MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **76** (2016) 61-68

ISSN 0340 - 6253

Inequalities for the Number of Walks in Subdivision Graphs

Hanjo Täubig

Computer Science Dept., TU München,
D-85748 Garching, Germany,
taeubig@in.tum.de

(Received September 18, 2015)

Abstract

We consider an undirected graph G with n vertices and m edges that is modified by introducing an intermediate vertex on every edge. It has been shown by Ilić and Stevanović that this subdivision graph S_G satisfies the Zagreb indices inequality $M_1(S_G)/(m+n) \le M_2(S_G)/(2m)$. This inequality can also be expressed in the form $w_1(S_G) \cdot w_2(S_G) \le w_0(S_G) \cdot w_3(S_G)$, where $w_k(G)$ denotes the number of k-step walks in G. Besides trees, this is another class of bipartite graphs where the inequality holds true.

In this paper, we prove the inequalities $w_1(S_G) \cdot w_4(S_G) \le w_0(S_G) \cdot w_5(S_G)$ and $w_2(S_G) \cdot w_3(S_G) \le w_0(S_G) \cdot w_5(S_G)$. This raises the question whether the generalization $w_a(S_G) \cdot w_b(S_G) \le w_0(S_G) \cdot w_{a+b}(S_G)$ is satisfied for subdivision graphs.

1 Introduction

We consider an undirected (multi-)graph $G = (V, E)$ with $n := |V|$ vertices and $m := |E|$ edges. The degree of a vertex $v \in V$ is denoted by d_v. A *walk* in a multigraph $G = (V, E)$ is an alternating sequence $(v_0, e_1, v_1, \ldots, v_{k-1}, e_k, v_k)$ of vertices $v_i \in V$ and edges $e_i \in E$ where each edge e_i of the walk must connect vertex v_{i-1} to vertex v_i in G, that is, $e_i = \{v_{i-1}, v_i\}$ for all $i \in \{1, \ldots, k\}$. Vertices and edges can be used repeatedly in the same walk. If the multigraph has no parallel edges, then the walks could also be specified by the sequence of vertices $(v_0, v_1, \ldots, v_{k-1}, v_k)$ without the edges. The *length* of a walk is the number of edge traversals. That means, the walk $(v_0, \ldots, v_k)$ consisting of $k+1$ vertices and k edges is a walk of length k. Mostly, we will call it a *k-step walk*. Our main concern will be the investigation of the *number of walks* of a specified length. Let $w_k(v)$ denote the number of k-step walks starting at vertex $v \in V$. Since G is undirected, this is the same as the number of k-step walks ending at v. The total number of k-step walks is denoted by w_k. For walks of length 0, we have $w_0(v) = 1$ for each vertex v and $w_0 = n$. For walks of length 1, we have $w_1(v) = d_v$ and $w_1 = \sum_{v \in V} d_v = 2m$ by the handshake lemma. The total number of walks can be decomposed as

$$w_{a+b} = \sum_{v \in V} w_a(v) \cdot w_b(v) \qquad \text{and} \qquad w_{a+b+1} = 2 \sum_{\{x,y\} \in E} w_a(x) \cdot w_b(y) \ ,$$

where the total number of walks is divided into summands representing the walks with fixed vertex v or fixed edge traversals (x, y) and (y, x) after a steps. That means, partial walks of length a and b are attached to a certain vertex or edge traversal. In particular, we will use the special cases $w_2(G) = \sum_{v \in V} d_v^2$, $w_3(G) = 2\sum_{\{x,y\} \in E} d_x \cdot d_y$, $w_4(G) = \sum_{v \in V} w_2(v)^2$, and $w_5(G) = 2\sum_{\{x,y\} \in E} w_2(x) \cdot w_2(y)$.

For a given graph $G = (V, E)$, the *subdivision graph* S_G is obtained from G by introducing for each edge $e \in E$ a new vertex v_e that splits the old edge $e = \{v_1, v_2\}$ and replaces it by two new edges $e_1 = \{v_1, v_e\}$ and $e_2 = \{v_e, v_2\}$.

