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SHORT COMMUNICATION

Matrices and orthogonal polynomials

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ABSTRACT

The Lanczos algorithm of minimized iterations shows that a polynomial verifying a three-term recurrence relation can be written as the determinant of a tridiagonal matrix, here we exhibit examples of this property. Besides, for several orthogonal polynomials, Cohen proved that their roots are the proper values of symmetric tridiagonal matrices; here we give examples of this Cohen's result for the Legendre, Laguerre, and Hermite polynomials, which are important in applications to numerical analysis and quantum mechanics.

***Keywords*:** Chebyshev, Hermite, Laguerre and Legendre polynomials, Leverrier-Takeno's method, Lanczos algorithm, Three-member recurrence

1. INTRODUCTION

In the Lanczos technique of minimized iterations [1-5] we learn that polynomials satisfying the three-member recurrence:

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$$p_m(x) = (x - \alpha_{m-1})\, p_{m-1}(x) - \beta_{m-2}\, p_{m-2}(x), \quad m \geq 2,$$
$$p_0(x) = 1, \quad p_1(x) = x - \alpha_0, \tag{1}$$

can be interpreted as determinants of tridiagonal matrices:

$$p_r(x) = \det(x\, I_{rxr} - L_{rxr}), \quad r = 1, 2, 3, \dots; \quad L = \begin{pmatrix} \alpha_0 & \beta_0 & 0 & \cdots & 0 \\ 1 & \alpha_1 & \beta_1 & \cdots & 0 \\ 0 & 1 & \alpha_2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 1 & \alpha_{r-1} \end{pmatrix}, \tag{2}$$

that is:

$$L_{1X1} = (\alpha_0), \quad L_{2X2} = \begin{pmatrix} \alpha_0 & \beta_0 \\ 1 & \alpha_1 \end{pmatrix}, \quad L_{3x3} = \begin{pmatrix} \alpha_0 & \beta_0 & 0 \\ 1 & \alpha_1 & \beta_1 \\ 0 & 1 & \alpha_2 \end{pmatrix}, \quad L_{4x4} = \begin{pmatrix} \alpha_0 & \beta_0 & 0 & 0 \\ 1 & \alpha_1 & \beta_1 & 0 \\ 0 & 1 & \alpha_2 & \beta_2 \\ 0 & 0 & 1 & \alpha_3 \end{pmatrix},$$

etc. (3)

We notice that the recurrence relation (1) is exactly of the type which is characteristic for all the classical kinds of orthogonal polynomials [1]. In Sec. 2 we apply the expressions (1), (2) and (3) to the Legendre, Hermite and Chebyshev polynomials.

On the other hand, for the Legendre polynomials $P_n(x)$ [6, 7]:

$$P_0(x) = 1, \quad P_1(x) = x, \quad P_2(x) = \tfrac{1}{2}(3x^2 - 1), \quad P_3(x) = \tfrac{1}{2}(5x^3 - 3x), \dots \tag{4}$$

which verify the differential equation $(1 - x^2)y'' - 2xy' + l(l+1) = 0,\ l = 0, 1, 2, \dots,$ Cohen [8, 9] showed that the roots of $P_n(x)$ are the proper values of the following symmetric tridiagonal matrix:

$$\boldsymbol{P}_n = \begin{pmatrix} 0 & \frac{1}{\sqrt{3}} & & & & \\ \frac{1}{\sqrt{3}} & 0 & \frac{2}{\sqrt{15}} & & & \\ & \frac{2}{\sqrt{15}} & 0 & \frac{3}{\sqrt{35}} & & \\ & & \frac{3}{\sqrt{35}} & 0 & \ddots & \\ & & & \ddots & \ddots & \ddots \\ & & & & \ddots & 0 & g(n) \\ & & & & & g(n) & 0 \end{pmatrix}, \quad g(n) = \frac{n-1}{\sqrt{(2n-1)(2n-3)}}. \tag{5}$$

Since the eigenvalues of a symmetric matrix are all real, it follows that the roots of the Legendre polynomials must all be real [6, 10, 11]. Moreover, the absence of nonzero terms along the leading diagonal of the matrix $\boldsymbol{P}_n$ implies that the eigenvalues are symmetrically distributed about the origin. Let's remember that the roots of $P_n(x)$ are important in the Gaussian quadrature [6, 12].

