# Graphical and Combinatorial Aspects of Some Orthogonal Polynomials

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(Received September 7, 1981)

## 1. Introduction

The present author has defined the topological index $Z_G$,

(1) $$Z_G=\sum_{k=0}^{m} p(G,k),$$

for characterizing a graph $G$ as the sum of the non-adjacent number, $p(G, k)$, which is the number of ways for choosing $k$ disjoint lines from $G$, or the number of $k$-matchings in $G$ [1]. The set of numbers $p(G, k)$'s can easily be obtained by the aid of the $Z$-counting polynomial

(2) $$Q_G(x)=\sum_{k=0}^{m} p(G,k)x^k,$$

for which several recursion relations have been found [1, 2]. With this polynomial $Z_G$ can be expressed as

(3) $$Z_G=Q_G(1).$$

These quantities, $Z_G$, $p(G, k)$, and $Q_G(x)$, have been shown to be closely related to a number of chemical and physical properties of certain series of molecules [1, 3-6]. They can also be applied to the coding and classification of molecules [7]. It was pointed out that the $Z_G$ values of path graphs $\{P_n\}$ and cycle graphs $\{C_n\}$, respectively, from the Fibonacci and Lucas numbers [1, 2]. These series of numbers have been known to be associated with the Chebyshev polynomial, one of the most typical orthogonal polynomials.

Recently several authors have independently proposed the matching polynomial*

(4) $$M_G(x)=\sum_{k=0}^{m}(-1)^k p(G,k)x^{n-2k}$$

by using the $p(G, k)$ numbers for a given graph both from chemical and graph-theoretical points of view [8-10]. It is obvious, however, that

* Aihara [8] calls $M_G(x)$ as the reference polynomial, while Gutman *et al.* [9, 11] prefer to use the term acyclic polynomial. The term "matching polynomial" is due to the suggestion by Harary [12].

(5) $$M_G(x)=x^n Q_G(-x^{-2})$$

(6) $$Q_G(x)=(-i\sqrt{x})^n M_G(i/\sqrt{x})\,.$$

The matching polynomial for a tree graph is identical to the corresponding characteristic polynomial

(7) $$P_G(x)=(-1)^n \det(\boldsymbol{A}-x\boldsymbol{E})$$
$$=M_G(x)\,. \qquad (G\in\text{tree})$$

Note also that

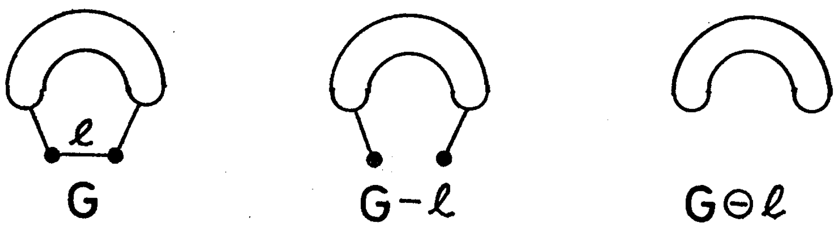
(9) $$M_G(i)=i^n Z_G$$

for all graphs, *i.e.*, the sum of the absolute values of the coefficients of the matching polynomial is equal to the topological index.

Recently Gutman discovered that the matching polynomials of certain series of graphs are closely related to some of the orthogonal polynomials, such as Hermite, Laguerre, and associated Laguerre polynomials [13]. All these findings are the outcomes of the important features of the non-adjacent numbers, $p(G, k)$'s. In this report the graphical and combinatorial aspects of several orthogonal polynomials will be surveyed.

## 2. Recursion Relations

Two different kinds of subgraphs of a given graph $G$ are defined as follows [2, 5]:




$G-l$ is obtained from $G$ by deleting a given line $l$, and $G\ominus l$ is obtained by deleting $l$ together with all the lines adjacent to $l$.