2 Related Work

2.1 General graphs and chemical graphs

Lagarias, Mazo, Shepp, and McKay [6] posed the following question: what are the numbers $a, b \in N$ such that $w_a(G) \cdot w_b(G) \leq n \cdot w_{a+b}(G)$ is satisfied for all graphs G? Later, they proved the inequality for the case of an even sum $a + b$ [7]. Hence, it could be stated in the following way.

Theorem 1 (Lagarias et al.)**.** *For all $a, b \in N$, every graph G on n vertices satisfies the inequality*

$$w_{2a+b}(G) \cdot w_b(G) \leq n \cdot w_{2(a+b)}(G) \ .$$

More general forms of these inequalities were proposed in [10, 11].

Lagarias et al. presented counterexamples showing $w_a(G) \cdot w_b(G) \nleq n \cdot w_{a+b}(G)$ whenever $a + b$ is odd and $a, b \geq 1$. This means that the inequalities $w_1(G) \cdot w_2(G) \leq$

$w_0(G) \cdot w_3(G)$ and $w_1(G) \cdot w_4(G) \leq w_0(G) \cdot w_5(G)$ are *not* satisfied in general (not even for bipartite graphs, see [11]). Recently, these counterexamples were generalized by Täubig [8] to the more general form

$$w_{2a+c}(G) \cdot w_{2a+2b+c+1}(G) \not\leq w_{2a}(G) \cdot w_{2a+2b+2c+1}(G)$$

for $a, b, c \in N$.

Probably unaware of the work by Lagarias et al., an inequality that is equivalent to $w_0(G) \cdot w_3(G) \geq w_1(G) \cdot w_2(G)$ was investigated again by Hansen and Vukičević [4]. The AutoGraphiX system [2] had been used to make a conjecture in the slightly different form $M_1(G)/n \leq M_2(G)/m$ using the Zagreb indices

$$M_1(G) := \sum_{v \in V} d_v^2 = w_2(G) \qquad \text{and} \qquad M_2(G) := \sum_{\{x,y\} \in E} d_x d_y = w_3(G)/2 \ .$$

Hansen and Vukičević again found counterexamples for the case of general graphs, but they also proved the inequality for graphs with maximum degree not exceeding 4. That includes most of the graphs that are interesting from the perspective of chemical structures. An undirected graph is called a *chemical graph* if its maximum degree Δ is bounded by $\Delta \leq 4$.

Theorem 2 (Hansen and Vukičević). *Every chemical graph G satisfies the inequality*

$$\frac{M_1(G)}{n} \leq \frac{M_2(G)}{m} \ .$$

2.2 Trees

Vukičević and Graovac [12] proved the same inequality for all trees. (Later, another proof appeared in the paper of Andova, Cohen, and Škrekovski [1].)

Theorem 3 (Vukičević and Graovac). *Let T be a tree with $n \geq 2$ vertices and m edges. Then,*

$$\frac{M_1(T)}{n} \leq \frac{M_2(T)}{m} \ .$$

The equality holds if and only if T is a star.

Unaware of this result, the following equivalent form of the inequality that uses the number of walks was proved in [11].

Corollary 4. *Every tree T satisfies the inequality*

$$w_1(T) \cdot w_2(T) \leq w_0(T) \cdot w_3(T) \qquad \text{or, equivalently,} \qquad \overline{d} \cdot w_2(T) \leq w_3(T) \ ,$$

where $\overline{d} = 2m/n$ denotes the average degree.

In the same paper, a similar inequality for walks of length 4 and 5 is shown.

Theorem 5. *Every tree T satisfies the inequality*

$$w_1(T) \cdot w_4(T) \leq w_0(T) \cdot w_5(T) \qquad \text{or, equivalently,} \qquad \overline{d} \cdot w_4(T) \leq w_5(T) \ .$$

2.3 Subdivision graphs

Ilić and Stevanović [5] proved the following theorem for subdivision graphs.

Theorem 6 (Ilić and Stevanović)**.** *For every graph G on n vertices and m edges, the corresponding subdivision graph S_G obeys the inequality*

$$\frac{M_1(S_G)}{n+m} \leq \frac{M_2(S_G)}{2m} \ .$$

If we translate this to walk numbers, the statement corresponds to the following.

