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MATRIX METHODS FOR CALCULATING ZEROS, COEFFICIENTS, CHRISTOFFEL NUMBERS, AND DERIVATIVES OF SOME ORTHOGONAL POLYNOMIALS

H. A. Luther and J. M. Nash

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(Abstract)

A computational technique is sketched, useful, for example, in the comparative study of various quadrature methods. Infinite Jacobian matrices are constructed having the property that the eigenvalues of successive leading submatrices are the zeros of successive orthogonal polynomials (or, if desired, their derivatives of any order). Symmetric and unsymmetric formulations are shown. ~~The unsymmetric version proves efficient in finding~~ coefficients for the polynomials. The determinants of leading submatrices of a matrix related to the above can be used to evaluate such polynomials without calculating coefficients. In particular, Christoffel numbers can be so calculated efficiently. The methods apply to any Sturm sequence.

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MATRIX METHODS FOR CALCULATING ZEROS, COEFFICIENTS, CHRISTOFFEL NUMBERS, AND DERIVATIVES OF SOME ORTHOGONAL POLYNOMIALS*

H. A. Luther† and J. M. Nash††

Introduction

It is known that a recursion relation exists involving any three consecutive orthonormal polynomials of a given class. This relation can be used to build a Jacobian matrix whose successive leading submatrices have as eigenvalues the zeros of these polynomials. This same matrix may be used to yield the coefficients of the polynomials in monic form.

In the case of Jacobi, Hermite and Laguerre polynomials, the concept extends simply to the derivatives of the polynomials.

More than one such matrix can be determined. A symmetric form can be devised, thus permitting, for example, the use of the method of Jacobi for finding eigenvalues. An unsymmetric form can be found better suited for finding the Frobenious normal form and better suited for evaluating the polynomials by a determinant method later explained in detail.

The scheme can be applied to any Jacobian matrix, and thus to any sequence of Sturm functions. It seems well adapted to a comparative

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*Sponsored in part by NASA Grant NGR 44-001-024.
†Mathematics Department, Texas A&M University, College Station, Texas.
††Mechanical Engineering Department, Texas A&M University.

study of quadrature and series developments for Jacobi polynomials.

The General Case for Orthogonal Polynomials

Let $p_n(x)$, $n \geq 0$, denote the orthonormal polynomials. Then (see [1], p. 41)

$$p_n(x) = (A_n x + B_n)p_{n-1}(x) - C_n\, p_{n-2}(x) \tag{1}$$

where $A_n > 0$ and $C_n > 0$. Let k_n denote the coefficient of the term of highest degree in $p_n(x)$. Then

$$p_n(x) = k_n\, q_n(x) \tag{2}$$

where $q_n(x)$ is monic. Also, since $q_n(x)$ and $q_{n-1}(x)$ are monic, $k_n = A_n\, k_{n-1}$. Thus

$$q_n(x) + (D_n - x)q_{n-1}(x) + E_n\, q_{n-2}(x) = 0 \tag{3}$$

where $D_n = -B_n/A_n$ and $E_n = C_n/(A_{n-1}\, A_n)$. E_n is positive, $q_o(x)$ is one, and we interpret $q_{-1}(x)$ as zero.

Now let M be the (infinite) tridiagonal matrix $[m_{ij}]$ such that $m_{ii} = D_i$, $m_{i,i+1} = m_{i+1,i} = \sqrt{E_{i+1}}$. It may be displayed as

$$M = \begin{bmatrix} D_1 & \sqrt{E_2} & 0 & 0 & --- \\ \sqrt{E_2} & D_2 & \sqrt{E_3} & 0 & --- \\ 0 & \sqrt{E_3} & D_3 & \sqrt{E_4} & --- \\ 0 & 0 & \sqrt{E_4} & D_4 & --- \\ - & - & - & - & --- \end{bmatrix} \tag{4}$$

Let the corresponding characteristic functions be $F_1(x)$, $F_2(x)$, etc. Then as a Jacobian matrix (see [2], p. 30) it is known that by taking

$F_o = 1$, $F_{-1} = 0$, the functions $F_n(x)$ satisfy

(5) $$F_n(x) - (D_n - x)F_{n-1}(x) + E_n F_{n-2}(x) = 0 .$$

Thus

(6) $$q_n(x) = (-1)^n F_n(x) .$$

The matrix M is known at least for the case of Legendre polynomials (see [3], p.127). Its more general use for the derivatives in the three following sections may have been unobserved.