The inclusion-exclusion principle ensures the following relation,

(10) $$p(G, k)=p(G-l, k)+p(G\ominus l, k-1)\,.$$

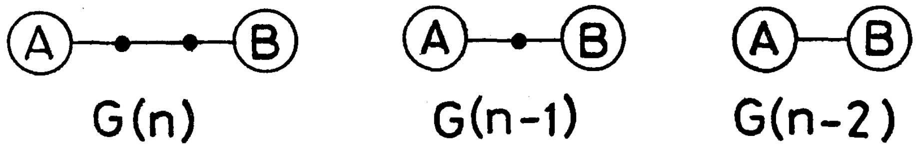
It is straightforward to get the recursion relations,

(11.1) $$Q_G(x)=Q_{G-l}(x)+x\cdot Q_{G\ominus l}(x)$$

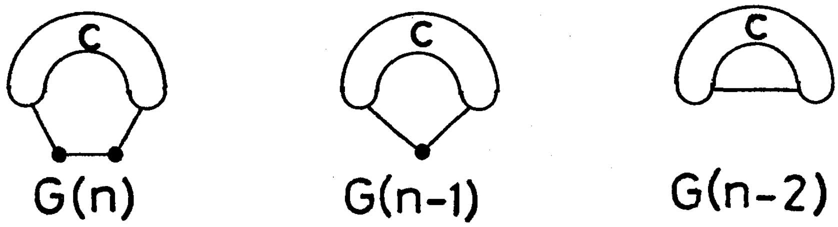
(11.2) $$Z_G=Z_{G-l}+Z_{G\ominus l}$$

(11.3) $$M_G(x)=M_{G-l}(x)-M_{G\ominus l}(x)\,.$$

Next consider the following three graphs in which the numbers of the lines joining the subgraphs $A$ and $B$ are, respectively, three, two, and one, as




The subgraphs $A$ and $B$ may be joined each other to give $C$ as



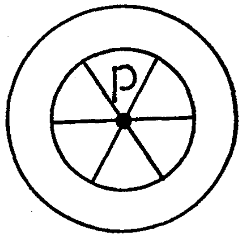

For these series of graphs we get the following relations,

(12.1) $$Q_{G(n)}(x)=Q_{G(n-1)}(x)+x\cdot Q_{G(n-2)}(x)$$

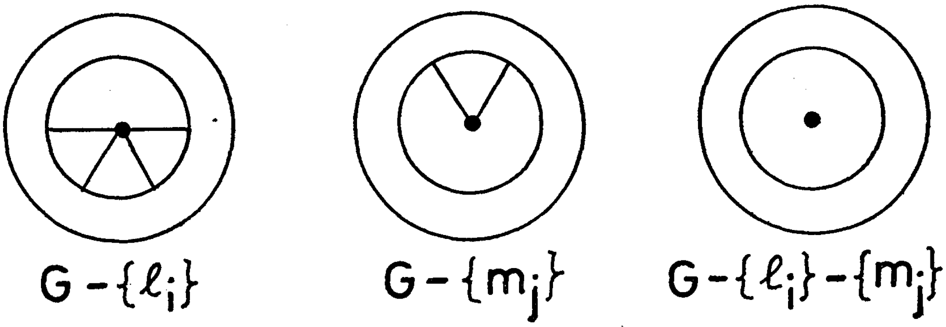
(12.2) $$Z_{G(n)}=Z_{G(n-1)}+Z_{G(n-2)}$$

(12.3) $$M_{G(n)}(x)=x\cdot M_{G(n-1)}(x)-M_{G(n-2)}(x)\,.$$

Consider a graph with a wheel structure as




where more than two lines radiate from a point $p$ toward the perimeter of the graph. Divide these lines into two groups of lines $\{l_i\}$ and $\{m_j\}$. Then consider the following three subgraphs




With these subgraphs another set of the recursion formulas can be obtained.

