THREE EXAMPLES OF A GROUND-BREAKING IMPACT OF THE VARIABLE NEIGHBORHOOD SEARCH ON INVESTIGATIONS IN GRAPH THEORY

Dedicated to Professor Pierre Hansen

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Content

The variable neighbourhood search is a meta heuristic in optimization problems. It uses several distances and neighbourhoods in the same set of basic objects. Once a search ends in a local extremum, you change the neighbourhood and continue to global extremum.

Hansen P., Mladenović N., *An introduction to variable neighborhood search*, In: Voss S., et al. (Ed.), Meta-Heuristics: Advances and Trends in Local Search Paradigms for Optimization, Kluwer Academic Publishers, Dordrecht, 1998, 433-458.

The variable neighbourhood search is exploited in the programming package AutoGraphiX (briefly AGX) for finding graphs with extremal values of a graph invariant chosen by the user. The system starts from a random graph or from a graph given by the user. The graph is perturbed to some extent using the variable neighbourhood search and a new graph is chosen which improves maximally the considered graph invariant. The system AGX is very useful in formulating some conjectures which are later treated by theoretical means.

Caporossi G., Hansen P., *Variable neighborhood search for extremal graphs, The Auto-GraphiX system*, Discrete Math., 212(2000), 29-44.

System AGX has generated (among other things):

1. several conjectures for the energy of a graph

Caporossi G., Cvetković D., Gutman I., Hansen P., *Variable neighborhood search for extremal graphs*, 2. *Finding graphs with extremal energy*, J. Chem. Inform. Comp. Sci., 39(1999),984-996,

2. thirty conjectures concerning signess Laplacian eigenvalues

Cvetković D., Rowlinson P., Simić S., *Eigenvalue bounds for the signless Laplacian*, Publ. Inst. Math. (Beograd), 81(95)(2007), 11-27

and 3. some difficult conjectures on the index of a graph

Aouchiche M., Bell F.K., Cvetković D., Hansen P., Rowlinson P., Simić S., Stevanović D., *Variable neighborhood search for extremal graphs*, 16. *Some conjectures related to the largest eigenvalue of a graph*, Europ. J. Oper. Res., 191(2008), No. 3, 661-676.

There is a series of over twenty papers with a common subtitle

Variable neighborhood search for extremal graphs.

Case 1: Graph Energy

System AGX has generated several conjectures for the energy of a graph

Caporossi G., Cvetković D., Gutman I., Hansen P., *Variable neighborhood search for extremal graphs*, 2. *Finding graphs with extremal energy*, J. Chem. Inform. Comp. Sci., 39(1999),984-996.

The story behind the publication of this paper is as follows. I met Professor Pierre Hansen at an International Colloquium for Graph Theory in April 1997 in Dornföld a.d. Heide, Germany. The colloquium was dedicated to H. Sachs on the occasion of his 70-th birthday. P. Hansen was presenting his AutoGraphiX system. Since there was no experience with this system, I suggested to Hansen some extremal eigenvalue problems with trees with known solutions as first test examples. The test was successful and Hansen invited me in March 1998 to visit his institut in Montreal to work with AGX.

I new that there had been no results on graph energy for many years, that it was difficult for a human to guess conjectures about it and that the existence of a new package AGX is a great opportunity to obtain conjectures. When AGX really produced very interesting and unexpected conjectures, we immediately contacted Ivan Gutman and this led, after some additional work, to publication of an influental paper.

The energy of a graph is the sum of absolute values of eigenvalues of the adjacency matrix of the graph:

$$E = |\lambda_1| + |\lambda_2| + \cdots + |\lambda_n|.$$

This definition was given by Ivan Gutman in 1978:

Gutman I., *The energy of a graph*, Berichte Math. Stat. Sekt. Forschungszentrum Graz, 103(1978), 1–22.

Motivation came from theoretical chemistry but the intention was to initiate mathematical studies of this graph invariant. No significant work on this subject appeared in about next twenty years.

Among other things, AGX generated a conjecture on unicyclic graphs with maximal energy which attracted much attention. The conjecture was difficult to prove (22 pages in a book). This conjecture was unusual and attractive for a mathematician. While a mathematician (perhaps not a chemist) would expect that the cycle is extremal, the computer found that, with a finite number of exceptions, the graph consisting of a hexagon with an appended path is extremal.

In addition, the paper established that among graphs on 10 vertices maximal energy has a strongly regular graph (complement of the Petersen graph). This attracted researchers working in the area of strongly regular and related graphs and we now have the Koolen-Moulton upper bound for the energy of graphs with n vertices:

Koolen J., Moulton V., *Maximal energy graphs*, Advances Appl. Math., 26(2001), 47–52.

The order of magnitude in this bound ($n^{2/3}$) was numerically predicted by AGX.

For $n = 4k^2$, k integer, extremal graphs should be strongly regular with parameters
$(n, (n + \sqrt{n})/2, (n + \sqrt{n})/4, (n + \sqrt{n})/4)$
if they exist. It has been proved by W. Haemers that such graphs exist for $n = 4, 16, 36$ and they are unique while for $n = 64, 100, 144$ these extremal graphs are not unique.

Haemers W.,*Strongly regular graphs with maximal energy*, Linear Algebra Appl., 429(2008), 2719-2723.

After our paper was published "a dramatic change occurred, and graph energy started to attract the attention of a remarkably large number of mathematicians, all over the globe".
The number of published papers on graph energy is nowadays of order of several hundred, perhaps already approaching one thousand. Only in years 2008-2011 the average number of such papers was around 50 per year. Also the following monograph was published:

Li X., Shi Y., Gutman I., *Graph Energy*, Springer, New York, 2012, XII + 266.

