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A Piecewise Modified Matrix Padé-type Approximation of Hybrid Order in the Interval [0, 1]

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Abstract. In this paper, we introduce a piecewise modified matrix Padé-type approximation of hybrid order in the interval [0, 1]. It yields highly accurate results and exact values at some given points. The accuracy of this approximation increases as the order or the node increases. This method can be applied to approximate the exponential function. The explicit formula for computing the matrix exponential is presented. A numerical example is given to illustrate the effectiveness of this method.

Keywords: matrix Padé-type approximation, piecewise interpolation, matrix exponential.

1. Introduction

Padé-type approximation has been widely used in various fields of mathematics, physics, and engineering since it was first introduced by Brezinski [1, 2]. In the last thirty years, it has received a lot of attention and has been generalized to many cases by some authors, for example, Arioka [3], Daras [4], Salam [8], Thukral [9], Gu and Shen [6].

Following the idea of scalar Padé-type approximation [2], Gu [5] gave a matrix Padé-type approximation whose denominator is a scalar polynomial by means of a matrix-valued linear functional on the polynomial space. The matrix Padé-type approximation [5, 7] is a good approximation in a region near the origin, but may not be accurate at other points. To improve the accuracy of such approximation, we develop an interpolation technique for generating a new rational approximation with high accuracy.

In this paper, matrix Padé-type approximation is modified by an interpolation polynomial. Based on the modified matrix Padé-type approximation, we construct a piecewise modified matrix Padé-type approximation of hybrid order in the interval [0, 1]. This new rational approximation to a matrix function gives more accurate results and exact values at certain selected points in the interval [0, 1]. In addition, we use this new method to approximate the matrix exponential. The practical formula for computing the matrix exponential is presented. It is shown by a numerical example of the matrix exponential that the accuracy of the approximation increases as the order or the node increases.

2. Main Results

Let $F(t)$ be a given power series at t_k with $s \times s$ matrix coefficients

$$F(t) = \sum_{i=0}^{\infty} C_i^{(t_k)} (t - t_k)^i, \quad C_i^{(t_k)} \in C^{s\times s}, \quad C_0^{(t_k)} \neq 0, \quad k \in \mathrm{N}. \tag{1}$$

Denote P the set of scalar polynomials in one real variable whose coefficients belong to the complex field C. Let $\phi^{(l)} : \mathrm{P} \to C^{s\times s}$ be a matrix-valued linear functional on P, acting on $(x - t_k)$, defined by

$$\phi^{(l)}((x - t_k)^i) = C_{l+i}^{(t_k)}, \quad i, l = 0, 1, \cdots,$$

where

$$\phi^{(0)}((x - t_k)^i) = \phi((x - t_k)^i) = C_i^{(t_k)}, \quad i = 0, 1, \cdots, \tag{2}$$

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with $C_i^{(t_k)} = 0$ for $i < 0$.

For the given power series (1), it follows from (2) that

$$\begin{aligned} &\phi((1-(x-t_k)(t-t_k))^{-1}) \\ &= \phi(1+(x-t_k)(t-t_k)+(x-t_k)^2(t-t_k)^2+\cdots) \\ &= C_0^{(t_k)} + C_1^{(t_k)}(t-t_k) + C_2^{(t_k)}(t-t_k)^2 + \cdots \\ &= F(t). \end{aligned} \tag{3}$$

Let v be an arbitrary polynomial of degree n

$$v(t) = b_0 + b_1(t-t_k) + \cdots + b_n(t-t_k)^n, \quad b_n \neq 0, \tag{4}$$

and define the matrix polynomial W_{mn} by

$$W_{mn}(t) = \phi\left(\frac{(x-t_k)^{m-n+1}v(x) - (t-t_k)^{m-n+1}v(t)}{x-t}\right). \tag{5}$$

