Discrete Orthogonal Polynomials on Equidistant Nodes

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Abstract

In this paper we give an alternative and, in our opinion, more simple proof for the orthonormal discrete polynomials on a set of equidistant nodes. Such a proof provides a unifying explicit formulation of discrete orthonormal polynomials on an equidistant grid and an explicit formula for the coefficients of the “three-term recurrence relation”. We show how to efficiently apply these formulas to the problem of least-squares fitting on equidistant nodes. Finally we investigate the problem to determine the effect of adding a new basis function or taking one away. This is useful in the process of trying to discover the optimal set of basis functions and the problem to update them when a moving window over the time series/data stream is used.

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1 Introduction

Although orthogonal polynomials over discrete sets were considered as early as the middle of the nineteenth century by Chebyshev [5, 6, 10, 11], comparatively little attention had been paid to them until now. They appear naturally in combinatorics, genetics, statistics and various areas in applied mathematics (see, for example, [7, 11]). Expansion in orthogonal polynomials is used, for example, to avoid the difficulties with ill-conditioned systems of equations which occur in a least squares applications [1]. The Gram polynomials [3, 1], orthonormal on the set of equidistant nodes in $[-1, 1]$, are used

in all the applications in which equidistant measures must be used. In this paper we focus our attention on discrete orthonormal polynomials. We derive an analytic expression for orthonormal polynomials on a discrete grid $Z_n = \{z_r | z_r = a + hr, r = 0, 1, \dots, n-1\}$ and the coefficients of the “three-term recurrence relation” by using some results of the pseudoinverse on integer nodes [4]. We show how to efficiently apply these formulas to the problem of least-squares fitting on equidistant nodes. Finally we investigate the problem to determine the effect of adding a new basis function or taking one away as part of a process of trying to discover the optimal set of basis functions and the problem to update the basis functions when a moving window over the time series/data stream is used.

We want to emphasize that although high degree approximations on equidistant nodes have a bad reputation in numerical analysis, a lot of researches have been made for the design of accurate algorithms for polynomial approximation on such a set of nodes. There is a considerable interest on equidistant nodes because this choice frequently occurs in many applications.

2 Preliminary results

Let f_1 and f_2 be real valued functions defined on the set of nodes $X_n = \{x_1, x_2, \dots, x_n\}$ and introduce the inner product:

$$\langle f_1(x), f_2(x) \rangle = \sum_{k=1}^n f_1(x_k) f_2(x_k). \quad (1)$$

A family $P = \{p_1(x), p_2(x), \dots, p_m(x)\}$ with $m \leq n$ of polynomials is orthogonal respect to this inner product if the following properties hold:

$$\begin{aligned} \langle p_k(x), p_q(x) \rangle &= 0, & k \neq q; \quad k, q = 1, 2, \dots, m \\ \langle p_k(x), p_k(x) \rangle &= \xi_k \neq 0, & k = 1, 2, \dots, m. \end{aligned} \quad (2)$$

If $\xi_k = 1$, $k = 1, 2, \dots, m$ then polynomials p_k are said orthonormal on the set of nodes X_n . A well known result from the general theory of orthogonal polynomials is that the orthogonal polynomials satisfy a three term recursion formula:

$$p_k(x) = (\alpha_k x + \beta_k) p_{k-1}(x) + \gamma_k p_{k-2}(x), \quad k = 3, 4, \dots, m. \quad (3)$$

Proposition 1 *Let X_n be a set of n nodes and let P be a family of m orthogonal polynomials on X_n , then*

$$p_i(x_j) = (-1)^{i+1} p_i(x_{n+1-j}), \quad j = 1, 2, \dots, n; \quad i = 1, 2, \dots, m \quad (4)$$

if and only if

$$\alpha_i(x_j + x_{n+1-j}) + 2\beta_i = 0, \quad i = 1, 2, \dots, m; \quad j = 1, 2, \dots, n. \quad (5)$$

Proof. The proof is made by induction on the polynomial index i . Suppose (5) is true for $i - 1$ and $i - 2$ then

$$p_{i-1}(x_j) = (-1)^i p_{i-1}(x_{n+1-j}), \quad j = 1, 2, \dots, n \quad (6)$$

and

$$p_{i-2}(x_j) = (-1)^{i+1} p_{i-2}(x_{n+1-j}), \quad j = 1, 2, \dots, n \quad (7)$$

- ($\rightarrow$) Taking into account (3), the (4) becomes:

$$\begin{aligned} &(\alpha_i x_j + \beta_i) p_{i-1}(x_j) + \gamma_i p_{i-2}(x_j) = \\ &(-1)^{i+1} [(\alpha_i x_{n+1-j} + \beta_i) p_{i-1}(x_{n+1-j}) + \gamma_i p_{i-2}(x_{n+1-j})] \end{aligned} \quad (8)$$

By using (6) and (7) the (5) follows.

