

THE CHROMATIC NUMBER OF GENERALIZED FIBONACCI PRIME DISTANCE GRAPH

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Abstract. Fibonacci numbers and distance graphs play a very important role in day to day applications. In this paper we construct the generalized Fibonacci prime distance graph and determine its chromatic number. We also indicate here an interesting application involving graph vertex coloring and Fibonacci numbers in the problem of sequence design of nucleic acids a wonderful work done by Von Mag.Ingrid G.Abfalter in [9].

Keywords: Prime distance graphs, Chromatic number, Fibonacci numbers, Generalized Fibonacci Numbers.

2000 AMS Subject Classification: 05C15

1. Introduction

Graph Theory is a branch of mathematics that investigates the properties of graphs and their relations. Structures that can be presented as graphs are ubiquitous and many problems of practical interest can thus be modeled as graph theoretical problems. In chemistry we find two main types of correspondency between graphs and chemical categories: (i) The structural or constitutional graph that corresponds to a molecule or a group of molecules, where the nodes symbolize the atoms and edges symbolize covalent

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bonds It was this type of graph that inspired Cayley to develop a procedure for counting the constitutional isomers of alkanes and (ii) the reaction graph that corresponds to a reaction mixture, where points symbolize chemical species and lines represent conversions between them. Graph coloring is a well known NP-complete problem [8]. The graphs considered in this paper are finite, simple and undirected.

An interesting motivation for writing this paper is the following: Fibonacci numbers work in everything from the microscopic materials like DNA molecule to the distance between our eyes, ears, hands, even the distance of the planets in the solar system and the way they move in the space, even the distance and pathway of the stars in the universe and finally in the currencies?prices and the way they move up and down. Fibonacci numbers can be found anywhere in the world. The Fibonacci numbers can be used to approximately convert from miles to kilometers and back. Take two consecutive Fibonacci numbers, for example 5 and 8. And you're done converting. There are 8 kilometers in 5 miles. To convert back just read the result from the other end - there are 5 miles in 8 km! Again consider the consecutive Fibonacci numbers 21 and 34. What this tells us is that there are approximately 34 km in 21 miles and vice versa. (The exact answer is 33.79 km. If you need to convert a number that is not a Fibonacci number, just express the original number as a sum of Fibonacci numbers and do the conversion for each Fibonacci number separately. For example, how many kilometers are there in 100 miles? Number 100 can be expressed as a sum of Fibonacci numbers 89 + 8 + 3. Now, the Fibonacci number following 89 is 144, the Fibonacci number following 8 is 13 and the Fibonacci number following 3 is 5. Therefore the answer is 144 + 13 + 5 = 162kilometers in 100 miles. This is less than 1% off from the precise answer, which is 160.93 km. Another example, how many miles are there in 400 km? Well, 400 is 377 + 21 + 212. Since we are going the opposite way now from miles to km, we need the preceding Fibonacci numbers. They are 233, 13 and 1. Therefore there are 233 + 13 + 1 = 247miles in 400 km. (The correct answer is 248.55 miles.). If the distance to be converted can be expressed as a single Fibonacci number, then for numbers greater than 21 the error is always around 0.5%. However, if the distance needs to be composed as a sum

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THE CHROMATIC NUMBER OF GENERALIZED FIBONACCI PRIME DISTANCE GRAPH 1453 of n Fibonacci numbers, then the error will be around $\operatorname{sqrt}(n)$?.5%. We know that Fibonacci numbers have a property that the ratio of two consecutive numbers tends to the Golden ratio as numbers get bigger and bigger. The Golden ratio is a number and it happens to be approximately 1.618. Coincidentally, there are 1.609 kilometers in a mile, which is within 0.5% of the Golden ratio. Now that we know these two key facts, we can figure out how to do the conversion. If two consecutive Fibonacci numbers, are F_{n+1} and F_n , then F_{n+1}/F_n is approximately 1.618. Since the ratio is also almost the same as kilometers per mile, we can write $F_{n+1}/F_n = [\text{mile}]/[\text{km}]$. It follows that $F_n[\text{mile}] =$ $F_{n+1}?[km]$, which translates to Englishas" n-th Fibonacci number inmiles is the same as (n+1)-th Fibona

