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Genome Sequencing Using Graph Theory Approach

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Abstract

Genome sequencing is the process of determining in which order the nitrogenous bases also known as nucleotides within a DNA molecule are arranged. Every organism's genome consists of a unique sequence of nucleotides. These nucleotides bases provide the phenotypes and genotypes of a cell. In mathematics, Graph theory is the study of mathematical objects known as graphs which are made of vertices (or nodes) connected by either directed edges or indirect edges. Determining the sequence in which these nucleotides are bonded can help scientists and researchers to compare DNA between organisms, which can help show how the organisms are related. In this research, we study how graph theory plays a vital part in genome sequencing and different types of graphs used during DNA sequencing. We are going to propose several ways graph theory is used to sequence the genome. We are as well, going to explore how the graphs like Hamiltonian graph, Euler graph, and de Bruijn graphs are used to sequence the genome and advantages and disadvantages associated with each graph.

Keywords

DNA Sequencing, Hamiltonian Graph, Euler Graph, de Bruijn Graph, Nucleotide

1. Introduction

In 1953, two scientists, J.D. Watson and F.H.C. Crick [1] established the double-helix model for the DNA molecule after combining chemical and physical data. DNA is a short name for DeoxyriboNucleic Acid and according to this proposed model, the DNA molecule is made out of two antiparallel strands which are connected together by two or three hydrogen bonds and helically twisted. Within these nucleotides encode the genetic information of all living

matter, the human beings included.

There are four different types of *nucleotides* bases in DNA which are guanine (G), thymine (T), adenine (A) and cytosine (C). Within these bases, adenine bonds with thymine and guanine bonds with cytosine. *Genome sequencing* hence is the process of figuring out in which order are these nucleotides bases arranged in the genome. Rapid advancements in genome sequencing have made understanding genome sequencing essential for many biological studies, other research areas that use genome sequencing and a variety of applied fields like biotechnology, forensic biology, and diagnostics. The journey with genome sequencing began in 1977 [2] when Frederick with his colleagues proposed a method on chain-termination inhibitors. Sanger sequencing is known to deliver 99.99% base accuracy that is crucial for optimum validation in the field of genetics. It is considered the gold standard when the job is to understand how the genes carry out information (The Genomic Services Company, 2020).

Sanger sequencing was used in the Human Genome Project to determine the sequences of relatively small fragments of human DNA (900 bp or less). These fragments were used to assemble larger DNA fragments and, eventually, entire chromosomes. Edwin Southern [3] introduced a new genome sequencing approach where the genome is sequenced by hybridization (SBH). SBH is an approach whereby a collection of overlapping oligonucleotide sequences is assembled together to determine an organism's DNA sequence. Through the efficient method of SBH, scientists are able to gather information on the genomes of different species and organisms for the future development of biological sciences, medicine, and agriculture. Among the scientists of algorithmic approaches to SBH we can distinguish Y.P. Lysov with his colleagues [4] and Pevzner [5], who formulated the problem as finding a Hamiltonian path and an Eulerian path, respectively. Next Generation Sequencing is yet another genome sequencing method and is a powerful platform that has enabled the sequencing of thousands to millions of DNA molecules simultaneously (Margulies, Egholm, & Altman [6]).

The methods of sequencing have become a game-changer in modern biological and medical fields. DNA sequencing has accelerated not only biological research and discovery but also enhanced medical diagnostics and treatment of diseases. This article will focus more on methods for DNA sequencing which use concepts of graph theory.

Before we dive into the graph theory approaches in genome sequencing, let's briefly understand what graph theory is and definitions of key words used in graph theory.

Graph Theory is a mathematical representation of a network and it describes the relationship between lines and points. A graph consists of some points and lines between them. The length of the lines and position of the points do not matter. Each object in a graph is called a node. A graph G is a set of vertices, called nodes v which are connected by edges, called links e . Thus $G = (v, e)$.

Vertex is an intersection point of a graph. It denotes a location such as a city, a road intersection, or a transport terminal (stations, harbors, and airports). Edge is a link between two nodes. An edge denotes movements between nodes. It has a direction that is generally represented as an arrow. If an arrow is not used, it means the link is bi-directional.

2. Genome Sequencing Using Hamiltonian Graph

In this section, we show the genome sequencing by using Hamiltonian graph. A connected graph G is called Hamiltonian graph if there is a cycle which includes every vertex of G and the cycle is called Hamiltonian cycle. Hamiltonian walk-through graph G is a walk that passes through each vertex exactly once. We first show two very famous Theorems for Hamiltonian graph, which the proofs can be found in [7].

Theorem 2.1. (Dirac's Theorem) states that if G is a simple graph with n vertices, where $n \geq 3$, If $\deg(v) \geq \frac{n}{2}$ for each vertex v , then the graph G is Hamiltonian graph.

Theorem 2.2. (Ore's Theorem) states if G is a simple graph with n vertices, where $n \geq 2$ if $\deg(x) + \deg(y) \geq n$ for each pair of non-adjacent vertices x and y , then the graph G is Hamiltonian graph.

Objective. Use overlapping DNA reads in order to reconstruct the original genome sequence.

When having our fragments of the genome they often overlap. We are able to make use of this overlap and stitch them together. Assuming our fragments (often referred as mers) are 3 molecules long (3-mer). For instance, we could have fragments such as AAT, GCG, CAA. By also assuming they overlap with two molecules. This means the fragment AAT must be followed by a fragment beginning with AT e.g., ATT. We create a Hamiltonian graph where each node is a fragment. And there is an edge going from a node to another when they only overlap by two nucleotides bases. So, the node AAT would have an edge connecting it to ATT.

Example 1: Let $S = \{AAT, GCG, GCA, ATG, TGG, TGC, GGC, GTG, CGT, CAA\}$ be a multiset of all 3-long nucleotides of a DNA sequence. Let's construct a network that represents the overlap information in our reads. Each k -mer nucleotide from the multiset becomes a vertex (as depicted in **Figure 1**); two vertices are connected by a directed vertex if the $k - 1$ rightmost nucleotides of first vertex overlap with the $k - 1$ leftmost nucleotides of the second one.

First, we create a node for each read. e.g., GTG. Prefix: First two nucleotide of a read (GTG). Suffix: Last two nucleotide of a read (GTG). Note: Different 3-mers may share a prefix/suffix: ATG, TGA, CTG. As shown from **Figure 1** DNA reads are aligned and ready to be joined using overlap reads from prefix to suffix.

Figure 2 shows how to connect these DNA nodes based on the prefix and suffix. As illustrated from **Figure 2** with nodes ATG and GTG connecting to nodes TGC and TGG based on the overlapping part of the nucleotide.

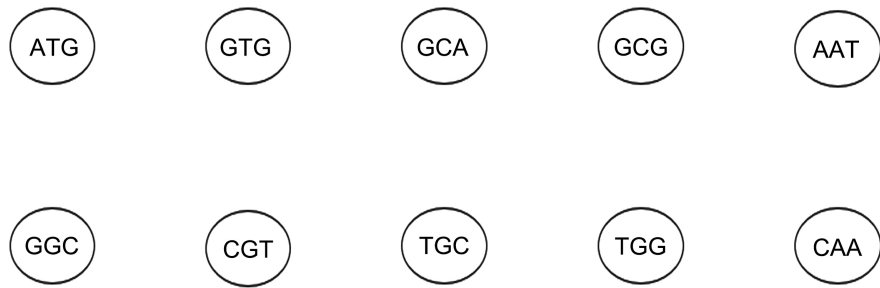


Figure 1. Aligning the 3-mer nodes.