- ($\leftarrow$) Taking into account (6) and (7), $p_i(x_{n+1-j})$ can be written as

$$\begin{aligned} p_i(x_{n+1-j}) &= (-1)^i (\alpha_i x_{n+1-j} + \beta_i) p_{i-1}(x_j) + \\ &+ (-1)^{i+1} p_{i-2}(x_j). \end{aligned} \quad (9)$$

Considered that $(\alpha_i x_{n+1-j} + \beta_i) = -(\alpha_i x_j + \beta_i)$ then (4) follows.

■

Here we review a result useful in the sequel. Let B_k be the matrix defined as follows:

$$B_k(i, j) = \sum_{p=1}^n p^{i+j-2}, \quad i, j = 1, 2, \dots, k \quad (10)$$

then its inverse can be factorized as [4]:

$$B_k^{-1} = W_k \Lambda_k^{-1} W_k^T. \quad (11)$$

In (11), W_k and Λ_k^{-1} have the following expressions:

$$W_k(i, j) = \frac{(j-1)!}{\binom{2j-2}{j-1}} \sum_{s \geq 1}^n \frac{(-1)^{i+j}}{(s-1)!} \binom{s+j-2}{s-1} \binom{n-s}{n-j} \begin{bmatrix} s \\ i \end{bmatrix}, \quad i, j = 1, 2, \dots, k, \quad (12)$$

where $\begin{bmatrix} i \\ j \end{bmatrix}$ are the Stirling numbers of the first kind [8], and

$$\Lambda_k^{-1} = \text{diag} \left\{ \frac{\binom{2i-2}{i-1}}{[(i-1)!]^2 \binom{n+i-1}{2i-1}} \right\}_{i=1,2,\dots,k}. \quad (13)$$

3 Discrete orthogonal polynomials

Let $P = \{p_1(x), p_2(x), \dots, p_m(x)\}$ be the set of polynomials defined as

$$p_k(x) = \sum_{i=1}^k c_{k,i} x^{i-1}, \quad k = 1, 2, \dots, m. \quad (14)$$

The set P is orthogonal on the set of nodes $X_n = \{1, 2, \dots, n\}$ if the following equalities hold:

$$\langle p_k(x), x^{q-1} \rangle = 0, \quad k = 2, 3, \dots, m; \quad q = 1, 2, \dots, k-1, \quad (15)$$

$$\langle p_k(x), x^{k-1} \rangle = \rho_k \neq 0, \quad k = 1, 2, \dots, m. \quad (16)$$

Let $\bar{c}_k$ and $\bar{b}_k$ ($k = 1, 2, \dots, m$), be two vectors defined as follows:

$$\begin{aligned} \bar{c}_k(i) &= c_{k,i}, \quad i = 1, 2, \dots, k \\ \bar{b}_k(i) &= \rho_k \delta_{k,i}, \quad i = 1, 2, \dots, k \end{aligned} \quad (17)$$

then by (15) and (16) and taking into account (11), it must be

$$\bar{c}_k = W_k \Lambda_k^{-1} W_k^T \bar{b}_k. \quad (18)$$

It is straightforward to note that:

$$W_k^T \bar{b}_k = \bar{b}_k \quad (19)$$

and

$$[\Lambda_k^{-1} W_k^T \bar{b}_k]_i = \rho_k \frac{\binom{2k-2}{k-1}}{[(k-1)!]^2 \binom{n+k-1}{2k-1}} \delta_{k,i}, \quad i = 1, 2, \dots, k. \quad (20)$$

