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Variable neighbourhood search for connected graphs of fixed order and size with minimal spectral radius

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ABSTRACT

In this study we consider connected graphs of fixed order n and size m that minimize the largest eigenvalue of the adjacency matrix, also known as the spectral radius. Such graphs are called minimizers. The motivation for this research lies in the fact that the spectral radius plays a significant role in modelling virus propagation in complex networks, in the sense that a smaller spectral radius ensures a better virus protection in the network modelled by the corresponding graph. We conjecture that vertex degrees of a minimizer are as equal as possible, i.e. belong to $\{\lfloor 2m/n \rfloor, \lceil 2m/n \rceil\}$. The conjecture is confirmed for graphs with at most 10 vertices by the total enumeration, and some classes of graphs are resolved theoretically. In general, exact determining of minimizers is quite difficult and computationally exhaustive, and thus we propose a long-scale variable neighbourhood search as an alternative approach. We employ this heuristic search for selected instances concerning graphs with at most 100 vertices, and as a result we always obtain a graph with required vertex degrees. The search efficiently results in solutions that are (in a precise sense) close to the optimal ones, i.e. to minimizers.

Introduction

We consider only simple graphs, i.e. those that are finite, undirected and without loops or multiple edges. The *order* (resp. the *size*) of such a graph is the number of its vertices (resp. edges). The *spectrum* of a graph G is the spectrum of its standard $(0, 1)$ -adjacency matrix. Since this matrix is symmetric, its eigenvalues are real. The largest eigenvalue $\rho = \rho(G)$ is known as the *spectral radius* or the *index* of G . If G is connected, $\rho(G)$ is a simple eigenvalue. Following (Cvetković and Rowlinson, 1990; Simić et al., 2004), we denote the class of connected graphs with order n and size m by $H(n, m)$.

In this study we are interested in graphs that minimize the spectral radius in $H(n, m)$. Such a graph is called a *minimizer* and denoted by $H_{n,m}$. We recall the reader that the famous Perron–Frobenius Theorem (see Stanić 2015, Theorem 1.1) yields that the spectral radius of a connected graph strictly decreases when we remove any vertex or any edge. This justifies the approach in which we restrict ourselves to graphs with fixed order and size, since if the order is not fixed then the minimizer is a connected graph with the smallest allowed order, and similarly for the size. On the basis of the computer search and exhaustive computational experiments that include variable neighbourhood search (VNS) metaheuristic, we conjecture that vertex degrees of a minimizer are as equal as possible, i.e. they belong to $\{\lfloor 2m/n \rfloor, \lceil 2m/n \rceil\}$ (During the production of this paper, Sebi Cioabă has informed us that the same was conjectured by Hong in 1993.).

There are many efficient applications of the VNS in the spectral graph theory and related disciplines. Notably, the central place is reserved for the AutoGraphiX computer system developed by GERAD group from Montréal (Caporossi and Hansen, 2000, 2004): An interactive user-friendly software designed to help finding conjectures in graph theory which uses the VNS metaheuristic along with data analysis methods to find extremal graphs with respect to one or more graph invariants. Many research papers are devoted to conjectures generated by this system. Some of them are (Aouchiche et al., 2008) where the authors treated the three conjectures related to the spectral radius, Aouchiche et al. (2009) where the interaction between the spectral radius and selected structural invariants is considered or (Hansen et al., 2019) where one can find a review of results in which VNS was very successful in resolutions of many conjectures related to various graph invariants. For more applications of the VNS metaheuristic in graph theory we refer the reader to the list of references of Hansen et al. (2019), while for the related topics one may consult (Djukanović et al., 2022; Grbić et al., 2019; Mladenović et al., 2016, 2022; Mrkela and Stanimirović, 2021).

In our study, due to the enormous number of graphs that should be considered, an extensive search over all graphs is possible only for graphs with at most 10 vertices. However, a metaheuristic approach enables to find optimal or nearly optimal solutions for graphs with up to 100 vertices.

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We know from a broad literature, see [Stanić \(2015, p. 28\)](#), that the spectral radius of every connected graph is bounded from below by the average vertex degree $2m/n$, and it attains this bound if and only if the graph is regular (i.e. all its vertices are equal in degree). It follows that for a regular graph we have $\lfloor 2m/n \rfloor = 2m/n$ and this is the common vertex degree. In other words, the conjecture is confirmed for regular graphs. Moreover, the ‘regular case’ tells us that a minimizer is not necessarily unique. A connected graph with minimum number of edges is known as a *tree*, and here we have $n = m + 1$. There is a classical result, conjectured in [Collatz and Sinogowitz \(1957\)](#) and proved in [Lovász and Pelikán \(1973\)](#), stating that $2 \cos \frac{\pi}{n+1} \leq \rho(G)$ holds, along with equality if and only if G is the n -vertex path. This confirms the conjecture in case of trees, as the path has 2 vertices of degree $\lfloor 2m/n \rfloor = 1$ and $n - 2$ vertices of degree $\lfloor 2m/n \rfloor = 2$. This case also tells us that the minimizer can be unique. More known results that consider classes of graphs for which the conjecture is addressed positively are given in Section “Background”.

In this paper we confirm the conjecture for another class and give theoretical results that support it in general case. An experienced reader is probably aware of the complexity of the proposed problem and that it is hard to believe that it can be resolved in a close future; more details on this are given in Section “Background”. For example, the opposite problem concerning graphs that maximize the spectral radius in the same class (that is, $\mathcal{H}(n, m)$) is one of the major problems in the entire theory of graph spectra. Over the last six decades it was considered in tens of references (possibly, more than hundred), many results are obtained, but we are still far away from the complete resolution; again, more details are given in Section “Background”. Our problem seems to be more difficult which leads to the idea that it could be considered by methods that are not the exact ones, say by heuristic searches (at least in seeking for the structure of corresponding minimizers). Accordingly, in this paper we also report the result of a long-scale variable neighbourhood search on instances that cover some cases for $n \leq 100$. We point out that, for every instance, the computer search results in a graph with the foregoing structure related to vertex degrees.

The paper is organized as follows. A strong motivation (faced in the framework of virus propagation) for this research is separated in Section “Motivation”. In Section “Background” we quote some related results and describe the complexity of the problem we are dealing with. Theoretical results are reported in Section “Theoretical results”. A detailed description of variable neighbourhood search for minimizers is described in Section “Variable Neighbourhood Search”, while the corresponding experimental results are reported in Section “Experimental results”. The analysis of the experimental results is given in Section “Analysis of the experimental results”. Concluding remarks are collected in Section “Conclusions”. The latter five sections figure as our main contribution. The additional data obtained by the metaheuristic search is given in Appendix.

Motivation

The influence of a network structure on a virus spread has attracted a great deal of attention in the last two decades. Some examples include the spread of particularly transmitted diseases through contact networks ([Miller, 2017](#); [Rocha et al., 2010](#)), the spread of malware on wireless networks ([Hu et al., 2009](#)), the spread of e-mail worms or other viruses ([Chakrabarti et al., 2008](#); [Jamaković et al., 2006](#); [Daley and Gani, 1999](#); [Van Mieghem et al., 2009](#); [Newman et al., 2002](#); [Pastor-Satorras and Vespignani, 2001](#)), the propagation of faults or failures ([Daley and Gani, 1999](#); [Van Mieghem et al., 2009](#)), the spread of offensive and repetitive information on the computer network ([Chakrabarti et al., 2008](#); [Van Mieghem et al., 2009](#)), and similar.

Contacts between the network nodes are modelled by a simple undirected graph G whose vertices and edges represent nodes and direct contacts between them, respectively. An infectious node transmits

infectious doses with rate β . Simultaneously, infected nodes recover as a one-step process with rate γ . The quotient $\frac{\beta}{\gamma}$ is called the *effective spreading rate*. In simple words, it measures how quickly the virus spreads through the network. An *epidemic threshold* τ is the critical $\frac{\beta}{\gamma}$ quotient beyond which epidemics ensue. In other words, for $\frac{\beta}{\gamma} > \tau$ the virus persists, whereas for $\frac{\beta}{\gamma} < \tau$ the epidemic dies out.

There are two standard models for virus infections. In the SIS (*Susceptible–Infected–Susceptible*) viral model, a node can be susceptible or infective, where a susceptible node can be infected in a contact with an infective node and then healed with some probability to become susceptible again. In the SIR (*Susceptible–Infected–Removed*) viral model, once healed node is removed from the others and considered immune for the same infection. As the authors of [Chakrabarti et al. \(2008\)](#) plastically explained: SIS models the flu, while SIR models mumps.

There are several theoretical methods for predicting epidemic thresholds surveyed in [Wang et al. \(2016\)](#). One of them is the so-called *quenched mean-field (QMF) method* in which the epidemic threshold of a SIS virus is equal to $\frac{1}{\rho}$, where ρ is the spectral radius of G . Recently, a *non-linear dynamical system (NLDS)* that accurately models viral propagation in any network, including real and synthesized network graphs, has been developed ([Chakrabarti et al., 2008](#)). According to this model, we again have $\tau = \frac{1}{\rho}$. In simple words, a smaller ρ yields a better virus protection! Since the effective threshold of the SIR model is larger than that of SIS, $\frac{1}{\rho}$ acts as the lower bound for the effective threshold of the SIR model ([Daley and Gani, 1999](#); [Wang et al., 2016](#)). On the basis of a sequence of experiments, it conjectured in [Chakrabarti et al. \(2008\)](#) that smaller ρ yields a better protection in this model, as well.