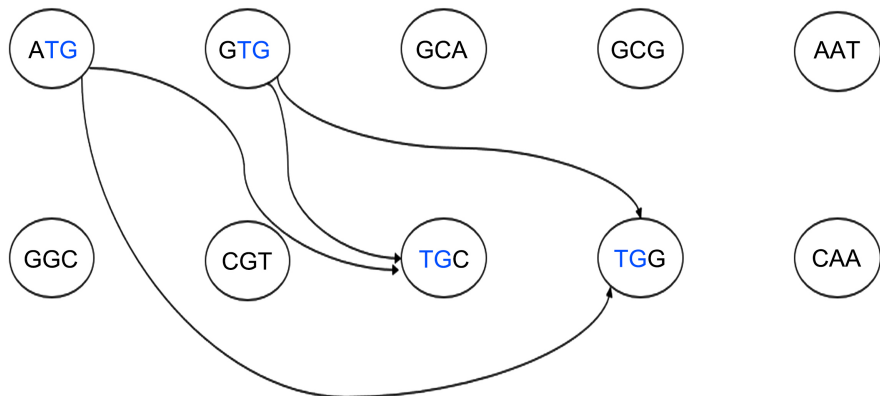


Figure 2. Connecting DNA nodes based on prefix and suffix.

From the diagram in **Figure 3**, we can clearly see a completed graph when connecting all nodes with the same prefix to the node with the same suffix and shows how the genome sequencing is done using the Hamiltonian approach. Now we need to deduce the order of the DNA and for us to do so we need to follow the path on the diagram that takes us from where we started. Our Hamiltonian cycle will be: ATG → TGG → GGC → GCG → CGT → GTG → TGC → GCA → CAA → AAT → ATG. Therefore, our genome from this reconstruction is ATGGCGTGCAAT.

Example 2: Let $H = \{TGC, TTC, GCT, TCC, CTA, CCA, TAG, CAA, AGT, GTT, AAT, TTT, ATA\}$ be a multiset of all 3-long nucleotides of a DNA sequence. From the given reads of DNA above, let's reconstruct the original gene sequence using Hamiltonian cycle.

Using the steps in example 1, constructing a network that represents the overlap information in our DNA reads will give the diagram above, as depicted in **Figure 4**. Therefore, from the re-arranged graph above, as depicted in **Figure 5**, Graph H has Hamiltonian path: TGC → GCT → CTA → TAG → AGT → GTT → TTT → TTC → TCC → CCA → CAA → AAT. From reconstructing Graph H, our genome is TGCTAGTTTCCAAT.

If we find a path that visits every node once (a Hamiltonian path) we have a found an ordering of the fragment that makes up the whole DNA sequence. Sadly, finding a Hamiltonian path isn't easy (it is classed as an NP-Complete problem).

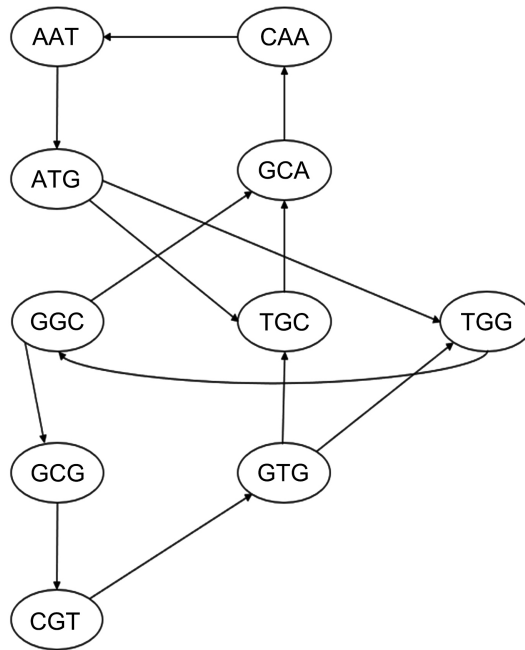


Figure 3. Complete Hamiltonian Graph of example 1.

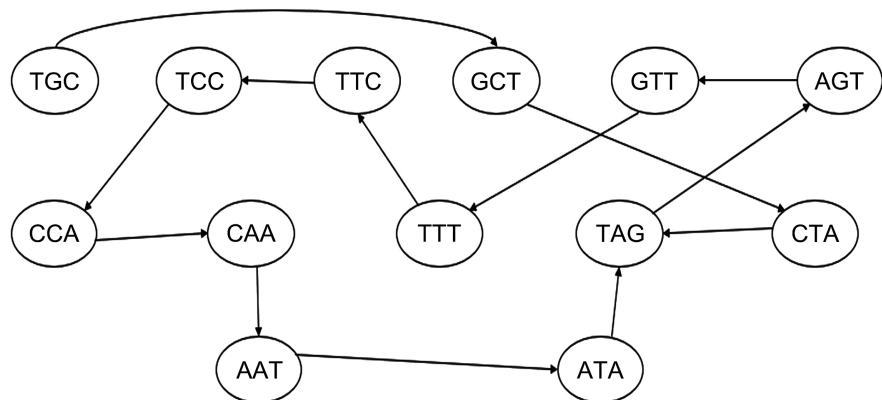


Figure 4. Hamiltonian graph of H.

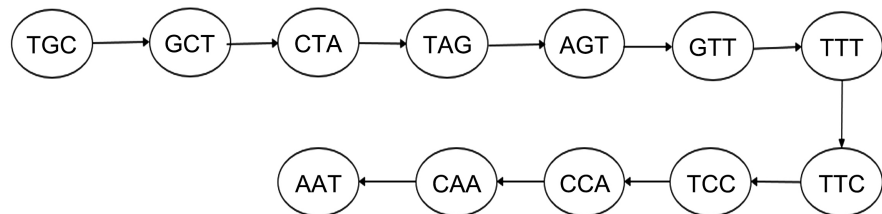


Figure 5. Re-arranged Hamiltonian path of H.

3. Genome Sequencing Using Eulerian Graph

In this section, we show the genome sequencing by using Eulerian graph.

A connected graph G is called a Euler graph, if there is a closed trail which includes every edge of the graph G . A Euler path is a path that uses every edge of a graph exactly once. A Euler path starts and ends at different vertices. A Euler

circuit is a circuit that uses every edge of a graph exactly once. A Euler circuit always starts and ends at the same vertex.

A connected graph G is a Euler graph if and only if all vertices of G are of even degree, and a connected graph G is Eulerian if and only if its edge set can be decomposed into cycles. Objective: From a given set, S , in reads, use Eulerian approach to reconstruct the genome sequence.

Using genome reads, make a node for each unique prefix or suffix. From the set of $(l-1)$ -mers, which are substrings of some of the l -mers in our set S , will make up the vertices. Whenever there is a node which has a prefix v and suffix is w , connect the node v to node w . If the final $l-1$ elements of node v and first $l-2$ elements of node w match and the union of node v and node w is in set S , then node v and node w are connected by a directed edge.

In order to reconstruct the shortest sequence string using the Eulerian path, a set of $(l-1)$ mer strings (*i.e.*, strings having length less by one from given strings) are taken into account.

