Reinforcement learning for graph theory, I. Reimplementation of Wagner's approach*

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Abstract

We reimplement here the recent approach of Adam Zsolt Wagner [arXiv:2104.14516], which applies reinforcement learning to construct (counter)examples in graph theory, in order to make it more readable, more stable and much faster. The presented concepts are illustrated by constructing counterexamples for a number of published conjectured bounds for the Laplacian spectral radius of graphs.

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1 Introduction

We are witnessing yet another computational revolution through proliferation of applications of artificial intelligence (AI) methods in everyday tasks. Besides being very publicly scrutinised through the ongoing development of self-driving vehicles, defeating world champions in Go, achieving superhuman performance in recognising images and playing video games, or generating multimedia content, AI models are trained and used to an even greater extent in science, engineering and technology to provide surrogate models for predicting values of functions that are hard to compute or simulate numerically. Our goal here is to elaborate on a recent application of a particular AI method——reinforcement learning——in construction of (counter)examples in graph theory.

A few specialised software packages have been used as auxiliary tools in graph theoretical research for four decades already, either to help with posing new conjectures or to help refute existing conjectures by providing counterexamples. Two earliest examples of such packages are GRAPH and Graffiti, which were special types of expert systems. GRAPH, written by Dragoš Cvetković and Laszlo Kraus in the 1980s [1–3], provided a closed environment for visually editing individual graphs and computing their invariants, and implemented certain AI methods for automatically proving simplest theorems in graph theory. Graffiti, written by Siemion Fajtlowicz in 1986 [4–7], was geared more toward automatic conjecture making than enabling researcher to test his own conjectures. Graffiti was used to produce many conjectures, some of which attracted attention of well-known graph theorists [8]. It is interesting to note that these old packages have been rewritten and modernised a few times in the forms of newGRAPH [9–11], Graffiti.pc [12–15] and Grinvin [16, 17]. A relatively recent addition to this group is graph6java [18, 19], which builds upon the power of existing programs for exhaustive generation of different types of graphs and is capable, for a selected graph invariant, to answer the questions such as which graphs have extremal values or which pairs of graphs have equal values of this invariant. Another approach is taken by AutoGraphiX (AGX), written by Gilles Caporossi and Pierre Hansen in the 2000s [20–24]. AGX considered expressions made up of graph invariants as instances of an optimisation

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problem and consequently applied variable neighbourhood search (VNS) metaheuristic to search for extremal graphs for these expressions over a search space that consists of a predefined set of graphs (which is too big to perform an exhaustive search in it). AGX has been used to refute some of the conjectures of Graffiti, and in a lengthy series of papers its authors posed several new conjectures as well.

Most recently, in the pioneering work [25] Adam Zsolt Wagner used reinforcement learning (RL) to construct counterexamples for several conjectures in graph theory. Although RL is present for a long time in AI community, it experienced recent rise in popularity after it was used by DeepMind in programs AlphaGo, AlphaZero and MuZero that managed to reach superhuman level of performance in go, chess and visually complex Atari games, all without knowing the game rules in advance [26]. RL is based on an interplay between an agent and an environment (see Fig. 1): at each step, the agent receives the observation on the state of the environment, performs an action in the environment, for which it then receives the reward from the environment. The goal of the RL agent is to learn how to maximise the cumulative reward received from the environment.

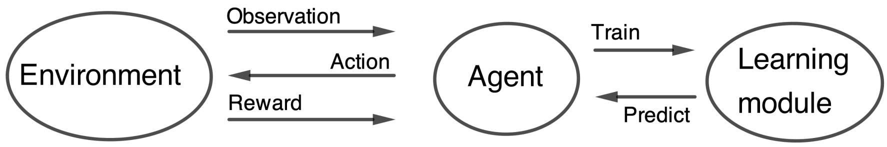


Figure 1: General process of reinforcement learning.

In Wagner's approach, simple graphs are constructed by an agent as a sequence of 0-1 actions which represent the entries of the upper part of the adjacency matrix. The environment responds with zero intermediate rewards, while the final reward, when the graph is fully constructed, is equal to a specified graph invariant. Setting the final reward to represent the difference of two sides of a conjectured inequality between graph invariants, Wagner [25] was able to find counterexamples for several published conjectures. Among others, this includes a 19-vertex counterexample for an AGX conjecture on the sum of the matching number and the spectral radius [20], for which one of the authors previously showed the existence of counterexamples on more than 600 vertices [27]. One of the authors [28] also tested Wagner's approach on a recent conjecture of Akbari, Alazemi and Andjelić [29]. Although RL did not manage to explicitly find counterexamples in this case, it was still very useful by suggesting their proper structure.

Our goal here is to offer the reimplementation of Wagner's approach that is more readable, more stable, much faster and as a result, more useful. Wagner's initial RL implementation runs only for very specific combinations of python and tensorflow versions, which is probably a consequence of pre-existing code that it is based on (see [30]). To avoid this, we reimplement his approach here from scratch. We separate the learning agent from the reward computation, so that interested researchers need only define the final reward in a separate python file in order to adapt and reuse this implementation. We pay particular attention to computation performance, since RL must compute invariants for at least several hundred thousands of graphs before reaching a satisfactory level of convergence in its learning. While final rewards may certainly be computed by using networkX and/or numpy, our experience shows that computing them by calling Java code directly from Python offers a significant speedup. For example, computation of eigenvalues of graphs on 20–30 vertices with graph6java (which internally uses EJML library [31]) is 3–5 times faster than computing them with numpy. Overall, the new implementation enables interested researchers to see learning results in a matter of minutes instead of hours or even days.

In the next section we briefly overview the principles used in Wagner's approach and the details of our reimplementation, which also serves as a short manual for its use. In Section 3 we then apply it to find counterexamples to a number of older conjectured bounds on the Laplacian spectral radius of graphs from [39].

2 Wagner's simple graph environment and the cross-entropy method

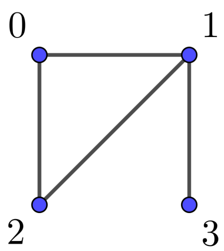
Wagner's most profound observation from [25] is that construction of a simple graph and computation of its invariant can be treated as a sequence of consecutive observations, actions and rewards. For an

n-vertex graph G, let $L\colon l_1, \dots, l_{\binom{n}{2}}$ be the part of adjacency matrix above the diagonal, listed in the row-wise order. Since G is fully determined by L, the agent constructs G simply by issuing actions equal to the consecutive elements of L. All rewards given by the environment before G is fully constructed are equal to zero, while the final reward is equal to the graph invariant $r(G)$ that is of interest to us.