Summa summarum, there is a natural question asking for graphs of fixed order and size having the minimal spectral radius, since such graphs would give a good network model. One may consider a relaxed problem asking for a graph with a comparatively small spectral radius, that is a graph whose spectral radius is (in some sense) close to the minimal one.

We will see in the next section that certain particular classes of graphs with above properties are considered in the recent past. In this paper, we provide theoretical and computational results concerning the minimizer(s) for $\mathcal{H}(n, m)$ and the graphs related to the relaxed variant of the problem. According to our results, vertex degrees of graphs with a small spectral radius (including the minimizers) are as equal as possible. Such graphs appear in *homogeneous epidemiological models* which assume that every node has equal contact to others and that the rate of infection is largely determined by the density of infected nodes. More details on these and other models can be found in [Chakrabarti et al. \(2008\)](#) and [Daley and Gani \(1999\)](#).

Background

We have mentioned in the introductory section that minimizers are known for the class $\mathcal{H}(n, n - 1)$, $n \in \mathbb{N}$, as well as for the class $\mathcal{H}(n, m)$, whenever $2m \equiv 0 \pmod{n}$. The latter, in particular, means that the class $\mathcal{H}(n, n)$ is resolved with the n -vertex cycle in the role of the unique minimizer. The next natural step is the class $\mathcal{H}(n, n + 1)$ (containing the so-called bicyclic graphs). It occurs that this class is also resolved with exactly two minimizers for every $n \geq 7$, see [Simić \(1989\)](#). The first is obtained by inserting the three disjoint paths between a pair of vertices, two of length $\lceil n/3 \rceil$ and one of length $n + 1 - 2\lceil n/3 \rceil$. The second is obtained by taking 2 copies of the $\lceil n/3 \rceil$ -vertex cycle and inserting the path of length $n + 1 - 2\lceil n/3 \rceil$ between a vertex in the first copy and a vertex in the second copy.

Concerning large values for m , we get that $\mathcal{H}(n, \binom{n}{2})$ and $\mathcal{H}(n, \binom{n}{2} - 1)$ both contain a single graph (for a fixed n) which is simultaneously the minimizer. The classes $\mathcal{H}(n, \binom{n}{2} - i)$ for a small i , say $i \leq 5$, contain just few non-isomorphic graphs and can be inspected by hand. For example, the minimizer for $\mathcal{H}(n, \binom{n}{2} - 2)$ is obtained by deleting two non-adjacent edges of the n -vertex complete graph.

The remaining known results refer to graphs that minimize the spectral radius within classes that are more or less related to the one considered in this paper. First, there is a sequence of results concerning connected graphs of fixed order and diameter. In [Van Dam and Kooij \(2007b\)](#) the minimizers for diameter in $\{2, \lfloor n/2 \rfloor, n-3, n-2\}$ are identified. To the best of our knowledge, this is the first reference concerning graphs with minimal spectral radius under the motivation described in the previous section. The result is extended to diameter $n-i, 4 \leq i \leq 8$, in [Cioabă et al. \(2010\)](#), [Yuan et al. \(2008\)](#), [Lan et al. \(2012\)](#). In the latter reference one can find the structure of a minimizer with diameter $n-i$, for any admissible i and sufficiently large n . Additional notable results concern graphs with minimal spectral radius within particular subclasses of $\mathcal{H}(n, n-1)$ ([Belardo et al., 2009](#)), $\mathcal{H}(n, n)$ and $\mathcal{H}(n, n+1)$ ([Guo, 2005](#)), and classes of graphs with prescribed subgraphs ([Kim et al., 2020](#); [Stevanović and Hansen, 2008](#)).

We mention once again the opposite problem of maximizing the spectral radius in $\mathcal{H}(n, m)$. According to [Friedland \(1985\)](#), the problem was posed by Schwarz in 1965, and extensively studied during the decades. Several significant results were obtained by Brualdi and Solheid ([Brualdi and Solheid, 1986a](#)), and consequently the problem is also known as the Brualdi–Solheid problem, see [Stevanović \(2015a, p. ix\)](#). The results obtained before 1990 are surveyed in [Cvetković and Rowlinson \(1990\)](#). The majority of the monograph ([Stevanović, 2015a](#)) is devoted to this problem, and some additional results can be found in [Stanić \(2015, Subsection 2.3.2\)](#). Of notable results, we mention the one concerning particular relocations of graph edges that necessarily increase the spectral radius ([Simić et al., 2004](#)). (It is worth mentioning that there is no result that provides similar transformations which would decrease the spectral radius; such a result would be of great interest in the study of the ‘problem of minimizers’.) The next significant result can be found in the same reference and states that a graph which maximizes the spectral radius within $\mathcal{H}(n, m)$ belongs to the class of the so-called threshold graphs (also known as nested split graphs). The definition can be found in any of [Anđelić and Simić \(2010\)](#), [Simić et al. \(2004\)](#), [Stanić \(2015\)](#), [Stevanović \(2015a\)](#); both names describe the structure of graphs in question. (Again, there is no similar class that would help in the study of our problem.) In [Stevanović \(2015b\)](#) one may find a quite different approach based on counting walks in graphs. Due to the mentioned results, many particular subclasses of $\mathcal{H}(n, m)$ are resolved positively, many conjectures on resulting maximizers are posed (apart from the foregoing references, see [Bell, 1991](#); [Brualdi and Solheid, 1986b](#); [Van Dam, 2007a](#)), but after more than 60 years the problem persists open. On the basis of the previous discussion, one may imagine that the problem of minimizing the spectral radius in $\mathcal{H}(n, m)$ is even more difficult, and therefore more challenging, especially in the light of the mentioned viral motivation.

Theoretical results

We pointed out that the spectral radius is bounded from below by the average vertex degree $2m/n$. There is an other lower bound offered by Hofmeister (see [Stanić 2015, p. 32](#)) which reads

$$\sqrt{\frac{1}{n} \sum_{i=1}^n d_i^2} \leq \rho, \tag{1}$$

where d_i stands for degree of the vertex i . Even more, this bound is never less than $2m/n$. To see this, we use the Cauchy–Schwarz inequality to get

$$\left(\frac{2m}{n}\right)^2 = \left(\frac{1}{n} \sum_{i=1}^n d_i\right)^2 \leq \frac{1}{n^2} \left(n \sum_{i=1}^n d_i^2\right) = \frac{1}{n} \sum_{i=1}^n d_i^2,$$

which leads to the desired conclusion. The Hofmeister bound is attained if and only if the graph is regular or semiregular bipartite, where the latter one is a bipartite graph and vertices belonging to the same part share the same degree, see [Stanić \(2015, Remark 2.5\)](#).

Example 1. There are exactly 2 bipartite graphs in $\mathcal{H}(10, 24)$: the complete bipartite graph $K_{4,6}$ and the graph $K_{5,5} - e$ obtained by deleting an edge of the complete bipartite graph $K_{5,5}$. Both are illustrated in [Fig. 1](#). (We believe that the reader knows that the complete bipartite graph has an edge between every vertex in one colour class and every vertex in the other colour class.) Since $K_{4,6}$ is semiregular bipartite, its spectral radius attains the bound (1), and so $\rho(K_{4,6}) = \sqrt{24}$. The other one is not semiregular bipartite, and so its spectral radius does not attain the mentioned bound. In this light, one might expect that $K_{4,6}$ is a minimizer for $\mathcal{H}(10, 24)$, but it is not. The computer search found exactly 46 minimizers, one is $K_{5,5} - e$, an other is the third graph of [Fig. 1](#) (also given in the forthcoming [Table 3](#)). All minimizers have 8 vertices of degree 5 and 2 vertices of degree 4.

We proceed with the two upper bounds for ρ . It is well-known that the spectral radius of every graph does not exceed its maximum vertex degree Δ , with equality if and only if the graph is regular (for example, see [Stanić 2015, p. 28](#)). Another upper bound expressed in terms of order, size and the minimum vertex degree δ , obtained by Hong et al. and independently by Nikiforov (see [Stanić 2015, Theorem 2.19](#)), states that

$$\rho \leq \frac{\delta - 1 + \sqrt{(\delta + 1)^2 + 4(2m - \delta n)}}{2}. \tag{2}$$

In case of connected graphs, equality in (2) is attained if and only if the graph is regular or bidegreed in which each vertex is of degree δ or $n-1$. Observe that the right hand side of (2) and Δ are uncomparable: A direct algebraic computation yields that (2) gives a better estimation if and only if $2m + n - 1 < (n + 1)\lfloor 2m/n \rfloor$.

Let further H denote a non-regular graph of $\mathcal{H}(n, m)$ with vertex degrees in $\{\lfloor 2m/n \rfloor, \lceil 2m/n \rceil\}$. Since H is non-regular, we have $\lceil 2m/n \rceil = \lfloor 2m/n \rfloor + 1$. Moreover, it follows that $2m - n\lfloor 2m/n \rfloor$ vertices of H have degree $\lceil 2m/n \rceil$ and $n - 2m + n\lfloor 2m/n \rfloor$ vertices have degree $\lfloor 2m/n \rfloor$. By setting $\delta_H = \lfloor 2m/n \rfloor$, we find that the left hand side of (1) reduces to

$$\begin{aligned} &\sqrt{\frac{1}{n} \left((2m - \delta_H n)(\delta_H + 1)^2 + (n - 2m + \delta_H n)\delta_H^2 \right)} \\ &= \sqrt{(2\delta_H + 1)\frac{2m}{n} - \delta_H(\delta_H + 1)}. \end{aligned}$$

Together with (2) and the previous discussion, this gives the following range for the spectral radius of H .

