Continuant, caterpillar, and topological index Z. Fastest algorithm for degrading a continued fraction

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Abstract Manipulation of continued fraction, either finite and infinite, was shown to be greatly simplified and systematized by introducing the topological index *Z* and caterpillar graph. The continuant which was introduced by Euler in 18 century for solving continued fraction problems was shown to be identical to the *Z*-index of the caterpillar graph derived from the continued fraction concerned. Then the fastest algorithm for solving the Pell equations was obtained. Further, graph-theoretical interpretation for Fibonacci and Lucas numbers, and generalized Fibonacci numbers was obtained.

1. Introduction

According to the standard recipe developed by Lagrange simple continued fractions, either finite or infinite periodic, are known to play a key role in solving the Pell equation $x^2 - Dy^2 = \pm 1$.[1,2] For degrading a given continued fraction the so-called "continuants" were proposed by Euler.[3-6] It was recently found that instead of following iterative steps for this degradation Bhaskara II found more efficient jumping algorithm for reaching the final result 600 years before these European giants in mathematics.[7]

In this paper the continuant is shown to be identical to the topological index Z,[8,9] of a caterpillar graph[10,11] composed solely of the terms of the continued fraction concerned. Further by using graph-theoretical technique developed by the present author the smallest solution of the above Pell equation can be represented by a 2×2 or 3×3 determinant whose elements are the Z-indices of four subgraphs of the caterpillar.

Although all these techniques come from the elementary graph theory,[12] in which the present author has been engaged to solve physicochemical problems for more than three decades,[13] all of them are easy enough for those with no prior knowledge of the graph theory to follow. This method can be applied not only to solve quickly the Pell equation but also to get rational number approximant of quadratic irrational or even some transcendental numbers efficiently. Application to information sciences and physics is also open.

2. Preliminaries

2.1. Continued fraction

In this paper simple(st) continued fractions are treated, which may be finite or infinite.[14] A finite continued fraction Q_N is expressed and denoted by a finite set of elements a_n with all positive integers as

$$Q_N = a_0 + \cfrac{1}{a_1 + \cfrac{1}{a_2 + \cfrac{1}{\cdots + \cfrac{1}{a_{N-1} + \cfrac{1}{a_N}}}}} = [a_0; a_1, a_2, \cdots, a_{N-1}, a_N]. \tag{2.1}$$

In principle a_0 can be negative, but as will be shown in the following discussion, only non-negative values are assumed here. One may denote an infinite continued fraction Q as

$$Q = [a_0; a_1, a_2, \cdots], \tag{2.2}$$

but a recursive one is expressed as $[a_0; \overline{a_1, a_2, \cdots, a_k}]$ by using a finite number of elements. Although other types of recursion are possible, generality of the present discussion is not lost by ignoring those cases. The purpose of this paper is to introduce the fastest algorithm for calculating the value of Q_N and finite convergents of Q by transforming the continuant polynomials into a 2×2 or 3×3 determinant obtained from simple manipulation of a_n's from a_0 to a certain point.

2.2 Continuant and the related determinant

[Def. 1] The continuant polynomial, or simply continuant, which was extensively discussed by Euler, can be defined recurrently, as follows:[3-5]

$$\mathrm{K}_0() = 1;$$

$$\mathrm{K}_1(x_1) = x_1;$$

$$\mathrm{K}_2(x_1, x_2) = x_1 x_2 + 1;$$

$$\mathrm{K}_n(x_1, x_2, \cdots, x_n) = x_n \mathrm{K}_{n-1}(x_1, x_2, \cdots, x_{n-1}) + \mathrm{K}_{n-2}(x_1, x_2, \cdots, x_{n-2}). \tag{2.3}$$

The continuant has been known to be reversible as shown in the following three theorems whose proofs may not be necessary here.

[Theorem 1] Reversible character.

$$\mathrm{K}_n(x_1, x_2, \cdots, x_n) = \mathrm{K}_n(x_n, \cdots, x_2, x_1). \tag{2.4}$$

This can be proved by mathematical induction. □

[Theorem 2] Recursive relation (cf. (2.3)).

$$\mathrm{K}_n(x_1, x_2, \cdots, x_n) = x_1 \mathrm{K}_{n-1}(x_2, x_3, \cdots, x_n) + \mathrm{K}_{n-2}(x_3, x_4, \cdots, x_n). \tag{2.5}$$

This can also be proved by mathematical induction. □

[Theorem 3] Tridiagonal determinantal expression.

$$\mathrm{K}_n(x_1, x_2, \cdots, x_n) = \begin{vmatrix} x_1 & 1 & 0 & 0 & \cdots & 0 \\ -1 & x_2 & 1 & 0 & \cdots & 0 \\ 0 & -1 & x_3 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & -1 & x_{n-1} & 1 \\ 0 & 0 & \cdots & 0 & -1 & x_n \end{vmatrix} . \qquad (2.6)$$

This can also be proved by mathematical induction. □

It is to be remembered that a tridiagonal determinant is easy to be degraded, and Theorem 3 will actually play a very important role in the present theory. More complicated theorems for the reversibility of the continuant are known but they are practically unnecessary in our discussion.