On the other hand, environment observations have to support the goal of the agent to learn which actions should be issued at which stage of graph construction in order to maximise the final (=cumulative) reward. Hence each observation has to inform the agent what part of the graph has been already constructed so far. For this reason, each observation represents the current state of L, followed by the one-hot encoding of the next entry of L to be determined. The initial observation, before any action is issued, is thus

$$\underbrace{0\dots0}_{\binom{n}{2}}\,\underbrace{10\dots0}_{\binom{n}{2}}.$$

Subsequent actions are collected in the first part of the observation which builds up to L, while the single 1 in the second part travels from left to right, indicating the index of the entry of L that will store the next action, until it should pass over the right end, which indicates that the graph is fully constructed and that $r(G)$ can be computed. This process of interaction between the agent and the environment while constructing a small graph is illustrated in Fig. 2.



$$\begin{bmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}$$

Environment Observation	Agent Action	Environment Reward
000000 100000		
	1	
100000 010000		0
	1	
110000 001000		0
	0	
110000 000100		0
	1	
110100 000010		0
	1	
110110 000001		0
	0	
110110 000000		$r(G)$

Figure 2: Illustration of the sequence of observations, actions and rewards issued while constructing the graph shown in top left part. Entries of the adjacency matrix above the diagonal, which yield the sequence L, are shown in red. Red-coloured entries of observations represent the entry in the left part which will store the next action and the single 1 in the right part which indicates the index of this entry. Note that both the list of actions issued and the left part of the last observation are equal to L.

Wagner [25] used the *cross-entropy method* [32, 33] to enable the agent to learn how to construct graphs with large rewards. This is one of the simplest reinforcement learning methods, which usually works well for environments that do not require discovery of complex, multistep policies [34, Chapter 4]. In this method the agent employs as a learning module the neural network (initialised randomly at the beginning) which accepts a graph observation as the input and outputs a probability distribution over the set of possible actions (0 and 1 in this case), according to which the agent selects the next action. The cross-entropy method successively iterates through the *generation* and the *learning* phases. In the generation phase, the agent uses the neural network to simultaneously construct a batch of N graphs, for a fixed value of N. While each graph in the batch starts with the same initial observation $\underline{0\dots0}\,\underline{10\dots0}$, the agent's actions are selected at random according to the probability distribution provided by the neural network for each observation, so that the fully constructed graphs in the batch will not necessarily be mutually isomorphic. In the learning phase, the agent selects L graphs (for some $L \ll N$) with the largest rewards and trains its neural network on the pairs of observations and actions used in their construction (see Fig. 3). The goal of training is to minimise the cross-entropy between the actions used and the probability distributions that the network outputs for the corresponding observations. After training is done, the agent selects S graphs (for some $S < L$) with the largest rewards that are forwarded as survivors to the next generation phase.

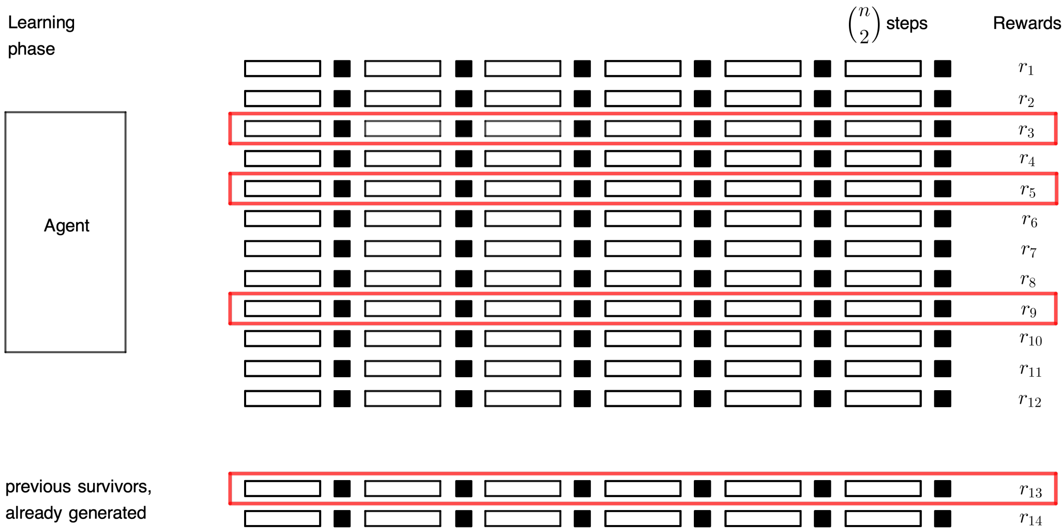


Figure 3: Illustration of the learning phase in the cross-entropy method. White-coloured rectangles symbolise observations of graph environments, while black-coloured boxes represent subsequent actions issued by the agent. Construction of each graph is completed after $\binom{n}{2}$ actions, after which the rewards r_i are computed. Constructed graphs with a specified percentage of largest rewards are selected (framed in red rectangles). The agent's neural network is retrained on the set of observation/actions pairs used in construction of most rewarding graphs, with the aim of minimising the cross-entropy between the action probability distributions that the neural network provides for these observations and the actual actions used in their construction.

Note that the only purpose of rewards in the cross-entropy method is to select the subsets of elite graphs, as the actual value of rewards is not used in training of the agent's underlying neural network. Nevertheless, the network learns the common characteristics of the structure of elite graphs, so that the graphs constructed in the following generation phases will tend to have higher rewards. Survivor graphs serve to speed up the learning process in the beginning, directing neural network toward imitating construction of particularly rewarding graphs. However, as the learning process converges, the graphs constructed in each new generation will begin to share more and more similarities, to the point when majority of them will actually be mutually isomorphic to the same locally optimal graph. At such moment either the learning should be stopped or the actions issued by the agent should be additionally randomised in an effort to avoid this local optimum.

2.1 New reimplementation

Our reimplementation of the cross-entropy method employing Wagner's simple graph environment is freely available online at

`github.com/dragance106/cema-for-graphs`

and it consists of three independent files:

- `cema_train_simple_graph.py`,
- `graph6java.jar` and
- `training_runner.py`,

that we briefly discuss here.

The file `cema_train_simple_graph.py` contains implementation of the methods for successively generating batches of simple graphs and training the agent's neural network to maximize the reward function. The main method in this file is:

```
train(compute_reward,
      n=20,
      batch_size=200,
      num_generations=1000,
      percent_learn=90,
      percent_survive=97.5,
      neurons=[72,12],
      learning_rate=0.003,
      act_rndness_init=0.005,
      act_rndness_wait=10,
      act_rndness_mult=1.1,
      act_rndness_max=0.025,
      verbose=True,
      output_best_graph_rate=25)
```

Let us quickly discuss the parameters of this method:

- compute_reward: denotes the method that computes a real-valued reward for each constructed graph. This method has to be provided by the user and it has the signature `my_reward(n, A)`, where `n` is the number of vertices and `A` is the adjacency matrix;
- n: the number of vertices of graphs to be constructed;
- batch_size: the number of graphs in each batch;
- num_generation: the number of generations over which to train the agent;
- percent_learn: the best (100-percent_learn) percents of graphs from each batch are used to train the agent's neural network;
- percent_survive: the best (100-percent_survive) percents of graph from each batch are transferred to the next generation as survivors;
- neurons: the list determining the numbers of neurons in hidden layers of the agent's neural network. The neural network has $n(n-1)$ inputs to accommodate a simple graph observation, and two outputs representing raw scores for the possible actions (0=skip this edge, 1=add this edge). The structure of hidden layers (together with their number) is defined by this parameter;
- learning_rate: the learning rate of the agent's neural network;
- act_rndness_init: the initial value for the action randomness act_rndness. In order to increase exploration of different graphs and avoid being stuck in a local optimum from overexploitation of acquired knowledge, the agent will issue random actions at this rate, i.e., this percent of adjacency matrix entries will be random;
- act_rndness_wait: the number of generations without an increase in the maximum reward to wait before act_rndness should be increased;
- act_rndness_mult: the factor used to multiply act_rndness when there are no increases in the maximum reward for act_rndness_wait generations;
- act_rndness_max: the maximum allowed act_rndness value, since we do not want to have too many random edges in constructed graphs;
- verbose: True or False, describing whether to print on the console the summary information for each generation: generation number, maximum reward seen, reward used to select survivors, reward used to select graphs for learning, processing time for the generation, and act_rndness value
- output_best_graph_rate: the number of generations at which to produce the drawing of the best graph so far, which is then reported in the external runs/event file for TensorBoard consumption.

When the learning starts to converge, the train method tries to prevent mutual isomorphism of constructed graphs by randomising a certain percentage of actions issued by the agent. This percentage is represented by the internal variable act_rndness, while the four act_rndness_... parameters above serve to control it in a way that is inspired by the variable neighborhood search [35]: whenever act_rndness_wait generations pass without improving the maximum reward, act_rndness is multiplied by act_rndness_mult (with the waiting counter reset), but it is not allowed to surpass the value of act_rndness_max. On the other hand, as soon as the maximum reward increases in the next generation, act_rndness is returned back to act_rndness_init. Such varying action randomness can somewhat postpone convergence towards generating isomorphic graphs, depending on the combination of these four parameters.

After training is completed, the train method returns the maximum reward obtained, as well as the adjacency matrix of a graph that attains it. However, in order to check up on the progress of learning during training, the train method reports both short textual summary information on the console after each generation (when verbose is set to True) and writes this data, together with a drawing of the best graph each output_best_graph_rate generations, to an external event file in the runs subfolder. This event file may be visualised already while it is being populated during training, by starting TensorBoard application from the same folder with:

```
tensorboard --logdir runs
```

and then opening the web page indicated by TensorBoard in the browser. In this way, the user can effectively visualise the evolution of both the maximum reward and the best graphs during training, which helps her/him to judge whether training is going in a good direction or whether it should be stopped or restarted. Note, however, that there is not a simple recipe for determining the proper combination of training parameters—at the end, it boils down to experimentation through trial and error.

The values indicated after the equality signs in the signature of the train method above represent the default values for the corresponding parameters (which need not be mentioned in the method call if they are not changed). Hence the minimum way of calling the train method is as follows:

```
from cema_train_simple_graph import train
r, A = train(compute_reward=my_reward)
```

where my_reward is a method that has to be provided by the user. This method accepts the number of vertices `n` and the adjacency matrix `A` for each constructed graph, and returns a real number that represents its reward. If we are looking for a counterexample to a conjectured inequality $a(G) \leq b(G)$, Wagner's suggestion [25] was to return the reward $a(G) - b(G)$, since in this way we can easily recognise counterexamples through the positive value of their reward.

While it is quite standard in the Python community to use networkX [36] and numpy [37] for computation of graph invariants, we have found that using our existing Java framework graph6java [18, 19] directly from Python offers significant performance speedup—between three and five times—without the need for any compilation. This is enabled by the package JPype [38], which starts the Java virtual machine parallel to the Python virtual machine and sharing the same memory, so that with a small overhead, one can call Java methods directly from the Python code. In order not to interfere with the implementation details in `cema_train_simple_graph.py`, it is customary to write the reward method and start the training from another python file. Here is a minimal example that implements the reward for the conjectured inequality

$$\mu \leq \max_{v \in V(G)} \sqrt{\frac{4d_v^3}{m_v}}$$

from [39], where μ is the largest Laplacian eigenvalue of the graph, d_v is the degree of vertex v and m_v is the average degree of the neighbours of v:

```
import jpype.imports
from jpype.types import *
jpype.startJVM(classpath=['*'], convertStrings=False)
from graph6java import Graph

import numpy as np
import math
MINUS_INF = -1000000        # reward signifying unwanted graphs
```

```
def auto_lapla_1(n, A):
    g = Graph(JInt[:,:](A))
    if g.numberComponents()>1:
        return MINUS_INF

    mu = max(g.Lspectrum())
    deg = np.array(g.degrees())
    avd = np.array(g.averageDegrees())

    return mu - max(np.sqrt(4*deg*deg*deg/avd))

from cema_train_simple_graph import train
r, A = train(compute_reward=auto_lapla_1)

jpype.shutdownJVM()
```

The above code makes an important assumption that Java archive `graph6java.jar` (available at `github.com/dragance106/cema-for-graphs`) is located in the current folder. The list of invariants currently implemented in its Graph class is given in Appendix A. When needed, new invariants can be added to the Graph class directly in the graph6java source files, available at `github.com/dragance106/graph6java`, and the newly compiled jar file can then be used instead.

Finally, the file `training_runner.py` contains many further examples of implemented reward functions and different ways of inviting the train method.

3 Automated conjectures on the Laplacian spectral radius of graphs

Brankov, Hansen and Stevanović observed in [39] that a large number of upper bounds on the Laplacian spectral radius μ of graphs published in the literature so far have very similar form: they are a maximum taken either over the vertices or over the edges of functions that depend on the degree d_v of the vertex and the average degree m_v of the neighbors of v, and that evaluate to $2x$ when all the d_v and m_v terms in the functional expression are replaced by x. Based on this observation, they proposed a procedure for automatically creating new conjectured bounds of increasing complexity. Out of 361 vertex-maximum bounds and 1138 edge-maximum bounds of small complexity generated in [39], it turned out that 190 vertex-maximum and 297 edge-maximum bounds hold for connected graphs with up to 9 vertices, as well as on stars and windmills (triangles sharing one common vertex). This is a fairly large ratio of the total number of generated bounds, suggesting that the way of generating the bounds is likely meaningful. The 68 conjectured bounds from [39], having either small complexity or being most interesting, are listed here in Appendix B.

Here we apply the previously described reimplementation of Wagner's approach to reinforcement learning on graphs to all 68 conjectured automated bounds on the Laplacian spectral radius of graphs. The training was run mostly for graphs on 20 vertices, ocassionally going up to 24 vertices, and it managed to find counterexamples for 25 of the conjectured bounds: for 8 out of 32 vertex-maximum bounds and for 17 out of 36 edge-maximum bounds, as indicated in Table 1. Tensorboard's event files, from which one can see the actual counterexamples and the evolution of maximum, learning and surviving rewards for all of these conjectures, can be downloaded from [40].