Proposition 2. *The spectral radius $\rho(H)$ of a non-regular graph $H \in \mathcal{H}(n, m)$ whose vertex degrees belong to $\{\lfloor 2m/n \rfloor, \lceil 2m/n \rceil\}$ satisfies the following inequalities*

$$\begin{aligned} &\sqrt{(2\delta_H + 1)\frac{2m}{n} - \delta_H(\delta_H + 1)} \leq \rho(H) \\ &\leq \min \left\{ \frac{\delta_H - 1 + \sqrt{(\delta_H + 1)^2 + 4(2m - \delta_H n)}}{2}, \delta_H + 1 \right\}. \end{aligned}$$

Now, we prove that the spectral radius of a minimizer belongs to the same range.

Proposition 3. *The spectral radius of a non-regular minimizer $H_{n,m}$ for $\mathcal{H}(n, m)$ satisfies the inequalities of [Proposition 2](#).*

Proof. Since $\rho(H_{n,m}) \leq \rho(H)$, the upper bound follows.

The remainder of the proof relies on the following claim: For $x_1 \geq x_2 \geq \dots \geq x_n \in \mathbb{N}$, if $\sum_{i=1}^n x_i = 2m$ is fixed, then the sum $\sum_{i=1}^n x_i^2$ is minimized if x_1, x_2, \dots, x_n coincide with vertex degrees of H . This result is known from literature, but for the sake of completeness we give a short proof. Assume by way of contradiction that the minimizing integers x_1, x_2, \dots, x_n are not the corresponding vertex degrees. We compute

$$(x_1 - 1)^2 + x_2^2 + x_3^2 + \dots + x_{n-1}^2 + (x_n + 1)^2 = \sum_{i=1}^n x_i^2 + 2(x_n + 1 - x_1) \geq \sum_{i=1}^n x_i^2,$$

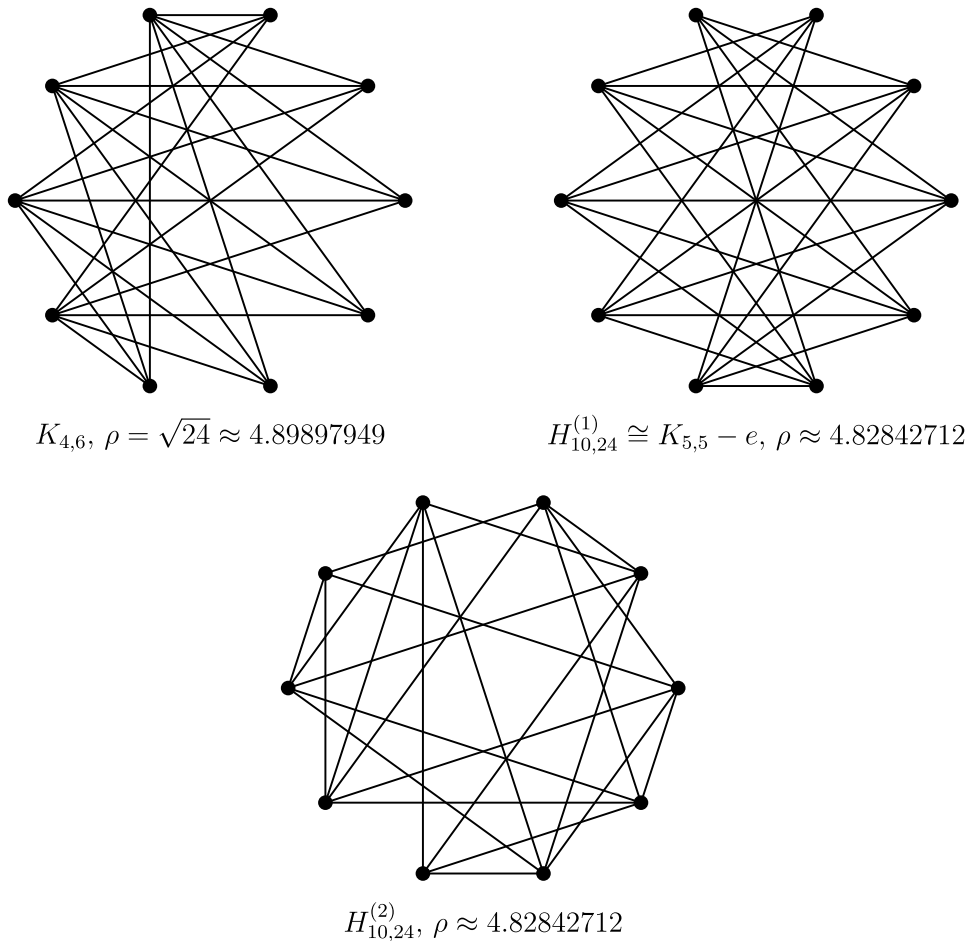


Fig. 1. The complete bipartite graph $K_{4,6}$ and the two (of 46 in total) minimizers for $\mathcal{H}(10,24)$.

but the previous inequality holds only if $2(x_n + 1 - x_1) \geq 0$, i.e. $x_1 \in \{x_n, x_n + 1\}$. The former possibility implies that $2m \equiv 0 \pmod n$, but this would mean that H is regular, while it is not the statement assumption. The latter possibility implies that $x_1, x_2, \dots, x_n \in \{\lfloor 2m/n \rfloor, \lceil 2m/n \rceil\}$, but then they coincide with vertex degrees of H , and we are done.

Now, since vertex degrees of $H_{n,m}$ satisfy the inequality (1), to conclude the proof, it is sufficient to show that the sum of squares of vertex degrees of $H_{n,m}$ is not less than the lower bound of Proposition 2. This follows by the previous part of the proof since H and $H_{n,m}$ are equal in size and the value under the square root in the lower bound is precisely the sum of squares of vertex degrees of H multiplied by $\frac{1}{n}$. \square

In other words, the spectral radius of a minimizer never falls below the lower bound of Proposition 2. We remark that the upper bound of the same proposition is comparatively close to the lower one (numerical data that confirms this is given in Section “Experimental results”). This means that even if H is not a minimizer for $\mathcal{H}(n, m)$, $\rho(H)$ is close to the spectral radius of a minimizer in the sense that both belong to the same range given in Proposition 3. Therefore, even if H is not a minimizer, its spectral radius may be sufficiently small so that $\frac{\beta}{\gamma} < \frac{1}{\rho(H)}$ holds, and then H can be considered as a model for the corresponding network. Finally, observe that we can always construct a graph like H ; for example, there are exactly 720 connected graphs in $\mathcal{H}(10, 26)$ with required vertex degrees.

We proceed with a simple proposition that restricts the search for minimizers just by examining the spectral radius or vertex degrees (polynomially computed invariants).

Proposition 4. Let $G \in \mathcal{H}(n, m)$, for $2m \not\equiv 0 \pmod n$.

- If $\rho(G)$ is greater than the upper bound of Proposition 2, then G is not a minimizer.
- If, for vertex degrees d_1, d_2, \dots, d_n of G , $\sqrt{\frac{1}{n} \sum_{i=1}^n d_i^2}$ is greater than the upper bound of Proposition 2, then G is not a minimizer.
- If, for $n < m$, G has a vertex of degree 1, then G is not a minimizer.

Proof. The assumptions of the first two items lead to $\rho(G) > \rho(H_{n,m})$, and the result follows. For the third item, deletion of a vertex of degree 1 decreases the spectral radius (by the mentioned Perron–Frobenius Theorem), and inserting a vertex into the edge of a cycle have the same effect to the spectral radius (Stanić, 2015, Theorem 1.8). Therefore, a graph obtained in this way belongs to $\mathcal{H}(n, m)$ and has a smaller spectral radius, which completes the proof. \square

This was a very simple statement, but useful because it eliminates many candidates for minimizers in the sense that many with a sufficiently large $\max_{i,j} |d_i - d_j|$ would not pass given tests.

In the end of this section, we resolve a subclass of $\mathcal{H}(n, m)$. We denote by $\mathcal{B}(s, t)$ the class of connected semiregular bipartite graphs in which all vertices in one colour class have degree s and all vertices in the other class have degree t . Observe that for the graphs in $\mathcal{B}(s, t)$ the order and the size are not fixed.

Proposition 5. The following statements hold true.

- (i) For $2m \not\equiv 0 \pmod n$, if $\mathcal{H}(n, m) \cap \mathcal{B}(\lfloor 2m/n \rfloor, \lceil 2m/n \rceil) \neq \emptyset$, then a graph is minimizer for $\mathcal{H}(n, m)$ if and only if it belongs to the previous intersection.
- (ii) The graph $K_{s,s+1}$ is the unique minimizer for $\mathcal{H}(2s + 1, s(s + 1))$.

Proof. (i): Every graph of $\mathcal{H}(n, m) \cap \mathcal{B}(\lfloor 2m/n \rfloor, \lceil 2m/n \rceil)$ attains the lower bound of (1), and therefore it is a minimizer. We denote an arbitrary graph of the previous intersection by $H_{n,m}$, and assume by way of contradiction that $G \notin \mathcal{H}(n, m) \cap \mathcal{B}(\lfloor 2m/n \rfloor, \lceil 2m/n \rceil)$ is also a minimizer. Let G have vertex degrees d_1, d_2, \dots, d_n .