Case 2: Inequalities for Signless Laplacian Eigenvalues

By a spectral graph theory we understand, in an informal sense, a theory in which graphs are studied by means of the eigenvalues of some graph matrix M. This theory is called *M–theory*.

Recall that, given a graph, the matrix $Q = D + A$ is called the *signless Laplacian*, where A is the adjacency matrix and D is the diagonal matrix of vertex degrees. The matrix $L = D - A$ is known as the *Laplacian* of G.

Together with Q–theory we shall frequently consider the relevant facts from A–theory and L–theory as mostly developed spectral theories and therefore useful in making comparisons between theories.

System AGX has generated thirty conjectures concerning signless Laplacian eigenvalues

Cvetković D., Rowlinson P., Simić S., *Eigenvalue bounds for the signless Laplacian*, Publ. Inst. Math. (Beograd), 81(95)(2007), 11-27.

The paper contains the following acknowledgement: "We are grateful to P. Hansen who accepted our challenge to create some conjectures related to signless Laplacian eigenvalues using the programming package AGX, and to his collaborator M. Aouchiche whose experiments led to the formulation of the conjectures."

Paper is devoted to inequalities involving Q–eigenvalues. It presents 30 computer generated conjectures in the form of inequalities for Q–eigenvalues. The conjectures were obtained by the system AGX and the paper contributed substantially in building the spectral graph theory based on the signless Laplacian.

Conjectures that are confirmed by simple results already recorded in the literature, explicitly or implicitly, are identified. Some of the remaining conjectures have been resolved by elementary observations; for some quite a lot of work had to be invested. The conjectures left unresolved appear to include some difficult research problems.

One of difficult conjectures (Conjecture 24) has been confirmed in

Cardoso D., Cvetković D., Rowlinson P., Simić S., *A sharp lower bound for the least eigenvalue of the signless Laplacian of a non-bipartite graph*, Linear Algebra Appl., 429(2008), 2770-2780,

by a long sequence of lemmas. The corresponding result reads:

Theorem. *The minimal value of the least Q–eigenvalue among connected non–bipartite graphs with prescribed number of vertices is attained for the odd–unicyclic graph obtained from a triangle by appending a hanging path.*

Cvetković D., Rowlinson P., Simić S.K., Signless Laplacians of finite graphs, *Linear Algebra Appl.*, 423(2007), No. 1, 155–171.

Cvetković D., Simić S.K.,*Towards a spectral theory of graphs based on the signless Laplacian, I*, Publ. Inst. Math. (Beograd), 85(99)(2009), 19-33.

Cvetković D., Simić S.K.,*Towards a spectral theory of graphs based on the signless Laplacian, II*, Linear Algebra Appl., 432(2010), 2257-2272.

Cvetković D., Simić S.K.,*Towards a spectral theory of graphs based on the signless Laplacian, III*, Appl. Anal. Discrete Math., 4(2010), 156-166.

After these papers and other several hundred by other authors we can say: THE Q-THEORY REALLY EXISTS !

Case 3: Some Difficult Conjectures on the Largest Eigenvalue

System AGX has generated some difficult conjectures on the index of a graph

Aouchiche M., Bell F.K., Cvetković D., Hansen P., Rowlinson P., Simić S., Stevanović D., *Variable neighborhood search for extremal graphs*, 16. *Some conjectures related to the largest eigenvalue of a graph*, Europ. J. Oper. Res., 191(2008), No. 3, 661-676.

The conjectures are related to the maximal value of the irregularity and spectral spread in n-vertex graphs and to a Nordhaus-Gaddum type upper bound for the index. None of the conjectures has been resolved so far. We present partial results and provide some indications that the conjectures are very hard.

The difference between the index and the average vertex degree is called the *irregularity* of a graph.

A *pineapple* with parameters n, q $(q \leq n)$, denoted by $PA(n, q)$, is a graph on n vertices consisting of a clique on q vertices and a stable set on the remaining $n - q$ vertices in which each vertex of the stable set is adjacent to a unique vertex of the clique.

Conjecture 1. *The most irregular connected graph on* n $(n \geq 10)$ *vertices is a pineapple* $PA(n, q)$ *in which the clique size* q *is equal to* $\lceil \frac{n}{2} \rceil + 1$.

The quantity $\lambda_1 - \lambda_n$ is called the *spectral spread* of the graph.

A *complete split graph* with parameters n, q ($q \leq n$), denoted by $CS(n, q)$, is a graph on n vertices consisting of a clique on q vertices and a stable set on the remaining $n - q$ vertices in which each vertex of the clique is adjacent to each vertex of the stable set.

Conjecture 2. *Given n, the maximal value of the spectral spread of a graph on n vertices is obtained for a complete split graph* $CS(n, q)$ *with an independent set of size* $n - q = \lceil \frac{n}{3} \rceil$.

Conjecture 3. *Maximal graphs on n vertices for the function* $\lambda_1 + \overline{\lambda}_1$ *are complete split graphs* $CS(n, q)$ *with the clique size equal or close to* $n/3$.

Conclusion

We have described three examples of a ground-breaking impact of the variable neighborhood search, implemented within the system AutoGraphiX (AGX), on investigations in graph theory, in particular, in spectral graph theory.

The paper *Finding graphs with extremal energy* enabled a ground-breaking development of research in the area of graph energy with several hundreds of papers published as a consequence.

The paper *Eigenvalue bounds for the signless Laplacian* helped very much in creating the spectral graph theory based on the signless Laplacian, again with several hundreds of papers published.

The paper *Some conjectures related to the largest eigenvalue of a graph* is of somewhat different character. It provided conjectures difficult to resolve. The papers published on these conjectures are not numerous because the conjectures are really difficult.

Thank you for your attention