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Variable Neighborhood Search for Extremal Graphs 12. A note on the variance of bounded degrees in graphs.

Pierre Hansen
GERAD
HEC Montréal
Canada
Pierre.Hansen@gerad.ca

Hadrien Mélot*
Department of Computer Science
University of Mons-Hainaut
Belgium,
hadrien.melot@umh.ac.be

Ivan Gutman
Faculty of Science
University of Kragujevac
Serbia and Montenegro,
gutman@knez.uis.kg.ac.yu

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Abstract

An upper bound is given on the variance of degrees of graphs with n vertices, m edges and maximum degree Δ. Particular cases of chemical interest, i.e., graphs with $\Delta = 3$ or 4 and at most 2 cycles are examined, and conditions for the bound to be sharp derived.

1 Introduction

Graphs are extensively used to model molecules. Chemical graphs designed for that purpose have bounded degrees, with a maximum degree Δ usually equal to 4. Irregularity of graphs has been studied intensively [1] – [5] through a variety of indices. A comparison of the most prevalent ones for chemical trees was done in [6]. We consider here a classic index, i.e., the variance of degrees. A best possible bound and corresponding families of extremal graphs have been found by Bell [2] when the number of vertices n and the number of edges m are given and degrees are unbounded, i.e., $\Delta \leq n-1$. We consider here values of $\Delta < n-1$, and particulary $\Delta = 3$ and 4, which appear to be the most relevant to chemistry. Experiments with the *AutoGraphiX* (AGX) system [7] [8] gave presumably optimal graphs, and are described in the next section. These graphs pointed the way to formulate and then prove the general result, given in Section 3. Special cases are considered in Section 4 and conclusions drawn in Section 5

*Corresponding author

2 Experiments

The *variance of degrees* of a graph G is defined by

$$\mathrm{VAR}(G) = \frac{1}{n}\sum_{i=1}^{n-1} n_i \left(i - \frac{2m}{n}\right)^2 \tag{1}$$

where n is the number of vertices and n_i is the number of vertices of degree i in G. This definition shows that the variance of degrees depends only on the values of the n_i, i.e., on the sequence of degrees.

We first used the system *AGX* [7] [8] to find graphs with a fixed Δ and optimal or near-optimal values for the maximum variance of degrees. In order to get an idea of the dependence of the maximum degree Δ on these extremal graphs, we launched the system on different problem fixing the value of Δ and number of edges m. For example, Figure 1 shows the extremal graphs obtained by the system for $m = n - 1$ (trees) and $\Delta = 3$ and Figure 2 when $m = n$ (unicyclic graphs) and $\Delta = 5$.

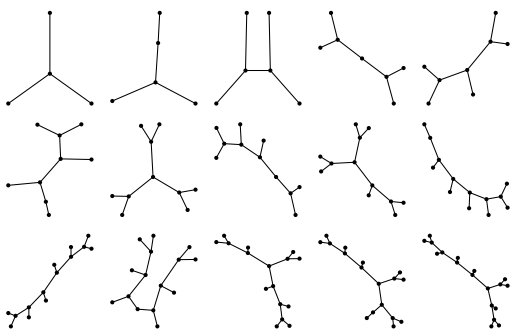

Figure 1: Some extremal trees with $\Delta = 3$ found by *AGX*

As the variance depends only on the sequence of degrees, the observation of these extremal graphs leads quickly to the following conjecture : the extremal graphs have only vertices of degree Δ and 1 if this is compatible with the existence of a graph. We also observe that all extremal graphs, found by the system for different values of m and Δ, have at most one vertex which has a degree different from 1 or Δ.

3 Results

For a fixed value of n, there are only two connected graphs with $\Delta = 2$, the path P_n and the cycle C_n; the variance of their degrees is readily computed as $\mathrm{VAR}(P_n) = (2n-4)/n^2$ and $\mathrm{VAR}(C_n) = 0$. Hence, it is not restrictive to assume that $\Delta > 2$ in the following theorem.