Example 3: Let $H = \{AAT, TGC, CAA, GCT, CCA, CTA, TCC, TAG, AGT, TCC, TTT, TTC\}$ be a multiset of all 3-long nucleotides of a DNA sequence. We create a node for each distinct prefix/suffix *i.e.*, CTA we get the prefix CT and the suffix TA. By completing finding the distinct prefix and suffix we get the following $V = \{AT, GC, CT, CC, AA, TG, TT, CA, AG, GT, TC, TA\}$.

As illustrated above, (as depicted in **Figure 6**), prefix AA connects to the suffix AT with an edge AAT as the DNA read also prefix CT connects to the suffix TA with an edge CTA as the DNA read. By completing the diagram connecting these prefixes to suffix we can show in **Figure 7**.

From the diagram above (as depicted in **Figure 7**), the numbers mark the Eulerian path that we will be followed when reconstructing this genome from k -mer DNA reads and by using the overlaps DNA reads we can produce the path table (as depicted in **Figure 8**).

The path table above (as depicted in **Figure 8**) illustrates how we can reconstruct our original genome using DNA reads overlaps and we got our genome using Eulerian path TGCTAGTTCCAAT.

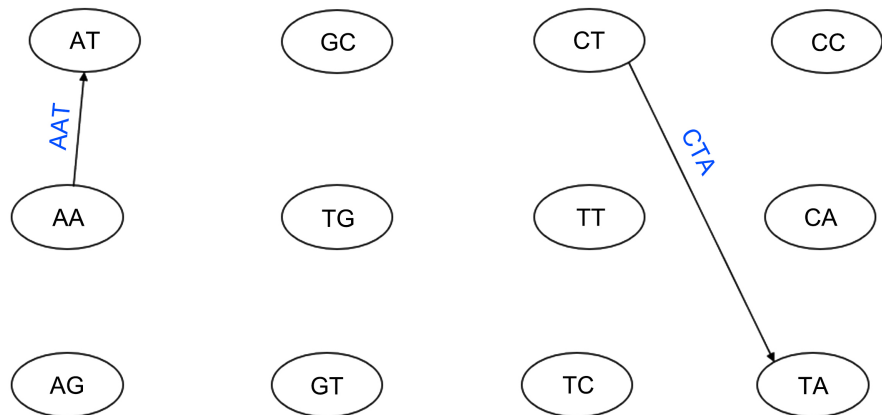


Figure 6. Multigraph with AAT and CTA.

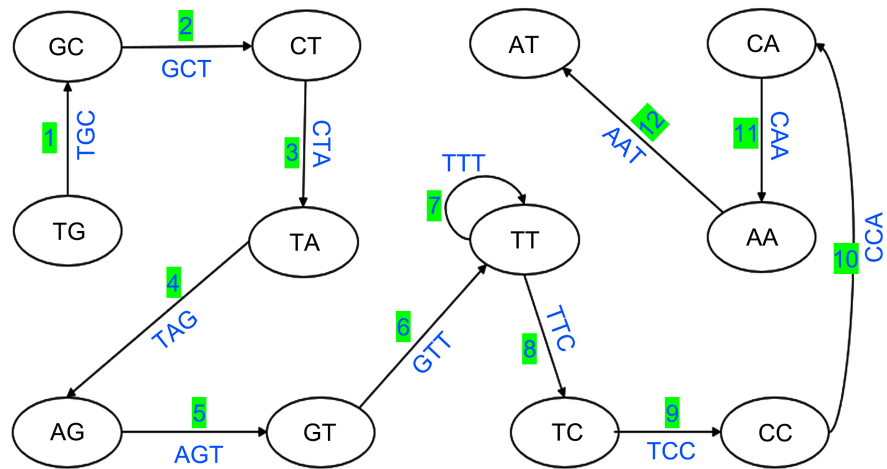


Figure 7. Complete Eulerian path of H.

	T	G	C																	
		G	C	T																
			C	T	A															
				T	A	G														
					A	G	T													
						G	T	T												
							T	T	T											
								T	T	C										
									T	C	C									
										C	C	A								
											C	A	A							
												A	A	T						
genome	T	G	C	T	A	G	T	T	T	C	C	A	A	T						

Figure 8. Eulerian path table of H.

Comparing between Hamiltonian approach and Eulerian approach, the only difference is when using a computer, it can easily find the Eulerian cycle very fast compared to when using Hamiltonian cycle.

4. Genome Sequencing Using de Bruijn Graph

A sequence’s k -mer components can be efficiently represented using a de Bruijn graph. Despite the fact that de Bruijn graphs can be applied to a variety of issues, we will focus on nucleotide sequences in this article. Around the 1940s, Nicolaas de Bruijn, a Dutch mathematician, became interested in finding the shortest circular string of characters that encompasses all conceivable substrings of the same length in a particular alphabet. He came up with a solution that entailed creating a graph with all of the possible $(k - 1)$ -mers as the nodes. If the $(k - 1)$ -mer in node A is a prefix and that in node B is a suffix of the k -mer, then each

k -mer was an edge directed from node A to node B. Finding a path through the graph that passes over each edge exactly once, or an Eulerian trail, was the suggested answer. Our genome reads are fragmented into smaller fragments of a given size k . A node for each $(k - 1)$ -mer from k -mers for each k -mer in k -mers is formed and an edge is used to connect its prefix node with its suffix node.

Let's illustrate with an example below.

Example 4: Let $M = \{TGT, AAT, TGG, ATG, TGC, ATG, TAA, ATG, GTT, CAT, CCA, GGA, GCC, GAT, GGG\}$ be a multiset of all 3-long nucleotides of a DNA sequence. Take all distinct $(k - 1)$ -mers from the set of k -mers, here $k = 3$. *i.e.*, $TGC, TGG \rightarrow TG, GC, GG$. Construct a multi-graph with nodes being $(k - 1)$ -mers; draw an edge between two $(k - 1)$ -mers only if the two $(k - 1)$ -mers are taken from the same read. *i.e.*, AAT & ATG (as depicted in **Figure 9**).

This method guarantees that the graph will have a Eulerian trail, by following the Eulerian trail and joining the nodes will thereby reconstruct our original genome sequence. A graph similar to this will be displayed (as depicted in **Figure 10**).

As illustrated in **Figure 10**, each edge in this graph corresponds to a length-3 length input string. Through this network, a Eulerian path is traced, and therefore as a result, we are able to reconstruct our original genome sequence table (as depicted in **Figure 11**).

Using a Eulerian walk crossing each edge exactly once gives a reconstruction of the genome. After funding the walk, our genome will be TAATGCCATGGGATGTT.



Figure 9. Multigraph with AAT and ATG.