Then, by simple algebraic manipulations we have:

$$c_{k,i} = \mu_k (-1)^{i+k} \sum_{s=1}^k \frac{1}{(s-1)!} \binom{s+k-2}{s-1} \binom{n-s}{n-k} \begin{bmatrix} s \\ i \end{bmatrix}, \quad i = 1, 2, \dots, k, \quad (21)$$

where

$$\mu_k = \frac{\rho_k}{(k-1)! \binom{n+k-1}{2k-1}}, \quad k = 1, 2, \dots, m. \quad (22)$$

By using the identity [8]:

$$\sum_i (-1)^i \begin{bmatrix} s \\ i \end{bmatrix} x^{i-1} = (-1)^s (s-1)! \binom{x-1}{s-1} \quad (23)$$

polynomial $p_k(x)$ becomes:

$$p_k(x) = \mu_k \sum_{s=1}^k (-1)^{s+k} \binom{s+k-2}{s-1} \binom{n-s}{n-k} \binom{x-1}{s-1}, \quad k = 1, 2, \dots, m. \quad (24)$$

If we put

$$\rho_k = (k-1)! \binom{n+k-1}{2k-1}, \quad k = 1, 2, \dots, m \quad (25)$$

then the family P of polynomials

$$p_k(x) = \sum_{s=1}^k (-1)^{s+k} \binom{s+k-2}{s-1} \binom{n-s}{n-k} \binom{x-1}{s-1}, \quad k = 1, 2, \dots, m. \quad (26)$$

is orthogonal on the set $X_n = \{1, 2, \dots, n\}$. By an affine transformation on the variable x in (26) we have that the polynomials

$$p_k(x) = \sum_{s=1}^k (-1)^{s+k} \binom{s+k-2}{s-1} \binom{n-s}{n-k} \binom{\frac{x-a}{h}}{s-1}, \quad k = 1, 2, \dots, m. \quad (27)$$

are orthogonal on the set

$$Z_n = \{z_r | z_r = a + hr, \quad r = 0, 1, \dots, n-1\} \quad (28)$$

Such polynomials satisfy the following three-term recurrence relation:

$$p_k(x) = (\alpha_k x + \beta_k) p_{k-1}(x) + \gamma_k p_{k-2}(x), \quad k = 3, 4, \dots, m \quad (29)$$

where

$$\begin{cases} \alpha_k = \frac{4k-6}{h(k-1)^2}, \\ \beta_k = -\frac{[(2k-3)(2a+h(n-1))]}{h(k-1)^2}, \\ \gamma_k = \frac{(k-2)^2 - n^2}{(k-1)^2}, \end{cases} \quad k = 3, 4, \dots, m \quad (30)$$

Proposition 2 *The set of polynomials $Q = \{q_1(x), q_2(x), \dots, q_m(x)\}$ where*

$$q_k(x) = \frac{1}{\sqrt{\binom{n+k-1}{2k-1} \binom{2k-2}{k-1}}} \sum_{s=1}^k (-1)^{s+k} \binom{s+k-2}{s-1} \binom{n-s}{n-k} \binom{x-1}{s-1}, \quad (31)$$

$$k = 1, 2, \dots, m$$

is orthonormal on the set of nodes $X_n = \{1, 2, \dots, n\}$.

Proof. It is straightforward to note that

$$\langle p_k(x), p_k(x) \rangle = c_{k,k} \rho_k, \quad (32)$$

then by using (21) and the expression (25) for ρ_k , we have

$$\langle p_k(x), p_k(x) \rangle = \binom{n+k-1}{2k-1} \binom{2k-2}{k-1} \quad (33)$$

and the (31) follows. ■

Corollary 3.1 *The generic polynomial $t_k(x)$ in the family of orthonormal polynomials $T = \{t_1(x), t_2(x), \dots, t_m(x)\}$ on the set of nodes*

$$Z_n = \{z_r | z_r = a + hr, \quad r = 0, 1, \dots, n-1\} \quad (34)$$

can be written as

$$t_k(x) = \frac{1}{\sqrt{\binom{n+k-1}{2k-1} \binom{2k-2}{k-1}}} \sum_{s=1}^k (-1)^{s+k} \binom{s+k-2}{s-1} \binom{n-s}{n-k} \left(\frac{x-a}{h} \right)_{s-1}, \quad (35)$$