Note that ϕ acts on $(x-t_k)$ and W_{mn} is a matrix polynomial of degree m. Define

$$\begin{aligned} q_{mn}^{t_k}(t) &= (t-t_k)^n v((t-t_k)^{-1}+t_k), \\ P_{mn}^{t_k}(t) &= (t-t_k)^m W_{mn}((t-t_k)^{-1}+t_k). \end{aligned} \tag{6}$$

Theorem 1. If $q_{mn}^{t_k}(t_k) \neq 0$, then

$$F(t) - \frac{P_{mn}^{t_k}(t)}{q_{mn}^{t_k}(t)} = O((t-t_k)^{m+1}), \quad t \to t_k.$$

Proof. Note that ϕ is a matrix-valued linear functional on P, acting on $(x-t_k)$. From (3), (5) and (6), we get

$$\begin{aligned} P_{mn}^{t_k}(t) &= (t-t_k)^m W_{mn}((t-t_k)^{-1}+t_k) \\ &= (t-t_k)^m \phi\left(\frac{(t-t_k)^{-(m-n+1)}v((t-t_k)^{-1}+t_k) - (x-t_k)^{m-n+1}v(x)}{((t-t_k)^{-1}+t_k)-x}\right) \\ &= \phi\left(\frac{(t-t_k)^n v((t-t_k)^{-1}+t_k) - (t-t_k)^{m+1}(x-t_k)^{m-n+1}v(x)}{1-(x-t_k)(t-t_k)}\right) \\ &= q_{mn}^{t_k}(t)F(t) - (t-t_k)^{m+1}\phi^{(m-n+1)}\left(\frac{v(x)}{1-(x-t_k)(t-t_k)}\right). \end{aligned}$$

Thus, the result follows if $q_{mn}^{t_k}(t_k) \neq 0$.

Definition 1. Let $R_{mn}^{t_k}(t) = P_{mn}^{t_k}(t)/q_{mn}^{t_k}(t)$. Then $R_{mn}^{t_k}(t)$ is called a matrix Padé-type approximation of order (m,n) for $F(t)$ at $t = t_k$ and is denoted by $(m/n)_F^{t_k}(t)$, where $v(t)$ in (4) is called a generating polynomial of $(m/n)_F^{t_k}(t)$.

Note that the definition of matrix Padé-type approximation given in [5] is a special case of Definition 1 here for $t_k = 0$. We can also denote $(m/n)_F^0(t)$ simply by $(m/n)_F(t)$.

Definition 2. Let $F(t)$ defined on the interval $[t_0, t_1] \subset [0,1]$ be given the values at $t = t_0$ and $t = t_1 (t_0 \neq t_1)$. Then a modified matrix Padé-type approximation (MMPTA) for $F(t)$ in the interval $[t_0, t_1]$ is defined by

$$(m/n)_F^{[t_0,t_1]}(t) = (m/n)_F^{t_0}(t) + \varepsilon_{mn}^{t_0}(t-t_0)^{m+1}, \tag{7}$$

where the matrix parameter $\varepsilon_{mn}^{t_0}$ is determined by

$$(m/n)_F^{[t_0,t_1]}(t_1) = F(t_1). \tag{8}$$

By the condition (8) of Definition 2, we have

$$\varepsilon_{mn}^{t_0} = \frac{F(t_1) - (m/n)_F^{t_0}(t_1)}{(t_1 - t_0)^{m+1}}.$$

For $n = 0, t_0 = 0, t_1 = 1$ in Definition 2, we get

$$(m/0)_F^{[0,1]}(t) = \sum_{i=0}^{m} C_i^{(0)} t^i + (F(1) - \sum_{i=0}^{m} C_i^{(0)}) t^{m+1}.$$

