On cubic Padé Approximation to the exponential function and its application in solving diffusion-convection equation

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Abstract

Diagonal cubic Hermite-Padé approximation to the exponential function with coefficient polynomials of degree at most m is considered. Explicit formulas and differential equations are obtained for the coefficient polynomials. An exact asymptotic expression is obtained for the error function and it is also shown that these generalized Padé-type approximations can be used to asymptotically minimize the expressions on the unit disk. As an application, a class of local analytical difference schemes based on diagonal cubic Padé approximation for diffusion-convection equation with constant coefficients is proposed.

Keywords: Padé-type approximant; Cubic Hermite-Padé approximation; Asymptotic formula; Differential equation

1 Introduction

The Padé approximation theory has been widely used in problems of theoretical physics[1][3][4][5], numerical analysis[9][10], and electrical engineering, especially in modal analysis model[2], order reduction of multivariable systems[6][11][13][14].

We consider approximations of e^{-x} generated by finding polynomials P_m, Q_m, R_m and S_m so that

$$E_m(x) := P_m(x)e^{-3x} + Q_m(x)e^{-2x} + R_m(x)e^{-x} + S_m(x)$$
$$= O(x^{4(m+1)-1}), \tag{1}$$

where $P_m, Q_m, R_m, S_m \in \pi_m$ (the vector space of all algebraic polynomials of degree at most m), and P_m has leading coefficient 1. The approximation of e^{-x} is given by one of the following three functions (j = 0, 1, 2)

$$\delta_{jm}(x) := \omega_1^j \sqrt[3]{-\frac{b}{2} + \sqrt{\left(\frac{b}{2}\right)^2 + \left(\frac{a}{3}\right)^3}} + \omega_2^j \sqrt[3]{-\frac{b}{2} - \sqrt{\left(\frac{b}{2}\right)^2 + \left(\frac{a}{3}\right)^3} - \frac{Q_m}{3P_m},$$

which is real and closest to 0, where

$$a = \frac{3P_m R_m - Q_m^2}{3P_m^2},$$

$$b = \frac{2Q_m^3 - 9P_m Q_m R_m + 27P_m^2 S_m}{27P_m^3};$$

$$\omega_1 = \frac{-1 + \sqrt{3}i}{2}, \ \omega_2 = \frac{-1 - \sqrt{3}i}{2}.$$

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Obviously, $\delta_{jm}(x)$ is the natural cubic generalization of the main diagonal Padé approximant $-\hat{Q}_m/\hat{P}_m$ satisfying

$$\hat{P}_m(x)e^{-x} + \hat{Q}_m(x) = O(x^{2(m+1)-1})$$

and the diagonal quadratic Hermite-Padé approximant [7] $\left(-q_m + \sqrt{q_m^2 - 4p_m r_m}\right) / (2p_m)$ satisfying

$$p_m(x)e^{-2x} + q_m(x)e^{-x} + r_m(x) = O(x^{3(m+1)-1}).$$
 (2)

Our primary aim is to derive the exact asymptotic formula for $\{E_m\}$, the explicit formulae of $\{P_m\}, \{Q_m\}, \{R_m\}, \{S_m\}, \{E_m\}$ and to treat some minimization problems concerning related approximations on the unit disk in **C**.

Exact results concerning best rational approximation to the exponential function, particularly the Meinardus conjecture, have attracted much attention ([8]). Theorem 4 can be viewed as a cubic version of this conjecture on the disk. A linear version, due to Trefethen appeared in [15]; a quadratic version on the disk given by Borwein can be found in [7].

As an application, this paper proposes a class of local analytical difference schemes based on cubic Padé approximation to e^{-x} for the following diffusion-convection equation

$$\frac{\partial u}{\partial t} = a \frac{\partial u}{\partial x} + \varepsilon \frac{\partial^2 u}{\partial x^2} \tag{3}$$

with the initial condition $u(x, 0) = \phi(x)$, $0 \le x \le 1$; and the boundary condition $u(0,t) = \alpha$, $u(1,t) = \beta$; where $\varepsilon > 0, a \ne 0, \alpha, \beta$ are all real constants.