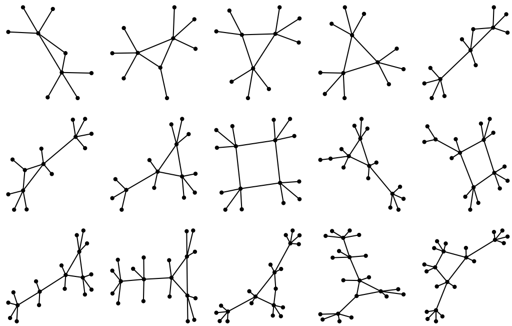

Figure 2: Some extremal unicyclic graphs with $\Delta = 5$ found by *AGX*

Theorem 1 *For all connected graphs G with maximum degree $\Delta \geq 3$, n vertices and m edges,*

$$VAR(G) \leq \frac{2m(\Delta+1) - n\Delta + (1-k)(\Delta-k)}{n} - \left(\frac{2m}{n}\right)^2, \tag{2}$$

where

$$k = \Big[(2m-n)(mod\ \Delta - 1)\Big] + 1.$$

with equality in (2) attained if and only if at most one vertex of G has degree different from 1 *and* Δ*.*

Proof. A simple rearrangement of the definition of VAR(G) yields

$$\text{VAR}(G) = (M_1)/n - (2m/n)^2 \tag{3}$$

where $M_1 = \sum\limits_{i=1}^{n-1} i^2 n_i$ is the *first Zagreb index* [9] – [14] and n_i denotes the number of vertices of degree i. Eq. (3) shows that for fixed values of Δ, m and n, VAR will be maximum if M_1 is maximum.

By definition of Δ and n_i,

$$M_1 = \sum_{i=1}^{\Delta} i^2\ n_i. \tag{4}$$

For all connected graphs with n nodes, m edges and bounded degree Δ, summing numbers of vertices of all degrees yields

$$n_1 + n_\Delta + \sum_{i=2}^{\Delta-1} n_i = n, \tag{5}$$

and summing degrees :

$$n_1 + \Delta n_\Delta + \sum_{i=2}^{\Delta-1} i\ n_i = 2m. \tag{6}$$

Solving (5) and (6) in n_1 and n_Δ gives

$$n_1 = \frac{1}{\Delta-1}\left[n\Delta - 2m + \sum_{i=2}^{\Delta-1}(i-\Delta)n_i\right], \tag{7}$$

and

$$n_\Delta = \frac{1}{\Delta-1}\left[2m - n + \sum_{i=2}^{\Delta-1}(1-i)n_i\right]. \tag{8}$$

Then, substituting (7) and (8) into (4) yields

$$\begin{aligned} M_1 &= \tfrac{1}{\Delta-1}\left[n\Delta - 2m + 2m\Delta^2 - n\Delta^2 + \sum_{i=2}^{\Delta-1}\left(i - \Delta + \Delta^2 - i\Delta^2 + i^2\Delta - i^2\right)n_i\right] \\ &= \tfrac{1}{\Delta-1}\left[\Big(\Delta-1\Big)\Big(2m(\Delta+1) - n\Delta\Big) + \sum_{i=2}^{\Delta-1}\Big((\Delta-1)(1-i)(\Delta-i)\Big)n_i\right] \end{aligned}$$

As $\Delta > 1$,

$$M_1 = 2m(\Delta+1) - n\Delta + \sum_{i=2}^{\Delta-1} f(i)n_i, \tag{9}$$

where $f(i)$ is the quadratic function

$$f(i) = (1-i)(\Delta-i). \tag{10}$$

Observe that $f(i)$ is strictly negative for $2 \le i \le \Delta - 1$. This implies that, for fixed values of n, m and Δ, the first Zagreb index M_1 (and VAR also) will be maximum if $n_i = 0$ for $i = 2, 3, \ldots, \Delta - 1$.

In this case, Eqs (8) and (7) lead to

$$n_1 = \frac{n\Delta - 2m}{\Delta - 1}, \tag{11}$$

and

$$n_\Delta = \frac{2m - n}{\Delta - 1}. \tag{12}$$

However, n_1 and n_Δ should have integer values which, as $n\Delta - 2m = n - 2m + n(\Delta - 1)$, is true in (11) and (12) if $2m - n$ is a multiple of $\Delta - 1$, i.e., if

$$(2m - n)(\bmod\ \Delta - 1) = 0. \tag{13}$$

Suppose now that condition (13) is not respected. In this case, we have to maximize $\sum_{i=2}^{\Delta-1} f(i)n_i$. Let k denote the value of the left-hand side of (13) plus 1; then k is an integer between 2 and $\Delta - 1$. It is always possible to choose the n_i such that

$$\begin{aligned} n_k &= 1, \\ n_i &= 0 \qquad \forall i (\neq k) = 2, 3, \ldots, \Delta - 1. \end{aligned}$$

and Eqs. (5) and (6) are satisfied. Indeed, as

$$k = \Big[(2m - n)(\text{mod } \Delta - 1)\Big] + 1, \tag{14}$$

Eqs. (7) and (8) become

$$n_1 = \frac{n\Delta - 2m + k - \Delta}{\Delta - 1}, \tag{15}$$

and

$$n_\Delta = \frac{2m - n + 1 - k}{\Delta - 1}, \tag{16}$$

which then have integer values.