Corollary 7. *For every graph G, the corresponding subdivision graph S_G obeys the inequality*

$$w_1(S_G) \cdot w_2(S_G) \leq w_0(S_G) \cdot w_3(S_G) \ .$$

Proof. We give a short alternative proof. We have

$$\begin{aligned}
w_0(S_G) &= n+m = w_0(G) + w_1(G)/2 \qquad \text{(There are } m \text{ new vertices.)} \\
w_1(S_G) &= 4m = 2w_1(G) \qquad \text{(Every edge is split into two parts.)} \\
w_2(S_G) &= \Big(\sum\nolimits_{v\in V} d_v^2\Big) + m \cdot 2^2 = w_2(G) + 4m = w_2(G) + 2w_1(G) \\
w_3(S_G) &= 2 \sum_{\{x,y\}\in E(S_G), x\in V} 2d_x = 4 \sum_{x\in V} d_x^2 = 4w_2(G)
\end{aligned}$$

The formulas for $w_2(S_G)$ and $w_3(S_G)$ use the fact that old vertices have the same degree in G and in S_G while new vertices have always degree 2. Then the inequality corresponds to

$$\begin{aligned}
2w_1(G) \cdot [w_2(G) + 2w_1(G)] &\leq [w_0(G) + w_1(G)/2] \cdot 4w_2(G) \\
w_1(G)^2 &\leq w_0(G) \cdot w_2(G) \ .
\end{aligned}$$

Thus the inequality is valid by Theorem 1. In principle, this inequality can also be found (without reference to walks) in the slightly different form $1 + c_v^2 = \frac{n}{4m^2} \sum_{i=1}^{n} d_i^2$ within the paper of Edwards [3]. ■

3 Main Results

Now, it would be interesting to know whether similar inequalities hold for longer walks in subdivision graphs, e.g., for the number of 5-step walks. For the next step towards a proof of the general inequality, we will use the following lemma.

Lemma 8. *Given n nonnegative numbers a_k and an exponent $p \in R$, the following inequality holds:*

$$\left(\sum_{k=1}^{n} a_k\right)^p \leq n^{p-1} \cdot \sum_{k=1}^{n} a_k^p \qquad \text{for } p \leq 0 \text{ or } p \geq 1 .$$

The inequality is reversed for $0 \leq p \leq 1$.

Proof. For $p \leq 0$ or $p \geq 1$, the inequality is equivalent to $\left(\frac{1}{n} \sum_{k=1}^{n} a_k\right)^p \leq \frac{1}{n} \sum_{k=1}^{n} a_k^p$. The basic form of Jensen's inequality states that $f(\frac{1}{n} \sum_{i \in [n]} x_i) \leq \frac{1}{n} \sum_{i \in [n]} f(x_i)$ for any real convex function f and all $x \in R^n$. The inequality is reversed if f is concave. The lemma is correct for $a_k \geq 0$ since the function $f(x) = x^p$ (with $x \geq 0$) is convex for $p \leq 0$ or $p \geq 1$ and it is concave for $0 \leq p \leq 1$. ■

3.1 General graphs

Lemma 9. *Every graph $G = (V, E)$ satisfies the inequality*

$$w_2(G)^2 \leq m \sum_{\{x,y\} \in E} (d_x + d_y)^2 .$$

Proof. By application of Lemma 8, we have

$$\left(\sum_{\{x,y\} \in E} (d_x + d_y)\right)^2 \leq m \sum_{\{x,y\} \in E} (d_x + d_y)^2 .$$

The proof is complete by observing $w_2(G) = \sum_{v \in V} d_v^2 = \sum_{\{x,y \in E\}} (d_x + d_y)$. ■

Now we show our main results. For convenience, we use the abbreviation $w_k = w_k(G)$.

Theorem 10. *Every graph $G = (V, E)$ satisfies the inequality*

$$2w_1 w_2 \leq w_0 \sum_{\{x,y\} \in E} (d_x + d_y)^2 = w_0 \left(w_3 + \sum_{v \in V} d_v^3\right) .$$

Proof. For the proof, we use the equivalent form

$$2\frac{w_1}{w_0} \;\leq\; \frac{1}{w_2}\sum\nolimits_{\{x,y\}\in E}(d_x+d_y)^2 \;\; .$$