First, if $d_i \in \{\lfloor 2m/n \rfloor, \lceil 2m/n \rceil\}$ for every i , then G shares vertex degrees with $H_{n,m}$, and therefore it attains the same lower bound if and only if it is semiregular bipartite or regular. In the former case we get $G \in \mathcal{H}(n, m) \cap \mathcal{B}(\lfloor 2m/n \rfloor, \lceil 2m/n \rceil)$, and in the latter case we get that, under the assumption that $2m \not\equiv 0 \pmod{n}$, G cannot simultaneously be regular and share vertex degrees with $H_{n,m}$. Thus, we have established a contradiction in both cases.

Now, if $d_i \notin \{\lfloor 2m/n \rfloor, \lceil 2m/n \rceil\}$ for some i , the proof is essentially the same as the corresponding part of the proof of Proposition 3. Indeed, here we have that the sum of squares of vertex degrees is minimized by vertex degrees of $H_{n,m}$, which yields

$$\rho(G) \geq \sqrt{\frac{1}{n} \sum_{i=1}^n d_i^2} > \sqrt{\lfloor 2m/n \rfloor \lceil 2m/n \rceil} = \rho(H_{n,m}),$$

and the proof of (i) is completed.

(ii): This result follows from the previous item and the fact that $K_{s,s+1}$ is the unique semiregular bipartite graph of $\mathcal{H}(2s+1, s(s+1))$. \square

Variable neighbourhood search

The number of non-isomorphic graphs with n vertices is asymptotically $\frac{2^{\binom{n}{2}}}{n!}$. Since the share of disconnected graphs is comparatively small, the previous estimation tells us that the number of non-isomorphic connected graphs with n vertices grows extremely rapidly with increase of n . For example, for $n = 18$ there is more than $1.7 \cdot 10^{30}$ connected graphs which implies that the number of candidates for minimizers for a fixed m is close to 10^{28} . This numerical data forces us to employ a particular metaheuristic search for connected graphs with a small spectral radius.

The *Variable Neighbourhood Search* (Mladenović, 1995; Mladenović and Hansen, 1997) has been approved as successful in dealing with a large number of discrete optimization problems. The motivation for applying this metaheuristic came from the fact that, unlike many other metaheuristics, the VNS has a very simple implementation requiring only a few (or none) parameters to be setted in advance. Also, it occurs that a final solution obtained by the VNS does not depend significantly on an initial solution. Finally, this metaheuristic is very efficient when deals with binary vectors (as in our case). Other desirable advantages in comparison to the other metaheuristic algorithms can be found in Brimberg et al. (2000) and Mladenović et al. (2016).

The main idea of the VNS algorithm is the systematic change of predefined different neighbourhoods of the currently best solution in order to find a better solution. At the beginning of the algorithm, one should define a set of different neighbourhood structures \mathcal{N}_k , $1 \leq k \leq k_{\max}$, where k_{\max} is a predefined number, and choose an arbitrary initial solution \mathbf{x} from the set of all feasible solutions X . Let $\mathcal{N}_k(\mathbf{x})$ denote the k th neighbourhood of the solution \mathbf{x} and $f(\mathbf{x})$ the objective function value in \mathbf{x} .

In each step of the algorithm, VNS starts from the incumbent solution \mathbf{x} and performs the shaking procedure which randomly generates a feasible solution \mathbf{x}' in the current neighbourhood $\mathcal{N}_k(\mathbf{x})$ of the incumbent. Some local search procedure is applied around the generated feasible solution \mathbf{x}' in order to obtain a possibly better solution \mathbf{x}'' . If the local search encounters a better solution, i.e. if $f(\mathbf{x}'')$ is smaller than $f(\mathbf{x})$, \mathbf{x}'' becomes the new incumbent ($\mathbf{x} \leftarrow \mathbf{x}''$) and the search procedure continues in the first neighbourhood of the new incumbent solution $\mathcal{N}_1(\mathbf{x})$. Otherwise, the neighbourhood which will be explored in next step is changed from $\mathcal{N}_k(\mathbf{x})$ to $\mathcal{N}_{k+1}(\mathbf{x})$. The entire VNS procedure is given in the following pseudo-code.

Algorithm VNS

```

/* Initialization */
01 Select the set of neighbourhood structures  $\mathcal{N}_k$ ,
    $1 \leq k \leq k_{\max}$ 
02 Choose an arbitrary initial solution  $\mathbf{x} \in X$ 
/* Main loop */
03 repeat the following steps until the stopping condition is
   met
04   Set  $k \leftarrow 1$ 
05   repeat the following steps until  $k > k_{\max}$ 
     /*Shaking*/
06     Generate at random a solution  $\mathbf{x}' \in \mathcal{N}_k(\mathbf{x})$ 
     /*Local search*/
07     Apply a local search method to  $\mathbf{x}'$  and obtain a local
       minimum  $\mathbf{x}''$ 
08     if  $f(\mathbf{x}'') < f(\mathbf{x})$  then
09       Set  $\mathbf{x} \leftarrow \mathbf{x}''$  and goto line 05
10     endif
11     Set  $k \leftarrow k + 1$ 
12   endrepeat
13 endrepeat
14 stop  $\mathbf{x}$  is an approximate solution of the problem.

```

The main concept of the VNS metaheuristic applied to the problem of finding the minimizer $H_{n,m}$ for $\mathcal{H}(n, m)$ is explained in more details as follows.

Solution representation. For a graph G , the adjacency matrix A is symmetric, so only the upper triangle (with the main diagonal neglected) of this matrix needs to be stored. The VNS solution is represented by a single vector obtained by a row-by-row concatenation of the upper triangle. Such a vector has $\binom{n}{2}$ entries and is denoted by \mathbf{x} . During the execution, the VNS algorithm records the incumbent solution \mathbf{x} , while in the end it returns the best found solution. To ease language, we use the term solution for both the incumbent and the best solution. It will be clear from the context which one it refers to.

The set of feasible solutions. For each combination $n = |V|$ and $m = |E|$, the set of feasible solutions X contains all the vectors \mathbf{x} of length $\binom{n}{2}$ such that:

- $x_i \in \{0, 1\}$, $1 \leq i \leq \binom{n}{2}$,
- $\sum_{i=1}^{\binom{n}{2}} x_i = m$ and
- the graph G , represented by the vector \mathbf{x} , is connected.

The objective function. For a vector \mathbf{x} , the objective function $f(\mathbf{x})$ is the spectral radius of the corresponding graph G , i.e. $f(\mathbf{x}) = \rho(G)$. The eigenvalue problem is solved using the *Spectra C++ library* for the large-scale eigenvalue problems (Qiu et al., 2015).

The initial solution. In order to generate an initial solution, we use the *NetworkX package* (Hagberg et al., 2008) for obtaining a random d -regular graph with n vertices. We choose $d = \lfloor 2m/n \rfloor$ or $d = \lceil 2m/n \rceil$, so that nd is even. If the resulting graph is disconnected, we repeat the same procedure.

The connectivity of a graph is decided by a Depth First Search (DFS) algorithm which takes an arbitrary vertex and checks whether the remaining vertices belong to the same component.

Once we get a random connected regular graph, we have to add or remove some edges to obtain a graph with exactly m edges. Adding edges does not violate the connectivity condition, so if $d = \lfloor 2m/n \rfloor$ we add $m - \lfloor 2m/n \rfloor \frac{n}{2}$ edges by the following rule. Starting from the first vertex v_1 we add the first missing edge and continue the same with vertices v_i , $2 \leq i \leq m - \lfloor 2m/n \rfloor \frac{n}{2}$. Otherwise, if $d = \lceil 2m/n \rceil$ we

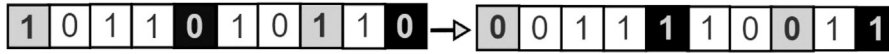


Fig. 2. An example of the shaking procedure for $k = 2$.

delete one-by-one the first $\lceil 2m/n \rceil \frac{n}{2} - m$ edges that does not violate the connectivity condition.

The idea for such an initial solution is inspired by the fact that the conjecture about minimizers is confirmed for $n \leq 10$ and for some additional classes. In general, the initial solution constructed in such a way has more than two vertices with distinct degrees, but its vertex degrees are close to $2m/n$.

The neighbourhood structure. For $1 \leq k \leq k_{\max}$, we define the k th neighbourhood of a solution \mathbf{x} as $\mathcal{N}_k(\mathbf{x}) = \{\mathbf{x}' \in X : d(\mathbf{x}, \mathbf{x}') = 2k\}$, where $d(\cdot, \cdot)$ stands for the Hamming distance between vectors. Since the set X contains only vectors with exactly m ones, we find that $\mathcal{N}_k(\mathbf{x})$ contains all vectors $\mathbf{x}' \in X$ which differ from \mathbf{x} in exactly $2k$ entries. This means that graphs represented by \mathbf{x} and \mathbf{x}' agree in $m - k$ edges.