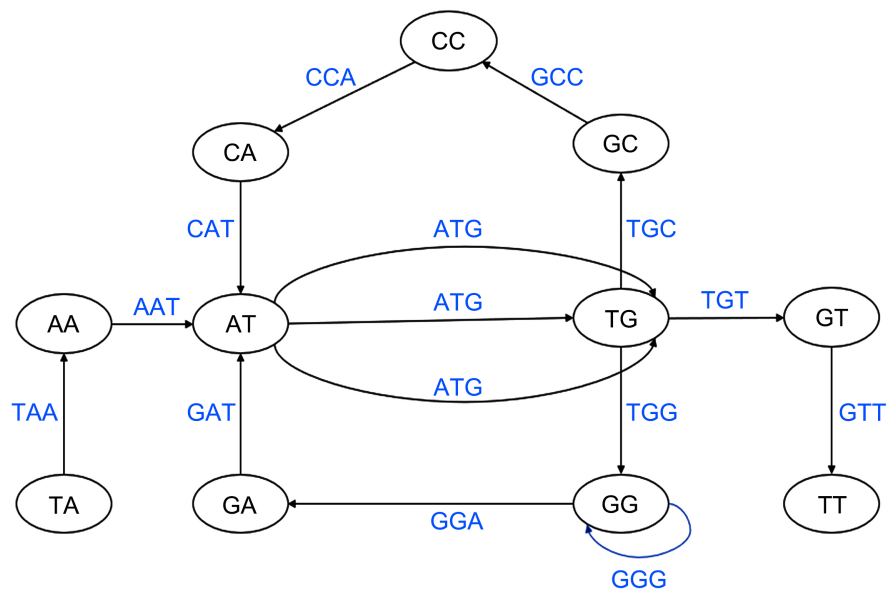


Figure 10. Complete de Bruijn graph of M.

	T	A	A																
		A	A	T															
			A	T	G														
				T	G	C													
					G	C	C												
						C	C	A											
							C	A	T										
								A	T	G									
									T	G	G								
										G	G	G							
											G	G	A						
												G	A	T					
													A	T	G				
														T	G	T			
															G	T	T		
																T	T		
genome	T	A	A	T	G	C	C	A	T	G	G	G	A	T	G	T	T		

Figure 11. The reconstruction of the original genome sequence table of M.

5. Conclusions

When it comes to solving biological problems and making medicine, graph theory plays a vital role and it's necessary for this generation to understand it. DNA sequencing was critical in mapping out the human genome, which was finished in 2003, and is now a crucial tool for many fundamental and practical research applications.

This paper discussed how graph theory is used in genome sequencing and showed some of the graph theory graphs that are used and showed some graphical representation of those methods and some step by step on how the methods are used.

When using Hamiltonian approach, as the DNA reads increase, finding a Hamiltonian path is not easy (it is classed as an NP-Complete problem). Euler approach is a better approach than Hamiltonian approach in genome sequencing because nowadays with massive growth in genetics finding the Euler cycle does not take a long time. Sadly, in real life there are some other problems that make this process harder. One example is if a fragment occurs multiple times in a sequence.

The de Bruijn graph approach has proven to be a better method in genome reconstruction compared to Euler approach and Hamiltonian approach.

True, assembly approaches based on de Bruijn graphs start rather counter-intuitively, by replacing each read with a collection of all-overlapping sequences of a shorter, fixed length, but this is a popular way for genome assembly. Although the de Bruijn assembler is a famous way to perform assembling, there are significant obstacles for de Bruijn genome assembly, including sequence error, unequal sequencing depth, repetitive parts, and processing expense.

Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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A Relationship between the Partial Bell Polynomials and Alternating Run Polynomials

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Abstract

In this note, we first derive an exponential generating function of the alternating run polynomials. We then deduce an explicit formula of the alternating run polynomials in terms of the partial Bell polynomials.

Keywords

Alternating Run Polynomials, Bell Polynomials, Permutations

1. Introduction

Let \mathfrak{S}_n be the symmetric group of all permutations of $[n]$, where $[n] = \{1, 2, \dots, n\}$. An *alternating run* of a permutation $\sigma = \sigma(1)\sigma(2)\cdots\sigma(n) \in \mathfrak{S}_n$ is a continuous maximal monotone increasing or decreasing sequence. For example, the permutation 3175246 has four alternating runs 31, 17, 752 and 246. Let $R(n, k)$ denote the number of permutations in \mathfrak{S}_n with k alternating runs. The study of alternating runs of permutations was initiated by André [1], who found that the numbers $R(n, k)$ satisfy the recurrence relation

$$R(n, k) = kR(n-1, k) + 2R(n-1, k-1) + (n-k)R(n-1, k-2) \quad (1)$$

for $n, k \geq 1$, where $R(1, 0) = 1$ and $R(1, k) = 0$ for $k \geq 1$. The reader is referred to [2] [3] [4] for the recent studies on this topic. For $n \geq 1$, we define $R_n(x) = \sum_{k=1}^{n-1} R(n, k)x^k$. Then by using (1), one can deduce the following recurrence relation

$$R_{n+2}(x) = x(nx+2)R_{n+1}(x) + x(1-x^2)R'_{n+1}(x), \quad (2)$$

with initial value $R_1(x) = 1$. The first few terms of $R_n(x)$'s are given as follows:

$$R_2(x) = 2x,$$

$$R_3(x) = 2x + 4x^2,$$

$$R_4(x) = 2x + 12x^2 + 10x^3,$$

$$R_5(x) = 2x + 28x^2 + 58x^3 + 32x^4.$$

In a series of papers [5] [6] [7], Carlitz studied the generating functions for the numbers $R(n, k)$. In particular, Carlitz [5] proved that

$$\sum_{n=0}^{\infty} \frac{z^n}{n!} \sum_{k=0}^n R(n+1, k) x^{n-k} = \frac{1-x}{1+x} \left(\frac{\sqrt{1-x^2} + \sin(z\sqrt{1-x^2})}{x - \cos(z\sqrt{1-x^2})} \right)^2. \tag{3}$$

As a dual of (3), the first result of this note is the following.

Theorem 1. Let $R(x, t) = \sum_{n=0}^{\infty} R_{n+1}(x) \frac{t^n}{n!}$, we have

$$R(x, t) = \frac{(x-1)(1 + \cosh z)}{(x+1)(1 - \cosh z)},$$

where $z = \operatorname{arccosh}\left(\frac{1}{x}\right) - t\sqrt{1-x^2}$.

Let $\{x_i\}_{n \geq 1}$ be a sequence of variables. The *partial Bell polynomials* $B_{n,k} = B_{n,k}(x_1, x_2, \dots, x_{n-k+1})$ are defined by the generating function

$$\sum_{n \geq k} B_{n,k} \frac{t^n}{n!} = \frac{1}{k!} \left(\sum_{i \geq 1} x_i \frac{t^i}{i!} \right)^k,$$

or equivalently defined by the series expansion

$$\exp\left(u \sum_{j \geq 1} x_j \frac{t^j}{j!}\right) = 1 + \sum_{n \geq 1} \frac{t^n}{n!} \sum_{k=1}^n u^k B_{n,k}(x_1, x_2, \dots, x_{n-k+1}),$$

with $B_{0,0} = 1$ and $B_{n,0} = 0$ for $n > 0$. We refer the reader to [8] [9] [10] for some applications of the partial Bell polynomials.