Definition 3. Let $F(t)$ defined on the interval $[0,1]$ be stored in a tabular form (t_k, F_{t_k}), $k = 0,1,\cdots,N$, where $F_{t_k} = F(t_k)$ and the points t_k form an ordered sequence $0 \le t_0 < t_1 < \cdots < t_N \le 1$. Then a piecewise modified matrix Padé-type approximation of hybrid order (PMMPTAHO) for $F(t)$ in the interval $[t_0, t_N]$ is denoted by $P(m_1/n_1,\cdots,m_N/n_N)_F^{[t_0,t_N]}(t)$ and is defined by

$$P(m_1/n_1,\cdots,m_N/n_N)_F^{[t_0,t_N]}(t) = \begin{cases} (m_1/n_1)_F^{[t_0,t_1]}(t), & t \in [t_0,t_1], \\ (m_2/n_2)_F^{[t_1,t_2]}(t), & t \in [t_1,t_2], \\ \quad\vdots & \\ (m_N/n_N)_F^{[t_{N-1},t_N]}(t), & t \in [t_{N-1},t_N], \end{cases} \tag{9}$$

where for $i = 1,\cdots,N$,

$$(m_i/n_i)_F^{[t_{i-1},t_i]}(t) = (m_i/n_i)_F^{t_{i-1}}(t) + \frac{F(t_i) - (m_i/n_i)_F^{t_{i-1}}(t_i)}{(t_i - t_{i-1})^{m_i+1}} (t - t_{i-1})^{m_i+1}, \tag{10}$$

which is called the ith approximant of the piecewise modified matrix Padé-type approximation of hybrid order $P(m_1/n_1,\cdots,m_N/n_N)_F^{[t_0,t_N]}(t)$.

It is easy to get

$$P(m_1/n_1,\cdots,m_N/n_N)_F^{[t_0,t_N]}(t_k) = F(t_k), \quad k = 0,1,\cdots,N. \tag{11}$$

Theorem 2. Let $T = \{t_0, t_1, \cdots, t_N\}$, then

$$P(m_1/n_1,\cdots,m_N/n_N)_F^{[t_0,t_N]}(t) - F(t) = \begin{cases} O((t-t_0)^{m_1+1}), & t \in (t_0,t_1), \\ O((t-t_1)^{m_2+1}), & t \in (t_1,t_2), \\ \quad\vdots & \\ O((t-t_{N-1})^{m_N+1}), & t \in (t_{N-1},t_N), \\ 0, & t \in T. \end{cases} \tag{12}$$

Proof. The result follows immediately form Definition 3, Theorem 1 and (11).

Remark 1. If $N = 1$ in Definition 3, then the piecewise modified matrix Padé-type approximation of hybrid order will reduce to the modified matrix Padé-type approximation. For $m_1 = \cdots = m_N = m$, $n_1 = \cdots = n_N = n$, we denote $P(m_1/n_1,\cdots,m_N/n_N)_F^{[t_0,t_N]}(t)$ simply by $P(m/n)_F^{[t_0,t_N]}(t)$.

3. Application for the Matrix Exponential

Expand e^{At} at $t = t_k$ into a power series

$$\begin{aligned} e^{At} &= e^{At_k} e^{A(t-t_k)} \\ &= e^{At_k} (\sum_{i=0}^{\infty} C_i (t-t_k)^i), \quad A \in C^{s\times s}, \end{aligned} \tag{13}$$

where $C_i = A^i / i!, \quad i = 0,1,\cdots.$

Assume that the coefficients b_i in (4) satisfy the following linear system of equations

$$\sum_{i=0}^{n} b_i trC_{m-n+1+k+i} = 0, \quad k = 0,1,\cdots,n-1, \tag{14}$$

where tr indicates the trace of a matrix, that is, the sum of its diagonal elements. Note that one of the b_i 's is arbitrary, and then let us choose $b_n = 1$ so that $v(t)$ has the exact degree $n.$ It follows that

$$\sum_{i=0}^{n-1} b_i trC_{m-n+1+k+i} = -trC_{m+1+k}, \quad k = 0,1,\cdots,n-1. \tag{15}$$

Thus $b_0, b_1, \cdots b_{n-1}$ are obtained as the unique solution of the above linear system of equations if the determinant of the coefficient matrix in (15) is different from zero. Knowing the b_i 's, (5) and (6) directly give $(m/n)_{e^A}^{t_k}(t).$