Here we illustrate two particular conjectures

$$31: \quad \mu \leq \max_{v\in V} \frac{4m_v^2}{m_v+d_v}$$

and

$$65: \quad \mu \leq \max_{v_i\sim v_j} \frac{(m_i+m_j)(d_im_i+d_jm_j)}{2m_im_j}$$

for which RL managed to properly prove itself by converging toward graphs with clearly identifiable and nontrivial structure. Evolution of learning rewards for these two conjectures is shown in Fig. 4, while evolutions of graphs with maximum rewards are shown in Figs. 5 and 6. Learning rewards tend to oscillate after reaching a plateau due to increases in action randomness, which randomly adds or deletes

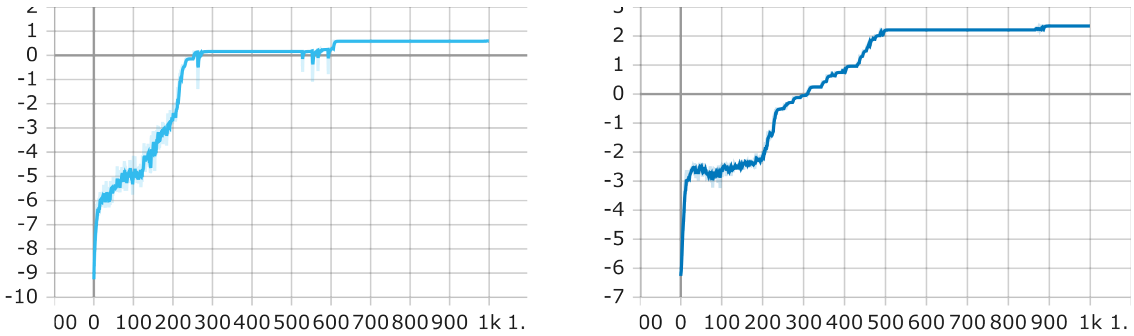


Figure 4: Evolution of learning rewards for the conjecture **(left)** 31: $\mu \leq \max_{v \in V} \frac{4m_v^2}{m_v + d_v}$ and **(right)** 65: $\mu \leq \max_{v_i \sim v_j} \frac{(m_i+m_j)(d_i m_i + d_j m_j)}{2 m_i m_j}$.

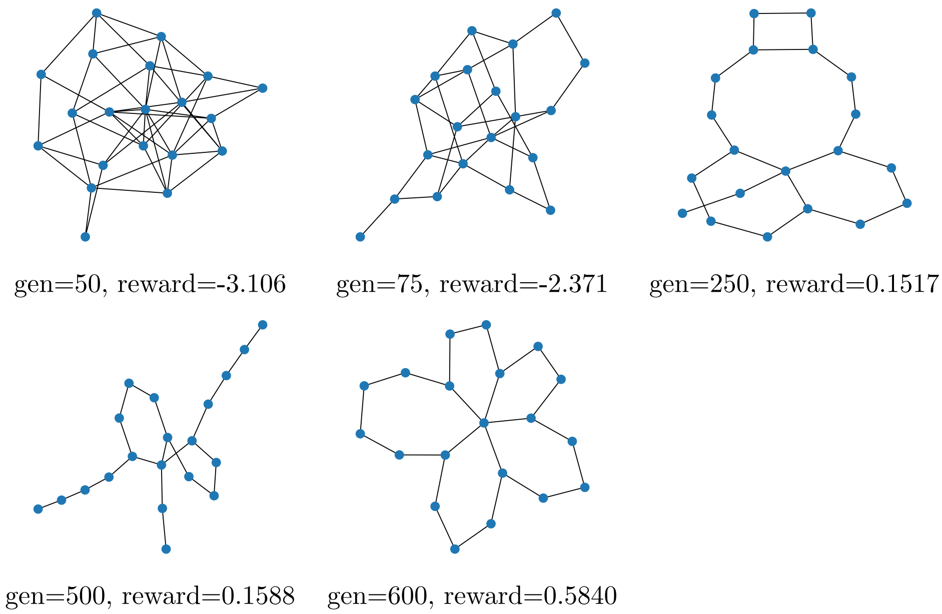


Figure 5: Evolution of graphs with maximum rewards for the conjecture 31: $\mu \leq \max_{v \in V} \frac{4m_v^2}{m_v + d_v}$.

edges to graphs constructed by the RL agent. While the counterexamples for these two conjectures were found relatively early (after 250–500 generations), we see that RL managed to further improve their rewards in later generations (after 600–900 generations). A look at the maximum reward graphs shows that this prolonged learning was worthwile, as it gave time to RL to make minor adjustments to its learning strategy and produce a more evident structure.

Certainly, not all RL runs produce counterexamples with an easily identifiable structure, as can be noted from the counterexamples shown in Fig. 7. RL is, after all, an optimization algorithm that can get stuck in a local optimum. Slow and steady increase of action randomness, which is incorporated in our reimplementation, may help it to get out of the local optimum if training is left to work over a larger number of generations. While this was indeed the case with conjectured bounds 31 and 65, there can be no upfront guarantee of success, so it is up to the user to decide based on his/her intuition when is the proper time to stop training that is unlikely to make further progress.

Nevertheless, the learning that does occur during the training of RL agent can often suggest appropriate directions for further study. For example, while the counterexamples from Fig. 7 do not necessarily have clearly identifiable structure (except obviously for a counterexample to bound 68), they do suggest that counterexamples are most often subquartic graphs.

Subquartic graphs are not too numerous, compared to connected graphs in general, so we were able to perform an exhaustive search among subquartic graphs with up to 14 vertices. It turned out that among them subquartic graphs on 12 vertices were most successful, disproving 26 of the conjectured bounds, including some for which RL did not find counterexamples, as indicated in Table 1. Interestingly, one

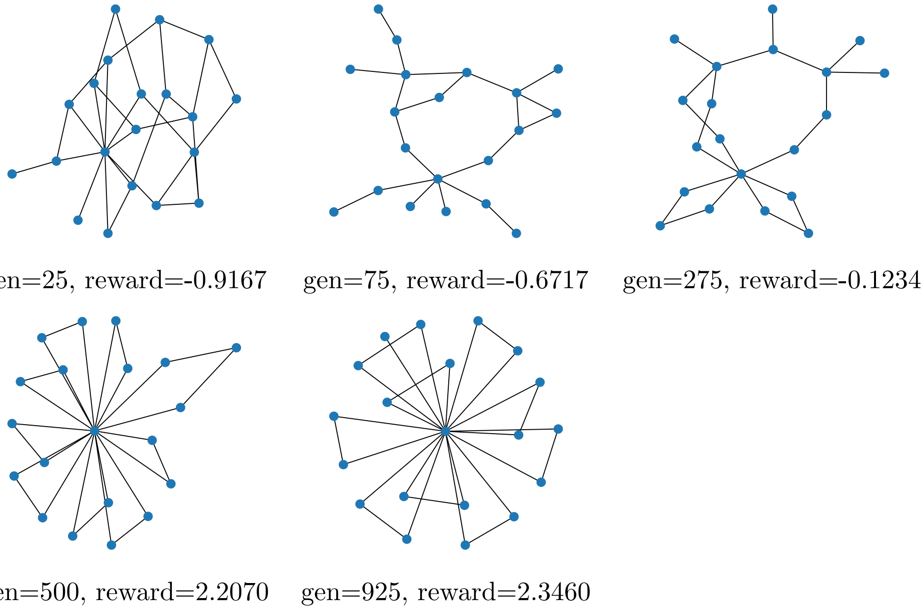


Figure 6: Evolution of graphs with maximum rewards for the conjecture 65: $\mu \leq \max_{v_i \sim v_j} \frac{(m_i+m_j)(d_i m_i + d_j m_j)}{2 m_i m_j}$.