2 Explicit Formulae of the Polynomial Coefficients

Let

$$p_m(x) = m! \sum_{j=0}^m \frac{c_j x^j}{j!},$$
$$q_m(x) = -2^{m+1} m! \sum_{j=0}^m \frac{d_j x^j}{j!},$$
$$r_m(x) = (-1)^m p_m(-x),$$

with

$$c_{j} = \sum_{k=0}^{m-j} \frac{1}{2^{k}} \binom{2m - (k+j)}{m} \binom{m+k}{m};$$
$$d_{j} = \sum_{k=0}^{m-j} (-1)^{k-j} \binom{2m - (k+j)}{m} \binom{m+k}{m}.$$

Then $\left(-q_m + \sqrt{q_m^2 - 4p_m r_m}\right) / (2p_m)$ is the diagonal quadratic Hermite-Padé approximant [7] to e^{-x} . Also, p_m, q_m and r_m satisfy (2) and

$$p_m(x)e^{-2x} + q_m(x)e^{-x} + r_m(x)$$

= $\frac{2^{m+1}x^{3m+2}}{m!m!} \int_0^1 \int_0^1 (1-u)^m u^m$
 $\times e^{-uvx}(1-v)^m v^{2m+1}e^{-vx} du dv.$ (4)

Now let

$$P_m(x) := \frac{e^{3x} 3^{m+1}}{m!} \int_x^\infty (t-x)^m p_m(t) e^{-3t} \mathrm{d}t.$$
 (5)

Then

$$P_m(x) = \frac{e^{3x}3^{m+1}}{m!} \int_x^\infty (t-x)^m e^{-3t} m! \sum_{j=0}^m \frac{c_j t^j}{j!} dt$$
$$= m! \sum_{i=0}^m \sum_{j=i}^m \frac{c_j}{3^{j-i}} \binom{m+j-i}{m} \frac{x^i}{i!}.$$

If we set

$$a_i := \sum_{j=i}^m 3^{i-j} c_j \binom{m+j-i}{m},$$

then

$$P_m(x) = m! \sum_{i=0}^{m} \frac{a_i x^i}{i!}.$$
 (6)

Note that P_m is a polynomial of degree m with highest coefficient 1.

Let

$$Q_m(x) = \frac{e^{2x} 3^{m+1}}{m!} \int_x^\infty (t-x)^m q_m(t) e^{-2t} dt \qquad (7)$$

$$:= -3^{m+1}m! \sum_{i=0}^{m} \frac{b_i x^i}{i!},$$
(8)

with

$$b_i = \sum_{j=i}^m d_j 2^{i-j} \binom{m+j-i}{m}.$$

Then $Q_m(x)$ is a polynomial with integer coefficients. Let

$$R_m(x) := \frac{e^x 3^{m+1}}{m!} \int_x^\infty (t-x)^m r_m(t) e^{-t} dt \quad (9)$$

$$= (-1)^m 3^{m+1} m! \sum_{i=0}^m \frac{e_i x^i}{i!}, \qquad (10)$$

where

$$e_i := \sum_{j=i}^m c_j (-1)^j \binom{m+j-i}{m},$$

then $R_m(x)$ is a polynomial with integer coefficients.

Define S_m by

$$S_m(x) = -\frac{3^{m+1}}{m!} \int_0^\infty (t-x)^m e^{-t} \\ \times \left\{ p_m(t) e^{-2t} + q_m(t) e^{-t} + r_m(t) \right\} \mathrm{d}t,$$

then

$$S_m(x) = m! \sum_{i=0}^m \frac{s_i x^i}{i!},$$
(11)

with

$$s_i = (-1)^{i+1} \sum_{j=0}^{m-i} \binom{2m-j-i}{m}$$
$$\times \sum_{k=0}^j \binom{m+k}{m} \binom{m+j-k}{m} \frac{1}{3^k 2^{j-k}}.$$

Finally, let

$$E_m(x) = -\frac{3^{m+1}}{m!} \int_0^x (t-x)^m e^{-t}$$
$$\cdot \frac{2^{m+1}t^{3m+2}}{m!m!} \int_0^1 \int_0^1 u^m (1-u)^m$$



$$e^{-uvt}(1-v)^{m}v^{2m+1}e^{-vt}dudvdt$$
(12)
= $(-1)^{m+1}\frac{6^{m+1}x^{4m+3}}{m!m!m!}$
 $\cdot \int_{0}^{1}\int_{0}^{1}\int_{0}^{1}(1-u)^{m}u^{m}e^{-uvwx}$
 $\cdot (1-v)^{m}v^{2m+1}e^{-vwx}w^{3m+2}$
 $\cdot (1-w)^{m}e^{-wx}dudvdw (t=wx).$ (13)

Now we may establish the basic theorem.