2. Fibonacci Sequences

Fibonacci sequences are interesting sequences in all of mathematics. Fibonacci numbers F_k is defined by the second-order linear recurrence formula and initial terms:

$$F_{k+1} = F_k + F_{k-1}, F_0 = 0, F_1 = 1.$$

The generalization of this sequence $F_k^{(n)}$, the Fibonacci *n*-step sequence is defined by a linear recurrence formula of order n > 1:

$$F_{k+1}^{(n)} = F_k^{(n)} + F_{k-1}^{(n)} + \dots + F_{k-n+1}^{(n)} \dots (1)$$

and initial terms

$$F_{1-n}^{(n)} = 1, F_k^{(n)} = 0, \ k = -n+2, ..., 0....(2)$$

Let us indicate the generation of generalized Fibonacci n-step sequences for certain values of n and k.

n = 2 $F_0^{(2)} = 0, F_{-1}^{(2)} = 1; F_1^{(2)} = F_0^{(2)} + F_{-1}^{(2)} = 0 + 1 = 1 ; F_2^{(2)} = F_1^{(2)} + F_0^{(2)} = 1 + 0 = 1;$ $F_3^{(2)} = F_2^{(2)} + F_1^{(2)} = 1 + 1 = 2 \text{ and so on.}$ n = 3

$$\begin{split} F_{0}^{(3)} &= 0, F_{-1}^{(3)} = 0, F_{-2}^{(3)} = 1; \ F_{1}^{(3)} = F_{0}^{(3)} + F_{-1}^{(3)} + F_{-2}^{(3)} = 0 + 0 + 1 = 1; \ F_{2}^{(3)} = F_{1}^{(3)} + F_{0}^{(3)} + F_{-1}^{(3)} = 1 + 0 + 0 = 1; \ F_{3}^{(3)} = F_{2}^{(3)} + F_{1}^{(3)} + F_{0}^{(3)} = 1 + 1 + 0 = 2 \text{ and so on.} \end{split}$$

n = 6

$$\begin{split} F_{0}^{(6)} &= 0, F_{-1}^{(6)} = 0, F_{-2}^{(6)} = 0, F_{-3}^{(6)} = 0, F_{-4}^{(6)} = 0, F_{-5}^{(6)} = 1; \ F_{1}^{(6)} = F_{0}^{(6)} + F_{-1}^{(6)} + F_{-2}^{(6)} + F_{-3}^{(6)} + F_{-4}^{(6)} + F_{-4}^{(6)} + F_{-3}^{(6)} + F_{-4}^{(6)} + F_{-3}^{(6)} + F_{-4}^{(6)} +$$

The sequence generated by equations (1) and (2) is also known as the k-generalized Fibonacci numbers, which are discussed by Flores[5]. Observe that equation (1) is equivalent to the three-term recursions $F_{k+1}^{(n)} = 2F_k^{(n)} - F_{k-n}^{(n)}$ which are computationally superior for large n, and which show that n-step sequence grow at a rate less than 2^k . This recursion requires one more initial term, which we can take to be $F_1^{(n)} = 1$.

Dickson[3] cites a long history of generalized of the Fibonacci numbers. Miles[6] used equation (1) in 1960. Benjamin and Quinn [1] briefly discussed a combinatorial interpretation of these n-step sequences.

The usual Fibonacci numbers are obtained for n = 2. For small values of n, these sequences are called tribonacci (n = 3), tetranacci or quadranacci (n = 4), Pentanacci or pentacci (n = 5), hexanacci or esanacci (n = 6), heptanacci (n = 7) and octanacci (n = 8).

	k	1	2	3	4	5	6	7	8	9	10	11	12	13	14
n															
2		1	1	2	3	5	8	13	21	34	55	89	144	233	377
3		1	1	2	4	7	13	24	44	81	149	274	504	927	1705
4		1	1	2	4	8	15	29	56	108	208	401	773	1490	2872
5		1	1	2	4	8	16	31	61	120	236	464	912	1793	3525
6		1	1	2	4	8	16	32	63	125	248	492	976	1936	3840
7		1	1	2	4	8	16	32	64	127	253	504	1004	2000	3984
8		1	1	2	4	8	16	32	64	128	255	509	1016	2028	4048
9		1	1	2	4	8	16	32	64	128	256	511	1021	2040	4076

Table 1:

Table 1 shows Fibonacci *n*-step sequences where the primes are in **bold** letters.