2.3 Fibonacci and Lucas numbers

Either from Def. 1 or Theorem 3, the Fibonacci (F_n) and Lucas (L_n) numbers can directly be obtained, respectively, to be

$$F_n = \mathrm{K}_n(1, 1, \cdots, 1) \qquad (n\ 1\text{'s}), \qquad (2.7)$$

and

$$L_n = \mathrm{K}_n(1, 2, 1, \cdots, 1) \qquad (1 \text{ and } n-2\ 1\text{'s}), \qquad (2.8)$$

both of them obey the following recursion formula:

$$f_n = f_{n-1} + f_{n-2} \quad (f: F \text{ and } L) . \qquad (2.9)$$

However, notice that in this paper the initial conditions of F_n are chosen to be

$$F_0 = F_1 = 1, \qquad (2.10)$$

contrary to the conventional ones as $F_0 = 1, F_1 = 2,$ [15,16] while for L_n the widely accepted

$$L_0 = 2, L_1 = 1, \qquad (2.11)$$

are adopted. In Table 1 the lower members of F_n and L_n are given for convenience of the later discussion.

Table 1. Fibonacci and Lucas numbers

n	0	1	2	3	4	5	6	7	8	9	10
F_n	1	1	2	3	5	8	13	21	34	55	89
L_n	2	1	3	4	7	11	18	29	47	76	123

Advantage of our definition for F_n will be shown several times later in this paper. Here let us enjoy to see the following pairs of expressions in terms of hypergeometric functions,[17]

$$F_n = {}_2F_1\,(-n/2, (1-n)2; -n; -4) \qquad (2.12)$$

and

$$L_n = {}_2F_1\,(-n/2, (1-n)2; 1-n; -4), \qquad (2.13)$$

where our initial conditions are adopted.

Next consider the sequence $\{G_n\}$ with the following properties: $G_1=a$, $G_2=b$, and $G_n=G_{n-1}+G_{n-2}$ ($n\geq3$). The ensuing sequence

$$a, b, a+b, a+2b, 2a+3b, 3a+5b, 5a+8b, \cdots \tag{2.14}$$

is called the generalized Fibonacci numbers or generalized Fibonacci sequence.[16)]

[Theorem 4] Recursive relation of G_n.

$$G_{m+n} = G_m F_n + G_{m-1} F_{n-1} \tag{2.15}$$

From (2.14) the following relations can directly be derived:

$$G_n = G_1 F_{n-3} + G_2 F_{n-2}$$
$$= G_2 F_{n-4} + G_3 F_{n-3} = \cdots$$
$$= G_{l-1} F_{n-l-1} + G_l F_{n-l}.$$

Then by putting n=m+n and l=m into the above identity we get (2.15). □

2.4 Rational number and continued fraction

If a (positive) rational number $Q_N = p_N/q_N$, with $(p_N, q_N)=1$, is given, it is straightforward to get its continued fraction expressions as in (2,1). In reverse it is well known that if the set of all the elements of a continued fraction $[a_0;a_1,a_2,\cdots,a_{N-1},a_N]$ are given, the parent rational number can be expressed by the ratio of a pair of continuants as in the following theorem:

[Theorem 5] For rational number $Q_N > 1$ we have

$$Q_N = \frac{\mathrm{K}_{N+1}(a_0,a_1,\cdots,a_N)}{\mathrm{K}_N(a_1,a_2,\cdots,a_N)}, \tag{2.16}$$

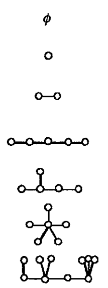
while for $Q_N < 1$ we have

$$Q_N = \frac{\mathrm{K}_{N-1}(a_2,a_3,\cdots,a_N)}{\mathrm{K}_N(a_1,a_2,\cdots,a_N)}. \quad \Box \tag{2.17}$$

Notice that (2.16) becomes to be equal to (2.17) by putting $a_0 = 0$ (from Theorem 2). Then in this sense (2.16) suffices for all positive values of Q_N.

2.5 Graphs G and its topological index *Z*

A graph is a mathematical object composed of vertices and edges.[10-12)] In this paper only those graphs with no directed edge, no multiple edge, and no cycle are concerned, i.e., non-directed tree graph. In Fig. 1 several examples of small trees are shown.



		$p(\mathrm{G},k)$ $k=0$	1	2	3	Z
vacant graph	S_0	1				1
vertex	S_1	1				1
edge	S_2	1	1			2
path	S_5	1	4	3		8
tree	$C_4(1,2,1,1)$	1	4	2		7
star	$K_{1,5}$	1	5			6
caterpillar	$C_4(2,3,1,4)$	1	9	22	11	43

Fig. 1. Various kinds of tree graphs, their notations, and *Z*-indices.

For characterizing a graph G the topological index Z was proposed to be defined by the present author as follows.[8,9] First define non-adjacent number $p(G,k)$ as the number of ways for choosing k disjoint edges from G. Here $p(G,0)$ is defined to be unity for all the graphs including the vacant graph, and $p(G,1)$ is equal to the number of edges in G. By using the set of $p(G,k)$'s the topological index $Z(G)$ is defined as

$$Z(G) = \sum_{k=0}^{m} p(G,k) \quad , \qquad (2,18)$$

Where m is the maximum number of k, or $m = \lfloor N/2 \rfloor$ with N being the number of vertices of G. In other words, $Z(G)$ is the total sum of perfect and imperfect matchings.

The characteristic polynomial of G with N vertices is defined as

$$P_G(x) = (-1)^N \det(\mathbf{A} - x\mathbf{I}), \qquad (2.19)$$

by using the $N \times N$ adjacency (**A**) and unit (**I**) matrices.