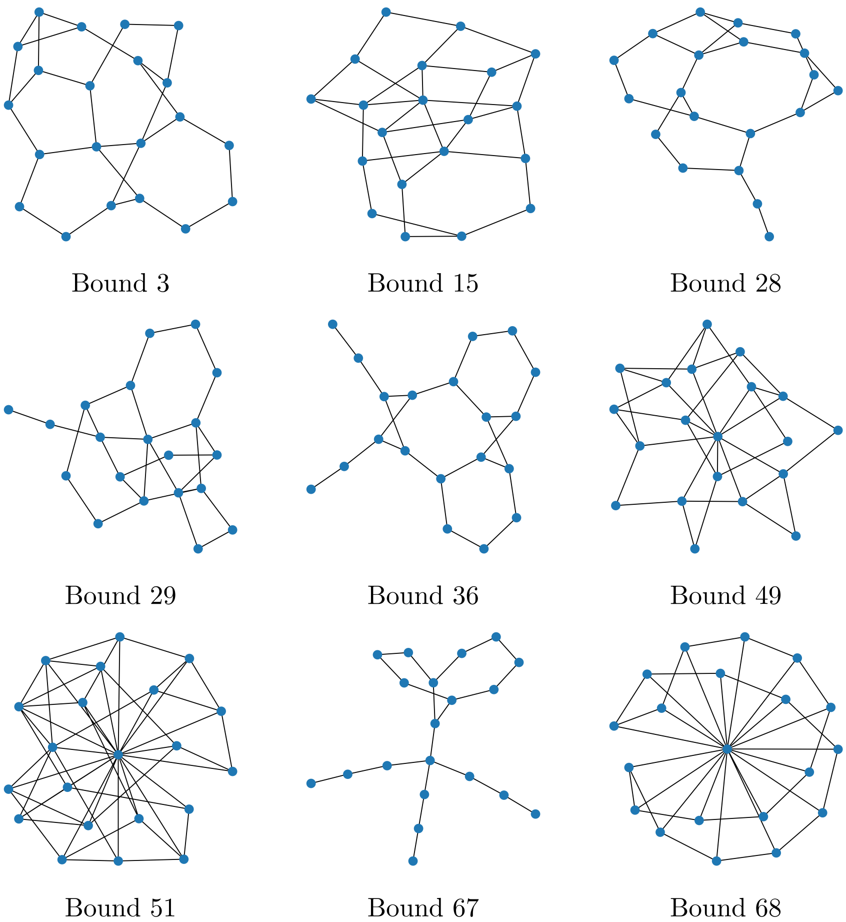
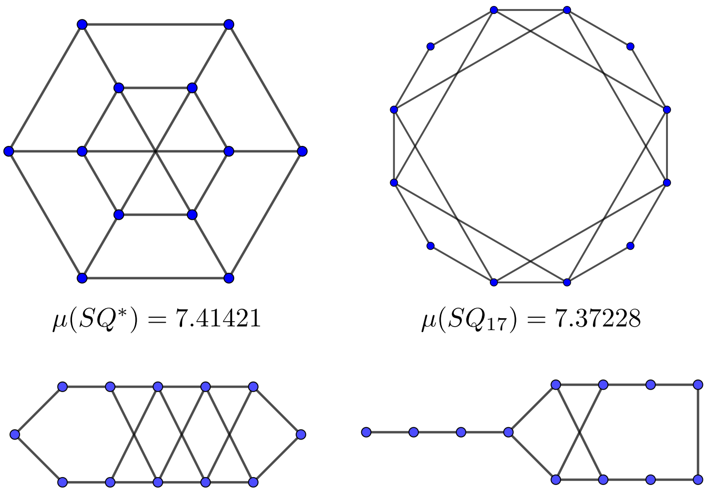


Figure 7: Counterexamples for several other conjectured bounds from Appendix B.



$\mu(SQ^*) = 7.41421$ $\mu(SQ_{17}) = 7.37228$

$\mu(SQ_{50}) = 7.06459$ $\mu(SQ_{66}) = 5.60286$

Figure 8: Counterexamples found among subquartic graphs on 12 vertices. SQ^* disproves 23 bounds: 2, 3, 15, 28, 29, 31, 32, 36, 43, 49, 52, 53, 54, 55, 57, 58, 59, 60, 61, 62, 63, 64 and 67, while SQ_{17}, SQ_{50} and SQ_{66} disprove only the bound indicated by their subscripts.

of these graphs serves as a counterexample for a total of 23 of these bounds, indicated as SQ^* in Fig. 8. The remaining graphs in this figure represent counterexamples for bounds 17, 50 and 66.

On the other hand, subquartic counterexamples have much more evident structure, so that they are easily generalizable, together with the two RL counterexamples for bounds 31 and 65 (see Figs. 5 and 6). However, while these generalizations do yield several further examples of graphs that disprove several conjectured bounds at once, they do not manage to disprove any other bound than those already disproved by RL training and subquartic graphs, so that we do not discuss them further here.

4 Concluding remarks

We have reimplemented here Wagner's approach of applying a cross-entropy method, a particular reinforcement learning technique, to an environment that represents simple graphs, in order to construct counterexamples in graph theory.

The reimplementation was applied to the set of 68 conjectured upper bounds on the Laplacian spectral radius of graphs from [39], which are listed in Appendix B. A total of 30 conjectured bounds was disproven: 25 directly by reinforcement learning and additional five by exhaustive search among subquartic graphs, which was largely suggested by the properties of counterexamples obtained through reinforcement learning. However, 38 conjectured bounds are still open after these computational attacks, suggesting that their automated way of generation may have had some merit. That appears to be especially true for vertex-based ones, as only 8 out of 32 conjectured bounds were disproved here. Probably due to the absence of symmetry in their expressions, none of the newly conjectured bounds from [39] has been proven in the last 18 years, yet they still resist being disproved computationally. We hope that new theoretical methods for proving at least a handful of these bounds will be discovered soon.

The reinforcement learning proved to be of valuable help in this study, and it is definitely a promising area for further work, either through the use of other available reinforcement learning methods, or by developing new environments for more specific graph classes or by applying it in new ways, e.g., to construct pairs of graphs at once in a single generation phase.

References

[1] D. Cvetković, L. Kraus, S. Simić, Discussing graph theory with a computer I, Implementation of graph theoretic algorithms, *Univ. Beograd, Publ. Elektrotehn. Fak., Ser. Mat. Fiz.* **716–734** (1981), 100–104.