Theorem 3. If $q_{mn}^{t_k}(t_k) \neq 0,$ then the matrix Padé-type approximant $(m/n)_{e^A}^{t_k}(t)$ of trace form for e^{At} in (13) at $t = t_k$ exists and is given by

$$(m/n)_{e^A}^{t_k}(t) = \frac{P_{mn}^{t_k}(t)}{q_{mn}^{t_k}(t)}, \tag{16}$$

where

$$q_{mn}^{t_k}(t) = \begin{vmatrix} trC_{m-n+1} & trC_{m-n+2} & \cdots & trC_{m+1} \\ \vdots & \vdots & \cdots & \vdots \\ trC_m & trC_{m+1} & \cdots & trC_{m+n} \\ (t-t_k)^n & (t-t_k)^{n-1} & \cdots & 1 \end{vmatrix}, \tag{17}$$

and

$$P_{mn}^{t_k}(t) = e^{At_k} \begin{vmatrix} trC_{m-n+1} & trC_{m-n+2} & \cdots & trC_{m+1} \\ \vdots & \vdots & \cdots & \vdots \\ trC_m & trC_{m+1} & \cdots & trC_{m+n} \\ \sum_{i=n}^{m} C_{i-n}(t-t_k)^i & \sum_{i=n-1}^{m} C_{i-n+1}(t-t_k)^i & \cdots & \sum_{i=0}^{m} C_i (t-t_k)^i \end{vmatrix}. \tag{18}$$

Proof. If $q_{mn}^{t_k}(t_k) \neq 0,$ then $v(t)$ can be solved out by Cramer's rule from the linear system of equations in (4) and (14). So Eq. (17) is shown by $q_{mn}^{t_k}(t) = (t-t_k)^n v((t-t_k)^{-1} + t_k).$ By replacing $v(t)$ in (5) and $P_{mn}^{t_k}(t) = (t-t_k)^m W_{mn}((t-t_k)^{-1} + t_k),$ Eq.(18) is obtained. Thus Eq. (16) is immediately got from Definition 1.

Corollary 1. If $q_{mn}^{t_k}(t_k) \neq 0,$ then

$$(m/n)_{e^A}^{t_k}(t_k) = e^{At_k}.$$

Replacing F by e^A in (7) and (9), respectively, the MMPTA of trace form for e^{At} is given by

$$(m/n)_{e^A}^{[t_0,t_1]}(t)=(m/n)_{e^A}^{t_0}(t)+\frac{e^{At_1}-(m/n)_{e^A}^{t_0}(t_1)}{(t_1-t_0)^{m+1}}(t-t_0)^{m+1}$$

and the PMMPTAHO of trace form for e^{At} is given by

$$P(m_1/n_1,\cdots,m_N/n_N)_{e^A}^{[t_0,t_N]}(t)=\begin{cases}(m_1/n_1)_{e^A}^{[t_0,t_1]}(t), & t\in[t_0,t_1],\\ (m_2/n_2)_{e^A}^{[t_1,t_2]}(t), & t\in[t_1,t_2],\\ \vdots & \\ (m_N/n_N)_{e^A}^{[t_{N-1},t_N]}(t), & t\in[t_{N-1},t_N],\end{cases}$$

where the approximants $(m_k/n_k)_{e^A}^{t_{k-1}}(t)$ are given by (16), (17) and (18).

4. Numerical Example

Three values of e^{At} with $A=\begin{bmatrix}0 & 1\\ 0 & -2\end{bmatrix}$ are given in Table 1.