Observe that k is the degree of the unique vertex of degree different from 1 and Δ. Indeed, the sum of all degrees is $2m$. Then consider a graph with all degrees equal to 1; this reduces this sum by n. Furthermore increase degrees one at a time up to Δ, as long as this is possible; this reduces the sum to $(2m - n)(\text{mod } \Delta - 1)$, which is equal to $k - 1$, so the degree of one more vertex can be increased, up to k.

Now assume there are at least two vertices of degree i and j, with i not greater than j and both i and j in the interval $[2, \Delta - 1]$. Reducing the degree of the first vertex by 1 changes (9) by

$$(1 - i)(\Delta - 1) - (1 - i - 1)(\Delta - i - 1) = \Delta - 2i;$$

augmenting the degree of the second vertex by 1 changes (9) by

$$(1 - j)(\Delta - j) - (1 - j + 1)(\Delta - j + 1) = -\Delta + 2j - 2.$$

The net effect of both operations leaves the sum of degrees unchanged and changes (9) by

$$\Delta - 2i - \Delta + 2j - 2 = 2(j - i + 1)$$

which is positive.

This means that the optimal choice for the n_i with $i \in \{2, \ldots, \Delta - 1\}$, if condition (13) is not respected, is to choose only one n_k positive and equal to 1. In this case, by Eq. (9),

$$M_1 \leq 2m(\Delta + 1) - n\Delta + (1 - k)(\Delta - k). \tag{17}$$

Observe that if condition (13) is respected, Eq. (14) gives $k = 1$, which expresses the fact that all n_i with $2 \leq i \leq \Delta - 1$ are then equal to zero. Hence, the bound (17) is still valid when $k = 1$.

Substituting (17) in (3) gives the result. $\square$

Note that in this proof we use a technique based on linear programming arguments which was first introduced in [15] and also used in Ref [6] and [16] – [18].

4 Particular cases

Theorem 1 is valid for all connected graphs. However, the bound is sharp only if the values of n, m and Δ are compatible with the existence of a graph which has the specific sequence of degrees described in the proof of this theorem. Given a general condition on n, analysing the dependence of the values of m and Δ requires a long discussion which break down in many particular cases. In this section, we restrict the graphs considered to some classes of chemical interest, and show how the theorem can be applied for such classes. In these cases, the bound is often sharp for reasonable values of n.

Again, we assume that $\Delta > 2$.

4.1 Trees

If T is a tree, as $m = n - 1$, Theorem 1 gives after simplifications :

$$\mathrm{VAR}(T) \leq \frac{1}{n^2}\Big[n^2\Big(\Delta - 2\Big) + n\Big(k^2 - k(\Delta+1) - \Delta + 6\Big) - 4\Big], \tag{18}$$

where

$$k = \Big[(n-2)(\mathrm{mod}\ \Delta - 1)\Big] + 1. \tag{19}$$

If $n \geq 4$, this bound is sharp because the smallest tree with $\Delta \geq 3$ is the star S_4. For fixed values of $n \geq 4$ and $\Delta \leq n - 1$, one can always construct a tree for which the equality holds. Starting from the star $S_{\Delta+1}$, add $\Delta - 1$ pending edges to a vertex of degree 1, until vertices are exhausted.

Trees with $\Delta \leq 3$

If T has degrees bounded by 3, Eqs. (18) and (19) give

$$\mathrm{VAR}(T) \leq \frac{1}{n^2}\Big[n^2 + n\Big(k^2 - 4k + 3) - 4\Big], \tag{20}$$

where

$$k = \Big[n(\mathrm{mod}\ 2)\Big] + 1. \tag{21}$$

Figure 3 shows some extremal trees with $\Delta \leq 3$ that can be obtained by applying the construction method explained above. Of course, for a given n, there can be more than one extremal graph, but they all share the following properties :

$$n_1 = \left\lfloor \frac{n+2}{2} \right\rfloor, \; n_2 = n(\mathrm{mod}\ 2) \;\text{ and }\; n_3 = \left\lfloor \frac{n-2}{2} \right\rfloor,$$

where $\lfloor a \rfloor$ denotes the largest integer not larger than a.