For tree graphs the coefficients of $P_G(x)$ exactly coincide with the set of $p(G,k)$'s as[8,9]

$$P_T(x) = \sum_{k=0}^{N} a_k x^{N-k}$$
$$= \sum_{k=0}^{m} (-1)^k p(T,k) x^{N-2k} \quad (T \in \text{tree}) \quad . \qquad (2.20)$$

These properties can be realized in Table 2, where the $p(G,k)$ and Z-values of the lower members of path graphs are shown. Further, the novel relation

$$Z(S_n) = F_n \qquad (2.21)$$

is also realized.

Table 2 $p(G,k)$ and Z-values of the lower members of path graphs (S_n)

		$p(G,k)$					
n	G	$k=$ 0	1	2	3	4	Z
1	•	1	1				1
2		1	1				2
3		1	2				3
4		1	3	1			5
5		1	4	3			8
6		1	5	6	1		13
7		1	6	10	4		21
8		1	7	15	10	1	34

A star graph $K_{1,n}$ is constructed from the central vertex and n edges of unit length emanating from it. Thus $K_{1,n}$ is composed of n+1 vertices and its Z-index is n+1. Before introducing the caterpillar graph the recursive relation of $p(G,k)$ and Z-index will be explained.

2.6 Recursive property of *Z* index

Suppose a tree graph G and an arbitrary chosen edge l in G, and define a pair of subgraphs, $G-l$ and $G\Theta l$, in the following way. Namely, as shown in Fig. 2, where comb graph M_3 is chosen for G, the subgraph $G-l$ is obtained by deleting l from G, while $G\Theta l$ is obtained by deleting l together with all the edges incident to l. As the non-adjacent number $p(G,k)$ is the number of ways for choosing k disjoint edges from G, it is the sum of $p(G-l,k)$ and $p(G\Theta l,k-1)$.

$$p(G,k) = p(G-l,k) + p(G\Theta l,k-1). \tag{2.22}$$

The former gives l-exclusive counting and the latter l-inclusive one.

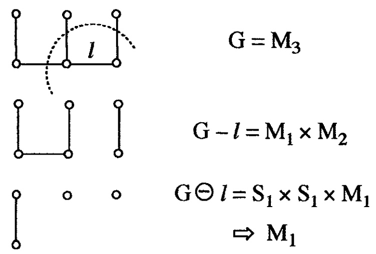


Fig. 2. Subgraphs, $G-l$ and $G\Theta l$, of comb graph M_3.

Since $Z(G)$ is the total sum of $p(G,k)$'s, the following identity is straightforwardly obtained.

$$Z(G) = Z(G-l) + Z(G\Theta l). \tag{2.23}$$

These recursive relations are just an outcome of the inclusion-exclusion principle.[11)]

In the case of Fig. 2, $G-l$ has two components, M_1 and M_2. The product of those Z-values gives the Z value of $G-l$. Since $G\Theta l$ is composed of a pair of isolated vertices (S_1's) and M_1, $Z(G\Theta l)$ is equal to $Z(M_1)$. Then $Z(M_3)$ can be obtained by using the values of $Z(M_1)$ and $Z(M_2)$ as

$$Z(M_3) = Z(M_1)\, Z(M_2) + Z(M_1) = 2\times 5 + 2 = 12.$$

Quite similarly, one can derive the following recursive formula,

$$Z(M_{m+n}) = Z(M_m)\, Z(M_n) + Z(M_{m-1})\, Z(M_{n-1}), \tag{2.24}$$

and $Z(M_n)$ values are found to be equal to the famous Pell numbers[11,16,18)] as shown below:

n	0	1	2	3	4	5	6	7	8
$Z(M_n)= P_n$	1	2	5	12	29	70	169	408	985

They are governed by the following recursive relation:

$$P_n = 2\,P_{n-1} + P_{n-2}\,. \tag{2.25}$$

However, again the initial conditions, P_0=1 and P_1=2, are different from the conventional ones,[11,16)] P_1=1 and

P_2=2. The reason for the superiority of our choice has already been documented elsewhere.[18)]

Note, however, that P_n can be expressed by the following continuant:

$$P_n = Z(\mathrm{M}_n) = \mathrm{K}_n(2, 2, \cdots, 2). \quad (n\ 2\text{'s}). \tag{2.26}$$

2.7 Caterpillar graphs

In the graph theory a caterpillar is defined as a tree that contains a path graph such that every edge has one or both endpoints in that path. Let us put it in another way. Suppose a path S_n and prepare the set of n stars, $X_n=\{x_1, x_2, \cdots, x_n\}$, where natural number x_n denotes K_{1,x_n-1}, whose Z-value is x_n. The set X_n has n x_n terms and each term x_n may take an arbitrary value. Then mount each element of X_n onto each vertex of S_n one by one either from left or right to another end (See Fig. 3). Let us call the resultant graph a caterpillar $\mathrm{C}_n(x_1, x_2, \cdots, x_n)$ composed of $|V|=\Sigma x_n$ vertices.

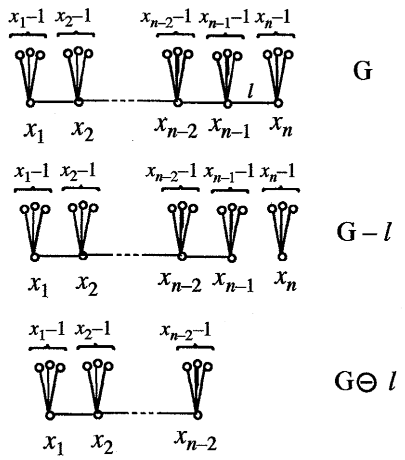


Fig. 3. Caterpillar $\mathrm{C}_n(x_1, x_2, \cdots, x_n)$ and its subgraphs. Isolated vertices are omitted from G⊖l.