The shaking step. The shaking procedure generates a new solution $\mathbf{x}' \in \mathcal{N}_k(\mathbf{x})$ by employing the following steps. For a fixed k , $1 \leq k \leq k_{\max}$, we first choose k random indices $\text{ind}0_1, \text{ind}0_2, \dots, \text{ind}0_k$ of the vector \mathbf{x} , in such a way that the entry of \mathbf{x} at the position $\text{ind}0_i$, $1 \leq i \leq k$, is 0 and another k random indices $\text{ind}1_1, \text{ind}1_2, \dots, \text{ind}1_k$ such that the entry of \mathbf{x} at the position $\text{ind}1_i$, $1 \leq i \leq k$, is 1. With a consistent choice of k_{\max} this is always possible. Next, we flip the values of each $x_{\text{ind}0_i}$ from 0 to 1, and of each $x_{\text{ind}1_i}$ from 1 to 0. This is equivalent to the deletion of k edges from the graph represented by \mathbf{x} combined with the insertion of k new edges into the resulting graph.

Example 6. Fig. 2 illustrates an example of the shaking step for $k = 2$ and a vector \mathbf{x} of length 10. First, from the list of indices $1 \leq i \leq 10$ such that $x_i = 0$ (that is $\{2, 5, 7, 10\}$) we chose randomly $k = 2$ of them. Let they be $\text{ind}0_1 = 5$ and $\text{ind}0_2 = 10$, coloured in black. Next, from the list of indices such that $x_i = 1$ (that is $\{1, 3, 4, 6, 8, 9\}$) we chose randomly another two, say $\text{ind}1_1 = 1$ and $\text{ind}1_2 = 8$, coloured in grey. The black and the grey entries flip their values which results in the solution \mathbf{x}' .

Although a disconnected solution obtained in a local search step may result in a connected solution in the end of the entire procedure, we eliminate this uncertainty, i.e. in case that \mathbf{x}' does not represent a connected graph, we discard that solution and obtain the new one until we get a feasible solution. Note that, in practice, disconnected solutions occur very rarely.

The local search step. Starting from the solution \mathbf{x}' , obtained in the shaking step, the local search procedure explores a small neighbourhood of \mathbf{x}' in search for a solution with a smaller objective function. Namely, if \mathbf{x}' has $s = \binom{n}{2}$ entries, the neighbourhood $\mathcal{N}_l(\mathbf{x}')$ consists of the $s - 1$ vectors obtained in the following way. For $1 \leq l \leq s - 1$, we split \mathbf{x}' into the first part containing the first $s - l$ entries and the second part containing the remaining entries. The vector \mathbf{x}'' is obtained by interchanging the roles of the two parts.

Example 7. Fig. 3 illustrates an example for the local search of a vector \mathbf{x}' of length 6 for $l = 1$ and $l = 2$. In the first case, we split the vector on the left hand side at the position $l = 1$, which results in the first part with the entries coloured in white and the second part with the entries coloured in grey. By interchanging, we obtain the vector \mathbf{x}'' on the right hand side. The local search for $l = 2$ is described in a similar way.

For the local search the best improvement strategy is used, which means that the best solution $\mathbf{x}'' \in \mathcal{N}_l(\mathbf{x}')$ is selected to be the result of the local search. The connectivity of the graph is checked only in the case when the solution with better objective function is obtained.

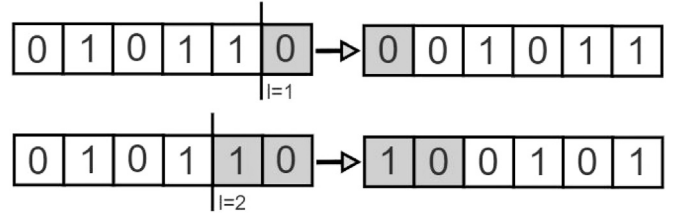


Fig. 3. An example of the local search procedure for $l = 1$ and $l = 2$.

Move or not. The solution \mathbf{x}'' obtained in the local search is compared to the currently best solution \mathbf{x} . If $f(\mathbf{x}'') < f(\mathbf{x})$, we move to the solution \mathbf{x}'' and continue the search in its first neighbourhood $\mathcal{N}_1(\mathbf{x}'')$. For $f(\mathbf{x}'') \geq f(\mathbf{x})$, we continue the search in the next neighbourhood $\mathcal{N}_{k+1}(\mathbf{x})$.

The stopping criterion. When the neighbourhood counter in the shaking step exceeds k_{\max} , the search continues with the first neighbourhood $\mathcal{N}_1(\mathbf{x})$. This procedure is repeated until the predefined stopping criterion is met. In this VNS implementation, for the stopping criterion we use the maximum CPU time allowed, meaning that the algorithm stops when the predefined maximum CPU time t_{\max} is exceeded.

Experimental results

In this section we report our experimental results obtained by the VNS metaheuristic algorithm described in the previous section. The algorithm was coded in C++ and executed on a laptop with AMD Ryzen 7 3700X with 32 GB RAM and Windows 10 OS.

Recently introduced *Less Is More Approach (LIMA)* (Mladenović et al., 2016) for solving optimization problems creates an algorithm for a particular problem to be as simple as possible, with as few as possible parameters that need to be defined in advance by the user, but without loosing the quality of obtained results. Following the main idea of the LIMA, for each test instance (n, m) , the only input parameter for our VNS implementation is the maximum CPU time allowed; the parameter t_{\max} .

Clearly, a test instance (n, m) represents the class $\mathcal{H}(n, m)$ treated by the VNS algorithm. A connected graph with n vertices may contain at least $n - 1$ edges and at most $\binom{n}{2}$ edges. On the basis of the discussion in Sections “Background” and “Theoretical results”, our test instances do not include the following cases:

- $m \in \{n-1, n, n+1, \binom{n}{2}, \binom{n}{2}-1, \binom{n}{2}-2\}$, since these cases are resolved;
- $2m \equiv 0 \pmod{n}$, since this case is resolved with regular minimizers;
- $(n, m) = (2s + 1, s(s + 1))$, since this case is resolved in Proposition 5(ii).

For $n \in \{3, 4, \dots, 10\}$, we take into consideration all pairs (n, m) that are not excluded by the previous restrictions. For instances with $n \in \{11, 12, \dots, 19, 20, 30, 40, 50, 60, 70, 80, 90, 100\}$, we take 5 random integer numbers $m \in \left[n + 2, \binom{n}{2} - 3 \right]$, again relative to the previous restrictions. For each test instance, we select the value for t_{\max} according to Table 1.

The parameter k_{\max} depends only on n and m , and is calculated as follows:

$$k_{\max} = \begin{cases} \min \left\{ \frac{n^2-n}{2} - m, \lfloor \frac{m}{2} \rfloor \right\} & \text{if } n < 9, \\ \min \left\{ \frac{n^2-n}{2} - m, \lfloor \frac{m}{2} \rfloor, 10 \right\} & \text{if } n \geq 9. \end{cases}$$

Since the number of zeros in the solution vector is $\frac{n^2-n}{2} - m$ and the number of ones is m , this is a natural choice for k_{\max} . The constraint

Table 1
Values for t_{\max} .

n	1–6	7	8	9	10	11–15	16–19
t_{\max}	1 s	10 s	50 s	300 s	600 s	1 h	1.5 h
n	20, 30	40, 50	60	70	80	90	100
t_{\max}	2 h	3 h	4 h	5 h	6 h	7 h	8 h

$k_{\max} \leq 10$ for larger instances is added in order to avoid situations in which the performances of the algorithm critically depend on the choice of the size and the number of neighbourhoods.

Due to its stochastic nature, the VNS algorithm has been run for 20 times for each pair (n, m) with different random seeds.

In order to verify the optimality of VNS solutions, for small instances ($n \leq 10$), we generate all connected graphs $G \in \mathcal{H}(n, m)$ and determine the corresponding minimizers. (As mentioned in previous section the number of graphs grows rapidly with n , but for $n \leq 10$ this procedure is performed in a reasonable time.)

The obtained results for instances with $n \leq 10$ are summarized in **Tables 2** and **3**. These tables are organized as follows:

- The first two columns contain the order n and the size m .
- The next column #opt contains the number of minimizers in $\mathcal{H}(n, m)$ found by computer search over all graphs in the corresponding class.
- The columns LB and UB contain the lower and the upper bound of **Proposition 2**.
- The column opt contains the spectral radius of a minimizer.
- The column VNS_{best} contains the best objective function found by VNS in 20 runs, i.e. $VNS_{\text{best}} = \min_{1 \leq i \leq 20} VNS_i$, where VNS_i is the objective function of VNS solution obtained in the i th run of the algorithm. If the obtained value is equal to the optimal one, we write ‘opt’ instead of the numerical value.
- Since the total execution time t_{\max} is the same for the instances with the same number of vertices, the column t_{first} contains the average VNS execution time until the best VNS solution is reached for the first time, given in seconds.
- The next two columns (agap and std) contain the information on the average VNS solution quality given in percentages. The value in agap column is the average relative percentage error of obtained solutions defined as $\text{agap} = \frac{1}{20} \sum_{i=1}^{20} \text{err}_i$, where $\text{err}_i = 100 \frac{VNS_i - VNS_{\text{best}}}{VNS_{\text{best}}}$. The value std is the standard deviation of err_i , computed as $\text{std} = \sqrt{\frac{1}{20} \sum_{i=1}^{20} (\text{err}_i - \text{agap})^2}$.
- The last column $H_{n,m}$ contains the first minimizer obtained by the VNS. The minimizer is represented in the nauty graph6 format **McKay and Piperno (2014)**; the basic idea for this format is to encode the graph size and the upper triangle of the adjacency matrix in ASCII-printable characters.