$$k = 1, 2, \dots, m$$

The t_k satisfies a three-term recurrence relation

$$t_1(x) = \frac{1}{\sqrt{n}}$$

$$t_2(x) = \frac{\sqrt{3}}{h\sqrt{n(n^2-1)}} [2x - h(n-1) - 2a]$$

$$t_k(x) = (\alpha_k x + \beta_k) t_{k-1}(x) + \gamma_k t_{k-2}(x) \quad k = 3, 4, \dots, n$$

where

$$\alpha_k = \frac{2}{h(k-1)} \sqrt{\frac{(2k-1)(2k-3)}{n^2-(k-1)^2}}$$

$$\beta_k = -\frac{1}{2} [2a + h(n-1)] \alpha_k \quad (36)$$

$$\gamma_k = -\frac{\alpha_k}{\alpha_{k-1}} \quad k = 3, 4, \dots, n$$

Such explicit formulas are particularly useful because they allow to compute efficiently the orthonormal polynomials without using the Stieltjes procedure which can be sensitive to roundoff errors [13].

4 Least squares application

In this section we consider the problem of least squares on a discrete set

$$Z_n = \{z_r | z_r = a + hr, \quad r = 0, 1, \dots, n-1\} \quad (37)$$

by using polynomials p_k defined in (27) which are orthogonal on Z_n . Such polynomials satisfies the three-term recurrence relation (29) with parameters (30). Note that $\langle p_k(x), p_k(x) \rangle$ is invariant under affine transformation, therefore its value can be computed by using the (33). Here we want to expand a given function $y = f(x)$ in terms of orthogonal polynomials [9, 12]:

$$\bar{f}(x) = \sum_{i=1}^m w_i q_i(x). \quad (38)$$

and to determine the coefficients $w_1, w_2, \dots, w_m$ in (38) such that the Euclidean norm of the error function $\bar{f} - f$ is minimized,

$$\|\bar{f} - f\| = \sum_{j=0}^{n-1} |\bar{f}(z_j) - f(z_j)|^2.$$

Since $q_1(x), q_2(x), \dots, q_m(x)$ form an orthogonal system, the coefficients are computed more simple by

$$w_j = \frac{\langle q_j(x), f(x) \rangle}{\langle q_j(x), q_j(x) \rangle}, \quad j = 1, 2, \dots, m. \quad (39)$$

If we define the following quantities:

$$b = H \cdot f \quad (40)$$

where

$$H(i, j) = q_i(z_j), \quad i = 1, 2, \dots, m; \quad j = 0, 1, \dots, n-1, \quad (41)$$

$$f = [f(z_0), f(z_1), \dots, f(z_{n-1})] \quad (42)$$

and

$$g(i) = \binom{2i-2}{i-1} \binom{n+i-1}{2i-1}, \quad i = 1, 2, \dots, m \quad (43)$$

then

$$w_i = \frac{b(i)}{g(i)}, \quad i = 1, 2, \dots, m. \quad (44)$$

Since the product $b = H \cdot f$ is also invariant under affine transformation, then it would be computed by considering, for example, the set of orthogonal polynomials on $[1, 2, \dots, n]$ for which the matrix H is

$$H(i, j) = \sum_{s=1}^i (-1)^{s+i} \binom{s+i-2}{s-1} \binom{n-s}{n-i} \binom{j-1}{s-1}, \quad (45)$$

$$i = 1, 2, \dots, m; \quad j = 1, 2, \dots, n.$$

The pseudo-code in Table 1 finds the coefficients w_i , $i = 1, 2, \dots, m$ in (38).

We compare our algorithm (**EF**) applied to the orthogonal polynomials on the set of n equidistant nodes in $[0, 1]$ with that proposed in [2] (**CB**) which costs $10mn$ flops and with the Mathematica built-in function *Fit* (**MA**) [15]. The first two algorithms have been implemented in Mathematica package, which allows arbitrary precision numbers. Our algorithm costs $3.5mn$ flops. Infact we build an half part of the matrix H by the three-term recurrence relation, and the product $H \cdot f$ by using the property in Proposition 1.