Next let N be the (infinite) tridiagonal matrix $[n_{ij}]$ such that $n_{ii} = D_i$, $n_{i,i+1} = 1$, $n_{i+1,i} = E_{i+1}$. It may be displayed as

(7) $$\begin{bmatrix} D_1 & 1 & 0 & 0 & --- \\ E_2 & D_2 & 1 & 0 & --- \\ 0 & E_3 & D_3 & 1 & --- \\ 0 & 0 & E_4 & D_4 & --- \\ - & - & - & - & --- \end{bmatrix}$$

Matrix N has, for its leading submatrices, the same characteristic functions as (4). Either (7) or (4) may be used with the method of Danilevskii to find the characteristic functions involved. It will be seen that for this purpose (7) leads to a simplified procedure of interest. Moreover, if x_ν is a number for which a polynomial value is desired, the determinants of the leading submatrices of $N - x_\nu I$ prove economical.

The three following sections give necessary details for the polynomials of Jacobi, Hermite and Laguerre. These sections are independent of each other and of the remaining sections.

Final sections discuss the evaluation procedure, in particular Christoffel numbers, then the simplified Danilevskii procedure, then the computation of eigenvalues.

The Polynomials of Jacobi

We consider the polynomials of Jacobi as defined by (see [1], p.61).

$$(8)\quad P_n^{(\alpha,\beta)}(x) = (1/n!)\sum_{\nu=0}^{n}\binom{n}{\nu}\left(\prod_{i=1}^{\nu}(\alpha+\beta+n+i)\right)\left(\prod_{j=1}^{\nu}(\alpha+\nu+j)\right)(x-1)^{\nu}2^{-\nu}$$

A direct consequence of (8) is the well-known differential relation

$$(9)\qquad D\,P_n^{(\alpha,\beta)}(x) = (1/2)(n+\alpha+\beta+1)P_{n-1}^{(\alpha+1,\beta+1)}(x)\ .$$

A familiar recurrence relation is

$$2(\alpha+\beta+2n)(\alpha+\beta+n+1)(n+1)P_{n+1}^{(\alpha,\beta)}(x)$$

$$(10)\quad +(\alpha+\beta+2n+1)[\beta^2-\alpha^2-(\alpha+\beta+2n)(\alpha+\beta+2n+2)x]P_n^{(\alpha,\beta)}(x)$$

$$+2(\alpha+\beta+2n+2)(\alpha+n)(\beta+n)P_{n-1}^{(\alpha,\beta)}(x) = 0\ .$$

It is seen that $P_o^{(\alpha,\beta)}(x) = 1$, $P_1^{(\alpha,\beta)}(x) = [(\alpha+\beta+2)x+\alpha-\beta]/2$. We define $P_{-1}^{(\alpha,\beta)}(x)$ to be zero. By requiring that α and β be each greater than minus one, not only is $P_1^{(\alpha,\beta)}(x)$ not constant, but the polynomials form an orthogonal set, relative to the weight function $(1-x)^{\alpha}(1+x)^{\beta}$, over the interval [-1, 1].

In (10) replace n by n − m, α by $\alpha + m$, β by $\beta + m$. The result is

$$2(\alpha + \beta + 2n)(\alpha + \beta + n + m + 1)(n - m + 1)P_{n+1-m}^{(\alpha+m,\beta+m)}(x)$$

$$+ (\alpha + \beta + 2n + 1)[(\beta - \alpha)(\beta + \alpha + 2m) - (\alpha + \beta + 2n)(\alpha + \beta + 2n + 2)x]P_{n-m}^{(\alpha+m,\beta+m)}(x)$$

$$+ 2(\alpha + \beta + 2n + 2)(\alpha + n)(\beta + n)P_{n-1-m}^{(\alpha+m,\beta+m)}(x) = 0 .$$

From (9) it is seen that

$$D^m P_n^{(\alpha,\beta)}(x) = 2^{-m}(\alpha + \beta + n + 1) \cdots (\alpha + \beta + n + m)P_{n-m}^{(\alpha+m,\beta+m)}(x) .$$