The numerical data in columns opt, VNS_{best} , LB and UB are rounded to 8 decimal places. We consider the values opt and VNS_{best} to be equal if $|\text{opt} - VNS_{\text{best}}| < 1.2 \cdot 10^{-14}$. This is justified due to the convergence tolerance for the algorithm computing the spectral radius.

The obtained results for $11 \leq n \leq 19$ are summarized in **Table 4**. There, we do not have columns related to the optimal result (#opt and opt) since they are not known due to the huge number of graphs in the search space. The last column, marked by $\tilde{H}_{n,m}$, contains the first best VNS solution such that $VNS_{\text{best}} = \min_{1 \leq i \leq 20} VNS_i$.

Similarly, **Table 5** summarizes the results for $20 \leq n \leq 100$. The only difference from **Table 4** is the absence of the last column containing the graph representation, since it is cumbersome. This information is given in Appendix.

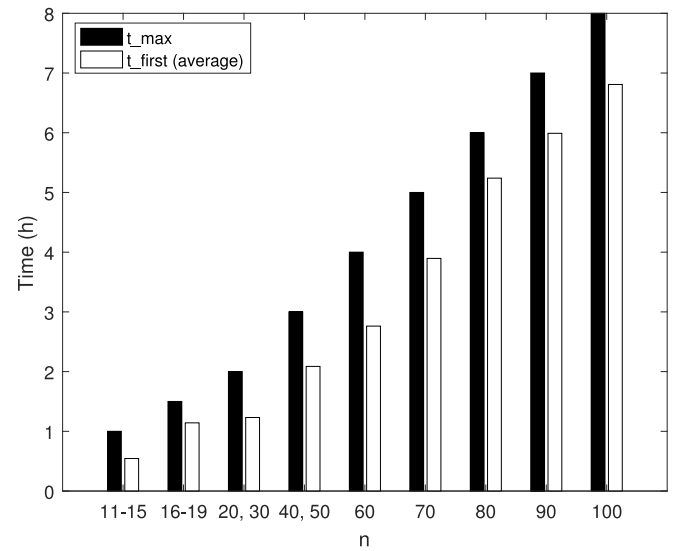


Fig. 4. Average values for t_{\max} and t_{first} .

Analysis of the experimental results

In this section we give the analysis of the VNS reported in the previous section, along with certain conclusions related to the efficiency of the algorithm and the resulting solutions.

The execution time. According to **Table 1**, the total execution time for 20 runs of the VNS algorithm for all instances is 5220 h. The simultaneous execution of different VNS runs are divided into 10 parallel tasks, and therefore the total testing time to obtain all results of **Tables 2–5** is reduced to 522 h.

Instances with $n \leq 10$. According to **Tables 2** and **3**, the VNS reached the optimal solution for all test instances with $n \leq 10$. For 63 out of 69 instances, the VNS reached the solutions with the same optimal value of the objective function in all 20 runs, and the parameters agap and std are both zero. When there are more than one optimal solution, a sufficiently large number of VNS runs returns all of them. (As mentioned before, in these cases, the last column in the tables contains the first obtained solution). The average value of t_{first} is approximately only three times smaller than the maximal execution time allowed. Since t_{first} has a comparatively small deviation on all test runs, it represents an indicator of the VNS algorithm robustness for this kind of problems.

Instances with $11 \leq n \leq 100$. As expected, in this settings the number of instances for which the same solution is obtained in all 20 VNS runs decreases (in other words, the parameters agap and std are greater than zero). Nevertheless, the obtained values for agap and std are still comparatively small, which indicates a high reliability of the obtained VNS solutions. For example, the instance $(n, m) = (50, 89)$ has the greatest values of $\text{agap} = 0.0660$ and $\text{std} = 0.0442$ among all 159 instances. One can also note that for larger values of n in almost all cases agap is greater than std, meaning that VNS solutions obtained in 20 runs which differ from the best solution are not significantly greater than VNS_{best} . The diagram on **Fig. 4** compares the total maximum execution time (t_{\max}) to the average time needed to obtain the best solution for the first time (t_{first}).

The best objective function. For all 159 instances, the obtained value of VNS_{best} lies in [LB, UB], so it can be justified to believe that we found either the optimal solutions or the solutions that are close to the optimal ones. In particular, this is confirmed for $n \leq 10$, where the VNS results in an optimal solution for each instance. The lower bound LB is reached

Table 2
Experimental results for $n \leq 9$.

n	m	# opt	LB	UB	opt	VNS _{best}	t_{first} (s)	agap(%)	std(%)	$H_{n,m}$
5	7	1	2.82842712	3.00000000	2.85577251	opt	0.0384	0.0000	0.0000	Dyk
6	8	2	2.70801280	3.00000000	2.73205081	opt	0.3754	0.0000	0.0000	EfNg
6	10	1	3.36650165	3.44948974	3.37228132	opt	0.3074	0.0000	0.0000	Ed~o
6	11	1	3.69684550	3.82842712	3.71358466	opt	0.3513	0.0000	0.0000	EYIO
7	9	2	2.61861468	3.00000000	2.64118648	opt	3.3895	0.0000	0.0000	FHFL
7	10	2	2.87849167	3.00000000	2.90321193	opt	5.4869	0.0000	0.0000	FIULG
7	11	1	3.16227766	3.23606798	3.17634100	opt	2.8398	0.0000	0.0000	F{IQw
7	13	1	3.74165739	4.00000000	3.75936551	opt	4.4459	0.0000	0.0000	Fmyzg
7	15	1	4.30945804	4.37228132	4.31662479	opt	3.6332	0.0000	0.0000	Fzu o
7	16	1	4.59813627	4.70156212	4.60555128	opt	4.4130	0.0000	0.0000	F ~_
7	17	1	4.86973159	5.00000000	4.88089912	opt	2.4301	0.0000	0.0000	F}~rw
7	18	1	5.15474816	5.16227766	5.16227766	opt	0.4758	0.0000	0.0000	FelHo
8	10	3	2.54950976	3.00000000	2.56155281	opt	16.4289	0.0000	0.0000	GBBSPS
8	11	1	2.78388218	3.00000000	2.81202496	opt	14.1195	0.0000	0.0000	Gicl?g
8	13	2	3.27871926	3.44948974	3.29074864	opt	21.0304	0.0000	0.0000	GhUV?w
8	14	1	3.53553391	3.82842712	3.54138127	opt	24.7107	0.0000	0.0000	GRKuMS
8	15	5	3.77491722	4.00000000	3.79128785	opt	16.1753	0.0000	0.0000	G O qW
8	17	1	4.27200187	4.37228132	4.28100496	opt	16.6949	0.0000	0.0000	Grv?S
8	18	1	4.52769257	4.70156212	4.53112887	opt	28.7646	0.0000	0.0000	Gniyw
8	19	1	4.76969601	5.00000000	4.78281596	opt	18.0809	0.0000	0.0000	Gq\\`dk
8	21	2	5.26782688	5.31662479	5.27491722	opt	16.4407	0.0000	0.0000	GnmZs
8	22	1	5.52268051	5.60555128	5.53112887	opt	19.7768	0.0000	0.0000	Glv~rk
8	23	1	5.76628130	5.87298335	5.77652737	opt	17.9738	0.0000	0.0000	Gnn}~s
8	25	1	6.26498204	6.27491722	6.27491722	opt	0.3519	0.0000	0.0000	Gv~j{
9	11	2	2.49443826	3.00000000	2.50350450	opt	126.5050	0.0000	0.0000	Ha_h'aC
9	12	7	2.70801280	3.00000000	2.73205081	opt	139.4653	0.0000	0.0000	H'EH@fC
9	13	1	2.90593263	3.00000000	2.92792296	opt	87.0698	0.0000	0.0000	HDPe?yg
9	14	4	3.12694384	3.23606798	3.14133612	opt	108.7500	0.0000	0.0000	HKhGsdC
9	15	3	3.36650165	3.64575131	3.37228132	opt	119.0251	0.0000	0.0000	HKpXT.q
9	16	1	3.59010987	4.00000000	3.60121938	opt	110.8347	0.0000	0.0000	H_BliK
9	17	2	3.80058475	4.00000000	3.81773414	opt	77.4653	0.0000	0.0000	Hjo'G
9	19	4	4.24264069	4.37228132	4.25259111	opt	134.6587	0.0000	0.0000	HwE'bp[
9	21	7	4.69041576	5.00000000	4.70156212	opt	115.4638	0.0000	0.0000	HBb~vR'
9	22	1	4.89897949	5.00000000	4.90852483	opt	126.5679	0.0002	0.0008	Himt'vN
9	23	1	5.12076383	5.16227766	5.12830161	opt	70.8098	0.0000	0.0000	H[-Vawn
9	24	2	5.35412613	5.46410162	5.35889894	opt	129.3736	0.0000	0.0000	H\\tj]mx
9	25	1	5.57773351	5.74165739	5.58257569	opt	162.1130	0.0064	0.0192	Huxztlx
9	26	2	5.79271573	6.00000000	5.80290835	opt	88.3704	0.0000	0.0000	Hs~rpv
9	28	2	6.23609564	6.27491722	6.24264069	opt	115.8175	0.0000	0.0000	H~uk~L~
9	29	1	6.46357314	6.53112887	6.47213596	opt	93.2913	0.0000	0.0000	H N~u n
9	30	1	6.68331255	6.77200187	6.69041576	opt	83.0973	0.0000	0.0000	H}~r }~
9	31	1	6.89605362	7.00000000	6.90235522	opt	101.4984	0.0000	0.0000	H~zZ~}
9	32	1	7.11805217	7.12310563	7.12310563	opt	30.0001	0.0000	0.0000	H}n~x~
9	33	1	7.34846923	7.35889894	7.35889894	opt	3.2729	0.0000	0.0000	H}~v~z~