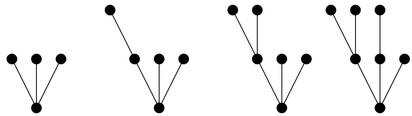

Figure 3: Some extremal trees with $\Delta \leq 3$

Chemical trees

If T is a chemical tree, i.e., $\Delta \leq 4$, Eqs. (18) and (19) gives

$$\mathrm{VAR}(T) \leq \frac{1}{n^2}\Big[2n^2 + n(k^2 - 5k + 2) - 4\Big], \tag{22}$$

where

$$k = \Big[(n-2)(\mathrm{mod}\ 3)\Big] + 1. \tag{23}$$

This problem was already solved in Ref [6] in which characterization of extremal chemical trees was also given.

4.2 Unicyclic graphs

If U is a unicyclic graph, as $m = n$, Theorem 1 leads to :

$$\mathrm{VAR}(U) \leq \frac{1}{n}\Big[n\Big(\Delta - 2\Big) + k^2 - k(\Delta + 1) + \Delta\Big], \tag{24}$$

where

$$k = \Big[n(\mathrm{mod}\ \Delta - 1)\Big] + 1. \tag{25}$$

If $n \geq 2\Delta - 1$, this bound is sharp because the smallest unicyclic graph with degrees bounded by Δ for which equality holds is the graph $U^*(\Delta)$ next described. This graph consists of a triangle of vertices $\{u, v, w\}$ with $\Delta - 2$ pending edges adjacent to v and $\Delta - 2$ pending edges adjacent to w. For example, the graph $U^*(5)$ is depicted in Figure 4. These graphs have $2\Delta - 1$ vertices.

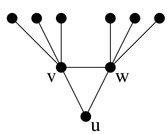

Figure 4: The graph $U^*(5)$

Starting from $U^*(\Delta)$, one can always construct a larger unicyclic graph for which the bound is sharp. It suffices to add $\Delta - 2$ pending edges to the vertex u, and then $\Delta - 1$ pending edges to a vertex of degree 1 until vertices are exhausted.

Unicyclic graphs with given girth

Unicyclic graphs with a triangle are not frequent in chemistry. Observe that it is possible to construct a unicyclic graph with maximum variance and given girth g (the length of the shortest cycle), if $n \geq g(\Delta - 1) - \Delta + 2$. One starts with a graph similar to U^* : a cycle of length g with all vertices (except one denoted by u) adjacent to $\Delta - 2$ pending edges. At this point $n = g(\Delta - 1) - \Delta + 2$ and this unicyclic graph with given girth is the smallest one for which the bound is sharp. The same reasoning than before can be applied to construct a larger unicyclic graph for which the girth will always be g : add $\Delta - 2$ pending edges to the vertex u, and then $\Delta - 1$ pending edges to a vertex of degree 1 until vertices are exhausted.

Unicyclic graphs with $\Delta \leq 3$

If U is a unicyclic graph with $\Delta \leq 3$,

$$\mathrm{VAR}(U) \leq \frac{1}{n}\Big[n + k^2 - 4k + 3\Big], \tag{26}$$

where

$$k = \Big[n (\mathrm{mod}\ 2)\Big] + 1. \tag{27}$$

From the discussion on the unicyclic graphs, if $n \geq 5$ (or $n \geq 2g - 1$ if the girth is given), the bound is sharp and all the extremal graphs have the following sequence of degrees :

$$n_1 = n_3 = \left\lfloor \frac{n}{2} \right\rfloor \quad \text{and} \quad n_2 = n (\mathrm{mod}\ 2).$$

Figure 5 shows some unicyclic graphs with $\Delta \leq 3$ and a girth equal to 6 for which the bound is sharp.

Unicyclic chemical graphs

If U is a unicyclic chemical graph,

$$\mathrm{VAR}(U) \leq \frac{1}{n}\Big[2n + k^2 - 5k + 4\Big], \tag{28}$$

where

$$k = \Big[n (\mathrm{mod}\ 3)\Big] + 1. \tag{29}$$

If $n \geq 7$ (or $n \geq 3g - 2$ for a fixed girth), the bound is sharp and the extremal graphs have :

$$n_1 = \left\lfloor \frac{2n}{3} \right\rfloor, \ n_4 = \left\lfloor \frac{n}{3} \right\rfloor,$$

$n_2 = n_3 = 0$ if $n (\mathrm{mod}\ 3) = 0$, $n_2 = 1, n_3 = 0$ if $n (\mathrm{mod}\ 3) = 1$ and $n_2 = 0, n_3 = 1$ if $n (\mathrm{mod}\ 3) = 2$.