For some values of m with $n = 1000$, we have generated one thousand vectors f , with entries uniformly distributed in $[-1, 1]$, and have computed the exact solution of the problem (38)

$$\bar{f}(x) = \sum_{i=1}^m h_i q_i(x) = \sum_{k=1}^m r_k x^{k-1} \quad (46)$$

using extended precision. For each algorithm we have computed the maximum componentwise relative errors

$$E_{EF} = \max_{1 \leq i \leq m} \frac{|\hat{r}_i^{EF} - r_i|}{|r_i|} \quad (47)$$

$$E_{CB} = \max_{1 \leq i \leq m} \frac{|\hat{r}_i^{CB} - r_i|}{|r_i|} \quad (48)$$

Table 1: Pseudo-code for least-square problem by discrete orthogonal polynomials.

function lmsOrt
Input: a, h, m, f
Output: w_i , $i = 1, 2, \dots, m$
Calculate the quantities α_k, β_k and γ_k in (30). Calculate g_k in (43).
Build the matrix C_P of the coefficients of the polynomials p_k by using the three-term recurrence relation (29).
Build the elements $i = 1, 2, \dots, m$, $j = 1, 2, \dots, \lfloor \frac{n}{2} \rfloor$ of the matrix H .
Build the two vectors $f_1 = \{f(i), i = 1, 2, \dots, \lfloor \frac{n}{2} \rfloor\}$ and $f_2 = \{f(n+1-i), i = 1, 2, \dots, \lfloor \frac{n}{2} \rfloor\}$.
Build the vector $b = \left\{ b(i) = \sum_{j=1}^{\lfloor \frac{n}{2} \rfloor} H(i, j)(f_1(j) + (-1)^{i+1}f_2(j)) \right\}$.
if n is odd then
$c_h = 1$
$b(1) = b(1) + f((n+1)/2)$
for $i = 3 : 2 : m$
$c_h = \gamma(i)c_h$; $b(i) = b(i) + c_h f((n+1)/2)$
end

$$E_{MA} = \max_{1 \leq i \leq m} \frac{|\hat{r}_i^{MA} - r_i|}{|r_i|} \quad (49)$$

where $\hat{r}^{EF}$, $\hat{r}^{CB}$ and $\hat{r}^{MA}$ are the approximate solutions computed by EF, CB and MA algorithms respectively in machine precision.

The mean and the maximum of E_{EF} , E_{CB} and E_{MA} over one thousand runs have then been computed and reported in Table 2. Table 2 reports also the fraction of trials in which the proposed algorithm gives equal or more accurate result than CB and MA algorithm. Note that the matrix H in (45) has integer entries that can be stored without rounding errors and this is probably the cause of the robustness of this algorithm.

5 Some properties

A common problem in least-square problems is to determine the effect of adding a new basis function, that is to determine the effect of using $m + 1$ basis in (38). This is important as part of a process of trying to discover the optimal set of basis functions. The effect can, of course, be calculated by restarting the algorithm in the previous section. However in our case, simple analytical formulas can be derived to cover this situation.

Let C_{P_m} be the matrix of the coefficients of the polynomial $p_k(x)$, $k = 1, 2, \dots, m$ in (27), that is

$$C_{P_m} = \left[\begin{array}{cccc|c} c_{1,1} & 0 & 0 & \dots & 0 \\ c_{2,1} & c_{2,2} & 0 & \dots & 0 \\ c_{3,1} & c_{3,2} & c_{3,3} & \dots & 0 \\ \vdots & \vdots & \vdots & \dots & \vdots \\ \hline c_{m,1} & c_{m,2} & c_{m,3} & \dots & c_{m,m} \end{array} \right] = \left[\begin{array}{c|c} C_{P_{m-1}} & 0 \\ \hline w_m^T & c_{m,m} \end{array} \right] \quad (50)$$

and let G_m be the matrix of the g_k , $k = 1, 2, \dots, m$ in (43):

$$G_m = \left[\begin{array}{ccc|c} g_1 & 0 & \dots & 0 \\ 0 & g_2 & \dots & 0 \\ \vdots & \vdots & \dots & 0 \\ \hline 0 & 0 & \dots & g_m \end{array} \right] = \left[\begin{array}{c|c} G_{m-1} & 0 \\ \hline 0^T & g_m \end{array} \right] \quad (51)$$

If we consider the matrix H in (41) as

$$H_m = \left[\begin{array}{c} H_{m-1} \\ \hline h_m^T \end{array} \right] \quad (52)$$

then the coefficients of the approximant polynomial can be expressed in matrix form as

$$C_{P_m}^T G_m H_m f = \begin{bmatrix} C_{P_{m-1}}^T G_{m-1} H_{m-1} f + g_m(h_m^T f) w_m \\ c_{m,m} g_m(h_m^T f) \end{bmatrix}. \quad (53)$$

Formula (53) is useful for the updating of the degree of the approximant polynomial in least square sense since it gives the coefficients of the approximant polynomial of degree $m - 1$ in terms of the approximant polynomial of degree $m - 2$.