Table 3
Experimental results for $n = 10$.

n	m	# opt	LB	UB	opt	VNS _{best}	t_{first} (s)	agap(%)	std(%)	$H_{n,m}$
10	12	2	2.44948974	3.00000000	2.44948974	opt	209.5693	0.0000	0.0000	I_aAH_BM?
10	13	4	2.64575131	3.00000000	2.67083940	opt	170.2813	0.0000	0.0000	IDN@CD@OG
10	14	7	2.82842712	3.00000000	2.85577251	opt	213.6797	0.0000	0.0000	IWC\\?JGCo
10	16	15	3.22490310	3.44948974	3.23606798	opt	228.5715	0.0000	0.0000	IcWecKkSG
10	17	1	3.43511281	3.82842712	3.43806940	opt	218.9503	0.0092	0.0400	I@DS'?Ry?
10	18	23	3.63318042	4.00000000	3.64575131	opt	222.0021	0.0000	0.0000	IKu?y?tXO
10	19	8	3.82099463	4.00000000	3.83802850	opt	239.1995	0.0000	0.0000	IKEXSpew_
10	21	4	4.21900462	4.37228132	4.22924699	opt	249.7656	0.0000	0.0000	IDVaTlaqG
10	22	1	4.42718872	4.70156212	4.42989680	opt	372.7327	0.0038	0.0165	IMerQXKgw
10	23	2	4.62601340	5.00000000	4.63522477	opt	207.1595	0.0000	0.0000	I_Lnuqs'W
10	24	46	4.81663783	5.00000000	4.82842712	opt	292.4264	0.0000	0.0000	IRginqnt_
10	26	2	5.21536192	5.31662479	5.22366226	opt	236.5811	0.0000	0.0000	ILna~YfTW
10	27	1	5.42217668	5.60555128	5.42442890	opt	318.4761	0.0561	0.0262	I@ Nnjsaw
10	28	2	5.62138773	5.87298335	5.62832392	opt	193.0858	0.0000	0.0000	IVpzRrJlg
10	29	4	5.81377674	6.00000000	5.82375494	opt	215.9554	0.0000	0.0000	I~Un'[N~W
10	31	1	6.21288983	6.27491722	6.21986828	opt	242.3106	0.0000	0.0000	Iyd }zilW
10	32	2	6.41872261	6.53112887	6.42442890	opt	315.6255	0.0062	0.0149	IFN~ryzO
10	33	2	6.61815684	6.77200187	6.62347538	opt	240.7775	0.0000	0.0000	IXsnnz~_
10	34	2	6.81175455	7.00000000	6.82003527	opt	187.0979	0.0000	0.0000	I~f z}vZw
10	36	3	7.21110255	7.24264069	7.21699057	opt	234.6396	0.0000	0.0000	I~b }vno
10	37	2	7.41619849	7.47213595	7.42442890	opt	217.8714	0.0000	0.0000	I }~r~{ w
10	38	1	7.61577311	7.69041576	7.62347538	opt	233.1308	0.0000	0.0000	I}~}~'fVw
10	39	1	7.81024968	7.89897949	7.81727139	opt	243.4793	0.0000	0.0000	I}nz~v~_
10	41	1	8.20975030	8.21699057	8.21699057	opt	210.5525	0.0000	0.0000	I~}~}vw
10	42	1	8.41427359	8.42442890	8.42442890	opt	16.0119	0.0000	0.0000	I~nn~}o

Table 4
Experimental results for $11 \leq n \leq 19$.

n	m	LB	UB	VNS _{best}	t_{first} (s)	agap(%)	std(%)	$\tilde{H}_{n,m}$
11	13	2.41209076	3.00000000	2.42023134	1352.0232	0.0000	0.0000	JE?H_GgIEA?
11	25	4.57264594	5.00000000	4.57919535	1395.6566	0.0000	0.0000	JlgpOpVrAe_
11	32	5.83095189	6.00000000	5.84045454	1715.8036	0.0000	0.0000	JqXAL}fnM{?
11	41	7.47115666	7.58257569	7.47722558	1367.4513	0.0100	0.0123	Jvy~rlnu[z_
11	47	8.55994902	8.62347538	8.56776436	1323.8369	0.0000	0.0000	Jz}~ v~Z_
12	23	3.85140667	4.00000000	3.86731111	1480.8976	0.0000	0.0000	KrHcOKX?gQqa
12	37	6.17791766	6.27491722	6.18499012	2015.9544	0.0000	0.0000	KbJdsX{vVEf[
12	39	6.51920241	6.77200187	6.52079729	2277.5045	0.0390	0.0148	KlMuXvLrRdxh
12	47	7.84219357	8.00000000	7.84884056	2153.9590	0.0001	0.0001	Knl""Xzk~Xu
12	52	8.67947771	8.81507291	8.68465844	1416.5034	0.0023	0.0055	KreV~z}z~yn
13	19	2.93519754	3.00000000	2.95270334	1824.8940	0.0000	0.0000	LoDC?gH?@b_Gc
13	36	5.56085218	6.00000000	5.56516294	3013.1901	0.0122	0.0167	Lbf_H}OQITKvS
13	38	5.85727687	6.00000000	5.86607157	2909.5240	0.0000	0.0000	LIW]Ozbh_pajhq
13	46	7.08193802	7.12310563	7.08631141	2460.9124	0.0003	0.0002	L{M]RluQzcvdb
13	53	8.16182483	8.21699057	8.16707927	2332.4706	0.0002	0.0001	Lymtr\ rnjjxk
14	19	2.75162290	3.00000000	2.77946795	1737.5023	0.0000	0.0000	Mgh?@_O?KCaA@O@g?
14	40	5.73211504	6.00000000	5.74165739	1995.0358	0.0007	0.0021	MMNQqHaJKeQilmgr?
14	51	7.29970645	7.47213595	7.30475498	3272.1196	0.0073	0.0087	M}gYdnKRsvvYw@_
14	81	11.58200580	11.63324960	11.58872340	1153.0190	0.0000	0.0000	Mz~v~n~}~v~^~
14	85	12.14789810	12.15206730	12.15206730	877.2795	0.0000	0.0000	M~^~n~ z~^~
15	24	3.22490310	3.64575131	3.23606798	2101.4709	0.0000	0.0000	Mg?}@?O?OD_IY?FGOA_
15	27	3.63318042	4.00000000	3.64575131	2335.6019	0.0016	0.0069	N@EACLW'S@D?K@ObGAO
15	37	4.93963561	5.00000000	4.94666514	2923.4900	0.0000	0.0000	NtU?CCg@g'KYOWT?fAG
15	51	6.81175455	7.00000000	6.81999696	3056.2283	0.0004	0.0004	NbX'srCfk}Bgx@_zkUo
15	98	13.06904740	13.07106780	13.07106780	513.3232	0.0000	0.0000	N}~vz~^~^~}~ ~zw
16	19	2.42383993	3.00000000	2.43026679	2501.8737	0.0000	0.0000	ODW?@??WAOPC?@_G?H?
16	21	2.66926956	3.00000000	2.69539996	1951.1639	0.0000	0.0000	O?G?_LG?@?Oc?ED?'QE?O
16	34	4.27200187	4.70156212	4.28100496	4606.1427	0.0008	0.0014	OOOHkaK[AOIH@GCCoOY@o
16	83	10.38628900	10.52079730	10.39104160	4663.0800	0.0053	0.0032	O ~tahlz}vrsk'rq z~\
16	100	12.50999600	12.58872340	12.51560980	3751.3471	0.0040	0.0013	Or~nzv~n}~V~ ~s~x}~
17	40	4.72788972	5.00000000	4.74045493	4640.2918	0.0014	0.0013	PK@HOUPc?x@W'@WG?JJGagD_
17	61	7.18658882	7.35889894	7.19268175	4694.9240	0.0003	0.0002	PqwRXoU_xLDiK\sAoVeYBTAs
17	91	10.71557420	11.00000000	10.72014910	4655.4214	0.0035	0.0032	Pt 'M'Fm j} [nRvNzJrNi{
17	97	11.42237230	11.55743850	11.42711020	4965.9882	0.0072	0.0033	Pbzd~LvU~^~Qn\ }vkvztxxmk
17	105	12.36218140	12.44622200	12.36708420	4732.3986	0.0037	0.0029	PvznuZv }mnjj }~uuvZz{
18	59	6.57436097	7.00000000	6.57938551	4552.0987	0.0207	0.0169	Q??kiPgCs\YaYmWV_QCxWURpo?
18	76	8.45905169	8.81507291	8.46443065	4645.0184	0.0081	0.0059	QvDdK gWR@'rfooXBfxywipLUG
18	78	8.67947771	9.00000000	8.68473675	4891.3250	0.0064	0.0043	QhKtZqXsrfMoxrix'tY'ssK\RG
18	86	9.56846673	9.91607978	9.57317932	4492.7089	0.0103	0.0061	Q@XSz~kmsZ~OoV cltVJ BeJiO
18	127	14.11461020	14.13216880	14.11726780	3834.0942	0.0000	0.0000	Ql ~m}v~nv v~^~x~jnv ~w ~ g
19	72	7.59501221	8.00000000	7.59978814	4456.2358	0.0165	0.0092	RYCGS{gw}iYVh_GEzoAVIHGwSjPodW
19	102	10.74586820	11.00000000	10.75070290	4699.9781	0.0015	0.0024	RHf{YTxunsXzh}yw[nFrHlmurxibiMw
19	112	11.79652040	12.00000000	11.80093640	4276.1009	0.0004	0.0002	RUVjBzm} ZwU~^~fs thiUnjJzNxo
19	150	15.79473600	15.88819440	15.79795900	3266.7790	0.0017	0.0007	Rrf~z~x~^~^}~^d~v~^~z~zz~^~zo
19	160	16.84605220	16.89414710	16.84885780	1937.8747	0.0000	0.0000	R~ ~ ~^~z~z~^~}~^n}~^}~ z~w

for the instance (10, 12), which by Proposition 5(i), means that $\mathcal{H}(10, 12)$ contains a semiregular bipartite graph with 4 vertices of degree 3 and 6 vertices of degree 2; in fact, there are exactly 2 such graphs and both are reached by the VNS.