Corollary 1. Let $B_{n,k}$ be the partial Bell polynomials. When $x_i = (1-x^2)^{\lfloor (i-1)/2 \rfloor}$ for each $i \geq 1$, we have

$$R_{n+1}(x) = 2x \sum_{k=1}^n (-1)^{n-k} k! (1+x)^{k-1} B_{n,k}.$$

Proof. Let $z = \operatorname{arccosh}(1/x) - t\sqrt{1-x^2}$. By Theorem 1, we get

$$\begin{aligned} & x(\cosh z - 1) \\ &= \cosh\left(-t\sqrt{1-x^2}\right) + x \sinh\left(-t\sqrt{1-x^2}\right) \sinh\left(\operatorname{arccosh}(1/x)\right) - x \\ &= \frac{1}{2} \left(e^{-t\sqrt{1-x^2}} + e^{t\sqrt{1-x^2}} \right) + \frac{\sqrt{1-x^2}}{2} \left(e^{-t\sqrt{1-x^2}} - e^{t\sqrt{1-x^2}} \right) - x \\ &= 1 - x + \sum_{i=1}^{\infty} (-1)^i y_i \frac{t^i}{i!}, \end{aligned}$$

where $y_i = (1-x^2)^{\lfloor (i+1)/2 \rfloor}$. Therefore,

$$\begin{aligned} R(x,t) &= \frac{(x-1)(1+\cosh z)}{(x+1)(1-\cosh z)} = \frac{1-x}{1+x} \left(1 + \frac{2x}{x(\cosh z - 1)} \right) \\ &= \frac{1-x}{1+x} \left(1 + \frac{2x}{1-x + \sum_{i=1}^{\infty} (-1)^i y_i \frac{t^i}{i!}} \right) \\ &= \frac{1-x}{1+x} + \frac{2x}{1+x} \sum_{k=0}^{\infty} (-1)^k (1+x)^k \left(\sum_{i \geq 1} (-1)^i x_i \frac{t^i}{i!} \right)^k, \end{aligned}$$

where $x_i = (1-x^2)^{\lfloor (i-1)/2 \rfloor}$, and the desired result follows immediately.

In the next section, we first prove Theorem 1 and then give an explicit formula of $R_n(x)$.

2. The Proof of Theorem 1 and an Explicit Formula of $R_n(x)$

A proof Theorem 1:

Proof. Multiplying both sides of (2) by $\frac{t^n}{n!}$ and summing over all $n \geq 0$, we get

$$\frac{\partial R(x,t)}{\partial t} = tx^2 \frac{\partial R(x,t)}{\partial t} + 2xR(x,t) + (x-x^3) \frac{\partial R(x,t)}{\partial x}.$$

Hence

$$(x-x^3) \frac{\partial R(x,t)}{\partial x} + (tx^2-1) \frac{\partial R(x,t)}{\partial t} = -2xR(x,t).$$

This is a non-homogeneous linear partial differential equation, and the corresponding characteristic equation is

$$\frac{dx}{x-x^3} = \frac{dt}{tx^2-1} = \frac{dR(x,t)}{-2xR(x,t)}.$$

It is easy to find that its two independent initial integrals are

$$\operatorname{arccosh}\left(\frac{1}{x}\right) - t\sqrt{1-x^2} = c_1, \quad \frac{x+1}{x-1} R(x,t) = c_2.$$

Since $R(x,0) = R_1(x) = 1$, we have

$$c_2 = \frac{1 + \cosh c_1}{1 - \cosh c_1},$$

which yields the desired formula.

Theorem 2. Let $b > a > 0$ be two constants. When $x_i = \left(\frac{a}{b}\right)^{\lfloor (i-1)/2 \rfloor}$ for each $i \geq 1$, we have

$$\begin{aligned}
 & B_{n,k} \left(1, 1, \frac{a}{b}, \frac{a}{b}, \dots, \left(\frac{a}{b} \right)^{\lfloor \frac{n-k}{2} \rfloor} \right) \\
 &= \frac{(-1)^k}{k!} \left(\frac{a}{b} \right)^{\frac{n-k}{2}} \sum_{l=0}^k \binom{k}{l} \left(-\frac{\sqrt{b-a}}{2\sqrt{b}} \right)^l \sum_{q=0}^l \binom{l}{q} (2q-l)^n \left(\frac{\sqrt{b} + \sqrt{a}}{\sqrt{b-a}} \right)^{2q-l}. \tag{4}
 \end{aligned}$$

Proof. By the definition of partial bell polynomial, let $x_i = \left(\frac{a}{b} \right)^{\lfloor (i-1)/2 \rfloor}$ have

$$\begin{aligned}
 & \sum_{n \geq k} B_{n,k} \left(1, 1, \frac{a}{b}, \frac{a}{b}, \dots, \left(\frac{a}{b} \right)^{\lfloor \frac{n-k}{2} \rfloor} \right) \frac{t^n}{n!} \\
 &= \frac{1}{k!} \left[\sum_{i \geq 1} \left(\frac{a}{b} \right)^{\lfloor \frac{i-1}{2} \rfloor} \frac{t^i}{i!} \right]^k = \frac{1}{k!} \left[\frac{\sqrt{b} \sinh \left(\frac{\sqrt{a}}{\sqrt{b}} t \right)}{\sqrt{a}} + \frac{b \cosh \left(\frac{\sqrt{a}}{\sqrt{b}} t \right)}{a} - \frac{b}{a} \right]^k \\
 &= \frac{\sqrt{b}^k}{k! a^k} \left[\sqrt{a} \sinh \left(\frac{\sqrt{a}}{\sqrt{b}} t \right) + \sqrt{b} \cosh \left(\frac{\sqrt{a}}{\sqrt{b}} t \right) - \sqrt{b} \right]^k \\
 &= \frac{\sqrt{b}^k}{k! a^k} \left[\sqrt{b-a} \cosh \left(\frac{\sqrt{a}}{\sqrt{b}} t + \ln \frac{\sqrt{a} + \sqrt{b}}{\sqrt{b-a}} \right) - \sqrt{b} \right]^k \\
 &= \frac{(-1)^k}{k!} \left(\frac{b}{a} \right)^k \sum_{l=0}^k \binom{k}{l} \left(\frac{\sqrt{b-a}}{\sqrt{b}} \right)^l (-1)^l \cosh^l \left(\frac{\sqrt{a}}{\sqrt{b}} t + \ln \frac{\sqrt{a} + \sqrt{b}}{\sqrt{b-a}} \right).
 \end{aligned}$$

Note that

$$\cosh^l(\alpha t + \beta) = \frac{1}{2^l} \left(e^{(\alpha t + \beta)} + e^{-(\alpha t + \beta)} \right)^l = \frac{1}{2^l} \sum_{q=0}^l \binom{l}{q} e^{q(\alpha t + \beta)} e^{-(l-q)(\alpha t + \beta)}.$$

So we get

$$\cosh^l(\alpha t + \beta) = \frac{1}{2^l} \sum_{q=0}^l \binom{l}{q} e^{(2q-l)(\alpha t + \beta)}.$$

It is clear that

$$\frac{d^m \cosh^l(\alpha t + \beta)}{dt^m} = \frac{1}{2^l} \sum_{q=0}^l \binom{l}{q} (2q-l)^m \alpha^m e^{(2q-l)(\alpha t + \beta)}.$$