Conjectured bound	RL counterexamples	Subquartic counterexamples
2		SQ^*
3	✓	SQ^*
15	✓	SQ^*
17		SQ_{17}
28	✓	SQ^*
29	✓	SQ^*
31	✓	SQ^*
32		SQ^*
36	✓	SQ^*
41	✓	
43	✓	SQ^*
49	✓	SQ^*
50		SQ_{50}
51	✓	
52	✓	SQ^*
53	✓	SQ^*
54	✓	SQ^*
55	✓	SQ^*
57	✓	SQ^*
58	✓	SQ^*
59	✓	SQ^*
60	✓	SQ^*
61		SQ^*
62	✓	SQ^*
63	✓	SQ^*
64	✓	SQ^*
65	✓	
66	✓	SQ_{66}
67	✓	SQ^*
68	✓	

Table 1: Disproved upper bounds on Laplacian spectral radius of graphs. (Refer to Appendix B for the actual bounds indicated here.)

[2] D. Cvetković, Discussing graph theory with a computer II, Theorems suggested by the computer, *Publ. Inst. Math. (Beograd)* **33(47)** (1983), 29–33.

[3] D. Cvetković, Discussing graph theory with a computer VI, Theorems proved by the aid of the computer, *Bull. Acad. Serbe Sci. Arts, Cl. Sci. Math. Natur., Sci. Math.* **47** (1988), 51–70.

[4] S. Fajtlowicz, On conjectures of Graffiti, *Discrete Math.* **72** (1988), 113–118.

[5] S. Fajtlowicz, On conjectures of Graffiti. II, Combinatorics, graph theory, and computing, Proc. 18th Southeast. Conf., Boca Raton, 1987, *Congr. Numerantium* **60** (1987), 189–197.

[6] S. Fajtlowicz, On conjectures of Graffiti. III, Combinatorics, graph theory, and computing, Proc. 19th Southeast. Conf., Boca Raton, 1988, *Congr. Numerantium* **66** (1988), 23–32.

[7] S. Fajtlowicz, On conjectures of Graffiti. IV, Combinatorics, graph theory, and computing, Proc. 20th Southeast Conf., Boca Raton, 1989, *Congr. Numerantium* **70** (1990), 231–240.

[8] S. Fajtlowicz, Written on the Wall, available at `independencenumber.files.wordpress.com/2012/08/wow-july2004.pdf`

[9] newGRAPH, available at `www.mi.sanu.ac.rs/newgraph`

[10] D. Stevanović, V. Brankov, An Invitation to newGRAPH, *Rend. Semin. Mat. Messina, Ser. II* **9(25)** (2003), 211–216.

[11] V. Brankov, D. Cvetković, S. Simić, D. Stevanović, Simultaneous editing and multilabelling of graphs in system newGRAPH, *Univ. Beograd. Publ. Elektr. Fak, Ser. Mat.* **17** (2006), 112–121.

[12] E. DeLaViña, Graffiti.pc, *Graph Theory Notes New York* **42** (2002), 26–30.

[13] E. DeLaViña, Graffiti.pc: a variant of Graffiti, in: S. Fajtlowicz, P.W. Fowler, P. Hansen, M.F. Janowitz, F.S. Roberts (eds.), *Graphs and Discovery*, DIMACS Series in Discrete Mathematics and Theoretical Computer Science, Vol. 69, American Mathematical Society, 2005, 71–79.

[14] E. DeLaViña, Some history of the development of Graffiti, in: S. Fajtlowicz, P.W. Fowler, P. Hansen, M.F. Janowitz, F.S. Roberts (eds.), *Graphs and Discovery*, DIMACS Series in Discrete Mathematics and Theoretical Computer Science, Vol. 69, American Mathematical Society, 2005, 81–118.

[15] E. DeLaViña, Written on the Wall II, Conjectures of Graffiti.pc, available at `cms.uhd.edu/faculty/delavinae/research/wowii/`

[16] Grinvin, available at `www.grinvin.org`

[17] A. Peeters, K. Coolsaet, G. Brinkmann, N. Van Cleemput, V. Fack, GrInvIn in a nutshell, *J. Math. Chem.* **45** (2009), 471–477.

[18] M. Ghebleh, A. Kanso, D. Stevanović, Graph6Java: a researcher-friendly Java framework for testing conjectures in chemical graph theory, *MATCH Commun. Math. Comput. Chem.* **81** (2019) 737–770.

[19] graph6java—Java templates for studying sets of graphs in g6 format, available at `github.com/dragance106/graph6java`

[20] G. Caporossi, P. Hansen, Variable neighborhood search for extremal graphs. I: The AutoGraphiX system, *Discrete Math.* **212** (2000), 29–44.

[21] M. Aouchiche, G. Caporossi, P. Hansen, M. Laffay, Autographix: a survey, Proc. 7th international colloquium on graph theory, Hyeres, France, September 12–16, 2005, *Electron. Notes Discrete Math.* **22** (2005), 515–520.

[22] M. Aouchiche, J.M. Bonnefoy, A. Fidahoussen, G. Caporossi, P. Hansen, L. Hiesse, J. Lacheré, A. Monhait, Variable neighborhood search for extremal graphs. XIV: The AutoGraphiX 2 system, in: L. Liberti, N. Maculan (eds.), *Global optimization—From theory to implementation*, Nonconvex Optimization and Its Applications 84, New York: Springer, 2006, pp. 281–310.

[23] M. Aouchiche, G. Caporossi, P. Hansen, Variable Neighborhood Search for Extremal Graphs 20. Automated Comparison of Graph Invariants, *MATCH Commun. Math. Comput. Chem.* **58** (2007), 365–384.

[24] M. Aouchiche, G. Caporossi, P. Hansen, N. Mladenović, C. Lucas, Finding conjectures in graph theory with AutoGraphiX, Le Cahiers du GERAD, G-2016-90, 2016.

[25] A.Z. Wagner, Constructions in combinatorics via neural networks, arXiv:2104.14516 (2021).

[26] DeepMind, AlphaGo, available at `deepmind.com/research/highlighted-research/alphago`

[27] D. Stevanović, Resolution of AutoGraphiX conjectures relating the index and matching number of graphs, *Linear Algebra Appl.* **433** (2010), 1674–1677.

[28] Dj. Stevanović, I. Damnjanović, D. Stevanović, Finding counterexamples for a conjecture of Akbari, Alazemi and Andjelić, arXiv: 2111.15303 (2021).

[29] S. Akbari, A. Alazemi, M. Andjelić, Upper bounds on the energy of graphs in terms of matching number, *Appl. Anal. Discrete Math.* **15** (2021) 444–459.

[30] A.Z. Wagner, Code accompanying the manuscript "Constructions in combinatorics via neural networks and LP solvers", available at `github.com/zawagner22/cross-entropy-for-combinatorics`

[31] P. Abeles, A fast and easy to use linear algebra library written in Java for dense, sparse, real, and complex matrices, available at `github.com/lessthanoptimal/ejml`

[32] R.Y. Rubinstein, Optimization of computer simulation models with rare events, *Eur. J. Oper. Res.* **99** (1997), 89–112.