If X_n is (1, 1,⋯, 1), the resultant $\mathrm{C}_n(1, 1, \cdots, 1)$ is identical to the parent S_n, whereas $\mathrm{C}_n(2, 2, \cdots, 2)$ is the comb graph M_n. With these preliminaries we can show that all the discussion on the degradation of simple continued fractions can be reduced to the manipulation of the topological indices of caterpillars, which are obtained from the terms of the continued fractions concerned.

3 Main Theorems

3.1 Continuant is Z-caterpillar

Let us choose a caterpillar $\mathrm{C}_n(x_1, x_2, \cdots, x_n)$, and calculate its Z-index $Z_n(x_1, x_2, \cdots, x_n)$. The Z-caterpillar is such a caterpillar whose $Z_n(x_1, x_2, \cdots, x_n)$ takes the specified value. Depending on the structure of C_n a variety of ways are available for efficient calculation of Z_n by the combined use of several recursive relations. Here let us attack from one end of the caterpillar toward another end. Instead of formulating the final result, let us extend the length of the caterpillar one by one from $C_1(x_1)$, $C_2(x_1, x_2)$ to $C_n(x_1, x_2, \cdots, x_n)$.

By applying the recursive relation (2.23) to Fig. 3 and following the recipe in Fig. 2 one gets stepwise

$$Z_1(x_1) = x_1, \quad Z_2(x_1, x_2) = x_1 x_2 + 1, \quad Z_3(x_1, x_2, x_3) = x_3 Z_2(x_1, x_2) + Z_1(x_1), \ \cdots. \tag{3.1}$$

This is nothing else but the recursive algorithm (2.3) for the continuant K_n. Moreover, as already explained, the Z-index of vacant graph is unity, i.e., $Z_0() = 1$. Then we get

[Theorem 5] Continuant is identical to Z-caterpillar, i.e., the Z-index of caterpillar $C_n(x_1, x_2, \cdots, x_n)$.

$$Z_n(x_1, x_2, \cdots, x_n) = K_n(x_1, x_2, \cdots, x_n). \tag{3.2}$$

∵ Both quantities have the same mathematical structure. □

Mathematically this is the most important theorem in the present theory, because all the difficulties in the calculation of the continuant which originates from solving continued fractions can be resolved quite easily by using the powerful recursive relation (2.23) of the Z-index after transforming K_n into C_n. For example, just in the similar way as the derivation of (2.24) we get

[Theorem 6]

$$K_{m+n}(x_1, x_2, \cdots, x_n) = K_m(x_1, \cdots, x_m)\, K_n(x_{m+1}, \cdots, x_{m+n}) + K_{m-1}(x_1, \cdots, x_{m-1})\, K_{n-1}(x_{m+2}, \cdots, x_{m+n}) \tag{3.3}$$

$$= \begin{vmatrix} K_m(x_1, \cdots, x_m) & K_{m-1}(x_1, \cdots, x_{m-1}) \\ -K_{n-1}(x_{m+2}, \cdots, x_{m+n}) & K_n(x_{m+1}, \cdots, x_{m+n}) \end{vmatrix}. \tag{3.4}$$

∵ The following relation for Z-index is directly derived from (2.23):

$$Z_{m+n}(x_1, x_2, \cdots, x_n) = Z_m(x_1, \cdots, x_m)\, Z_n(x_{m+1}, \cdots, x_{m+n}) + Z_{m-1}(x_1, \cdots, x_{m-1})\, Z_{n-1}(x_{m+2}, \cdots, x_{m+n}), \tag{3.5}$$

which automatically assures (3.3) and (3.4). □

By putting 1 into all x_n's in (3.3) one gets

$$F_{m+n} = F_m F_n + F_{m-1} F_{n-1}. \tag{3.6}$$

Note, however, that the initial conditions of the Fibonacci numbers are chosen as in (2.10). Otherwise, the conventionally used

$$F_{m+n} = F_m F_{n+1} + F_{m-1} F_n$$

is obtained.

Theorem 3 is also applicable to the Z-index.

[Theorem 7] Tridiagonal determinantal expression of Z-caterpillar.

$$Z_n(x_1, x_2, \cdots, x_n) = \begin{vmatrix} x_1 & 1 & 0 & 0 & \cdots & 0 \\ -1 & x_2 & 1 & 0 & \cdots & 0 \\ 0 & -1 & x_3 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & -1 & x_{n-1} & 1 \\ 0 & 0 & \cdots & 0 & -1 & x_n \end{vmatrix}. \tag{3.7}$$

This relation is obvious from (3.2). □

The rhs of (3.7) can be degraded as follows:

$$\begin{vmatrix} x_1 & 1 & 0 & 0 & \cdots & 0 \\ -1 & x_2 & 1 & 0 & \cdots & 0 \\ 0 & -1 & x_3 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & -1 & x_{n-1} & 1 \\ 0 & 0 & \cdots & 0 & -1 & x_n \end{vmatrix} = x_1 \begin{vmatrix} x_2 & 1 & 0 & \cdots & 0 \\ -1 & x_3 & 1 & \cdots & 0 \\ 0 & -1 & \ddots & 1 & \vdots \\ \vdots & \vdots & -1 & x_{n-1} & 1 \\ 0 & 0 & 0 & -1 & x_n \end{vmatrix} + \begin{vmatrix} x_3 & 1 & \cdots & 0 \\ -1 & \ddots & \ddots & \vdots \\ \vdots & \ddots & x_{n-1} & 1 \\ 0 & \cdots & -1 & x_n \end{vmatrix}$$