Differentiating the both sides of the following expression with respect to t ,

$$\begin{aligned}
 & \sum_{n \geq k} B_{n,k} \left(1, 1, \frac{a}{b}, \frac{a}{b}, \dots, \left(\frac{a}{b} \right)^{\lfloor \frac{n-k}{2} \rfloor} \right) \frac{t^n}{n!} \\
 &= \frac{(-1)^k}{k!} \left(\frac{b}{a} \right)^k \sum_{l=0}^k \binom{k}{l} \left(\frac{\sqrt{b-a}}{\sqrt{b}} \right)^l (-1)^l \cosh^l \left(\frac{\sqrt{a}}{\sqrt{b}} t + \ln \frac{\sqrt{a} + \sqrt{b}}{\sqrt{b-a}} \right),
 \end{aligned}$$

we arrive at

$$\begin{aligned} & \sum_{n \geq k} B_{n,k} \left(1, 1, \frac{a}{b}, \frac{a}{b}, \dots, \left(\frac{a}{b} \right)^{\lfloor \frac{n-k}{2} \rfloor} \right) \frac{t^{n-m}}{(n-m)!} \\ &= \frac{(-1)^k}{k!} \left(\frac{b}{a} \right)^k \sum_{l=0}^k \binom{k}{l} \left(\frac{\sqrt{b-a}}{\sqrt{b}} \right)^l (-1)^{kl} \frac{d^m \cosh^l \left(\frac{\sqrt{a}}{\sqrt{b}} t + \ln \frac{\sqrt{a} + \sqrt{b}}{\sqrt{b-a}} \right)}{dt^m} \\ &= \frac{(-1)^k}{k!} \left(\frac{b}{a} \right)^k \sum_{l=0}^k \binom{k}{l} \left(\frac{\sqrt{b-a}}{\sqrt{b}} \right)^l (-1)^{kl} \frac{1}{2^l} \sum_{q=0}^l \binom{l}{q} (2q-l)^m \left(\frac{\sqrt{a}}{\sqrt{b}} \right)^m \\ & \quad \cdot \exp \left[(2q-l) \left(\frac{\sqrt{a}}{\sqrt{b}} t + \ln \frac{\sqrt{a} + \sqrt{b}}{\sqrt{b-a}} \right) \right]. \end{aligned}$$

Taking the limit $t \rightarrow 0$, we get the desired result.

According to Corollary 1, we know that the coefficients of the corresponding Bell polynomials should be real numbers, so if formula (4) satisfies the conditions and is meaningful, we need to make $a > 0$, $b > 0$ and $\sqrt{b-a} > 0$. Therefore, we can obtain $b > a > 0$.

Set $\frac{a}{b} = 1 - x^2$. Then

$$\begin{aligned} -\frac{\sqrt{b-a}}{2\sqrt{b}} &= -\frac{1}{2} \sqrt{1 - \frac{a}{b}} = -\frac{x}{2}, \\ \frac{\sqrt{b+a}}{\sqrt{b-a}} &= \frac{1 - \sqrt{\frac{a}{b}}}{1 - \sqrt{\frac{a}{b}}} = \frac{1 + \sqrt{1-x^2}}{x}. \end{aligned}$$

Combining Corollary 1 and Theorem 2, we get the following result.

Corollary 2. We have

$$\begin{aligned} R_{n+1}(x) &= 2x \sum_{k=1}^n (-1)^k (x+1)^{k-1} \left(\frac{1}{1-x^2} \right)^{k-\frac{n}{2}} \sum_{l=0}^k \binom{k}{l} \left(-\frac{x}{2} \right) \\ & \quad \times \sum_{q=0}^l \binom{l}{q} (2q-l)^n \left(\frac{1 + \sqrt{1-x^2}}{x} \right)^{2q-l}. \end{aligned} \tag{5}$$

We note that the explicit formula of $R_{n+1}(x)$ given by Corollary 2 is very useful. With the use of formula (5), we can directly calculate the value of $R(n, k)$ for any given n and k , rather than relying on the recurrence relation. Here we provide an example to illustrate the application of Corollary 2, where all calculations are obtained using Mathematica 12.1.

Example 3. Let

$$W_{n,k} = \sum_{l=0}^k \binom{k}{l} \left(-\frac{x}{2} \right)^l \sum_{q=0}^l \binom{l}{q} (2q-l)^n \left(\frac{1 + \sqrt{1-x^2}}{x} \right)^{2q-l}.$$

Consider the case $1 \leq n \leq 4$, we have

$$\begin{aligned}
W_{1,1} &= -\sqrt{1-x^2}; \\
W_{2,1} &= -1, W_{2,2} = 2-2x^2; \\
W_{3,1} &= -\sqrt{1-x^2}, W_{3,2} = 6\sqrt{1-x^2}, W_{3,3} = -6(1-x^2)^{3/2}; \\
W_{4,1} &= -1, W_{4,2} = 14-8x^2, W_{4,3} = 36(-1+x^2), W_{4,4} = 24(-1+x^2)^2.
\end{aligned}$$

Thus

$$\begin{aligned}
R_2(x) &= -2x \sum_{k=1}^1 (x+1)^{k-1} \left(\frac{1}{1-x^2} \right)^{k-\frac{1}{2}} W_{1,k} = 2x; \\
R_3(x) &= 2x \sum_{k=1}^2 (x+1)^{k-1} \left(\frac{1}{1-x^2} \right)^{k-1} W_{2,k} = 2x + 4x^2; \\
R_4(x) &= -2x \sum_{k=1}^3 (x+1)^{k-1} \left(\frac{1}{1-x^2} \right)^{k-\frac{3}{2}} W_{3,k} = 2x + 12x^2 + 10x^3; \\
R_5(x) &= 2x \sum_{k=1}^4 (x+1)^{k-1} \left(\frac{1}{1-x^2} \right)^{k-2} W_{4,k} = 2x + 28x^2 + 58x^3 + 32x^4.
\end{aligned}$$

Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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A Remark on the Characterization of Triangulated Graphs

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Abstract

In this study, we consider the problem of triangulated graphs. Precisely we give a necessary and sufficient condition for a graph to be triangulated. This gives an alternative characterization of triangulated graphs. Our method is based on the so-called perfectly nested sequences.

Keywords

Triangulated Graphs, Perfect Set, Clique

1. Introduction

It is well known that graph theory provides simple, but powerful tools for constructing models and solving numerous types of interdisciplinary problems and possesses a wide range of applications [1]. Indeed graphs and graph theory can be used in several areas such as software designs, computer networks, social networks, communications networks, information networks, transportation networks, biological networks, managerial problems and others.

In 1736, the problem of the Königsberg bridges was considered as the first problem that laid the foundation of graph theory. Since the start of interest in this well-known problem several questions and problems have arisen.

Regarding the topic of this note, triangulated graphs form an important class among graphs. Since the end of the last century, a lot of work has been done in the theory of triangulated graphs (which we will define properly below). In some references triangulated graphs are variously called rigid circuit graphs [2], chordal graphs [3] or monotone transitive graphs, like in [4].

Triangulated graphs can be characterized in a number of different ways. See [2] [4] [5] [6] [7] [8]. We recall that a vertex v of a graph G is said to be simplicial if

v together with all its adjacent vertices induces a clique in G . An ordering v_1, v_2, \dots, v_n of all the vertices of G forms a perfect elimination ordering of G if each $v_i, 1 \leq i \leq n$, is simplicial in the subgraph induced by v_i, v_{i+1}, \dots, v_n . In [2], we find a necessary condition for a graph G to be triangulated which is the existence of simplicial vertex. In [6], Fulkerson and Gross, state that a graph G is triangulated if, and only if, it has a perfect elimination ordering. Precisely, Fulkerson and Gross showed that the class of triangulated graphs is exactly the class of graphs having perfect elimination orderings. Thus when the input graph G is not triangulated, no perfect elimination of it exists. Rose *et al.* in [9] treat the question of triangulated graphs and also give several characterizations of minimal triangulations. In [10] the author gives a new representation of a triangulated graph called the clique-separator graph, whose nodes are the maximal cliques and minimal vertex separators of the graph.