Note that every Mersenne prime- a prime of the form $2^p - 1$ appears in these sequences as $F_{p+2}^{(p)}$. THE CHROMATIC NUMBER OF GENERALIZED FIBONACCI PRIME DISTANCE GRAPH 1455 The above observation in Table 1 indicates that there are only small number of Fibonacci prime numbers in the respective sequences. The Fraction of odd numbers in the sequence $F_k^{(n)}$ is 2/(n+1). Hence, there are only a fewer prime numbers.

3. Chromaticity of the Fibonacci Graph

A prime distance graph is a graph G(Z, P) with the set of integers as vertex set and with an edge joining two vertices u and v if and only if $|u - v| \in P$ where P is the set of all prime numbers. We call a graph a Fibonacci prime distance graph, denoted $G_k^{(n)}(Z, D)$ if $D \subseteq P$ is a set of primes appearing in the Fibonacci *n*-step sequence.

A k-coloring of a graph G is an assignment of k different colors to the vertices of G such that adjacent vertices receive different colors. The minimum cardinality k for which G has a k-coloring is called the chromatic number of G and is denoted by $\chi(G)$.

By a chromatic subgraph of a graph G we mean a minimal subgraph of G with the same chromatic number as G. What class of graphs will include a chromatic subgraph of G(Z, D) for $D \subseteq Z$?.

A graph G is color critical if its only chromatic subgraph is G itself. For any positive integer m, n, let G(m, n) be the graph comprising (m + 1) distinct vertices $u_0, u_1, ..., u_m$ and m distinct subgraphs $H_1, ..., H_m$ each of which is a copy of K_n , (Where K_n is the complete graph on n vertices) such that u_0 is adjacent to u_m and each vertex of H_i is adjacent to u_{i-1} and u_i , for $1 \le i \le m$. $G(m, 1) \cong C_{2m+1}, G(1, n) \cong K_{n+2}$, where C_{2m+1} is the cycle on 2m+1 vertices.

Theorem 3.1.
$$\chi(G_k^{(n)}(Z,D)) = \begin{cases} 3, \text{ for all } n \geq 3, \text{ and } k \geq 1; \\ 4, \text{ if } n = 2 \text{ and } k \geq 1. \end{cases}$$

Proof. We divide the proof into the following Lemmas.

Lemma 1. For any positive integers m, n the graph G(m, n) is color critical with $\chi(G(m, n)) = n + 2$.

Proof of Lemma 1.

Suppose we had a proper coloring of G(m, n) using n + 1 colors. Without loss of generality let u_0 has color 0 and the vertices of H_1 have colors 1, 2, ..., n. Since u_1 is adjacent to all the vertices of H_1 it follows that u_1 has color 0. Iterating this argument shows that u_m has color 0. But this is impossible, since u_m is adjacent to u_0 . Hence any proper coloring of G(m, n) requires at least n + 2 colors. Clearly n + 2 colors are sufficient, so $\chi(G(m, n)) \leq n + 2$. Also if any edge is removed from G(m, n) the resulting graph has chromatic number n + 1, so G(m, n) is color critical.

We now compute the $\chi(G(Z, P))$.

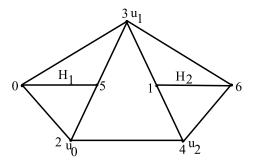


FIGURE 1. In the figure H_1 and H_2 are isomorphic to K_2

Lemma 2. $\chi(G(Z, \{2, 3, 5\})) = 4$ and hence $\chi(G(Z, P)) = 4$. **Proof of Lemma 2.**

Let each integer x be assigned a color class i precisely when $x \equiv i \pmod{4}$, for $0 \leq i \leq 4$. Since integers assigned to the same color differ by a multiple of 4, they are not adjacent in G(Z, P), so $\chi(G(Z, P)) \leq 4$. Since $G(Z, \{2, 3, 5\}) \subseteq G(Z, P)$ and χ is monotone, we have $\chi(G(Z, \{2, 3, 5\})) \leq \chi(G(Z, P))$. But as $G(Z, \{2, 3, 5\}) \supseteq G(2, 2)$ we have $\chi(G(Z, \{2, 3, 5\})) \geq 4$ where G(2, 2) is shown in the Figure determined by the vertices $u_0 = 2, u_1 = 3, u_2 = 4$ and the subgraphs H_1, H_2 with vertex sets $\{0, 5\}$ and $\{1, 6\}$ respectively. The proof now follows from the Lemma 1.