Similarly, the roots of the Laguerre polynomials $L_n(x)$ [13-15]:

$$L_0(x)=1, \quad L_1(x)=1-x, \quad L_2(x)=\frac{1}{2}(x^2-4x+2), \\ L_3(x)=\frac{1}{6}(-x^3+9x^2-18x+6), \ldots \tag{6}$$

which satisfy the differential equation $xy''+(1-x)y'+ny=0$, $n=0,1,2,\ldots$, are the eigenvalues of the symmetric matrix [8, 9]:

$$\boldsymbol{L}_n = \begin{pmatrix} 1 & 1 & & & & \\ 1 & 3 & 2 & & & \\ & 2 & 5 & \ddots & & \\ & & \ddots & \ddots & \ddots & \\ & & & n-2 & 2n-3 & n-1 \\ & & & & n-1 & 2n-1 \end{pmatrix}, \tag{7}$$

hence all solutions of $L_n(x)=0$ are real [16].

Besides, the Hermite polynomials $H_n(x)$ [17, 18]:

$$H_0(x)=1, \quad H_1(x)=2x, \quad H_2(x)=4x^2-2, \quad H_3(x)=8x^3-12x, \quad \ldots \tag{8}$$

which obey the differential equation $y''-2xy'+2ny=0$, $n=0,1,2,\ldots$, have real roots [19-21] corresponding to the proper values of [16]:

$$\boldsymbol{H}_n = \begin{pmatrix} 0 & \sqrt{\frac{1}{2}} & & & & \\ \sqrt{\frac{1}{2}} & 0 & \sqrt{\frac{2}{2}} & & & \\ & \sqrt{\frac{2}{2}} & 0 & \sqrt{\frac{3}{2}} & & \\ & & \ddots & \ddots & \ddots & \\ & & & \ddots & 0 & \sqrt{\frac{n-1}{2}} \\ & & & & \sqrt{\frac{n-1}{2}} & 0 \end{pmatrix}, \tag{9}$$

which are symmetrically distributed about the origin.

In Sec. 3 we employ the Leverrier-Takeno's technique [22-26] to realize applications of (5), (7) and (9).

2. POLYNOMIALS AS DETERMINANTS OF TRIDIAGONAL MATRICES

The Legendre polynomials satisfy a recurrence relation with the structure of (1):

$$P_m = \left(x - \frac{1-m}{m}\, x\right) P_{m-1} - \frac{m-1}{m}\, P_{m-2}\,, \qquad m \geq 2,\ P_0 = 1, \qquad P_1 = x, \tag{10}$$

hence for $r \geq 2$ we have that $\alpha_{r-1} = \frac{1-r}{r}\, x$ and $\beta_{r-2} = \frac{r-1}{r}$ with $\alpha_0 = 0$, thus from (2) and (3):

$$P_2(x) = det\begin{pmatrix} x & -\frac{1}{2} \\ -1 & \frac{3}{2}x \end{pmatrix}, \qquad P_3(x) = det\begin{pmatrix} x & -\frac{1}{2} & 0 \\ -1 & \frac{3}{2}x & -\frac{2}{3} \\ 0 & -1 & \frac{5}{3}x \end{pmatrix}, \quad \text{etc.} \tag{11}$$

in according with (4).