Combining these gives

(11)
$$2(\alpha + \beta + 2n)(\alpha + \beta + n)(\alpha + \beta + n + 1)(n - m + 1)D^m P_{n+1}^{(\alpha,\beta)}(x)$$
$$+ (\alpha + \beta + 2n + 1)(\alpha + \beta + n)[(\beta - \alpha)(\beta + \alpha + 2m)$$
$$- (\alpha + \beta + 2n)(\alpha + \beta + 2n + 2)x]D^m P_n^{(\alpha,\beta)}(x)$$
$$+ 2(\alpha + \beta + 2n + 2)(\alpha + \beta + n + m)(\alpha + n)(\beta + n)D^m P_{n-1}^{(\alpha,\beta)}(x) = 0 .$$

If we now let

$$f_{mm} = 2^{-m} \prod_{i=1}^{m} (\alpha + \beta + m + i)$$

(12)
$$f_{m,n+1} = f_{mn}(\alpha + \beta + 2n + 1)(\alpha + \beta + 2n + 2)/[2(n - m + 1)(\alpha + \beta + n + 1)]$$

$$D^m P_n^{(\alpha,\beta)}(x) = f_{mn} Q_{mn}^{(\alpha,\beta)}(x)$$

for $n \geq m \geq 0$, and choose $f_{oo} = 1$, the polynomials $Q_{mn}^{(\alpha,\beta)}(x)$ are monic. We have $Q_{mm}^{(\alpha,\beta)}(x) = 1$ and choose to set $Q_{m,m-1}^{(\alpha,\beta)}(x) = 0$. The recurrence formula of (11) then becomes

$$Q_{m,n+1}^{(\alpha,\beta)}(x) + [J_{m,n+1}^{(\alpha,\beta)} - x]Q_{mn}^{(\alpha,\beta)}(x) + K_{m,n+1}^{(\alpha,\beta)}\ Q_{m,n-1}^{(\alpha,\beta)}(x) = 0$$

(13)

$$J_{m,n+1}^{(\alpha,\beta)} = (\beta - \alpha)(\alpha + \beta + 2m)/[(\alpha + \beta + 2n)(\alpha + \beta + 2n + 2)]$$

$$K_{m,n+1}^{(\alpha,\beta)} = 4(\alpha + n)(\beta + n)(\alpha + \beta + n + m)(n - m)/$$

$$[(\alpha + \beta + 2n)^2\ (\alpha + \beta + 2n + 1)(\alpha + \beta + 2n - 1)] \ .$$

Here $n \geq m \geq 0$.

For application of final results, it is remarked that (12) yields

(14) $$f_{mn} = 2^{-n}\ [\prod_{i=1}^{n} (\alpha + \beta + n + i)]/(n - m)! \ .$$

Relation (13) has the form of (3).

The Polynomials of Laguerre

The definition of Laguerre polynomials is that in [1]. Concerning them it is known that (see [1], pp. 96-98)

(15)

$$n\, L_n^{(\alpha)}(x) + (x + 1 - 2n - \alpha)L_{n-1}^{(\alpha)}(x) + (n + \alpha - 1)L_{n-2}^{(\alpha)}(x) = 0$$

$$L_o^{(\alpha)}(x) = 1, \qquad L_1^{(\alpha)}(x) = \alpha + 1 - x, \qquad \alpha > -1 \ .$$

It can be observed that the coefficient of x^n in $L_n^{(\alpha)}(x) = (-1)^n/n!$. It is also known that

(16) $$D\ L_n^{(\alpha)}(x) = -L_{n-1}^{(\alpha+1)}(x) \ .$$

In (15) replace n by $n - m$ and α by $\alpha + m$. The result is

$$(n - m)L_{n-m}^{(\alpha+m)}(x) + (x + 1 - 2n - \alpha + m)L_{n-m-1}^{(\alpha+m)}(x)$$

$$+ (n + \alpha - 1)L_{n-2-m}^{(\alpha+m)}(x) = 0 \ .$$

By (16)

$$D^m L_n^{(\alpha)}(x) = (-1)^m L_{n-m}^{(\alpha+m)}(x) .$$

These last two in combination give

$$(17) \quad \begin{aligned} &(n - m)D^m L_n^{(\alpha)}(x) + (x + 1 - \alpha - 2n + m)D^m L_{n-1}^{(\alpha)}(x) \\ &\quad + (n + \alpha - 1)D^m L_{n-2}^{(\alpha)}(x) = 0 . \end{aligned}$$