(13.1) $$Q_G(x)=Q_{G-\{l_i\}}(x)+Q_{G-\{m_j\}}(x)-Q_{G-\{l_i\}-\{m_j\}}(x)$$

(13.2) $$Z_G=Z_{G-\{l_i\}}+Z_{G-\{m_j\}}-Z_{G-\{l_i\}-\{m_j\}}$$

(13.3) $$M_G(x)=M_{G-\{l_i\}}(x)+M_{G-\{m_j\}}(x)-M_{G-\{l_i\}-\{m_j\}}(x)\,.$$

## 3. Chebyshev Polynomial

The Chebyshev polynomials of the first and second kinds are defined for non-negative $n$ as

(14) $$T_n(\cos\theta)=\cos n\theta \qquad \text{(1st kind)}$$

(15) $$U_n(\cos\theta)=\sin(n+1)\theta/\sin\theta\,. \qquad \text{(2nd kind)}$$

It is convenient to define the modified polynomials $C_n(x)$ and $S_n(x)$ as [14]

(16) $$C_n(x)=2T_n(x/2) \quad \text{or} \quad T_n(x)=C_n(2x)/2$$

(17) $$S_n(x)=U_n(x/2) \quad \text{or} \quad U_n(x)=S_n(2x)\,.$$

By applying the addition theorems of the trigonometric functions to Eqs. (14) and (15), one gets the following recursion formulas

(18.1) $$T_n(x)=2xT_{n-1}(x)-T_{n-2}(x) \qquad (n\geqq 2)$$

(18.2) $$U_n(x)=2xU_{n-1}(x)-U_{n-2}(x) \qquad (n\geqq 2)$$

which give

(19.1) $$C_n(x)=xC_{n-1}(x)-C_{n-2}(x) \qquad (n\geqq 2)$$

(19.2) $$S_n(x)=xS_{n-1}(x)-S_{n-2}(x)\,. \qquad (n\geqq 2)$$

Now all these polynomials with any $n$ value can be calculated from Eqs. (18) and (19) with the following initial values:

(20.1) $$T_0(x)=1 \qquad T_1(x)=x$$

(20.2) $$U_0(x)=1 \qquad U_1(x)=2x$$

(21.1) $$C_0(x)=2 \qquad C_1(x)=x$$

(21.2) $$S_0(x)=1 \qquad S_1(x)=x\,.$$

In Tables 1 and 2 are given these Chebyshev polynomials for smaller $n$ values.

By using the de Moibre's theorem, Eqs. (14) and (15) can be converted into the closed forms

(22.1) $$T_n(x)=\{(x+\sqrt{x^2-1})^n+(x-\sqrt{x^2-1})^n\}/2$$

(22.2) $$U_n(x)=\{(x+\sqrt{x^2-1})^{n+1}-(x-\sqrt{x^2-1})^{n+1}\}/2\sqrt{x^2-1}\,.$$

Let the two roots of the following quadratic equation

$$x^2-x+1=0$$

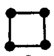
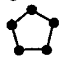
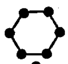
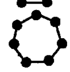
be $\alpha=(1+\sqrt{5})/2$ and $\beta=(1-\sqrt{5})/2$. Then by substituting $x=i/2$ into Eqs. (22), one gets

(23) $$2T_n(i/2)=C_n(i)=i^n(\alpha^n+\beta^n)/2=i^nL_n$$

Table 1.

| $n$ | $P_n$ | $M_{P_n}(x) = U_n(x/2) = S_n(x)$ | $U_n(x)$ | $Z_G$ |
|---|---|---|---|---|
| 0 | $\phi$ | $1$ | $1$ | 1 |
| 1 | • | $x$ | $2x$ | 1 |
| 2 |  | $x^2 - 1$ | $4x^2 - 1$ | 2 |
| 3 |  | $x^3 - 2x$ | $8x^3 - 4x$ | 3 |
| 4 |  | $x^4 - 3x^2 + 1$ | $16x^4 - 12x^2 + 1$ | 5 |
| 5 |  | $x^5 - 4x^3 + 3x$ | $32x^5 - 32x^3 + 6x$ | 8 |
| 6 |  | $x^6 - 5x^4 + 6x^2 - 1$ | $64x^6 - 80x^4 + 24x^2 - 1$ | 13 |
| 7 |  | $x^7 - 6x^5 + 10x^3 - 4x$ | $128x^7 - 192x^5 + 80x^3 - 8x$ | 21 |

Table 2.