For the instances (7, 18), (8, 25), (9, 32), (9, 33), (10, 41), (10, 42), (14, 85), (15, 98) and (20, 184), VNS_{best} attains the upper bound UB, the parameter t_{first} is significantly small (in comparison to the remaining instances) and agap and std are zero. This scenario was expected since in these instances we deal with graphs having a large number of edges, which reduces the entire computation and results in a fast convergence to the same solution in all 20 runs.

The structure of a solution. For all 159 instances, the solution obtained by the VNS has the desired structure; i.e. its vertex degrees belong to $\{\lfloor 2m/n \rfloor, \lceil 2m/n \rceil\}$. In addition, for $n \leq 10$ every solution is a minimizer. Due to the complexity of the problem, we cannot say whether the same holds for $n \geq 11$, unless we deal with instances that are resolved theoretically — they are listed in the beginning of Section “Experimental results” and excluded in further considerations. For the remaining instances, we can surely say that every obtained solution is close to the optimal one (the minimizer) in the sense that the corresponding spectral radius belongs to the range of Proposition 2 (in the notation of Section “Experimental results”, $VNS_{\text{best}} \in [LB, UB]$).

Conclusions

In this paper we considered connected graphs of fixed order n and size m that minimize the spectral radius, the so-called minimizers. We conjectured that vertex degrees of a minimizer are as equal as possible, i.e. belong to $\{\lfloor 2m/n \rfloor, \lceil 2m/n \rceil\}$. The conjecture is confirmed for graphs with at most 10 vertices and for certain particular classes of graphs as reported in Sections “Background” and “Theoretical results”. For larger n , we proposed the long-scale variable neighbourhood search metaheuristic following the LIMA approach, with only one parameter (the total execution time) defined in advance. All VNS procedures are designed and implemented specifically for this problem. We have checked that for instances up to 10 vertices the solution obtained by the VNS coincides with an optimal solution obtained by the brute force (i.e. by the total enumeration). For instances with up to 100 vertices, with various values of n and m , the VNS always results in a solution that has the required structure. Moreover, the solution always falls within the range of Proposition 2, which means that even if it is not the optimal one, it is close to it. According to the analysis of the previous section, we can say that the VNS has reached the best solution in a very reasonable time.

Future work may include determining new classes of graphs for which the conjecture can be confirmed theoretically and implementation of other heuristics. For example, due to the binary representation

Table 5
Experimental results for $20 \leq n \leq 100$.

<i>n</i>	<i>m</i>	LB	UB	VNS _{best}	<i>t</i> _{first} (s)	agap(%)	std(%)
20	46	4.62601340	5.00000000	4.63523802	5668.7270	0.0055	0.0052
20	66	6.61815684	7.00000000	6.62361473	5838.9678	0.0191	0.0113
20	104	10.41153210	10.68465840	10.41601080	6329.2307	0.0095	0.0041
20	113	11.30928820	11.48074070	11.31341370	6253.9712	0.0090	0.0036
20	184	18.40652060	18.41211380	18.41211380	2970.2854	0.0000	0.0000
30	200	13.34166410	13.68114580	13.34606840	3442.4696	0.0031	0.0017
30	295	19.67231560	19.95445120	19.67586290	3531.9771	0.0013	0.0008
30	351	23.40512760	23.48999600	23.40872260	3341.3151	0.0010	0.0006
30	401	26.73699060	26.79160590	26.73982770	3578.1932	0.0004	0.0002
30	418	27.86873990	27.89966440	27.87042620	3375.9415	0.0000	0.0000
40	166	8.31264098	9.00000000	8.31858787	6968.1729	0.0077	0.0054
40	330	16.50757400	17.00000000	16.51165260	7875.4863	0.0029	0.0013
40	525	26.25357120	26.36542460	26.25609850	7531.8366	0.0006	0.0004
40	563	28.15226460	28.20544120	28.15397430	6754.5594	0.0004	0.0002
40	590	29.50423700	29.65247580	29.50729850	7765.0548	0.0005	0.0003
50	89	3.59444015	4.00000000	3.60950788	7081.8768	0.0660	0.0442
50	422	16.88312770	17.00000000	16.88566650	7439.5205	0.0003	0.0002
50	565	22.60530910	23.00000000	22.60875610	7846.5760	0.0009	0.0005
50	866	34.64332550	34.89157420	34.64578970	8589.0167	0.0003	0.0001
50	1166	46.64246990	46.67126390	46.64461490	7288.0101	0.0001	0.0000
60	531	17.70593120	18.00000000	17.70957920	11,035.7343	0.0031	0.0011
60	821	27.37090910	27.76482310	27.37389630	11,684.1026	0.0006	0.0003
60	1165	38.83512160	39.00000000	38.83659110	10,385.1313	0.0001	0.0001
60	1273	42.43622670	42.59637980	42.43854230	10,385.3421	0.0001	0.0001
60	1351	45.03369110	45.04343720	45.03402640	6221.2467	0.0000	0.0000
70	594	16.97224630	17.00000000	16.97307430	8609.0675	0.0000	0.0000
70	867	24.77498740	25.00000000	24.77769220	15,180.2632	0.0006	0.0003
70	1003	28.66107360	29.00000000	28.66397610	15,926.5501	0.0007	0.0003
70	1442	41.20194170	41.33072900	41.20356720	14,829.6000	0.0002	0.0001
70	1832	52.34500930	52.44902600	52.34681630	15,578.5026	0.0001	0.0001
80	506	12.65898890	13.00000000	12.66523670	18,746.9368	0.0038	0.0031
80	539	13.48425010	14.00000000	13.49014610	18,353.9917	0.0060	0.0024
80	872	21.80366940	22.00000000	21.80650380	19,423.6818	0.0024	0.0026
80	1765	44.12623940	44.12713550	44.12735520	19,314.4195	0.0009	0.0007
80	2669	66.72649400	66.85476680	66.72782600	18,474.6976	0.0000	0.0000
90	859	19.09101010	19.39230480	19.09305920	19,586.7607	0.0072	0.0044
90	1072	23.82529000	24.00000000	23.82780850	21,980.1054	0.0031	0.0019
90	1466	32.58152170	33.00000000	32.58450280	22,968.8032	0.0005	0.0004
90	1943	43.17947040	43.36067980	43.18098660	21,301.0294	0.0011	0.0009
90	2501	55.57997240	55.91366460	55.58185030	21,989.2311	0.0001	0.0000
100	467	9.35200513	10.00000000	9.36146340	26,232.8503	0.0186	0.0111
100	1944	38.88135800	39.00000000	38.88262410	24,224.6026	0.0020	0.0009
100	2854	57.08064470	57.13760460	57.08126150	21,391.9699	0.0012	0.0005
100	3756	75.12070290	75.15756810	75.12136070	24,207.4165	0.0006	0.0003
100	3772	75.44163310	75.57460300	75.44310070	26,500.7736	0.0001	0.0001

of the solution, the genetic algorithm can be considered as a potentially suitable procedure.

In order to speed-up the entire procedure, a possible direction for future work is a parallelization of presented approach and its testing on powerful multiprocessor computers. Since the local search is the most time-consuming step, a parallel execution of this step figures as a natural strategy for larger instance. Another variant is the independent execution of the entire VNS procedure with different initial solutions.

Theoretical and experimental branches dealing with virus propagations should be included.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix.

Here are the first best solutions for instances with $n \geq 20$. As before, they are written in the graph6 format.

n = 20, m = 46

ST@CCECEaaC_AoQG??jK?AMGeE??RI?d?

n = 20, m = 66

SUCKr'SAYOdH@lgb]^_F?qP^AWV?KT_S

n = 20, m = 104

SBzffhjBTh@raNFtYUW_-HwFu_-G]p_-BMtO

n = 20, m = 113

S'R|tI{bxmY^||}PJsZEzfrpwoT^_}EG

n = 20, m = 184

S~n~^n~v~}~~~~~w

n = 30, m = 200

]inL'VK_ga'KbE{o}swqE[NC_lfMOc_jOUn[lvq][sIaQmHedhPzf? Xhwx@QweZML@roPpnF?

n = 30, m = 295

]drz}hun}^]]-QXvvBtjZ]liN} -ftNuBl|XZ{lvvVFxmX~M~Y}rul{hvv}mDVWZ} FXu_-\\Lvmjw

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