In real-time applications, which process a stream of continuously arriving data, it is often required a processing in moving time windows. More specific, let Z_1 and Z_2 be two discrete sets of nodes such as

$$Z_1 = \{a + h \cdot r, \quad r = 0, 1, \dots, n - 1\}, \quad (54)$$

$$Z_2 = \{a + p + h \cdot r, \quad r = 0, 1, \dots, n - 1, \quad p > 0\} \quad (55)$$

and C_{P_1} and C_{P_2} the matrix of the coefficients of the orthogonal polynomial on Z_1 and Z_2 respectively, then

$$C_{P_2} = C_{P_1} M^p \quad (56)$$

where

$$M(i, j) = (-1)^{i+j} \binom{i-1}{j-1}, \quad i, j = 1, 2, \dots, m. \quad (57)$$

Proposition 3 *The p -th power of the matrix M is*

$$M^p(i, j) = (-1)^{i+j} \binom{i-1}{j-1} p^{i-j}, \quad i, j = 1, 2, \dots, m. \quad (58)$$

The matrix M^p has the following useful recursive properties:

$$\begin{aligned} M^p(i, i) &= 1, & i &= 1, 2, \dots, m, \\ M^p(i, 1) &= -p M^p(i-1, 1), & i &= 2, 3, \dots, m, \\ M^p(i, j) &= -p M^p(i-1, j) + M^p(i-1, j-1), & i &= 3, 4, \dots, m, \quad j = 2, 3, \dots, i-1. \end{aligned} \quad (59)$$

m	CB		MA		EF		EF vs CB	EF vs MA
	max	mean	max	mean	max	mean		
2	9.53-13	6.15-15	1.92-13	4.30-15	4.19-13	3.26-15	0.85	0.75
3	1.17-09	1.82-12	4.46-11	9.57-14	4.62-12	8.06-15	1.00	0.98
4	9.57-11	1.06-12	2.22-11	3.16-13	6.94-13	6.53-15	1.00	0.99
5	5.56-10	2.43-12	4.60-10	1.61-12	3.76-13	5.64-15	1.00	1.00
6	2.97-10	2.79-12	1.14-09	9.37-12	1.80-12	1.37-14	1.00	1.00
7	2.70-08	8.85-11	4.56-09	3.29-11	4.70-12	1.66-14	1.00	1.00
8	4.05-07	1.61-09	8.20-08	2.48-10	1.41-11	4.95-14	1.00	1.00
9	3.13-07	5.85-10	5.72-07	1.80-09	4.97-12	2.55-14	1.00	1.00
10	9.89-07	1.14-08	5.99-07	5.82-09	1.16-11	2.79-14	1.00	1.00
20	5.34-01	5.75-03	2.02+03	2.01+01	1.08-11	1.34-13	1.00	1.00
30	3.27+07	2.08+05	1.14+03	5.49+00	4.51-11	2.89-13	1.00	1.00
40	4.06+60	8.45+57	3.75+02	3.11+00	2.76-10	7.88-13	1.00	1.00
50	4.51+173	3.49+171	5.10+03	8.74+00	5.82-11	4.28-13	1.00	1.00

Table 2: Maximum and mean value of E_{CB} , E_{MA} and E_{EF} over 1000 runs, $n = 1000$, $f \in [-1, 1]$. Success rate of EF algorithm.

6 Conclusions

In this paper we have given an alternative proof of the explicit formula for the discrete orthogonal polynomials on equidistant nodes. Such a formula, with its properties, allows us to design an efficient algorithm for solving least squares problem. The numerical experiments indicate that our approach is more stable compared with existing Conte-de Boor algorithm. We finally have shown some properties satisfied by these polynomials.

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