$$= (x_1 x_2 + 1) \begin{vmatrix} x_3 & 1 & \cdots & 0 \\ -1 & x_4 & \ddots & \vdots \\ \vdots & \ddots & \ddots & 1 \\ 0 & \cdots & -1 & x_n \end{vmatrix} + x_1 \begin{vmatrix} x_4 & 1 & \cdots \\ -1 & \ddots & 1 \\ \cdots & -1 & x_n \end{vmatrix}$$

$$= \begin{vmatrix} x_1 x_2 + 1 & x_1 & 0 & \cdots & 0 & 0 \\ -1 & x_3 & 1 & \cdots & 0 & 0 \\ 0 & -1 & x_4 & \ddots & \vdots & \vdots \\ \vdots & \vdots & \ddots & \ddots & 1 & 0 \\ 0 & 0 & \cdots & -1 & x_{n-1} & 1 \\ 0 & 0 & \cdots & 0 & -1 & x_n \end{vmatrix} = \begin{vmatrix} \mathrm{K}_2(x_1, x_2) & \mathrm{K}_1(x_1) & 0 & \cdots & 0 & 0 \\ -1 & x_3 & 1 & \cdots & 0 & 0 \\ 0 & -1 & x_4 & \ddots & \vdots & \vdots \\ \vdots & \vdots & \ddots & \ddots & 1 & 0 \\ 0 & 0 & \cdots & -1 & x_{n-1} & 1 \\ 0 & 0 & \cdots & 0 & -1 & x_n \end{vmatrix}$$

$$= \begin{vmatrix} \mathrm{K}_3(x_1, x_2, x_3) & \mathrm{K}_2(x_1, x_1) & 0 & \cdots & 0 & 0 \\ -1 & x_4 & 1 & \cdots & 0 & 0 \\ 0 & -1 & x_5 & \ddots & \vdots & \vdots \\ \vdots & \vdots & \ddots & \ddots & 1 & 0 \\ 0 & 0 & \cdots & -1 & x_{n-1} & 1 \\ 0 & 0 & \cdots & 0 & -1 & x_n \end{vmatrix}$$

$$= \begin{vmatrix} Z_3(x_1, x_2, x_3) & Z_2(x_1, x_1) & 0 & \cdots & 0 & 0 \\ -1 & x_4 & 1 & \cdots & 0 & 0 \\ 0 & -1 & x_5 & \ddots & \vdots & \vdots \\ \vdots & \vdots & \ddots & \ddots & 1 & 0 \\ 0 & 0 & \cdots & -1 & x_{n-1} & 1 \\ 0 & 0 & \cdots & 0 & -1 & x_n \end{vmatrix}.$$

By continuing similar degradation one can obtain the following pair of general expressions:

[Theorem 8]

$$Z_{m+n}(x_1, x_2, \cdots, x_{m+n}) = \begin{vmatrix} Z_{m-1}(x_1, \cdots, x_{m-1}) & Z_{m-2}(x_1, \cdots, x_{m-2}) & 0 \\ -1 & x_m & 1 \\ 0 & -Z_{n-1}(x_{m+2}, \cdots, x_{m+n}) & Z_n(x_{m+1}, \cdots, x_{m+n}) \end{vmatrix} \tag{3.8}$$

and

$$Z_{m+n}(x_1, x_2, \cdots, x_{m+n}) = \begin{vmatrix} Z_m(x_1, \cdots, x_m) & Z_{m-1}(x_1, \cdots, x_{m-1}) \\ -Z_{n-1}(x_{m+2}, \cdots, x_{m+n}) & Z_n(x_{m+1}, \cdots, x_{m+n}) \end{vmatrix}. \tag{3.9}$$

Note that without following the iterative degradation procedure (3.9) can be obtained directly from the application of (2.23) to caterpillar $C_{m+n}(x_1, x_2, \cdots, x_{m+n})$. Namely, $Z_m(x_1, \cdots, x_m)$ and $Z_n(x_{m+1}, \cdots, x_{m+n})$ in the diagonal are the Z-indices of the two components of G–*l*, whereas $Z_{m-1}(x_1, \cdots, x_{m-1})$ and $Z_{n-1}(x_{m+2}, \cdots, x_{m+n})$ in the off-diagonal are those of the two components of $G\Theta l$, where l is the edge between the central vertices of the mth and $(m+1)$th star moieties in the parent caterpillar G. Of course, (2.24) and (3.6) can be obtained also from (3.9). In principle (3.8) can further be changed into (3.9), but it will be shown later that it has a practical utility for solving some Pell equations. □

It is to be noted here that Balasubramanian and Randic developed the so-called "pruning technique" for efficient degradation of the characteristic determinant det(**A**−x**I**) (See (2.19)).[19,20] The essence of their algorithm is quite similar to that of Theorem 8.

[Collorary 1]

$$\mathrm{K}_{m+n}(x_1, x_2,\cdots, x_{m+n}) = \begin{vmatrix} \mathrm{K}_{m-1}(x_1,\cdots,x_{m-1}) & \mathrm{K}_{m-2}(x_1,\cdots,x_{m-2}) & 0 \\ -1 & x_m & 1 \\ 0 & -\mathrm{K}_{n-1}(x_{m+2},\cdots,x_{m+n}) & \mathrm{K}_n(x_{m+1},\cdots,x_{m+n}) \end{vmatrix} \tag{3.10}$$

and

$$\mathrm{K}_{m+n}(x_1, x_2,\cdots, x_{m+n}) = \begin{vmatrix} \mathrm{K}_m(x_1,\cdots,x_m) & \mathrm{K}_{m-1}(x_1,\cdots,x_{m-1}) \\ -\mathrm{K}_{n-1}(x_{m+2},\cdots,x_{m+n}) & \mathrm{K}_n(x_{m+1},\cdots,x_{m+n}) \end{vmatrix}. \tag{3.11}$$

are naturally valid from (3.2).