At the end of this section we mention that triangulated graphs have applications in several areas such as computer vision [11], the solution of sparse symmetric systems of linear equations [12], database management systems [13] and knowledge-based systems [14]. At the end of the paper, we collect two main consequences of triangulated graphs. Another consequence of triangulated graphs is the problem of finding a maximum clique. Indeed, in a triangulated graph we get the answer in polynomial time, while the same problem for general graphs is NP-complete. More generally, a triangulated graph can have only linearly many maximal cliques, while non-chordal graphs may have exponentially many [15].

Basic Concept of Graph Theory

In this section, we will enumerate and explain the basic definitions and the necessary terminology to make use of graph theory. There is a great variety in how different authors presented the basic definitions of the graph theory. Indeed there are many roughly equivalent definitions of a graph.

Most commonly, a graph G is defined as an ordered pair (V, E) , where $V = \{v_1, \dots, v_n, \dots\}$ is called the graph's vertex-set or some times the node set and $E = \{e_1, \dots, e_m, \dots\} \subset \{\{x, y\} \mid x, y \in V\}$ is called the edges set.

Given a graph G , we often denote the vertexset by $V(G)$ and the edgeset by $E(G)$. To visualize a graph as described above, we draw dots corresponding to vertices v_1, \dots, v_n, \dots . Then, for all $i, j \in \{1, \dots, n, \dots\}$ imagine a line between the dots corresponding to vertices v_i, v_j if and only if there exists an edge $\{v_i, v_j\} \in E$. Note that the placement of the dots is generally unimportant; many different pictures can represent the same graph as it is given in the example below **Figure 1**.

A subgraph is a concept akin to the subset. A subgraph has a subset of the vertex set $A \subseteq V$, a subset $E(A) = \{\{x, y\} \in E : x, y \in A\}$ of the edge set E , and each edge's endpoints in the larger graph has the same edges in the subgraph. We denote it by $G(A) = (A, E(A))$.

Example 1.

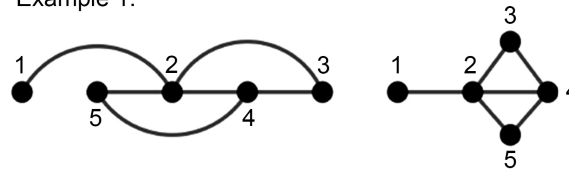


Figure 1. Two different representations of same graph.

Two vertices are said to be adjacent if there is an edge joining them. Given $x \in V$, the set of all adjacent vertices in G is denoted by $Adj(x)$,

$$Adj(x) = \{y \in V, \{x, y\} \in E\}. \tag{1}$$

The word incident has two meanings: On the one hand, an edge e is said to be incident to a vertex v if v is an endpoint of e . On the other hand, two edges are also incident to each other if both are incident to the same vertex. A set C of vertices is a clique if every pair of vertices in C are adjacent. A clique of a graph G is a complete subgraph of G .

A path is a sequence of edges $\langle e_1, \dots, e_N \rangle$ (also denoted (v_1, \dots, v_n)) such that e_i is adjacent to e_{i+1} for all i from 1 to $N-1$, e_i relates v_i to v_{i+1} . Two vertices are said to be connected if there is a path connecting them. A cycle is a path such that the last edge of the path is adjacent to the first and visits each vertices once (in some references they call this elementary cycle).

In a simple graph each edge connects two different vertices and no two edges connect the same pair of vertices. Multi-graphs may have multiple edges connecting the same two vertices. An edge that connects a vertex to itself is called a loop. Two graphs G and G' are said to be isomorphic if there is a one-to-one function from (or, if you prefer, one-to-one correspondence between) the vertex set of G to the vertex set of G' such that two vertices in G are adjacent if and only if their images in G' are adjacent. Technically, the multiplicity of the edges must also be preserved, but our definition suffices for simple graphs, which are graphs without multiple edges or loops.

Definitions

A graph is called triangulated if every cycle of length greater than three possesses a chord, *i.e.* an edge joining two non-consecutive vertices of the cycle. A vertex x of a graph $G = (V, E)$ is called perfect in G if $Adj(x) = \emptyset$ or $(\{x\} \cup Adj(x))$ is a clique. For $A \subseteq V$, we denote by $P(A)$ the set of all perfect vertices of A in $G(A)$ (Figure 2).

Let $G = (V, E)$, be a graph. A sequence $(U_n)_{n \in \mathbb{N}}$ of subsets of $\mathcal{P}(V)$, is said to be perfectly nested on $G = (V, E)$, if it satisfies the following three conditions

- 1) $U_0 = V$.
- 2) $\forall n \in \mathbb{N}$,

$$U_{n+1} \subseteq U_n.$$

- 3) $\forall n \in \mathbb{N}$, $P(U_n) \neq \emptyset$, and

$$U_n \setminus U_{n+1} \subseteq P(U_n).$$

Example 2.

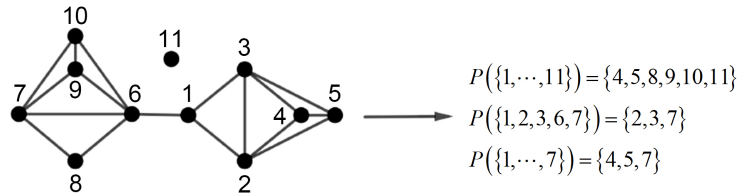


Figure 2. Perfect vertices.

We say that the sequence is stationary perfectly nested, if furthermore the three last conditions, there exists $n_0 \geq 0$ such that we have $P(U_n) = U_n$, for any $n \geq n_0$.

2. The Results

Proposition 1 Let $G = (V, E)$ be a graph and $A \subset P(X)$. Then the following items are equivalents:

- 1) $G = (V, E)$ is triangulated;
- 2) $G = (V \setminus A)$ is triangulated.

Proof. It is clear that 1) implies 2).

For the other sense, let us consider $A \neq \emptyset$. Let $C = (v_1, \dots, v_n)$ be a cycle in $G = (V, E)$. There are two possibilities [(a)].

- 1) If $C \subseteq V \setminus A$, then C has a chord.
- 2) If $C \cap A \neq \emptyset$, there exists $i_0 \in \{1, \dots, n\}$ such that $v_{i_0} \in A$. As v_{i_0} is a perfect vertex, then $Adj(v_{i_0}) \cap C$ is a clique and so, C has a chord. So $G = (V, E)$ is triangulated.

Theorem 2 Let $G = (V, E)$ be a graph. Suppose that there exists a perfectly nested sequence on $G = (V, E)$. Then $G = (V, E)$ is a triangulated graph.

Proof. Let $C = (v_1, v_2, \dots, v_n), n \geq 4$, be a cycle in the graph $G = (V, E)$. Let $(U_n)_n$ a perfectly nested sequences. There exists $n \in \mathbb{N}$, such that

$$C \subseteq U_n, C \not\subseteq U_{n+1}.$$

So,

$$C \cap P(U_n) \neq \emptyset.$$

This ensures that there exists a perfect vertices $x \in C \cap G(U_n)$. So C has a chord.

When V is infinite let us notice that we can construct triangulated graphs which do not have a perfectly nested sequence. Indeed for $V = \mathbb{Z}$ and $E = \{\{n, n+1\}, n \in \mathbb{Z}\}$, $G = (V, E)$ is triangulated and $P(V) = \emptyset$.