In view of Lemma 2, we can allocate the subsets D of P to four classes, according as G(Z, D) has chromatic number 1,2,3 or 4. Obviously empty set is the only member of class 1 and every singleton subset is in class 2. The following result addresses the classification of subsets with at least two elements.

First we prove the following Sub Lemma.

SubLemma 3.1. For any positive integer n, let $D = \bigcup_{k=0}^{\infty} [k(n+1)+1, k(n+1)+n]$. Then $\chi(G(R,D))$ is at most n+1.

Proof of Sublemma 3.1.

Let all points of the real line be assigned to color classes numbered 0, 1, ..., n such that x has color i precisely when $\lfloor x \rfloor \equiv i \pmod{n+1}$. We will show that this is a proper coloring of G(R, D). Let x, y be two reals assigned to each color class i with x < y. Then there are integers r, s such that $r \leq s$ and $r(n+1) + i \leq x < r(n+1) + i + 1$ and $s(n+1) + i \leq y < s(n+1) + i + 1$. If r = s then y - x < 1, so x is not adjacent to y in G(R, D). If r < s, let t = s - r. Then we have t(n+1) - 1 < y - x < t(n+1) + 1, so x and y will be adjacent only if there is some integer $k \geq 0$ such that [k(n+1) + 1, k(n+1) + n] has a non empty intersection with (t(n+1) - 1, t(n+1) + 1). This happens precisely when k(n+1) + 1 < t(n+1) + 1 and k(n+1) + n > t(n+1) - 1. But then we get k < t and k+1 > t, which then implies that t is not an integer, a contradiction. Therefore the distance between x and y is not in D, so they are not adjacent in G(R, D).

Proof of Lemma 3.

Now take n = 1 in Sub Lemma 3.1. We see that D is the set of odd positive integers and hence $\chi(G(Z, \{r, s\}))$ is at most 2. Since $G(Z, \{r, s\})$ contains $K_2, \chi \ge 2$ and hence the Sub Lemma 3.1.

Lemma 4. Let $D \subseteq P$, with $|D| \ge 2$. Then D may be classified as follows:

a) D is in class 2 if $2 \notin D$; otherwise D is in class 3 or class 4.

b)If $2 \in D$ and $3 \notin D$, then D is in class 3.

Proof of Lemma 4(a).

By the Lemma 3, if D is a subset of the odd primes then it is in class 2. If D contains 2 and any odd prime p, then G(Z, D) contains a cycle $v_0v_1...v_pwv_0$ where $v_i = 2i$ for $0 \le i \le p$, and w = p. This cycle has order p + 2, which is odd, so has chromatic number 3. Now with Lemma 2 we say that D is in class 3 or class 4.

Proof of Lemma 4(b).

Here a proper coloring of G(Z, D) is obtained by assigning the integer x to color class *i* precisely when $x \equiv i \pmod{3}$, for $0 \leq i < 3$. So in view of Lemma 4(a), D is in class 3.

Now as $G_k^{(n)}(Z,D) \subseteq G(Z,P)$ we have by Lemma 2 an easy lower and upper bound namely $1 \leq \chi(G_k^{(n)}(Z,D)) \leq 4$. First consider the graph $G_k^{(2)}(Z,D)$. As $\{2,3,5\} \subseteq D$ we have by Lemma $2 \chi(G_k^{(2)}(Z,D)) = 4$. But as $2 \in D$ and $3 \notin D$ for all n and k when $n \geq 3$ we deduce that $\chi(G_k^{(n)}(Z,D)) = 3$ for all $n \geq 3$ and all k.

4. An Interesting Application

Sequence design represents an integral part of research on nucleic acids and is equally important for industrial applications. The development of new theoretical approaches and hence the implementation of new program packages that assist with the rational design of nucleic acids is therefore of fundamental interest.