3.2 Fastest algorithm for solving Pell equations

The essence of the algorithm for solving the Pell equation

$$x^2 - Dy^2 = 1 \quad \text{(Pell-1)} \tag{3.12}$$

and Llep equation[18,21,22]

$$r^2 - Ds^2 = -1 \quad \text{(Llep-1)} \tag{3.13}$$

will be explained below. For the nomenclature about Pell and Llep see Ref. 21.

First obtain the continued fraction expansion of the square root of D. However, depending on the parity of the length k of the period of the infinite continued fractions the necessary procedures are a little different from each other.

1) Pell-1 with even k=2m

$$\begin{aligned}\sqrt{D} &= [a_0;\overline{a_1,a_2,\cdots,a_{m-1},a_m,a_{m+1},\cdots,a_{2m-1},a_{2m}}] \\ &= [a_0;\overline{a_1,a_2,\cdots,a_{m-1},a_m,a_{m-1},a_{m-2},\cdots,a_1,2a_0}] \\ &= [a\overline{\mathrm{L}c\mathrm{L}^- b}] = [a\overline{\mathrm{A}b}].\end{aligned} \tag{3.14}$$

where a, b, and c are, respectively, a_0, a_{2m}, and a_m, and L and L^- are, respectively, deemed as the caterpillar $C_{m-1}(a_1, a_2,\cdots, a_{m-1})$ and its reversed image $C_{m-1}(a_{m-1},\cdots, a_2, a_1)$. The latter two are essentially identical to each other, since they are graphs. The symbol A denotes the caterpillar $\mathrm{L}c\mathrm{L}^-$ with symmetrical structure beginning from and ending at the moiety of star K_{1,a_1-1}.

Now the smallest solution (x_1, y_1) of (3.12) is known to be expressed by the Z-indices of a pair of caterpillars, $C_{2m-1}(\mathrm{A})$ and $C_{2m}(a\mathrm{A})$, and all their family members can also be obtained as[18)]

$$x_1 = Z_{2m}(a\mathrm{A}), \quad x_2 = Z_{4m}(a\mathrm{A}b\mathrm{A}), \quad x_3 = Z_{6m}(a\mathrm{A}b\mathrm{A}b\mathrm{A}), \quad \text{etc.} \tag{3.15}$$

$$y_1 = Z_{2m-1}(\mathrm{A}), \quad y_2 = Z_{4m-1}(\mathrm{A}b\mathrm{A}), \quad y_3 = Z_{6m-1}(\mathrm{A}b\mathrm{A}b\mathrm{A}), \quad \text{etc.} \tag{3.16}$$

All these Z-values can be expressed by the determinantal form (3.7) and Theorem 8 can be applied. Then we get the following theorem.

[Theorem 9] Smallest solution of Pell-1 with even k.

$$x_1 = Z_{2m}(a\mathrm{A}) = Z_{2m}(a\mathrm{L}c\mathrm{L}^{-}) = \begin{vmatrix} aL & aM & 0 \\ -1 & c & 1 \\ 0 & -M & L \end{vmatrix} = \begin{vmatrix} Z_m(a\mathrm{L}) & Z_{m-1}(a\mathrm{M}) & 0 \\ -1 & a_m & 1 \\ 0 & -Z_{m-2}(\mathrm{M}) & Z_{m-1}(\mathrm{L}) \end{vmatrix} \tag{3.17}$$

$$y_1 = Z_{2m-1}(\mathrm{A}) = Z_{2m-1}(\mathrm{L}c\mathrm{L}^{-}) = \begin{vmatrix} L & M & 0 \\ -1 & c & 1 \\ 0 & -M & L \end{vmatrix} = \begin{vmatrix} Z_{m-1}(\mathrm{L}) & Z_{m-2}(\mathrm{M}) & 0 \\ -1 & a_m & 1 \\ 0 & -Z_{m-2}(\mathrm{M}) & Z_{m-1}(\mathrm{L}) \end{vmatrix}. \tag{3.18}$$

Higher family members f_{n-1} s can be obtained by using the recursion formula[22]

$$f_n = 2x_1 f_{n-1} - f_{n-2} \quad (f = x, y). \tag{3.19}$$

2) Llep-1 with odd $k=2m-1$

$$\begin{aligned}\sqrt{D} &= [a_0; \overline{a_1, a_2, \cdots, a_{m-1}, a_m, \cdots, a_{2m-2}, a_{2m-1}}] \\ &= [a_0; \overline{a_1, a_2, \cdots, a_{m-1}, a_{m-1}, a_{m-2}, \cdots, a_1, 2a_0}] \\ &= [a\overline{\mathrm{L}\mathrm{L}^{-}b}] = [a\overline{\mathrm{A}b}]\end{aligned} \tag{3.20}$$