| $n$ | $C_n$ | $M_{C_n}(x) = 2T_n(x/2) = C_n(x)$ | $T_n(x)$ | $Z_G$ |
|---|---|---|---|---|
| 0 | $\phi$ | $2$ | $1$ | 2 |
| 1 | • | $x$ | $x$ | 1 |
| 2 |  | $x^2 - 2$ | $2x^2 - 1$ | 3 |
| 3 |  | $x^3 - 3x$ | $4x^3 - 3x$ | 4 |
| 4 |  | $x^4 - 4x^2 + 2$ | $8x^4 - 8x^2 + 1$ | 7 |
| 5 |  | $x^5 - 5x^3 + 5x$ | $16x^5 - 20x^3 + 5x$ | 11 |
| 6 |  | $x^6 - 6x^4 + 9x^2 - 2$ | $32x^6 - 48x^4 + 18x^2 - 1$ | 18 |
| 7 |  | $x^7 - 7x^5 + 14x^3 - 7x$ | $64x^7 - 112x^5 + 56x^3 - 7x$ | 29 |

(24) $$U_n(i/2)=S_n(i)=i^n(\alpha^{n+1}-\beta^{n+1})/\sqrt{5}=i^nF_n\,,$$

where $F_n$ and $L_n$ are, respectively, the well-known Fibonacci and Lucas numbers, with the following properties:

(25) $$F_n=F_{n-1}+F_{n-2}\,,\qquad F_0=F_1=1^*$$

(26) $$L_n=L_{n-1}+L_{n-2}\,,\qquad L_1=1\,,\qquad L_2=3\,.$$

It has been shown by the present author that the topological indices $Z_G$'s

* Although another definition ($F_1=F_2=1$) is currently used, it will be clear that the present definition gives better graphical representation of the Fibonacci numbers.

of path graphs $\{P_n\}$ and cycle graphs $\{C_n\}$, respectively, from the Fibonacci and Lucas numbers [1, 2].

Note that the recursion formulas of $Z_G$'s of these series of graphs take the form of Eq. (12.2), which implies that the corresponding matching polynomials recur as Eq. (12.3), which is exactly the same as that of Eq. (19) including the set of the initial values in Eq. (21). Thus we have the relations

$$M_{P_n}(x)=U_n(x/2)=S_n(x) \tag{27}$$

$$M_{C_n}(x)=2T_n(x/2)=C_n(x)\,. \tag{28}$$

This means that the matching polynomial of a path graph $P_n$ is identical to the second kind of the Chebyshev polynomial with the degree $n$, while that of a cycle graph $C_n$ is to the first kind (See Tables 1 and 2). Once we know these relations, we can derive a number of recursion formulas of these orthogonal polynomials by using the graph-theoretical aspects of the matching polynomial. For example, suppose that the two path graphs, $P_m$ and $P_n$, are joined by a line $l$ to give a longer path graph $P_{m+n}$. Then the application of the relation (11.3) to $P_{m+n}$ gives

$$M_{P_{m+n}}(x)=M_{P_m}(x)\cdot M_{P_n}(x)-M_{P_{m-1}}(x)\cdot M_{P_{n-1}}(x)\,. \tag{29}$$

For the case where $m$ and $n$ are equal we have

$$M_{P_{2n}}(x)=\{M_{P_n}(x)\}^2-\{M_{P_{n-1}}(x)\}^2\,. \tag{30}$$

The following recursion relations for the $U$ polynomial are automatically obtained:

$$U_{m+n}(x)=U_m(x)\cdot U_n(x)-U_{m-1}(x)\cdot U_{n-1}(x) \tag{31}$$

$$U_{2n}(x)=\{U_n(x)\}^2-\{U_{n-1}(x)\}^2\,. \tag{32}$$

By using Eq. (9), Eq. (29) can be transformed into

$$Z_{P_{m+n}}=Z_{P_m}\cdot Z_{P_n}+Z_{P_{m-1}}\cdot Z_{P_{n-1}} \tag{33}$$

$$F_{m+n}=F_m\cdot F_n+F_{m-1}\cdot F_{n-1}\,. \tag{34}$$

Similarly the relation (11.3) is applied to a cycle graph $C_n$ to give

$$2T_n(x)=U_n(x)-U_{n-2}(x) \qquad (n\geqq 2)^* \tag{35}$$

$$C_n(x)=S_n(x)-S_{n-2}(x)\,, \qquad (n\geqq 2)^* \tag{36}$$

both of which can be transformed into

$$L_n=F_n+F_{n-2}\,. \qquad (n\geqq 2) \tag{37}$$

Next add up the both sides of Eq. (36) separately for the even and odd $n$

* If we extend Eqs. (35) and (36) down to $n=0$, we need to have

$$2T_1(x)=U_1(x) \qquad 2T_0(x)=2U_0(x)$$

and

$$C_1(x)=S_1(x) \qquad C_0(x)=2S_0(x)\,.$$

terms, and we are left with the following equations:

(38.1) $$C_{2n}(x)+C_{2n-2}(x)+\cdots+C_0(x)=S_{2n}(x)+S_0(x)$$

(38.2) $$C_{2n+1}(x)+C_{2n-1}(x)+\cdots+C_1(x)=S_{2n+1}(x),$$

which give the recursion relations of the Chebyshev polynomials [15],

(39.1) $$2\{T_{2n}(x)+T_{2n-2}(x)+\cdots+T_0(x)\}=U_{2n}(x)+U_0(x)$$

(39.2) $$2\{T_{2n+1}(x)+T_{2n-1}(x)+\cdots+T_1(x)\}=U_{2n+1}(x).$$

Similar treatment on the relations (19) gives

(40.1) $$x\{C_{2n}(x)-C_{2n-2}(x)+C_{2n-4}(x)-\cdots+(-1)^nC_0(x)\}$$
$$=C_{2n+1}(x)+(-1)^nC_1(x)$$

(40.2) $$x\{C_{2n+1}(x)-C_{2n-1}(x)+C_{2n-3}(x)-\cdots+(-1)^nC_1(x)\}$$
$$=C_{2n+2}(x)+(-1)^nC_0(x)$$

(40.3) $$x\{S_{2n}(x)-S_{2n-2}(x)+S_{2n-4}(x)-\cdots+(-1)^nS_0(x)\}=S_{2n+1}(x)$$

(40.4) $$x\{S_{2n+1}(x)-S_{2n-1}(x)+S_{2n-3}(x)-\cdots+(-1)^nS_1(x)\}$$
$$=S_{2n+2}(x)+(-1)^nS_0(x),$$

which give rather new types of the recursion relations of the Chebyshev polynomials:

(41.1) $$2x\{T_{2n}(x)-T_{2n-2}(x)+T_{2n-4}(x)-\cdots+(-1)^nT_0(x)\}$$
$$=T_{2n+1}(x)+(-1)^nT_1(x)$$

(41.2) $$2x\{T_{2n+1}(x)-T_{2n-1}(x)+T_{2n-3}(x)-\cdots+(-1)^nT_1(x)\}$$
$$=T_{2n+2}(x)+(-1)^nT_0(x)$$

(41.3) $$2x\{U_{2n}(x)-U_{2n-2}(x)+U_{2n-4}(x)-\cdots+(-1)^nU_0(x)\}=U_{2n+1}(x)$$

(41.4) $$2x\{U_{2n+1}(x)-U_{2n-1}(x)+U_{2n-3}(x)-\cdots+(-1)^nU_1(x)\}$$
$$=U_{2n+2}(x)+(-1)^nU_0(x).$$

## 4. Graphical Representation

Since all the Chebyshev polynomials, $T$, $U$, $S$, and $C$, are shown to be associated with either of the path or cycle graph through the matching polynomial, the recursion relations (29)-(39) can respectively be given their graphical representations as in Figs. 1-3, where the relations among the Fibonacci and Lucas numbers are also shown.

