwG	1.04350178
EpuG	1.04308838
Ez{G	1.04248210
EvsW	1.04127270
Et]G	1.04082858
Ev{W	1.04057352
EzPW	1.03944703
Elw_	1.03869527
EvcG	1.03802560
Dx_	1.03794998
Epo_	1.03760887
Eto_	1.03627677
Dto	1.03552399
ExPw	1.03508808
Exwo	1.03458078
EtUG	1.03375811
Edq_	1.03272839
EzZw	1.03266215
EpgG	1.03266215
Er{W	1.03197929
EzwG	1.03138546
Cx	1.03138184
Ev_G	1.03126091
Dxw	1.02998084
EpWG	1.02979441
E~TW	1.02813174
Bo	**1.02813174**
Ep_G	1.02808843
ErwG	1.02792587
E~{G	1.02768976
Dl_	1.02717603
E~SW	1.02636956
EzsG	1.02530775
Dlg	1.02465677
EvoW	1.02459474
ExOG	1.02421645
ExPW	1.02380968
D|c	1.02305146
EpSG	1.02303779
Elo_	1.02301009
ExoG	1.02253862
E~{W	1.02245280
EvwW	1.02150256
E~sW	1.02136937
EzZW	1.02039571
EzoG	1.02034616
D~c	1.02031933
ErcG	1.01998619
EzWW	1.01866302
EzOW	1.01862583
EpUG	1.01823188
Ez[W	1.01792742
E~sG	1.01775521
E|qW	1.01732826
Exoo	1.01710090
Ez{w	1.01709947
EzSW	1.01709947
Dxo	1.01695288
Ezww	1.01494232
E~OW	1.01436311
Cz	1.01417394
Cp	1.01417394
E|sW	1.01400371
EroG	1.01390539
E~cG	1.01337635
ErwW	1.01293228
E~}W	1.01273126
Edo_	1.01267470
Dh_	1.01213081
Dpo	1.01188403
E|SW	1.01133377
E~_G	1.01111110
E|TW	1.01090626
EzcG	1.01084213
E~oW	1.01073140
Er_G	1.01059866
Dxc	1.00995156
EpOG	1.00969514
E~wW	1.00956370
ExOW	1.00891795
EroW	1.00885018
Ez_G	1.00805939
D~s	1.00764077
EzYW	1.00741994
ErOW	1.00711468
Epoo	1.00711468
E~yW	1.00707898
ExSW	1.00696806
ErWW	1.00696806
E|oW	1.00662172
Ezsw	1.00608114
Ezow	1.00603467
Dzs	1.00499991
Dzc	1.00459536
E~}w	1.00451397
E~uw	1.00445419
E|OW	1.00293400
E~YW	1.00274201
E~~w	1.00000000
Ezuw	1.00000000
Erow	1.00000000
ErYW	1.00000000
EpOW	1.00000000
D~{	1.00000000
Dhc	1.00000000
C~	1.00000000
Cr	1.00000000
Bw	1.00000000
A_	**1.00000000**

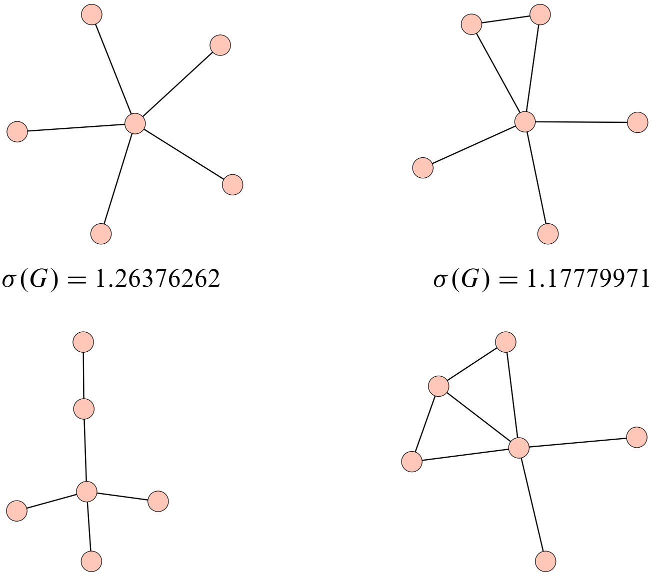
Table 1. The value of $\sigma(G)$ (to 8 decimal places) for every connected graph with at most 6 vertices, with the values of stars given in boldface.