Now let $g_{mn} = (-1)^n/(n-m)!$ and define $S_{mn}^{(\alpha)}(x)$ by

$$(18) \quad D^m L_n^{(\alpha)}(x) = g_{mn} S_{mn}^{(\alpha)}(x) .$$

Relation (17) becomes

$$(19) \quad \begin{aligned} &S_{mn}^{(\alpha)}(x) + (2n + \alpha - 1 - m - x)S_{m,n-1}^{(\alpha)}(x) \\ &\quad + (n + \alpha - 1)(n - m - 1)S_{m,n-2}^{(\alpha)}(x) = 0 . \end{aligned}$$

Here $0 \leq m \leq n - 1$ and $S_{m,m-1}^{(\alpha)}(x)$ is interpreted as zero. Clearly the polynomials $S_{mn}^{(\alpha)}(x)$ are monic.

It is seen that (19) has the form of (3).

The Hermite Polynomials

From [1] we find the Hermite polynomials characterized by the recurrence formula.

$$(20) \quad H_n(x) - 2x H_{n-1}(x) + 2(n - 1)H_{n-2}(x) = 0$$

and the relations $H_o(x) = 1$, $H_1(x) = 2x$. It is also known that (see [1], p. 102)

$$D\,H_n(x) = 2n\,H_{n-1}(x) \;, \tag{21}$$

thus $D^m H_n(x) = 2^m n(n-1) \cdots (n-m+1) H_{n-m}(x)$. When n is replaced by n-m in (20) and the result combined with the relation just above, we have

$$\begin{aligned}(n-m)D^m H_n(x) - 2n\,x\,D^m H_{n-1}(x)\\ + 2n(n-1)D^m H_{n-2}(x) = 0 \;.\end{aligned} \tag{22}$$

Now let $h_{mn} = 2^n\, n(n-1) \cdots (n-m+1)$ and define $T_{mn}(x)$ by

$$h_{mn}(x)\, T_{mn}(x) = D^m H_n(x) \;. \tag{23}$$

When this is used in (22) there results

$$T_{mn}(x) - xT_{m,n-1}(x) + [(n-m-1)/2]T_{m,n-2}(x) = 0 \;. \tag{24}$$

This is valid for $n - 1 \geq m \geq 0$, if $T_{m,m-1}$ is interpreted as zero. It is observed that $T_{mm}(x)=1$, so that $T_{mn}(x)$ is monic.

Evaluation of Polynomials and Christoffel Numbers

Polynomial evaluation can of course be accomplished by use of the polynomial itself; the technique following uses instead the matrix $N - x_\nu I$ directly (see (7)).

It is first of all clear that, except for a possible sign change, the determinants of the leading submatrices of $N - x_\nu I$ are the values $g_n(x_\nu)$ of the polynomials of (3). We choose to rewrite the matrix $N - x_\nu I$ as

$$\begin{bmatrix} a_{11} & 1 & 0 & 0 & 0 & ---- \\ a_{21} & a_{22} & 1 & 0 & 0 & ---- \\ 0 & a_{32} & a_{33} & 1 & 0 & ---- \\ 0 & 0 & a_{43} & a_{44} & 1 & ---- \\ 0 & 0 & 0 & a_{54} & a_{55} & ---- \\ - & - & - & - & - & ---- \end{bmatrix}$$

Note that $-a_{11}$ is $g_1(x_\nu)$. Now multiply column two by a_{11} and subtract from column one. The result is

$$\begin{bmatrix} 0 & 1 & 0 & 0 & 0 & ---- \\ a_{21}' & a_{22} & 1 & 0 & 0 & ---- \\ a_{31}' & a_{32} & a_{33} & 1 & 0 & ---- \\ 0 & 0 & a_{43} & a_{44} & 1 & ---- \\ 0 & 0 & 0 & a_{54} & a_{55} & ---- \\ - & - & - & - & - & ---- \end{bmatrix}$$

It is seen that $-a_{21}'$ is $q_2(x_\nu)$. If we continue in this fashion, next using a_{21}' times the elements of the third column to subtract from the first, we build in column one the negatives of $q_1(x_\nu)$, $q_2(x_\nu)$, $q_3(x_\nu)$, etc.