Theorem 1.

$$E_m(x) := P_m(x)e^{-3x} + Q_m(x)e^{-2x} + R_m(x)e^{-x} + S_m(x)$$
$$= O(x^{4(m+1)-1}),$$

where E_m , P_m , Q_m , R_m and S_m are given by (12), (6), (8), (10) and (11) respectively.

Proof By (12) and (4)

$$\begin{split} E_m(x) \\ &= -\frac{3^{m+1}}{m!} \int_0^x (t-x)^m e^{-t} \\ &\cdot \left\{ p_m(t) e^{-2t} + q_m(t) e^{-t} + r_m(t) \right\} \mathrm{d}t \\ &= \frac{3^{m+1}}{m!} \int_x^\infty (t-x)^m p_m(t) e^{-3t} \mathrm{d}t \\ &+ \frac{3^{m+1}}{m!} \int_x^\infty (t-x)^m q_m(t) e^{-2t} \mathrm{d}t \\ &+ \frac{3^{m+1}}{m!} \int_x^\infty (t-x)^m r_m(t) e^{-t} \mathrm{d}t \\ &- \frac{3^{m+1}}{m!} \int_0^\infty e^{-t} (t-x)^m \\ &\cdot \left\{ p_m(t) e^{-2t} + q_m(t) e^{-t} + r_m(t) \right\} \mathrm{d}t \\ &= P_m(x) e^{-3x} + Q_m(x) e^{-2x} + R_m(x) e^{-x} + S_m(x). \end{split}$$

With (13), the theorem has been proved.

3 Asymptotics and Exact Minimization

We now turn to asymptotic estimate for $\{E_m\}$. As usual, $i_m \sim j_m$ means $i_m/j_m \to 1 \ (m \to \infty)$. Throughout this paper the asymptotics are concerning the variable m.

In order to give the asymptotic, we need the following lemma.

Lemma 2 [15].

$$\int_0^1 (1-t)^{\alpha m} t^{\beta m} e^{-\gamma t} dt$$
$$\sim e^{-\frac{\beta \gamma}{\alpha+\beta}} \int_0^1 (1-t)^{\alpha m} t^{\beta m} dt$$
$$= e^{-\frac{\beta \gamma}{\alpha+\beta}} \frac{(\alpha m)!(\beta m)!}{((\alpha+\beta)m+1)!},$$

where α, β are positive numbers, $\alpha m, \beta m$ are positive integers.

Now we can give the asymptotic estimates of $\{E_m\}$.

Theorem 3.

$$E_m(x) \sim \frac{(-6)^{m+1}m!}{(4m+3)!} x^{4m+3} e^{-\frac{3}{2}x}.$$

The asymptotic is uniformly on the bounded subsets of **C**. **Proof** From (13)

$$E_m(x) \sim \frac{(-6)^{m+1}x^{4m+3}}{(2m+1)!m!} \int_0^1 \int_0^1 (1-v)^m \\ \cdot e^{-\frac{3}{2}vwx} v^{2m+1} (1-w)^m w^{3m+2} e^{-wx} dv dw \\ \sim \frac{(-6)^{m+1}x^{4m+3}}{(3m+2)!} \int_0^1 (1-w)^m \\ \cdot w^{3m+2} e^{-\frac{12m+5}{2(3m+1)}wx} dw \\ \sim \frac{(-6)^{m+1}m!}{(4m+3)!} x^{4m+3} e^{-\frac{(3m+2)(12m+5)}{2(4m+3)(3m+1)}x} \\ \sim \frac{(-6)^{m+1}m!}{(4m+3)!} x^{4m+3} e^{-\frac{3}{2}x}.$$

Both of the first two asymptotics follow from the elementary relation of Lemma 2. It is easy to check directly from (12) that $E_m(x)/\{(-6)^{m+1}m!x^{4m+3}e^{-\frac{3}{2}x}/(4m+3)!\}$ is uniformly bounded on a compact subsets of **C**. The uniformity of the asymptotic now follows from Vitali's theorem [7].