Theorem 3 Let $G = (V, E)$ be a graph, with V being a finite set. Then, $G = (V, E)$ is triangulated if and only if there exists a stationary perfectly nested sequence on $G = (V, E)$.

Proof. For the proof, we need the following two basic lemmas:

[4] Let $G = (V, E)$ be a triangulated finite graph. Then $P(V) = \emptyset$. The proof of the last lemma is given in [4] by using the notion of the minimal separators and elimination process. From a different point of view, we can see this by

noting that if we suppose that $P(V) = \emptyset$, starting with a non perfect point x it has necessary two adjacent points x_1, y_1 which themselves are non adjacent to each others. As V is a finite set, a typical end of the process should be in the form of **Figure 3**. At this step, as no point can be adjacent to a single point being a non perfect point it is adjacent to more than two points. This leads forcibly the existence of a non-chordal cycle of length of more than 3. So $G = (V, E)$ is not triangulated. Let $G = (V, E)$ be a connected graph. Let $A \subset P(V)$. Then, $G = (V \setminus A)$, is also a connected graph.

Proof. Let $A \subseteq P(V)$, and $v_1, v_n \in V \setminus A$. As $G = (V, E)$ is a connected graph, there exists a path $P = (v_1, \dots, v_n)$ in $G = (V, E)$, for any $v_{i_0} \in A \cap P$, as v_{i_0-1} and v_{i_0+1} are in $Adj(v_{i_0})$, we get that $v_{i_0-1} \in Adj(V_{i_0+1})$, by the definition of v_{i_0} being a perfect point. So we get a path $P' = (v_1, \dots, v_{i_0-1}, v_{i_0+1}, \dots, v_n)$ in $G = (V \setminus A, E(A))$.

Let us start by the proof of the necessary condition. By Lemma 2()@ we know that when $G = (V, E)$ is triangulated, then $P(V) \neq \emptyset$; For $V_1 \subsetneq P(V)$, we set

$$U_2 = U_1 \setminus V_1, \text{ with } U_1 = V.$$

By Proposition 1, $G(U_2, E(U_2))$ is a triangulated graph, so $P(U_2) \neq \emptyset$. Let $V_2 \subseteq P(U_2)$, we set

$$U_3 = U_2 \setminus V_2.$$

In the same way we construct the perfectly nested sequence. As the set V is finite by assumption we get the stationarity property using the result of Lemma 2, as at the end it remains only one or two perfect points.

For the sufficient condition it is given by Theorem 2.

Below we give an example where using our result we get the answer to the question of triangulated graph after only three steps.

Let us end this section with the following remark. In this particular case, if we take a perfectly nested sequence in Theorem 3 with the property that for any $1 \leq i < n$, $|U_i \setminus U_{i+1}| = 1$, $|U_n| = 1$ we get the characterization given in [4], by taking

$$\alpha : \{1, \dots, n\} \mapsto V.$$

$$\alpha^{-1}(U_i \setminus U_{i+1}) = \{i\}, \alpha^{-1}(U_n) = \{n\}.$$

Example 3.

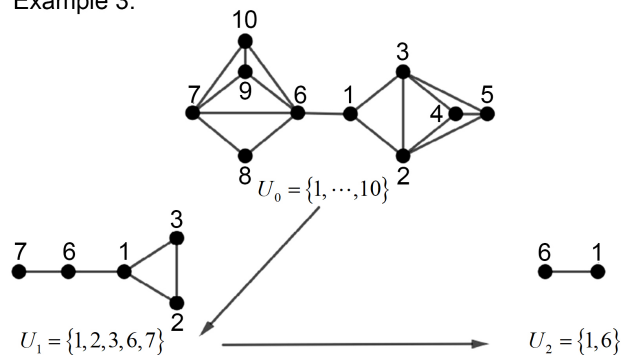


Figure 3. Triangulated graph.

3. Some Consequences of Triangulation

For completeness, below we collect some possible implications of our main result. In addition to the consequence given in the introduction which concerns the answer in polynomial time to some problems for triangulated graphs, the same problem for general graphs is NP-complete. Below we collect two more consequences of triangulated graphs.

3.1. Directed Acyclic Graphs

An orientation D of a finite graph G with n vertices is obtained by considering a fixed direction, either $x \rightarrow y$ or $y \rightarrow x$, on every edge $\{xy\}$ of G .

We call an orientation D acyclic if there does not exist any directed cycle. A directed graph having no directed cycle is known as a directed acyclic graph, we write DAG for short. DAGs provide frequently used data structures in computer science for encoding dependencies. The topological ordering is another way to describe a DAG. A topological ordering of a directed graph $G = (V, E)$ is an ordering of its vertices as v_1, v_2, \dots, v_n such that for every arc $v_i \rightarrow v_j$, we have $i < j$.

Let us consider an acyclic orientation D of G . An edge of D , is said to be dependent (in D) if its reversal creates a directed cycle in the resulted orientation. Note that $v_i \rightarrow v_j$ is a dependent arc if and only if there exists a directed walk of length at least two from v_i to v_j . We denote by $d(D)$, the number of dependent arcs in D . A graph G is called fully orientable if it has an acyclic orientation with exactly d dependent arcs for every number d between $dmin(G)$ and $dmax(G)$, the minimum and the maximum values of $d(D)$ overall acyclic orientations D of G . An acyclic orientation with 6 dependents arcs (**Figure 4**).

In [16], the authors show that all chordal graphs are fully orientable. Let us denote the complete r -partite graph each of whose partite sets has n vertices by $K_r(n)$. As it is also known [17] that $K_r(n)$ is not fully orientable when $r \geq 3$ and $n \geq 2$. One deduces that the acyclic orientation $K_3(2)$ given in the example is not a triangulated graph. If we consider the graph of example 3, as it is a triangulated graph we deduce that it is a fully orientable graph.

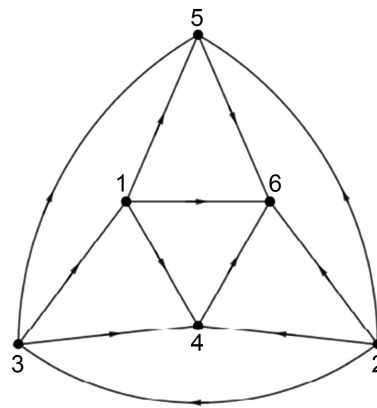


Figure 4. An acyclic orientation.

3.2. Chromatic Number

A graph coloring is an assignment of labels, called colors, to the vertices of a graph such that no two adjacent vertices share the same color.

- 1) A Clique number $\omega(G)$, is the maximum size of a clique in G .
- 2) A Chromatic number $\chi(G)$, is the minimum coloring number.

For a general graph G , we have

$$\chi(G) \geq \omega(G). \quad (2)$$

For triangulated graphs, we have equality instead of inequality in Equation (2).

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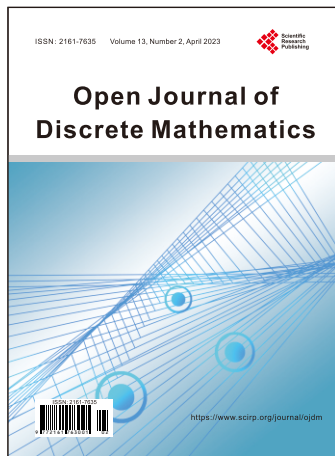
Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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