In practice, of course, there is no need to destroy any of the matrix N, nor is there need to establish the zeros. All computations can be done in terms of a column appended to N, and results left therein so that in the final stage the negative of $q_i(x_\nu)$ is the ith row of this column.

If the coefficients k_j are known (see (2)), and if x_ν is a zero of $q_n(x)$, then (see [1], p. 47), the Christoffel number λ_ν is given by

$$\lambda_\nu^{-1} = \sum_{i=0}^{n} \{p_i(x_\nu)\}^2 .$$

If a (finite) series involving the polynomials is under consideration, and if its value, or that of a derivative thereof, be desired for some x_ν, a similar technique can be employed.

In place of column manipulation to establish the values $g_n(x_\nu)$, row manipulation may be used. This is equally effective.

Polynomial Coefficients and Series Coefficients

Consider the use of a matrix of the type of N, together with the Method of Danilevskii (see [2], pp. 251-260) to find the coefficients of the successive polynomials. For simplicity, the matrix is rewritten as

$$\begin{bmatrix} b_{11} & 1 & 0 & 0 & 0 & --- \\ b_{21} & b_{22} & 1 & 0 & 0 & --- \\ 0 & b_{32} & b_{33} & 1 & 0 & --- \\ 0 & 0 & b_{43} & b_{44} & 1 & --- \\ 0 & 0 & 0 & b_{54} & b_{55} & --- \\ - & - & - & - & - & --- \end{bmatrix} .$$

To begin with, $x - b_{11}$ is the monic polynomial q_1. Now multiply on the right by the matrix $P_1 = [{}_1p_{ij}]$ where ${}_1p_{ij} = \delta_{ij}$ unless $i = 2$ and $j = 1$, in which event the value is $-b_{11}$, and on the left by its inverse $P_1^{-1} = [{}_1r_{ij}]$ where ${}_1r_{ij} = \delta_{ij}$ unless $i = 2$ and $j = 1$, in which event the value is b_{11}. The result is a matrix

$$\begin{bmatrix} 0 & 1 & 0 & 0 & 0 & --- \\ b_{21}' & b_{22}' & 1 & 0 & 0 & --- \\ b_{31}' & b_{32} & b_{33} & 1 & 0 & --- \\ 0 & 0 & b_{43} & b_{44} & 1 & --- \\ 0 & 0 & 0 & b_{54} & b_{55} & --- \\ - & - & - & - & - & --- \end{bmatrix}$$

and the monic polynomial q_2 is $x^2 - b_{22}'x - b_{21}'$.

In general, at the kth step we postmultiply by P_k and premultiply by P_k^{-1} to obtain q_{k+1}. $P_k = [{}_kp_{kj}]$ where ${}_kp_{ij} = \delta_{ij}$ unless $i = k + 1$, $j \leq k$, in which event ${}_kp_{ij}$ is the negative of the (i, j) entry of the current matrix. $P_k^{-1} = [{}_kr_{ij}]$ where ${}_kr_{ij} = \delta_{ij}$ unless $i = k + 1$, $j \leq k$, in which event ${}_kr_{ij}$ is the (i, j) entry of the current matrix. In the resulting matrix, the first $k + 1$ entries of the $(k + 1)^{th}$ row, with signs reversed, give the coefficients of q_{k+1}, in ascending order.

There is, of course, no need to construct the matrices P_k and P_k^{-1}, since all required members are simply obtained from the current matrix.

The above procedure is well adapted to finding the coefficients of powers of x in a finite series of such polynomials. At each step one needs only multiply the polynomial coefficients by the appropriate series coefficient and keep a cumulative total.

Polynomial Zeros

The zeros of the polynomials are the eigenvalues of successive leading submatrices. Thus several techniques are available for finding the zeros.

It was found that Jacobi's method, using a straight sweeping technique, was adequate for experimenting with different families of Jacobi polynomials.