$\sigma(G) = 1.17686828$ $\sigma(G) = 1.09692536$

$\sigma(G) = 1.05825411$ $\sigma(G) = 1.05543372$

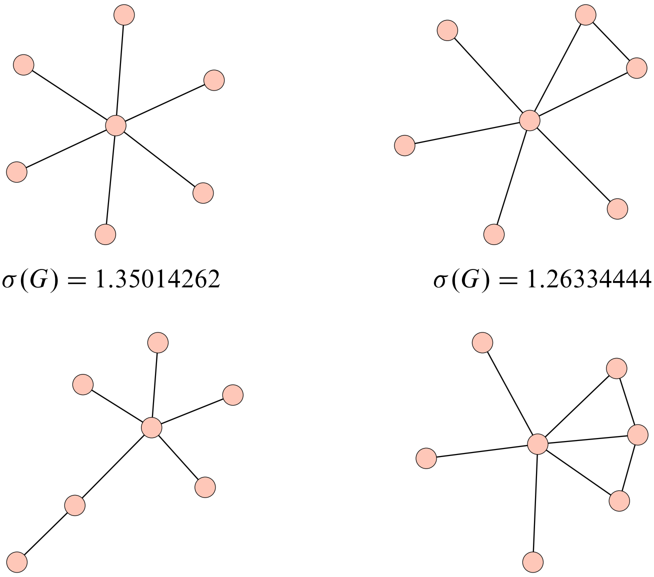
Figure 2. The graphs with the four highest singular values for $n = 5$.



$\sigma(G) = 1.26376262$ $\sigma(G) = 1.17779971$

$\sigma(G) = 1.12724256$ $\sigma(G) = 1.12719000$

Figure 3. The graphs with the four highest singular values for $n = 6$.



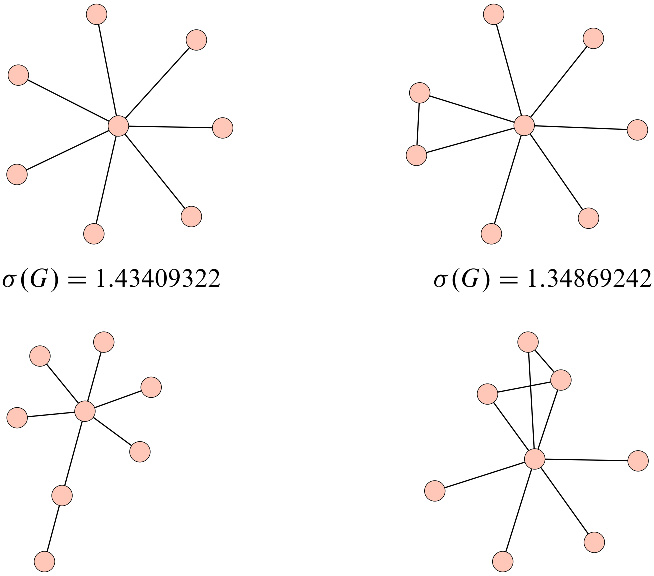
$\sigma(G) = 1.35014262$

$\sigma(G) = 1.26334444$

$\sigma(G) = 1.21280950$

$\sigma(G) = 1.20776980$

Figure 4. The graphs with the four highest singular values for $n = 7$.



$\sigma(G) = 1.43409322$

$\sigma(G) = 1.34869242$

$\sigma(G) = 1.30048331$

$\sigma(G) = 1.29185037$

Figure 5. The graphs with the four highest singular values for $n = 8$.

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crjohnso@math.wm.edu
Department of Mathematics, College of William & Mary,
Williamsburg, VA 23187, United States

blins@hsc.edu
Mathematics and Computer Science Department,
Hampden-Sydney College, Hampden Sydney, VA 23943,
United States

vdl1@williams.edu
Department of Mathematics and Statistics,
Williams College, 2899 Paresky, 39 Chapin Hall Drive,
Williamstown, MA 01267, United States

smeehan1@nd.edu
Department of Mathematics, University of Notre Dame,
Notre Dame, IN 46556, United States

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