We wish to uniformly minimize over $D := \{z \in \mathbf{C} : |z| \le 1\},\$

$$w_m(z) := s_m(z)e^{-3z} + t_m(z)e^{-2z} + u_m(z)e^{-z} + v_m(z),$$

where $s_m, t_m, u_m, v_m \in \pi_m$ and s_m has highest coefficient 1.

Firstly, we have **Theorem 4.** For |z| = 1,

$$\left| E_m \left(z + \frac{3}{2(4m+3)} \right) \right| \sim \frac{6^{m+1}m!}{(4m+3)!}$$

Proof This follows from Theorem 2 and the observation that

$$\left(z+\frac{3}{2(4m+3)}\right)^{4m+3} \sim z^{4m+3}e^{\frac{3}{2z}},$$

and the fact that for |z| = 1, $|e^{\frac{3}{2}(\frac{1}{z}-z)}| = 1$. Let

$$P_m^*(z) = P_m\left(z + \frac{3}{2(4m+3)}\right),$$
$$Q_m^*(z) = Q_m\left(z + \frac{3}{2(4m+3)}\right),$$

$$R_m^*(z) = R_m \left(z + \frac{3}{2(4m+3)} \right),$$
$$S_m^*(z) = S_m \left(z + \frac{3}{2(4m+3)} \right).$$

Let $|| \cdot ||_D$ denote the supremum norm on D.

Now we need the following lemma.

Lemma 5 [12] Suppose m_1, m_2, \dots, m_l are positive integers such that $m_1 + m_2 + \dots + m_l = n$ and $\lambda_1 < \lambda_2 < \dots < \lambda_l$ are real numbers. Let $f_1(z), f_2(z), \dots, f_n(z)$ denote $e^{\lambda_1 z}, ze^{\lambda_1 z}, \dots, z^{m_1-1}e^{\lambda_1 z}; e^{\lambda_2 z}, ze^{\lambda_2 z}, \dots, z^{m_2-1}e^{\lambda_2 z}; \dots, e^{\lambda_l z}, ze^{\lambda_l z}, \dots, z^{m_l-1}e^{\lambda_l z}$ respectively. If $|k_1| + |k_2| + \dots + |k_{m_1}| > 0$, $|k_{n-m_l+1}| + \dots + |k_{n-1}| + |k_n| > 0$, and N denotes the zero number of function $k_1 f_1(z) + k_2 f_2(z) + \dots + k_n f_n(z)$ in the region $\Omega = \{z : \xi \leq Imz \leq \eta\}$. Then

$$\frac{(\lambda_l - \lambda_1)(\eta - \xi)}{2\pi} - n + 1 \le N \le \frac{(\lambda_l - \lambda_1)(\eta - \xi)}{2\pi} + n - 1.$$

By this lemma, we can prove the main result of this section.

Theorem 6. (a)

$$\begin{split} ||P_m^*(z)e^{-3z} + Q_m^*(z)e^{-2z} + R_m^*(z)e^{-z} + S_m^*(z)||_D \\ &\sim \frac{6^{m+1}m!}{(4m+3)!}. \end{split}$$

(b) Let

$$w_m^* = \min_{s,t,u,v \in \pi_m} ||s_m e^{-3z} + t_m e^{-2z} + u_m e^{-z} + v_m ||_D,$$

where $s = z^m + \cdots$. Then

$$w_m^* \sim \frac{6^{m+1}m!}{(4m+3)!}.$$

Proof Part (a) is just a restatement of Theorem 4. Observe that P_m^* has leading coefficient 1.