A variation was tried, wherein the Jacobi technique was applied to the various leading submatrices in turn (a cascading scheme) and then moving on to the next submatrix. This was found to lose accuracy, so that as finally programmed, each set of zeros was found by returning to the original matrix.

Rutishauser's method might have been employed. In addition, because the matrix is tridiagonal, special techniques are available (see [2], pp. 283-284).

An Example

The "mixed" cases of Jacobi polynomials seem of interest. Here $\alpha = 1/2$, $\beta = -1/2$ or $\alpha = -1/2$, $\beta = 1/2$. It is not difficult to show that $P_n^{(1/2,-1/2)}(x) = (-1)^n P_n^{(-1/2,\ 1/2)}(-x)$. Because of this, knowledge of one case only is sufficient. However, both cases were treated computationally and results compared.

It is a simple matter to calculate exactly the polynomials of lower order. For $\alpha = 1/2$, $\beta = -1/2$, the monic polynomial of order 10 is $x^{10} + \frac{1}{2}x^9 - \frac{9}{4}x^8 - x^7 + \frac{7}{4}x^6 + \frac{21}{32}x^5 - \frac{35}{64}x^4 - \frac{5}{32}x^3 + \frac{15}{256}x^2 + \frac{5}{512}x - \frac{1}{1024}$.

The results following are for $\alpha = 1/2$, $\beta = -1/2$ and were computed, using single-precision arithmetic, on the IBM 7094. These and other computations indicate that through $n = 10$ the coefficients can be considered correct to seven significant figures (for n = 10 there were a few exceptions - one can be found for the polynomial exhibited above).

The zeros were checked in two ways - by evaluating the monic polynomials directly and by using the determinantal evaluation explained above. The two methods agreed nicely. In no instance did a functional value have a size in excess of 3×10^{-7}.

The polynomial coefficients listed below are in order of decreasing exponent.

For n = 1, 4, 7 and 10, the number -1/2 is a zero. This serves well enough to indicate the accuracy of the polynomial zeros.

n = 3. Coefficients are 1.0, 0.5, -0.49999999, -0.12499999.
Zeros are -0.90096878, -0.22252091, 0.62348974.

n = 4. Coefficients are 1.0, 0.5, -0.74999999, -0.24999999, 0.062499999.
Zeros are -0.93969247, -0.49999993, 0.17364815, 0.76604433.

n = 5. Coefficients are 1.0, 0.5, -0.99999997, -0.37499999, 0.18749999, 0.031249999.
Zeros are -0.95949273, -0.65486056, -0.14231480, 0.41541492, 0.84125329.

n = 6. Coefficients are 1.0, 0.5, -1.2499999, -0.49999999, 0.37499998, 0.093749998, -0.015624999.
Zeros are -0.97094148, -0.74851047, -0.35460476, 0.12053664, 0.56806450, 0.88545572.

n = 7. Coefficients are 1.0, 0.5, -1.4999999, -0.62499999, 0.62499996, 0.18749999, -0.062499996, -0.0078124997.

Zeros are -0.97814722, -0.80901659, -0.49999978, -0.10452841, 0.30901686, 0.66913024, 0.91354505.

n = 8. Coefficients are 1.0, 0.5, -1.7499999, -0.74999998, 0.93749993, 0.31249999, -0.15624999, -0.031249999, 0.0039062499.

Zeros are -0.98297261, -0.85021662, -0.60263427, -0.27366286, 0.092268316, 0.44573813, 0.73900845, 0.93247172.

n = 9. Coefficients are 1.0, 0.5, -1.9999999, -0.87499997, 1.3124999, 0.46874998, -0.31249997, -0.078124997, 0.019531249, 0.0019531249.

Zeros are -0.98636077, -0.87947316, -0.67728116, -0.40169515, -0.082579298, 0.24548535, 0.54694776, 0.78913999, 0.94581668.

n = 10. Coefficients are 1.0, 0.5, -2.2499999, -0.99999996, 1.7499998, 0.65624997, -0.54687494, -0.15624999, 0.058593743, 0.0097656245, -0.00097656245.

Zeros are -0.98883024, -0.90096820, -0.73305130, -0.49999968, -0.22252079, 0.074730041, 0.36534072, 0.62348928, 0.82623820, 0.95557211.

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