Similary, the Hermite polynomials verify (1) because:

$$H_m = 2x\, H_{m-1} - 2(m-1)\, H_{m-2} \quad \therefore \quad \alpha_r = -x\,, \quad \beta_r = 2(r+1), \quad r \geq 0, \tag{12}$$

hence:

$$H_2(x) = det\begin{pmatrix} 2x & -2 \\ -1 & 2x \end{pmatrix}, \qquad H_3(x) = det\begin{pmatrix} 2x & -2 & 0 \\ -1 & 2x & -4 \\ 0 & -1 & 2x \end{pmatrix}, \quad \ldots. \tag{13}$$

in harmony with (8). The Chebyshev polynomials [6, 27] satisfy a three-term recurrence relation:

$$T_m = 2x\, T_{m-1} - T_{m-2}\,, \quad T_0 = 1, \quad T_1 = x \quad \therefore \quad \alpha_0 = 0, \quad \alpha_{r+1} = -x, \quad \beta_r = 1, \quad r \geq 0, \tag{14}$$

then from (2) and (3):

$$T_2(x) = det\begin{pmatrix} x & -1 \\ -1 & 2x \end{pmatrix} = 2x^2 - 1,\ T_3(x) = det\begin{pmatrix} x & -1 & 0 \\ -1 & 2x & -1 \\ 0 & -1 & 2x \end{pmatrix} = 4x^3 - 3x, \ \ldots \tag{15}$$

The relations (15) are important because imply the existence of the associated polynomials of Chebyshev [28-30].

3. SOME APPLICATIONS OF THE COHEN'S RESULTS

The characteristic equation of a matrix $\boldsymbol{A}_{n\,x\,n}$:

$$\lambda^n + a_1\, \lambda^{n-1} + a_2\, \lambda^{n-2} + \cdots + a_n = 0, \tag{16}$$

can be constructed via the Leverrier-Takeno's procedure [22-26]:

$$a_1 = -s_1\,, \qquad a_2 = \frac{1}{2}[(s_1)^2 - s_2], \qquad a_3 = \frac{1}{6}[-(s_1)^3 + 3s_1\, s_2 - 2s_3], \ \ldots \quad (17)$$

where s_r is the trace of $\boldsymbol{A}^r$. Then we consider (5):

$$\boldsymbol{P}_2 = \begin{pmatrix} 0 & \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{3}} & 0 \end{pmatrix}, \qquad \boldsymbol{P}_2^2 = \begin{pmatrix} \frac{1}{3} & 0 \\ 0 & \frac{1}{3} \end{pmatrix}, \qquad s_1 = a_1 = 0, \quad s_2 = \frac{2}{3}, \quad a_2 = -\frac{1}{3}\,,$$

thus (16) implies the equation $3\lambda^2 - 1 = 0$ in agreement with $P_2(x) = 0$. Similarly:

$$\boldsymbol{P}_3 = \begin{pmatrix} 0 & \frac{1}{\sqrt{3}} & 0 \\ \frac{1}{\sqrt{3}} & 0 & \frac{2}{\sqrt{15}} \\ 0 & \frac{2}{\sqrt{15}} & 0 \end{pmatrix}, \qquad \boldsymbol{P}_3^2 = \begin{pmatrix} \frac{1}{3} & 0 & \frac{2}{3\sqrt{5}} \\ 0 & \frac{3}{5} & 0 \\ \frac{2}{3\sqrt{5}} & 0 & \frac{4}{15} \end{pmatrix}, \qquad \boldsymbol{P}_3^3 = \begin{pmatrix} 0 & \frac{\sqrt{3}}{5} & 0 \\ \frac{\sqrt{3}}{5} & 0 & \frac{6}{5\sqrt{15}} \\ 0 & \frac{6}{5\sqrt{5}} & 0 \end{pmatrix},$$

hence $s_1 = a_1 = 0$, $s_2 = \frac{6}{5}$, $a_2 = -\frac{3}{5}$, $s_3 = a_3 = 0$, and from (16) we obtain $5\lambda^3 - 3\lambda = 0$ in harmony with $P_3(x) = 0$. Let's remember that the roots of Legendre polynomials are important in the Gaussian quadrature [12], in the study of electromagnetic radiation and the angular function for the hydrogen atom.