To prove part (b) we use the fact that a nonzero expression of the form

$$h_1(z)e^{-3z} + h_2(z)e^{-2z} + h_3(z)e^{-z} + h_4(z)$$

where h_1, h_2, h_3, h_4 are polynomials, the sum of whose degrees is k, can have at most k + 3 zeros in D. This is winding number argument and is proved in Lemma 5 with l = 4, $\xi = -1$, $\eta = 1$, $\lambda_1 = -3$, $\lambda_2 = -2$, $\lambda_3 = -1$, $\lambda_4 = 0$ and n = k + 4. Thus

$$w_m^* \ge \min_{|z|=1} |P_m^*(z)e^{-3z} + Q_m^*(z)e^{-2z} + R_m^*(z)e^{-z} + S_m^*(z)|.$$

If this were not the case we could find $s, t, u, v \in \pi_m$ with s having leading coefficient 1 so that, for |z| = 1

$$|se^{-3z} + te^{-2z} + ue^{-z} + v|$$

$$<|P_m^*e^{-3z}+Q_m^*e^{-2z}+R_m^*e^{-z}+S_m^*|.$$

By Rouché's theorem this would imply that

$$(s - P_m^*)e^{-3z} + (t - Q_m^*)e^{-2z} + (u - R_m^*)e^{-z} + (v - S_m^*)$$
(14)

has at least 4m + 3 zeros in *D*. However, since $s - P_m^*$ has degree at most m - 1, the sum of the degrees of the coefficients in (14) is at most 4m - 1, and we have contradicted the above result from Lemma 5.

We note that

$$||P_m e^{-3z} + Q_m e^{-2z} + R_m e^{-z} + S_m||_D \sim e^{\frac{3}{2}} \frac{6^{m+1}m!}{(4m+3)!}$$

and so, up to a small constant, the cubic Hermite-Padé approximant is optimal in the sense of Theorem 6. The trick of shifting the center of the approximation to make the error curve have asymptotically constant norm on D is due to Braess [8] who used it to get the right constant in the Meinardus' conjecture.

It is easy to show that the coefficient polynomials of the diagonal cubic Hermite-Padé approximant are linked by the following fourth-order differential equations.

Theorem 7.

(a)
$$-6mP_{m-1}(x) = P_{m}^{''''} - 6P_{m}^{'''} + 11P_{m}^{''} - 6P_{m}^{'}.$$

(b) $-6mQ_{m-1}(x) = Q_{m}^{''''} - 2Q_{m}^{'''} - Q_{m}^{''} + 2Q_{m}^{'}.$
(c) $-6mR_{m-1}(x) = R_{m}^{''''} + 2R_{m}^{'''} - R_{m}^{''} - 2R_{m}^{'}.$
(d) $-6mS_{m-1}(x) = S_{m}^{''''} + 6S_{m}^{'''} + 11S_{m}^{''} + 6S_{m}^{''}.$

4 Local analytical difference schemes based on cubic Padé approximation

In order to investigate the application of the diagonal cubic Padé approximation to e^{-x} , we discuss the problem (1.6).

We rewrite the above equation (1.6) as

$$au_x + \varepsilon u_{xx} = c. \tag{15}$$

In the case that c is a constant, we get the solution of (15) after integration:

$$u = c_1 e^{\lambda x} + c_2 + \frac{c}{a} x, \quad \lambda = -\frac{a}{\varepsilon}.$$

After discretization, we have

$$u_{i} = \frac{u_{i+1} + e^{\lambda h} u_{i-1}}{1 + e^{\lambda h}} + c \frac{h(e^{\lambda h} - 1)}{a(1 + e^{\lambda h})},$$

where $h = \frac{1}{N}$ is the common step width. Therefore

$$c = \frac{a \left(u_{i+1} - (1 + e^{\lambda h}) u_i + e^{\lambda h} u_{i-1} \right)}{h(1 - e^{\lambda h})},$$
$$i = 1, 2, \dots, N - 1.$$

$$i = 1, 2, ..., N - 1$$

Now letting $c = \frac{\mathrm{d}u_i}{\mathrm{d}t}$, we have

$$\begin{cases} \frac{d\mathbf{u}}{dt} = -A\mathbf{u} + \mathbf{b}, \\ \mathbf{u}(0) = \mathbf{\Phi}, \end{cases}$$
(16)

where

$$\mathbf{u} = (u_1, u_2, ..., u_{N-1})^T,$$

$$\mathbf{b} = \left(\frac{a\alpha e^{\lambda h}}{h(1-e^{\lambda h})}, \ 0, ..., 0, \ \frac{\alpha\beta}{h(1-e^{\lambda h})}\right)^T,$$