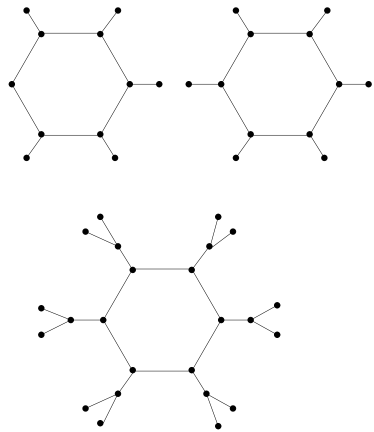

Figure 5: Some extremal unicyclic graphs with $\Delta \leq 3$ and $g = 6$

4.3 Bicyclic graphs

If B is a bicyclic graph, then $m = n + 1$. In this case, Theorem 1 leads to :

$$\mathrm{VAR}(B) \leq \frac{1}{n^2}\Big[n^2\Big(\Delta - 2\Big) + n\Big(k^2 - k(\Delta + 1) + 3\Delta - 6\Big) - 4\Big], \tag{30}$$

where

$$k = \Big[(n + 2)(\mathrm{mod}\ \Delta - 1)\Big] + 1. \tag{31}$$

The smallest bicyclic graph with degrees bounded by Δ for which equality holds is the graph $B^*(\Delta)$ which consists of a cycle of successive vertices (u, v, w, x) with a diagonal edge (v, x), $\Delta - 2$ pending edges adjacent to w and $\Delta - 3$ pending edges adjacent to v and x. Figure 6 shows $B^*(4)$ as an example. These graphs have $3\Delta - 4$ nodes.

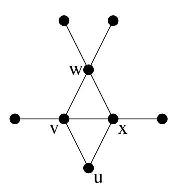

Figure 6: The graph $B^*(4)$

Again, one can construct a larger bicyclic graph for which the bound is sharp, starting from

$B^*(\Delta)$ and applying the same method than for the unicyclic graphs : add $\Delta - 2$ pending edges to the vertex u, and then $\Delta - 1$ pending edges to a vertex of degree 1 until vertices are exhausted.

Bicyclic graphs with given girth

If the girth g is fixed, one can starts with two cycles of length g (in place of triangles) such that these cycle have an edge in common, and construct a larger bicyclic graph. Hence, the smallest bicyclic graph with girth g and maximum degree Δ for which the bound (30) is sharp has $g(2\Delta - 2) - 3\Delta + 2$ nodes.

Figure 7 shows a smallest bicyclic chemical graph with girth 6 for which the bound is sharp.

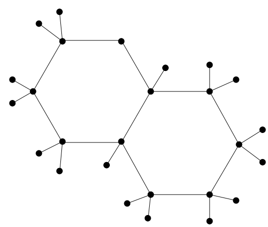

Figure 7: Extremal bicyclic chemical graph with $g = 6$

Bicyclic graphs with $\Delta \leq 3$

If B is a bicyclic graph with $\Delta \leq 3$,

$$\mathrm{VAR}(B) \leq \frac{1}{n^2}\Big[n^2 + n\Big(k^2 - k(\Delta+1) + 3\Delta - 6\Big) - 4\Big], \tag{32}$$

where

$$k = \Big[(n+2)(\mathrm{mod}\ 2)\Big] + 1, \tag{33}$$

and the bound is sharp if $n \geq 5$ (or $n \geq 4g - 7$ for a fixed girth).

Bicyclic chemical graphs

If B is a bicyclic chemical graph,

$$\mathrm{VAR}(B) \leq \frac{1}{n^2}\Big[2n^2 + n\Big(k^2 - 5k + 6\Big) - 4\Big], \tag{34}$$

where

$$k = \Big[(n+2)(\mathrm{mod}\ 3)\Big] + 1, \tag{35}$$

and the bound is sharp if $n \geq 8$ (or $n \geq 6g - 10$ for a fixed girth).

5 Conclusions

While a best upper bound for the variance of degrees of graphs has been available since 1992 [2], such a bound may provide values far from those observed for chemical graphs, where the maximum degree Δ is usually 3 or 4. We therefore provided a formula explicitly taking into account the fact that degrees are bounded. We also examined when it is sharp for trees, unicyclic and bicyclic graphs.

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