Besides, from (7):

$$\boldsymbol{L}_2 = \begin{pmatrix} 1 & 1 \\ 1 & 3 \end{pmatrix}, \qquad \boldsymbol{L}_2^2 = \begin{pmatrix} 2 & 4 \\ 4 & 10 \end{pmatrix}, \qquad s_1 = 4, \quad s_2 = 12, \quad a_1 = -4, \quad a_2 = 2,$$

then (16) gives $\lambda^2 - 4\lambda + 2 = 0$, equivalent to $L_2(x) = 0$; and:

$$\boldsymbol{L}_3 = \begin{pmatrix} 1 & 1 & 0 \\ 1 & 3 & 2 \\ 0 & 2 & 5 \end{pmatrix}, \qquad \boldsymbol{L}_3^2 = \begin{pmatrix} 2 & 4 & 2 \\ 4 & 14 & 16 \\ 2 & 6 & 29 \end{pmatrix}, \qquad \boldsymbol{L}_3^3 = \begin{pmatrix} 6 & 18 & 18 \\ 18 & 78 & 108 \\ 18 & 108 & 177 \end{pmatrix},$$

therefore $s_1 = 9$, $s_2 = 45$, $s_3 = 261$, $a_1 = -9$, $a_2 = 18$, $a_3 = -6$, and from (16) we deduce that $\lambda^3 - 9\lambda^2 + 18\lambda - 6 = 0$ in according with (6). The Laguerre polynomials participate in the radial function of hydrogen-like atoms [31] and diatomic molecules [32].

For the Hermite polynomials:

$$\boldsymbol{H}_2 = \begin{pmatrix} 0 & \sqrt{\frac{1}{2}} \\ \sqrt{\frac{1}{2}} & 0 \end{pmatrix}, \qquad \boldsymbol{H}_2^2 = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix}, \qquad s_1 = a_1 = 0, \quad s_2 = 1, \quad a_2 = -\frac{1}{2},$$

implying the characteristic equation $2\lambda^2 - 1 = 0$, equivalent to $H_2(x) = 0$; and:

$$\boldsymbol{H}_3 = \begin{pmatrix} 0 & \sqrt{\frac{1}{2}} & 0 \\ \sqrt{\frac{1}{2}} & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad \boldsymbol{H}_3^2 = \begin{pmatrix} \frac{1}{2} & 0 & \sqrt{\frac{1}{2}} \\ 0 & \frac{3}{2} & 0 \\ \sqrt{\frac{1}{2}} & 0 & 1 \end{pmatrix}, \quad \boldsymbol{H}_3^3 = \begin{pmatrix} 0 & \frac{3}{2}\sqrt{\frac{1}{2}} & 0 \\ \frac{3}{2}\sqrt{\frac{1}{2}} & 0 & \frac{3}{2} \\ 0 & \frac{3}{2} & 0 \end{pmatrix},$$

$s_1 = a_1 = 0,\ s_2 = 3,\ a_2 = -\frac{3}{2}\ ,\ s_3 = a_3 = 0$, thus (16) gives the expression $2\lambda^3 - 3\lambda = 0$ which is compatible with $H_3(x) = 0$. The Hermite polynomials are fundamental in the analysis of the harmonic oscillator in quantum physics.

4. CONCLUSIONS

Thus we have that the Leverrier-Takeno's process allows to see that the eigenvalues of the matrices (5), (7) and (9) are the roots of the Legendre, Laguerre [33, 34], and Hermite polynomials, respectively. Let's remember that the QR algorithm [35-38] is an efficient method to determine the proper values of a matrix. Besides, the interpretation of a polynomial as the determinant of certain tridiagonal matrix opens the possibility to define the corresponding associated polynomials.

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