[33] P.T. De Boer, D.P. Kroese, S. Mannor, R.Y. Rubinstein, A tutorial on the cross-entropy method, *Ann. Oper. Res.* **134** (2005), 19–67.

[34] M. Lapan, *Deep reinforcement learning hands-on*, Packt Publishing, Birmingham–Mumbai, 2020.

[35] P. Hansen, N. Mladenović, J. Brimberg, J.A.M. Pérez, *Variable Neighborhood Search*, in: M. Gendreau, J.Y. Potvin (eds.), Handbook of Metaheuristics, 3rd edition, Springer, Cham, 2019, 57–98.

[36] A.A. Hagberg, D.A. Schult, P.J. Swart, *Exploring network structure, dynamics, and function using NetworkX*, in: G. Varoquaux, T. Vaught, J. Millman (eds.), Proc. 7th Python in Science Conference SciPy2008, Pasadena, CA, USA, 2008, pp. 11–15.

[37] C.R. Harris, K.J. Millman, S.J. van der Walt, et al, Array programming with NumPy, *Nature* **585** (2020), 357—362.

[38] S. Menard, L. Nell, et al, JPype documentation, available at `jpype.readthedocs.io/en/latest/`

[39] V. Brankov, P. Hansen, D. Stevanović, Automated conjectures on upper bounds for the largest Laplacian eigenvalue of graphs, *Linear Algebra Appl.* **414** (2006), 407–424.

[40] S. Al-Yakoob, M. Ghebleh, A. Kanso, D. Stevanović, TensorBoard runs for reinforcement learning on automated conjectured bounds on Laplacian spectral radius of graphs, Zenodo (2024), doi: 10.5281/zenodo.10779251.

A Invariants implemented in Graph class in graph6java

The following list very briefly describes the invariants currently implemented in Graph class of the Java archive graph6java.jar from

`github.com/dragance106/cema-for-graphs`.

Further details on implemented invariants can be found in the source file of this class at `github.com/dragance106/graph6java`.

n() the number of vertices

m() the number of edges

degrees() the array of vertex degrees

averageDegrees() the array of average degrees of neighbours of vertices

isConnected() whether the graph is connected

numberComponents() the number of connected components

isIsomorphic(Graph h) whether the graph is isomorphic to another graph h

matchingNumber() The matching number of the graph

complement() the complement of the graph

Amatrix() the adjacency matrix A of the graph

Acharpoly() the characteristic polynomial of A, returned as the array of $n+1$ coefficients from the highest at index 0 to the lowest at index n

Aspectrum() the eigenvalues of A, sorted in non-decreasing order

Aeigenvectors() the eigenvectors of corresponding eigenvalues of A, returned as a double array with eigenvectors placed in columns

Acospectral(Graph h) whether the graph is cospectral to another graph h

Aintegral() whether all eigenvalues of A are integers

Aenergy() the energy of A, understood as the absolute deviation of the eigenvalues of A from their average value

Lmatrix() the Laplacian matrix

Qmatrix() the signless Laplacian matrix

Dmatrix() the distance matrix

DLmatrix() the distance Laplacian matrix

Mmatrix() the modularity matrix

Note that for each of the above matrices the Graph class also contains the corresponding methods for computing its spectral properties, i.e., Lcharpoly(), Qspectrum(), Deigenvectors(), DLenergy(), Mcospectral() etc.

Asingular() whether 0 is an eigenvalue of A

fiedlerVector() the eigenvector of the second smallest eigenvalue of L

LEL() Laplacian-like-energy invariant

estrada() Estrada index

Lestrada() Laplacian Estrada index

diameter() the diameter

radius() the radius

wiener() Wiener index

transmissions() the array of vertex transmissions, i.e., the sums of distances from a vertex to all other vertices

transmissionIrregular() whether the graph is transmission irregular

szeged() Szeged index

weightedSzeged() weighted Szeged index

randic() Randić index

zagreb1() The first Zagreb index

zagreb2() The second Zagreb index

B The list of conjectured upper bounds from [39]

The first group of bounds is of the form

$$\mu \le \max_{v\in V} f(d_v, m_v)$$

where μ is the spectral radius of Laplacian matrix of graph G, V is its vertex set, while d_v and m_v are, respectively, the degree of v and the average degree of the neighbours of v, for $v \in V$. In the following list we present only the right-hand side of these bounds. The symbol O after the ordinal number means that the conjecture is still open, while the symbol X means that the counterexample has been found in this paper, as indicated in Table 1.

1. O	$\max_{v\in V} \sqrt{\frac{4d_v^3}{m_v}}$	17. X	$\max_{v\in V} \sqrt[4]{5d_v^4 + 11m_v^4}$
2. X	$\max_{v\in V} \frac{2m_v^2}{d_v}$	18. O	$\max_{v\in V} \sqrt{\frac{2m_v^3}{d_v} + 2d_v^2}$

3. X $\max_{v\in V} \frac{m_v^2}{d_v} + m_v$
4. O $\max_{v\in V} \frac{2d_v^2}{m_v}$
5. O $\max_{v\in V} \frac{d_v^2}{m_v} + m_v$
6. O $\max_{v\in V} \sqrt{m_v^2 + 3d_v^2}$
7. O $\max_{v\in V} \frac{d_v^2}{m_v} + d_v$
8. O $\max_{v\in V} \sqrt{d_v(m_v + 3d_v)}$
9. O $\max_{v\in V} \frac{m_v+3d_v}{2}$
10. O $\max_{v\in V} \sqrt{d_v(d_v + 3m_v}$
11. O $\max_{v\in V} \frac{2m_v^3}{d_v^2}$
12. O $\max_{v\in V} \sqrt{2m_v^2 + 2d_v^2}$
13. O $\max_{v\in V} \frac{2m_v^4}{d_v^3}$
14. O $\max_{v\in V} \frac{2d_v^3}{m_v^2}$
15. X $\max_{v\in V} \sqrt{\frac{4m_v^3}{d_v}}$
16. O $\max_{v\in V} \frac{2d_v^4}{m_v^3}$
19. O $\max_{v\in V} \sqrt[4]{4d_v^4 + 12d_v m_v^3}$
20. O $\max_{v\in V} \frac{\sqrt{7d_v^2+9m_v^2}}{2}$
21. O $\max_{v\in V} \sqrt{\frac{d_v^3}{m_v} + 3m_v^2}$
22. O $\max_{v\in V} \sqrt[4]{2d_v^4 + 14d_v^2 m_v^2}$
23. O $\max_{v\in V} \sqrt{d_v^2 + 3d_v m_v}$
24. O $\max_{v\in V} \sqrt[4]{6d_v^4 + 10m_v^4}$
25. O $\max_{v\in V} \sqrt[4]{3d_v^4 + 13d_v^2 m_v^2}$
26. O $\max_{v\in V} \frac{\sqrt{5d_v^2+11d_v m_v}}{2}$
27. O $\max_{v\in V} \sqrt{\frac{3d_v^2+5d_v m_v}{2}}$
28. X $\max_{v\in V} \sqrt{\frac{2m_v^4}{d_v^2} + 2d_v m_v}$
29. X $\max_{v\in V} \sqrt{m_v^2 + \frac{3m_v^3}{d_v}}$
30. O $\max_{v\in V} \frac{m_v^3}{d_v^2} + \frac{d_v^2}{m_v}$
31. X $\max_{v\in V} \frac{4m_v^2}{m_v+d_v}$
32. X $\max_{v\in V} \frac{\sqrt{m_v^3(m_v+3d_v)}}{d_v}$