 $\boldsymbol{\Phi} = (\phi(x_1), \phi(x_2), ..., \phi(x_{N-1}))^T \quad \text{are} \quad \text{all} \quad (N - 1) \text{-} \\ \text{dimensional column vectors,}$

$$A = \frac{a}{h(1 - e^{\lambda h})}$$

$$\begin{pmatrix} 1+e^{\lambda h} & -1 & 0 & \cdots & 0\\ -e^{\lambda h} & 1+e^{\lambda h} & -1 & \ddots & \vdots\\ 0 & -e^{\lambda h} & 1+e^{\lambda h} & \ddots & 0\\ \vdots & \ddots & \ddots & \ddots & -1\\ 0 & 0 & \cdots & -e^{\lambda h} & 1+e^{\lambda h} \end{pmatrix}$$

is an $(N-1) \times (N-1)$ tridiagonal matrix. So the solution of problem (16) is

$$\mathbf{u}(t) = e^{-At}(\mathbf{\Phi} - A^{-1}\mathbf{b}) + A^{-1}\mathbf{b},$$
 (17)

where $e^{-At} = \sum_{n=0}^{\infty} \frac{1}{n!} (-At)^n$.

Equivalently, (17) can be written as the following forms:

$$\mathbf{u}(t+j\tau) = e^{-jA\tau} \{ \mathbf{u}(t) - A^{-1}\mathbf{b} \} + A^{-1}\mathbf{b} \ (j = 1, 2, 3),$$
(18)

where $\tau > 0$ is the increment.

Denoting

$$T_m(x) = -\frac{Q_m(x)}{P_m(x)}, \ \ U_m(x) = -\frac{R_m(x)}{P_m(x)},$$

 $V_m(x) = -\frac{S_m(x)}{P_m(x)},$

we have

$$e^{-3x} = T_m(x)e^{-2x} + U_m(x)e^{-x} + V_m(x) + O(x^{4m+3}).$$

Replacing $e^{-3A\tau}$ in (18) with $T_m(A\tau)e^{-2A\tau} + U_m(A\tau)e^{-A\tau} + V_m(A\tau)$, we get a class of 3-step local analytical difference schemes based on diagonal cubic Padé approximation:

$$\mathbf{u}(t+3\tau) = T_m(A\tau)\mathbf{u}(t+2\tau)$$
$$+U_m(A\tau)\mathbf{u}(t+\tau) + V_m(A\tau)\mathbf{u}(t)$$
$$+\{I - T_m(A\tau) - U_m(A\tau) - V_m(A\tau)\}A^{-1}\mathbf{b}.$$
 (19)

According to (19), we can list three simple schemes as follows:

Scheme 1. $m = 0, P_m = 1, Q_m = -3, R_m = 3, S_m = -1;$

$$\mathbf{u}(t+3\tau) = 3\mathbf{u}(t+2\tau) - 3\mathbf{u}(t+\tau) + \mathbf{u}(t).$$

Scheme 2. m = 1,

$$P_m = x + \frac{11}{3}, \ Q_m = 9(x+1),$$
$$R_m = 9(x-1), \ S_m = x - \frac{11}{3};$$
$$\mathbf{u}(t+3\tau) = \left(\frac{11}{3}I + \tau A\right)^{-1} \left\{ -9(I+\tau A)\mathbf{u}(t+2\tau) + 9(I-\tau A)\mathbf{u}(t+\tau) + \left(\frac{11}{3}I - \tau A\right)\mathbf{u}(t) + 20\tau \mathbf{b} \right\};$$

where I is the $(N-1) \times (N-1)$ unit matrix.

Scheme 3.
$$m = 2$$
,
 $P_m = x^2 + 11x + \frac{103}{3}, \ Q_m = 27(x^2 + 3x + 9),$
 $R_m = -27(x^2 - 3x + 9), \ S_m = x^2 - 11x + \frac{103}{3};$
 $\mathbf{u}(t + 3\tau) = \left(\frac{103}{3}I + 11\tau A + \tau^2 A^2\right)^{-1}$
 $\cdot \left\{27(9I + 3\tau A + \tau^2 A^2)\mathbf{u}(t + 2\tau) - 27(9I - 3\tau A + \tau^2 A^2)\mathbf{u}(t + 2\tau) + \left(\frac{103}{3}I - 11\tau A + \tau^2 A^2\right)\mathbf{u}(t) - 140\tau\mathbf{b}\right\}.$



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