Note that in this case the symmetrical caterpillar A=LL^{-} is different from case 1), and has an even number of star moieties. In this case the smallest solution $(r_1, s_1) = (t_1, u_1)$ of Llep-1 (3.13) is followed by the smallest solution $(x_1, y_1) = (t_2, u_2)$ of Pell-1 (3.12), and then alternately Llep-1 and Pell-1 appear to form the big family of Pellep-1.[18]

$$t_1 = r_1 = Z_{2m-1}(a\mathrm{A}), \quad t_2 = x_1 = Z_{4m-2}(a\mathrm{A}b\mathrm{A}), \quad t_3 = r_2 = Z_{6m-3}(a\mathrm{A}b\mathrm{A}b\mathrm{A}), \quad \text{etc.} \tag{3.21}$$

$$u_1 = s_1 = Z_{2m-2}(\mathrm{A}), \quad u_2 = y_1 = Z_{4m-3}(\mathrm{A}b\mathrm{A}), \quad u_3 = s_2 = Z_{6m-4}(\mathrm{A}b\mathrm{A}b\mathrm{A}), \quad \text{etc.} \tag{3.22}$$

Further, it was proved that once (r_1, s_1) is obtained, the larger members of Pellep-1 can be obtained by using the Chebyshev polynomials of the second kind.[22] Especially for (t_2, u_2) we have

$$\begin{aligned} t_2 &= 2r_1^2 + 1, \\ u_2 &= 2\, r_1 s_1 . \end{aligned} \tag{3.23}$$

Thus the following theorem can be obtained.

[Theorem 10] Smallest solution of Llep-1 with odd k.

$$r_1 = t_1 = Z_{2m-1}(a\mathrm{A}) = Z_{2m-1}(a\mathrm{L}\mathrm{L}^{-}) = \begin{vmatrix} aL & aM \\ -M & L \end{vmatrix} = \begin{vmatrix} Z_m(a\mathrm{L}) & Z_{m-1}(a\mathrm{M}) \\ -Z_{m-2}(\mathrm{M}) & Z_{m-1}(\mathrm{L}) \end{vmatrix} \tag{3.24}$$

$$s_1 = u_1 = Z_{2m-2}(\mathrm{A}) = Z_{2m-2}(\mathrm{L}\mathrm{L}^{-}) = \begin{vmatrix} L & M \\ -M & L \end{vmatrix} = \begin{vmatrix} Z_{m-1}(\mathrm{L}) & Z_{m-2}(\mathrm{M}) \\ -Z_{m-2}(\mathrm{M}) & Z_{m-1}(\mathrm{L}) \end{vmatrix}. \tag{3.25}$$

The smallest solution of Pell-1 with odd k is obtained by (3.22). Higher family members f_{n-1}'s can be obtained by using the recursion formula[22)]

$$f_n = 2x_1 f_{n-1} + f_{n-2} \quad (f = t, u). \tag{3.26}$$

The results (3.17-19) and (3.24-26) are the ever-proposed fastest algorithm for solving the Pell-1 and Llep-1 applicable to general D values. Examples will be demonstrated in another paper.[23)]

3.3 Generalized Fibonacci numbers

In **2.3** the explicit forms of Fibonacci- and Lucas-caterpillars are given. Namely, the Z-indices of some series of caterpillar graphs represent Fibonacci and Lucas numbers. Then what about the generalized Fibonacci numbers of the property (2.14)? In this case trivial star solutions are excepted. Although the present author has tried to pose a conjecture as a positive answer to this question, its mathematical proof could not be obtained.[24,25)] However, now we can prove it as follows:

[Theorem 11] Generalized Fibonacci-caterpillars.

For a given pair of natural numbers, $n_1 < n_2$, which are prime with each other, there exist a series of regularly growing Z-caterpillars $\{G_m\}$ of the property, $Z(G_m) = Z(G_{m-1}) + Z(G_{m-2})$ ($m \geq 3$), with $Z(G_1) = n_1$ and $Z(G_2) = n_2$.

(Proof) Prepare the continued fraction expression for n_1/n_2 as

$$n_1/n_2 = [0; a_1, a_2, \cdots, a_k] \tag{3.27}$$

By using these terms draw a pair of caterpillars as follows:

$$G_1 = C_{k-1}(a_2, a_3, \cdots, a_k) \quad \text{and} \quad G_2 = C_k(a_1, a_2, \cdots, a_k). \tag{3.28}$$

Then construct $G_3 = C_{k+1}(1, a_1, a_2, \cdots, a_k)$, $G_4 = C_{k+2}(1, 1, a_1, a_2, \cdots, a_k)$, etc. The equalities, $Z(G_1) = n_1$ and $Z(G_2) = n_2$, are proved from (2.23) and (3.2). The desired properties for G_m ($m \geq 3$) are proved from (2.23). □

A number of examples are given in Ref. 25. Theorem 11 can further be expanded to more general recursive relations.

[Theorem 12]

For a given pair of natural numbers, $n_1 < n_2$, which are prime with each other, and a natural number $d > 1$, there exist a series of regularly growing Z-caterpillars $\{G_m\}$ of the property, $Z(G_m) = d\,Z(G_{m-1}) + Z(G_{m-2})$ ($m \geq 3$), with $Z(G_1) = n_1$ and $Z(G_2) = n_2$.