Fibonacci sequences are used in the creation of a software tool to support the rational design of RNA molecules capable of forming two or more alternative metastable structures. This required the creation of a logical information model, isolating relevant aspects of the biological problem as posed, and incorporating these into a graph-based mathematical model. An appropriate design of an algorithm based on this model reduces the problem to vertex coloring the union of all prescribed outerplanar secondary structure graphs, called dependency-graph. Starting from a decomposition of this dependency graph, colorings can then be obtained by a dynamic programming procedure. The sequences so designed can then be optimized for particular properties by means of standard optimization heuristics. The connection between sequence design and vertex-colorings is interestingly worth probing. THE CHROMATIC NUMBER OF GENERALIZED FIBONACCI PRIME DISTANCE GRAPH 1459

Biopolymers such as RNA, DNA or proteins fold into well-defined three dimensional structures that are of the utmost importance for their biological functions. The most fundamental features of the 3D shape of these molecules are captured in so-called connection graphs which have the atoms of small molecules or the monomers of a biopolymer as their vertices and the connections between spatially adjacent objects as their edges. Obviously, this simplification discards many structural details, yet it retains and exposes a wealth of structural information that can be gained from a variety of experimental and computational methods. Biopolymers share a number of common features that distinguish them from other classes of molecular contact graphs. They have a spanning path that corresponds to the covalent backbone and the remaining non-covalent bonds determine the fold of the 3D structure of the molecule. Nucleic acids in particular form a special type of contact structure called secondary structure.

The primary structure of RNA is simply the sequence of nucleotides, the secondary structure is represented by a graph where the vertices are the bases and the edges depict the contacts (hydrogen bonds) between these bases and the backbone along the sequence. Thus the secondary structure is actually a topology that indicates which sequence positions are adjacent, but says nothing about the spatial distances between the positions. Therefore, it is not a real two-dimensional representation of the structure. The so-called tertiary structure depicts the spatial arrangement of the secondary structure elements, i.e. the real three dimensional fold of the molecule.

A nucleic acid secondary structure can be understood as the set Θ of base pairs. The graph of the secondary structure consists of a set of vertices (bases) V = 1, 2, ..., i, ..., n and a set E of edges $i?j, 1 \le i \le j \le n$ with the following constraints:

- (i) (backbone) for all $i < n : i?(i+1) \in E$ and
- (ii) (binary pairing) for each i there is at most one $k \neq i 1, i + 1$ where $i?k \in E$, and
- (iii) (pseudoknots are not allowed) if $i?j \in E$ and $k?l \in E$ and i < k < j then i < l < j.

According to this definition the set of vertices just contains the enumerated set of nucleotides of the sequence of the length n. The set of edges contains the backbone of the

chain and the base pairs where base pairing between consecutive positions i and i + 1 is ruled out. In practice, this does not represent a limitation, since steric reasons make it almost impossible for the bases i and i + 1 to form a base pair. To be able to compute secondary structures we now have to define a set $B \subset A \times A$ of allowed base pairs for the alphabet A of riobonucleotides. The dependency graph Ψ of a collection of secondary structures $\{\Theta_i\}$ with n nucleotides consists of n vertices and edges connecting k with l if and only if (k, l) is a base pair in at least one of the secondary structures Θ_i .

Given a secondary structure Θ , our choice of sequences compatible with Θ is restricted, since for each pair $i, j \in \Theta$ and each sequence x, the positions x_i and x_j must be able to form one of the permitted base pairs. We write $C[\Theta]$ for the set of all sequences that are compatible with Θ in the sense that every base pair $(i, j) \in \Theta$ is realized by a pair $(x_i, x_j) \in B$ of pairing nucleotides. It follows that the number of sequences compatible with a given structure $|C[\Theta]|$ is $|C[\Theta]| = |A|^{|\gamma|}|B|^{|\Theta|}$ (1) (where γ is the set of unpaired positions) since for each $i \in \gamma$ we can choose any random letter of the nucleic acid alphabet and for each pair we may choose one of the possible base pairs.

The first obvious question that arises when trying to design multi-stable sequences is: Can sequences be found that fold into two (and consequently more) predefined structures and if so, how many, i.e. what is the size of the cardinality of the intersection of two given secondary structures? This is answered by the Intersection Theorem.