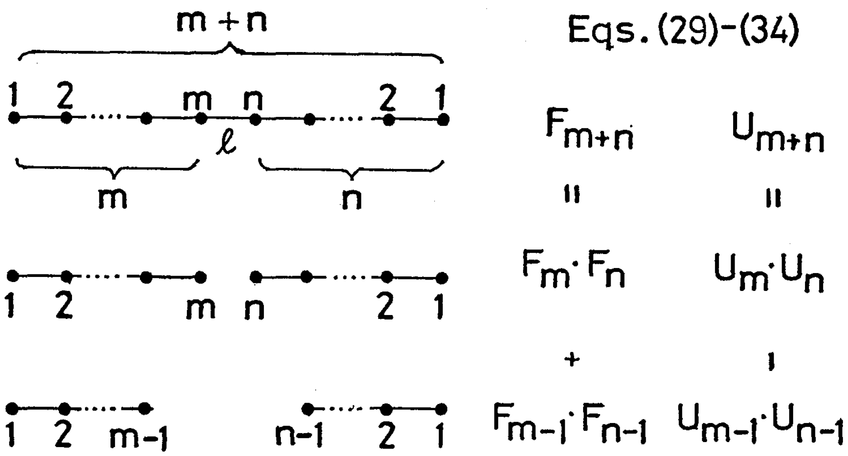



Fig. 1.

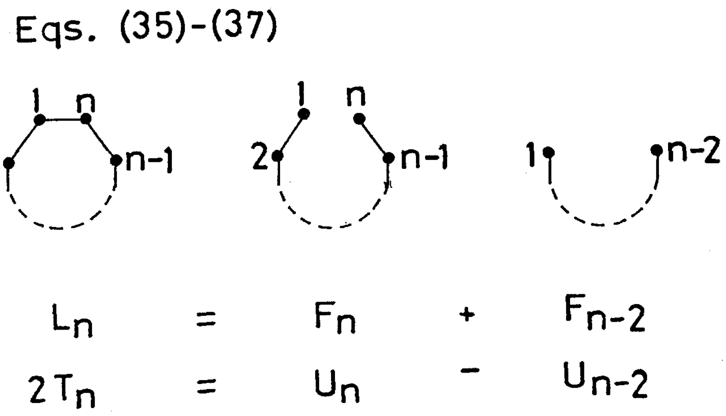



Fig. 2.

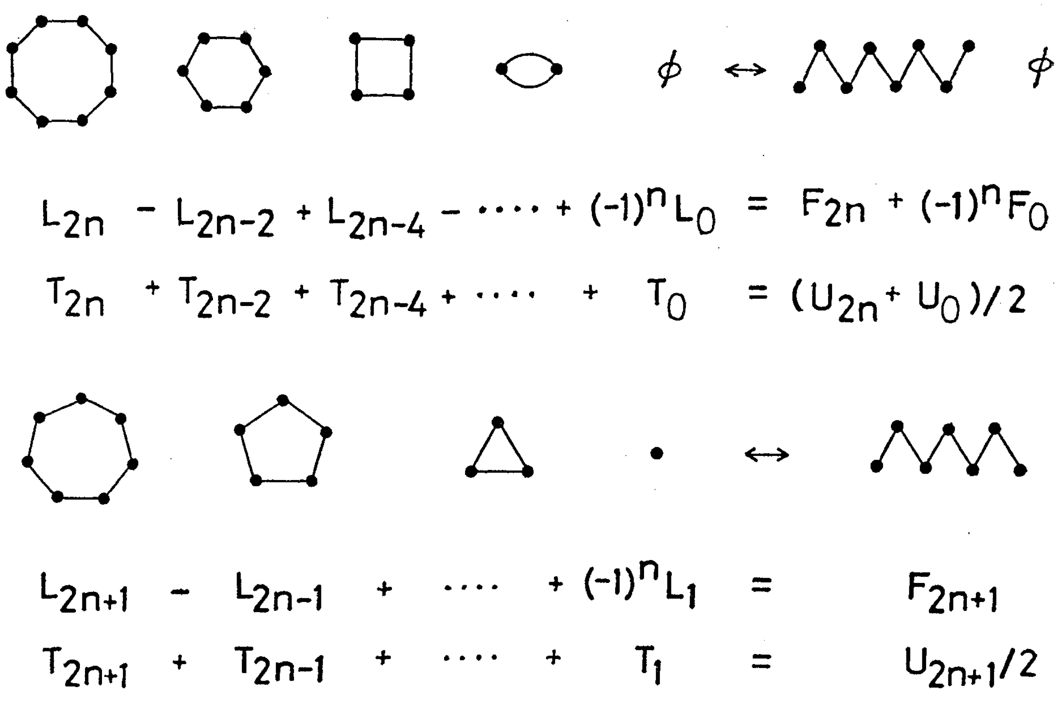



Fig. 3.