The second group of bounds is of the form

$$\mu \leq \max_{v_i \sim v_j} f(d_{v_i}, m_{v_i}, d_{v_j}, m_{v_j})$$

where the maximum is taken over all pairs of adjacent vertices v_i, v_j in V. Again, in the following list we present only the right-hand side of these bounds, with $d_{v_i}, m_{v_i}, d_{v_j}, m_{v_j}$ shortened as d_i, m_i, d_j, m_j, respectively.

33. O $\max_{v_i\sim v_j} 2(d_i + d_j) - (m_i + m_j)$
34. O $\max_{v_i\sim v_j} \frac{2(d_i^2+d_j^2)}{d_i+d_j}$
35. O $\max_{v_i\sim v_j} \frac{2(d_i^2+d_j^2)}{m_i+m_j}$
36. X $\max_{v_i\sim v_j} \frac{2(m_i^2+m_j^2)}{d_i+d_j}$
37. O $\max_{v_i\sim v_j} \sqrt{2(d_i^2 + d_j^2)}$
38. O $\max_{v_i\sim v_j} 2 + \sqrt{2(d_i-1)^2 + 2(d_j-1)^2}$
39. O $\max_{v_i\sim v_j} 2 + \sqrt{2(d_i^2 + d_j^2) - 4(m_i + m_j) + 4}$
40. O $\max_{v_i\sim v_j} 2 + \sqrt{2\left((m_i-1)^2 + (m_j-1)^2\right) + (d_i^2 + d_j^2) - (d_i m_i + d_j m_j)}$
41. X $\max_{v_i\sim v_j} 2 + (m_i + m_j) - (d_i + d_j) + \sqrt{2(d_i^2 + d_j^2) - 4(m_i + m_j) + 4}$
42. O $\max_{v_i\sim v_j} \sqrt{d_i^2 + d_j^2 + 2m_i m_j}$
43. X $\max_{v_i\sim v_j} 2 + \sqrt{3(m_i^2 + m_j^2) - 2m_i m_j - 4(d_i + d_j) + 4}$
44. O $\max_{v_i\sim v_j} 2 + \sqrt{2\left((d_i-1)^2 + (d_j-1)^2 + m_i m_j - d_i d_j\right)}$
45. O $\max_{v_i\sim v_j} 2 + \sqrt{(d_i - d_j)^2 + 2(d_i m_i + d_j m_j) - 4(m_i + m_j) + 4}$
46. O $\max_{v_i\sim v_j} 2 + \sqrt{2(d_i^2 + d_j^2) - 16\frac{d_i d_j}{m_i+m_j} + 4}$
47. O $\max_{v_i\sim v_j} \frac{2(d_i^2+d_j^2)-(m_i-m_j)^2}{d_i+d_j}$
48. O $\max_{v_i\sim v_j} \frac{2(d_i^2+d_j^2)}{2+\sqrt{2(d_i^2+d_j^2)-4(m_i+m_j)+4}}$
49. X $\max_{v_i\sim v_j} 2 + \sqrt{2(m_i^2 + m_j^2) + (d_i - d_j)^2 - 4(d_i + d_j) + 4}$
50. X $\max_{v_i\sim v_j} 2\frac{d_i^2+d_j^2+m_i m_j-d_i d_j}{d_i+d_j}$
51. X $\max_{v_i\sim v_j} 2(m_i + m_j) - 4\frac{m_i m_j}{d_i+d_j}$
52. X $\max_{v_i\sim v_j} 2 + \sqrt{\sqrt{8(m_i^4 + m_j^4) - 8(d_i^2 + d_j^2) + 4} - 4(d_i + d_j) + 6}$
53. X $\max_{v_i\sim v_j} 2 + \sqrt{\sqrt{8(m_i^4 + m_j^4) - 8(d_i m_i + d_j m_j) + 4} - 4(d_i + d_j) + 6}$
54. X $\max_{v_i\sim v_j} 2 + \sqrt{2(m_i^2 + m_j^2) + (d_i m_i + d_j m_j) - (d_i^2 + d_j^2) - 4(d_i + d_j) + 4}$
55. X $\max_{v_i\sim v_j} 2 + \sqrt{3(m_i^2 + m_j^2) - (d_i^2 + d_j^2) - 4(m_i + m_j) + 4}$

56. O $\max_{v_i \sim v_j} \frac{(d_i^2+d_j^2)(m_i+m_j)}{2d_id_j}$

57. X $\max_{v_i \sim v_j} 2+\sqrt{2(m_i^2+m_j^2)-8\frac{d_i^2+d_j^2}{m_i+m_j}+4}$

58. X $\max_{v_i \sim v_j} 2+\sqrt{2(m_i^2+m_im_j+m_j^2)-(d_im_i+d_jm_j)-4(d_i+d_j)+4}$

59. X $\max_{v_i \sim v_j} \frac{2(m_i^2+m_im_j+m_j^2)-(d_i^2+d_j^2)}{m_i+m_j}$

60. X $\max_{v_i \sim v_j} 2+\sqrt{2(m_i^2+m_im_j+m_j^2)-(d_i^2+d_j^2)-4(d_i+d_j)+4}$

61. X $\max_{v_i \sim v_j} \frac{2(m_i^2+m_j^2)}{2+\sqrt{2\left((d_i-1)^2+(d_j-1)^2\right)}}$

62. X $\max_{v_i \sim v_j} 2+\sqrt{m_i^2+4m_im_j+m_j^2-2d_id_j-4(d_i+d_j)+4}$

63. X $\max_{v_i \sim v_j} d_i+d_j+m_i+m_j-4\frac{d_id_j}{m_i+m_j}$

64. X $\max_{v_i \sim v_j} \frac{m_im_j(d_i+d_j)}{d_id_j}$

65. X $\max_{v_i \sim v_j} \frac{(m_i+m_j)(d_im_i+d_jm_j)}{2m_im_j}$

66. X $\max_{v_i \sim v_j} \frac{m_i^2+4m_im_j+m_j^2-(d_im_i+d_jm_j)}{d_i+d_j}$

67. X $\max_{v_i \sim v_j} \frac{(m_i+m_j)(d_im_i+d_jm_j)}{2d_id_j}$

68. X $\max_{v_i \sim v_j} 2+\sqrt{(m_i-m_j)^2+4d_id_j-4(m_i+m_j)+4}$