(Proof) After performing (3.27) and (3.28) construct $G_3 = C_{k+1}(d, a_1, a_2, \cdots, a_k)$, $G_4 = C_{k+2}(d, d, a_1, a_2, \cdots, a_k)$, etc. The desired properties for G_m ($m \geq 3$) are proved from (2.23). □

Finally graph-theoretical interpretation of (2.15) will be illustrated. See Fig. 4 where a series of graphs whose Z-values obey generalized-Fibonacci numbers. If a pair of natural numbers $a<b$ with $(a, b)=1$ are given, a pair of caterpillars , G_{m-1} and G_m, can be constructed so that $Z(G_{m-1})=a$ and $Z(G_m)=b$ according to Theorem 11. Then by extending an edge one by one as shown in Fig. 4a a series of generalized-Fibonacci graphs $\{G_{m+n}\}$ can be obtained. Now the Z-index of G_{m+n} can be obtained by cutting the edge marked with double bar as shown in Fig. 4b the recursive relation (2.15) can be obtained by using (2.23).

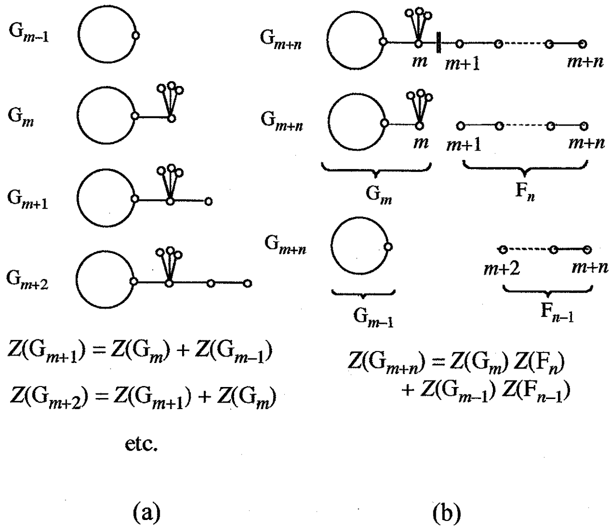


Fig. 4. (a) Construction of generalized-Fibonacci caterpillars, and (b) degradation of $Z(G_{m+n})$ by the use of recursive relation (2.15).

This example illustrates how the topological index Z works not only as a powerful proof technique in algebraic theorems but also gives us their geometrical or graph-theoretical interpretation. Many of the mathematical concepts and materials appearing in this paper, such as the continuant, Fibonacci numbers including generalized-Fibonacci sequences, caterpillars, and determinants, have been considered to belong to different categories. However, thanks to the Z-index they were found to be closely related with each other in the world of continued fractions. Thus by using the Z-index, many areas of elementary algebra and geometry can be combined more tightly and understood more easily.

References

1) A. H. Beiler, Recreations in the Theory of Numbers. The Queen of Mathematics Entertains. Dover, New York (1964), pp. 248.

2) E. J. Barbeau, Pell's Equation. Springer, New York (2002), pp.55.

3) T. Takagi, Elementary Number Theory (in Japanese), Kyoritsu, Tokyo (1931), pp. 124.

4) D. E. Knuth, The Art of Computer Programming, Vol. 1, Addison-Wesley, Reading, MS (1968), pp. 339.

5) R. L. Graham, D. E. Knuth, and O. Patashnik, Concrete Mathematics. A Foundation for Computer Science, Addison-Wesley, Reading, MS (1989), pp. 287.

6) A. T. Benjamin and J. J. Quinn, Proofs That Really Count. The Art of Combinatorial Proof, Mathematical Association of America, Washington, D. C., 2003, p. 57.

7) C.-O. Selenius, Historia Math., **2** (1975), 167.

8) H. Hosoya, *Bull. Chem. Soc. Jpn.*, **44** (1971) 2332-2339.

9) H. Hosoya, *Fibonacci Quart.*, **11** (1973) 255-266.

10) K. H. Rosen, J. G. Michaels, J. L. Gross, J. W. Grossman, and D. R. Shier (Eds.), Handbook of Discrete and Combinatorial Mathematics, CRC Press, Boca Raton, FL (2000), p. 498.

11) E. W. Weisstein, CRC Concise Encyclopedia of Mathematics, Chapman & Hall/CRC, Boca Raton, FL (2003), p. 351.

12) F. Harary, Graph Theory, Addison-Wesley, Reading, MS (1969).

13) H. Hosoya, *Internet Electronic. J. Mol. Design*, **1** (2002) 428.

14) A. Ya. Khintchine, Continued Fractions (Translated by P. Wynn), P. Noordhoff, Groningen, The Netherlands (1963).

15) V. E. Hoggatt, Jr., Fibonacci and Lucas Numbers, Houghton Mifflin, Boston (1969).

16) T. Koshy, Fibonacci and Lucas Numbers with Applications, Wiley, New York (2001).

17) B. G. S. Doman and J. K. Williams, *Math. Proc. Cambridge Phil. Soc.*, **90** (1981) 385.

18) H. Hosoya, *Natural Sci. Rept. Ochanomizu Univ.*, **57** (2006) (2) 35.

19) K. Balasubramanian, *Internatl. J. Quant. Chem.*, **22** (1982) 581.

20) K. Balasubramanian and M. Randic, Theor. Chim. Acta, **61** (1982) 307.

21) H. Hosoya and N. Asamoto, *Natural Sci. Rept. Ochanomizu Univ.*, **57** (2006) (1) 57.

22) H. Hosoya, *Natural Sci. Rept. Ochanomizu Univ.*, **57** (2006) (2) 19.

23) H. Hosoya, *Natural Sci. Rept. Ochanomizu Univ.*, **58** (2007) in press.

24) H. Hosoya, *Croat. Chem. Acta*, **80** (2007) 239.

25) H. Hosoya, *J. Chem. Inf. Model.*, **47** (2007) 744.