## 5. Orthogonal Polynomials

The Hermite polynomial is defined either as

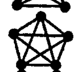
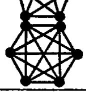
(42) $$H_n(x)=(-1)^n \exp(x^2)\frac{d^n}{dx^n}\exp(-x^2).$$

or as

(43) $$h_n(x)=2^{-n/2}H_n(x/\sqrt{2}) \quad [14].$$

In Table 3 are given the $H_n(x)$ and $h_n(x)$ for smaller $n$ values. The recursion relations have been known as

Table 3.

| n | $K_n$ | $M_{K_n}(x) = h_n(x)$ | $H_n(x)$ |
|---|---|---|---|
| 0 | $\phi$ | 1 | 1 |
| 1 | • | x | 2x |
| 2 |  | $x^2 - 1$ | $4x^2 - 2$ |
| 3 |  | $x^3 - 3x$ | $8x^3 - 12x$ |
| 4 |  | $x^4 - 6x^2 + 3$ | $16x^4 - 48x^2 + 12$ |
| 5 |  | $x^5 - 10x^3 + 15x$ | $32x^5 - 160x^3 + 120x$ |
| 6 |  | $x^6 - 15x^4 + 45x^2 - 15$ | $64x^6 - 480x^4 + 720x^2 - 120$ |

$$M_{K_n}(x) = \sum_{k=0}^{[n/2]} (-1)^k \frac{n!}{(n-2k)!\,k!\,2^k} x^{n-2k}$$

$$= \sum_{k=0}^{[n/2]} (-1)^k \binom{n}{2k} (2k-1)!!\, x^{n-2k}$$

$$H_n(x) = (-1)^n \exp(x^2)\frac{d^n}{dx^n}\exp(-x^2)$$

$$h_n(x) = 2^{-n/2} H_n(x/\sqrt{2})$$

(44) $$H_n(x)=2xH_{n-1}(x)-2(n-1)H_{n-2}(x)$$

(45) $$h_n(x)=xh_{n-1}(x)-(n-1)h_{n-2}(x).$$

Suppose a complete graph $K_n$ and its matching polynomial, which has already been shown by the present author to recur as

(46) $$M_{K_n}(x)=xM_{K_{n-1}}(x)-(n-1)M_{K_{n-2}}(x) \quad [11].$$

Note that Eqs. (45) and (46) have just the same form. The latter can be derived by a successive application of the recursion relation (13). It has also been shown that the closed form of $M_{K_n}(x)$ is given by

(47) $$M_{K_n}(x)=\sum_{k=0}^{[n/2]}(-1)^k\frac{n!}{(n-2k)!\,k!\,2^k}x^{n-2k} \quad [11],$$

which is identical to $h_n(x)$ [13], namely,

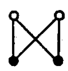
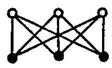
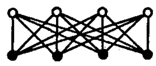
(48) $$M_{K_n}(x)=h_n(x)=2^{-n/2}H_n(x/\sqrt{2}).$$

Gutman has also shown that the matching polynomials of the complete bipartite graph $K_{n,n}$ and $K_{m,n}$ are, respectively, equivalent to the Laguerre and associated Laguerre polynomials as

(49) $$M_{K_{n,n}}(x)=(-1)^nL_n(x^2)$$

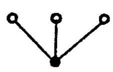
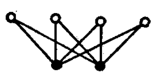
(50) $$M_{K_{m,n}}(x)=\frac{(-1)^n n!\,x^{m-n}}{m!}L_m^{m-n}(x^2). \qquad (m\geqq n)$$