Intersection Theorem: "If the nucleic acid alphabet admits at least one type of complementary base pairs, then, for any two secondary structures Θ_1 and Θ_2 there exists at least one sequence that is compatible with both structures, in symbols: $C[\Theta_1] \cap C[\Theta_2] \neq \Phi$ "...(2). This means whenever we have symmetric base pairs, i.e. $XY \in B$ implies $YX \in B$, we can always find sequences that can fold into both θ_1 and Θ_2 . An abstract group-theoretical proof can be found in [7], for a purely combinatorial proof see [2].

In order to determine the cardinality of the intersection of Θ_1 and Θ_2 we display the graph as the conjunct union of its connected components: $\Psi^* = \bigcup \Psi$. Depending on the predefined structures there can be found three kinds of components:

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(i) Positions that are unpaired in both structures correspond to isolated vertices in the graph.

(ii) Positions that are paired in both secondary structures correspond to paths of the length one.

(iii) Base-pairing positions that occur only in one of the two different structures are part of paths.

Using this definition we can write: $C[\Theta_1] \cap C[\Theta_2] = \prod_{\text{components}\Psi \text{of}\Psi^*} S(\Psi) \dots$ (3) where $S(\Psi)$ describes the number of sequences compatible with a connected component Ψ of Ψ^* . For (i) an isolated vertex K_1 we get $S(\{i\}) = S(K_1) = |A|$, i.e. the number of nucleotides in the alphabet, for (ii) paths of the length 1 $S(K_2) = |B|$, the number of allowed base pairs, for (iii) the compatible sequences of paths can be counted by using recursive formulae called Fibonacci numbers (paths): $S(P_n) = 2(F(n) + F(n+1)) = 2F(n+2)\dots$ (4).

The important observation is that a sequence that is compatible with all secondary structures can be viewed as a coloring of the vertices of the dependency graph such that adjacent vertices have colors $(a, b) \in B$, the alphabet of base-pairs. Then one can use a dynamic programming algorithm that counts the compatible sequences of a block and produces colorings during the backtracking procedure. Suppose that we have fully decomposited graph and obtained the ear decompositions of the blocks. Then we can initiate the counting and coloring routine of each connected component of the dependency graph. We start by colouring blocks and then proceed outwards towards the paths that are connected via cut-vertices until each connected component is completely coloured. The cut-vertices are treated just like attachment points. The compatible sequences of blocks are counted recursively starting from the utmost ear proceeding inwards to the central circle. In each step of the counting procedure while concatenating the ears, we have to compute and memorize the number of compatible colourings of paths given each consistent assignment of the attachment points. Then use recursive dynamic programming procedure for determining the number of sequences that start with a certain base i and end in a certain base

k for all path lengths l = n (n is the maximum path length in the graph). Next generate the matrix entries in the following manner: The number of paths with length l that start with base i and end in base k is the sum over all path matrix entries PM(i,j) of the path length l-1 times 1, if (j,k) is an allowed base pair, and times zero if (j,k) cannot form a base pair. The solution to the smallest sub problem of this dynamic programming algorithm finding assignments for paths of the length one- is clearly the base-pairing matrix. Proceeding bottom-up from this sub-instance we can generate the path matrices for paths of arbitrary length. The implementation of this counting procedure is very complex although it is based on a dynamic programming algorithm. It is the upkeep and update of the colouring matrices that store consistent assignments for attachment points and their multiplicity that result from each concatenation step which require a sophisticated table management. The reason is that as we concatenate the ears of the graph the table size does not always grow steadily but also decreases again when colourings become impossible due to constraints of attachment vertices in later steps. When counting on the blocks is finished, the counting procedure continues in an analogous manner on all remaining biconnected components of each connected component, with the exception that path concatenation now considers fixed assignments of cut vertices rather than attachment points. The result is a table of consistent assignments for all attachment points and cut vertices and the number of compatible sequences, given each assignment, which is then used to sample colourings with uniform distribution by means of stochastic backtracking.

From Table 1 we also infer that the generalized Fibonacci prime distance graph becomes sparser and sparser as n increases. However it is quite interesting to note that the presence of 2 in the distance set D somehow manage to induce a clique of size 3 in $G_k^{(n)}$ however large n is. Of course this is quite possible as primes are infinitely many. Lemmas 1,2,3,4 and Sub Lemma 3.1 are given in [4]. We have reproduced the proof here for the ease of reading and completeness. We wish to probe further the application of Theorem 1 to sequence design of nucleic acids elsewhere in the future.

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