We prove the inequality by separating both sides using the term w_2/m. First, we have $2w_1/w_0 \leq w_2/m$. This is obviously true since $w_1 = 2m$ and $w_1^2 \leq w_0 w_2$ by Theorem 1. It remains to show that

$$\frac{w_2}{m} \leq \frac{1}{w_2}\sum\nolimits_{\{x,y\}\in E}(d_x+d_y)^2 \;\; ,$$

which is true by Lemma 9. ■

It is interesting to see that the inequality

$$w_1 w_2 \;\leq\; w_0 \frac{w_3 + \sum_{v\in V} d_v^3}{2}$$

holds true although there are graphs with $w_1 w_2 \not\leq w_0 w_3$ and there are (other) graphs satisfying $w_3 = \sum_{v\in V} d_v^3$. Another interesting equivalent form uses arithmetic means:

$$\frac{1}{n}\sum_{x\in V} d_x^2 \;\leq\; \frac{1}{m}\sum_{\{x,y\}\in E}\left(\frac{d_x+d_y}{2}\right)^2 \;\; .$$

While arithmetic means appear on the left side (per vertex) and on the right side (per edge), there is also the squared mean of d_x and d_y on the right handside. Replacing this arithmetic mean $(d_x + d_y)/2$ by the smaller geometric mean $\sqrt{d_x d_y}$ would lead to the inequality $w_1 w_2 \leq w_0 w_3$, which is not valid for general graphs (as discussed earlier).

3.2 Subdivision graphs

The following theorem has been obtained in [9].[1]

Theorem 11. *For every graph G, the corresponding subdivision graph S_G obeys the inequality*

$$w_1(S_G)\cdot w_4(S_G) \;\leq\; w_0(S_G)\cdot w_5(S_G) \;\; .$$

Proof. The calculation starts by applying the formula $w_4(S_G) = \sum_{v\in V(S_G)} w_2(v)^2$. We need to distinguish two kinds of vertices: old vertices (corresponding to the vertices in the original graph G) and new vertices (corresponding to the edges of G). For each old vertex $v \in V$, the number of 2-step walks in S_G is $w_2^{S_G}(v) = 2d_v$. For every new vertex v_e corresponding to an edge $e = \{x, y\}$ in G, the number of 2-step walks in S_G is

[1] submitted to the faculty of computer science at TU München in April 2015

$w_2^{S_G}(v_e) = d_x + d_y$. Hence we obtain the following walk numbers in terms of the degrees and walks of the original graph G:

$$\begin{aligned} w_4(S_G) &= \sum_{v\in V}(2d_v)^2 + \sum_{\{x,y\}\in E}(d_x+d_y)^2 = 4w_2 + \sum_{\{x,y\}\in E}(d_x+d_y)^2 \\ w_5(S_G) &= 2\sum_{\{x,y\}\in E} 2d_x\cdot(d_x+d_y) + 2d_y\cdot(d_x+d_y) = 4\sum_{\{x,y\}\in E}(d_x+d_y)^2 \end{aligned}$$

We obtain the following equivalent inequalities:

$$\begin{aligned} (2w_1)\left(4w_2 + \sum\nolimits_{\{x,y\}\in E}(d_x+d_y)^2\right) &\le (w_0 + w_1/2)\left(4\sum\nolimits_{\{x,y\}\in E}(d_x+d_y)^2\right) \\ 8w_1w_2 &\le 4w_0\sum\nolimits_{\{x,y\}\in E}(d_x+d_y)^2 \\ 2\frac{w_1}{w_0} &\le \frac{1}{w_2}\sum\nolimits_{\{x,y\}\in E}(d_x+d_y)^2 \end{aligned}$$

The last inequality follows from Theorem 10. ■

Theorem 12. *For every graph G, the corresponding subdivision graph S_G obeys the inequality*

$$w_2(S_G)\cdot w_3(S_G) \le w_0(S_G)\cdot w_5(S_G) .$$

Proof. We have

$$\begin{aligned} (w_2+2w_1)(4w_2) &\le (w_0 + w_1/2)\left(4\sum\nolimits_{\{x,y\}\in E}(d_x+d_y)^2\right) \\ w_2^2 + 2w_1w_2 &\le (w_0 + w_1/2)\left(\sum\nolimits_{\{x,y\}\in E}(d_x+d_y)^2\right) \end{aligned}$$

The inequality follows from Lemma 9 and Theorem 10 after observing that $w_1/2 = m$.

■

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