Table 4.

| n | $K_{n,n}$ | $M_{K_{n,n}}(x) = (-1)^n L_n(x^2)$ |
|---|---|---|
| 0 | $\phi$ | 1 |
| 1 |  | $x^2 - 1$ |
| 2 |  | $x^4 - 4x^2 + 2$ |
| 3 |  | $x^6 - 9x^4 + 18x^2 - 6$ |
| 4 |  | $x^8 - 16x^6 + 72x^4 - 96x^2 + 24$ |

$$M_{K_{n,n}}(x) = \sum_{k=0}^{n}(-1)^k\frac{n!^2}{\{(n-k)!\}^2\,k!}x^{2n-2k}$$

Table 5.

| m | n | $K_{m,n}$ | $M_{K_{m,n}}(x)$ | $L_m^{m-n}$ |
|---|---|---|---|---|
| 2 | 1 |  | $x^3 - 2x$ | $2x - 4$ |
| 3 | 1 |  | $x^4 - 3x^2$ | $-6x + 18$ |
| 3 | 2 |  | $x^5 - 6x^3 + 6x$ | $-3x^2 + 18x - 18$ |
| 4 | 2 |  | $x^6 - 8x^4 + 12x^2$ | $12x^2 - 96x + 144$ |

$$M_{K_{m,n}}(x) = \sum_{k=0}^{\min(m,n)}(-1)^k\frac{m!\,n!}{(m-k)!\,(n-k)!\,k!}x^{m+n-2k}$$

In Tables 4 and 5 are given smaller $K_{n,n}$ and $K_{m,n}$ graphs and the corresponding polynomials.

By a successive application of the recursion relation (13) to Eqs. (49) and (50) Gutman has derived the following recursion relations of the Laguerre and associated Laguerre polynomials:

(51)
$$L_n(x)=nL_{n-1}(x)+\frac{x}{n}L_n^1(x)$$
$$L_{n+1}(x)=(2n+1-x)L_n(x)-n^2L_{n-1}(x) \quad [13].$$

## 6. Discussion

The matching polynomials for typical series of graphs are thus shown to be closely related to some of the orthogonal polynomials as summarized in Table 6. This fact suggests that the non-adjacent number $p(G, k)$ is not only an important graph-theoretical quantity but also may have some key role in the mathematical structure of the quantum mechanical eigenvalue problems. The Legendre, Laguerre, and Hermite polynomials are known to be the typical solutions of the Schrödinger equations for the problems where a wave-like particle is trapped in a potential well of various forms. The differential equations to be satisfied by the Chebyshev and Legendre polynomials are very similar, *i.e.*,

Table 6.

| Orthogonal Polynomial | | Graph | |
|---|---|---|---|
| Chebyshev (1st kind) | $T_n$, $C_n$ | Cycle graph | $C_n$ |
| Chebyshev (2nd kind) | $U_n$, $S_n$ | Path graph | $P_n$ |
| Hermite | $H_n$, $h_n$ | Complete graph | $K_n$ |
| Laguerre | $L_n$ | Complete bipartite graph | $K_{n,n}$ |
| Associated Laguerre | $L_m^{m-n}$ | Complete bipartite graph | $K_{m,n}$ |
| Legendre | $P_n$ | ----- | |

(47.1)
$$(1-x^2)T_n''(x)-xT_n'(x)+n^2T_n(x)=0$$

(47.2)
$$(1-x^2)U_n''(x)-xU_n'(x)+n^2U_n(x)=0$$

(47.3)
$$(1-x^2)P_n''(x)-2xP_n'(x)+n(n+1)P_n(x)=0$$

However, no eigenvalue problem has been known whose solution takes the Chebyshev polynomial, whose matching polynomial is identical to the Legendre polynomial. These questions are open.

## Acknowledgement

The author deeply thanks Professor Ivan Gutman of the Kragujevac University, Yugoslavia, for showing his unpublished materials on this topics. Thanks are also given to Professor Frank Harary of the University of Michigan for his discussion, suggestion, and encouragement.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