Table 1. The interpolation nodes and values

t	0	1/2	1
e^{At}	$\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix}$	$\begin{bmatrix}1 & (1-e^{-1})/2\\ 0 & e^{-1}\end{bmatrix}$	$\begin{bmatrix}1 & (1-e^{-2})/2\\ 0 & e^{-2}\end{bmatrix}$

To compute the approximant $(2/1)_{e^A}^{[0,1]}(t)$ for the interpolation nodes $t_0=0,t_1=1,$ and the approximants $P(2/1)_{e^A}^{[0,1]}(t), P(2/1,3/1)_{e^A}^{[0,1]}(t),$ and $P(3/1)_{e^A}^{[0,1]}(t)$ for the interpolation nodes $t_0=0,t_1=1/2,t_2=1.$

Solution. Expand e^{At} into a power series at $t=t_k(k=0,1,2),$

$$\begin{aligned}e^{At}&=e^{At_k}(C_0+C_1(t-t_k)+C_2(t-t_k)^2+\cdots+C_n(t-t_k)^n+\cdots)\\ &=e^{At_k}(\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix}+\begin{bmatrix}0 & 1\\ 0 & -2\end{bmatrix}(t-t_k)+\begin{bmatrix}0 & -1\\ 0 & 2\end{bmatrix}(t-t_k)^2\\ &+\begin{bmatrix}0 & \frac{2}{3}\\ 0 & -\frac{4}{3}\end{bmatrix}(t-t_k)^3+\begin{bmatrix}0 & -\frac{1}{3}\\ 0 & \frac{2}{3}\end{bmatrix}(t-t_k)^4+\begin{bmatrix}0 & \frac{2}{15}\\ 0 & -\frac{4}{15}\end{bmatrix}(t-t_k)^5+\cdots).\end{aligned}$$

Then we have

$$(2/1)_{e^A}^{[0,1]}(t)=(2/1)_{e^A}(t)+(e^A-(2/1)_{e^A}(1))t^3,$$

$$P(2/1)_{e^A}^{[0,1]}(t)=\begin{cases}(2/1)_{e^A}(t)+8(e^{A/2}-(2/1)_{e^A}(1/2))t^3,\\ (2/1)_{e^A}^{1/2}(t)+8(e^A-(2/1)_{e^A}^{1/2}(1))t^3,\end{cases}$$

$$P(2/1,3/1)_{e^A}^{[0,1]}(t)=\begin{cases}(2/1)_{e^A}(t)+8(e^{A/2}-(2/1)_{e^A}(1/2))t^3,\\ (3/1)_{e^A}^{1/2}(t)+16(e^A-(3/1)_{e^A}^{1/2}(1))t^4,\end{cases}$$

$$P(3/1)_{e^A}^{[0,1]}(t)=\begin{cases}(3/1)_{e^A}(t)+16(e^{A/2}-(3/1)_{e^A}(1/2))t^4,\\ (3/1)_{e^A}^{1/2}(t)+16(e^A-(3/1)_{e^A}^{1/2}(1))t^4,\end{cases}$$

where

$$(2/1)^{t_k}_{e^A}(t)=\frac{e^{At_k}\begin{bmatrix}2(t-t_k)+3 & -(t-t_k)^2+3(t-t_k)\\ 0 & 2(t-t_k)^2-4(t-t_k)+3\end{bmatrix}}{2(t-t_k)+3},\quad k=0,1,2,$$

$$(3/1)^{t_k}_{e^A}(t)=\frac{e^{At_k}\begin{bmatrix}(t-t_k)+2 & 1/3(t-t_k)^3-(t-t_k)^2+2(t-t_k)\\ 0 & -2/3(t-t_k)^3+2(t-t_k)^2-3(t-t_k)+2\end{bmatrix}}{(t-t_k)+2},\quad k=0,1,2.$$

Table 2. Some errors of the approximants for the $\infty-$norm

t	0.2	0.6	0.95
$\left\|e^{At}-(2/1)^{[0,1]}_{e^A}(t)\right\|_\infty$	2.49128×10^{-4}	8.76076×10^{-4}	9.15101×10^{-5}
$\left\|e^{At}-P(2/1)^{[0,1]}_{e^A}(t)\right\|_\infty$	1.87527×10^{-4}	1.38755×10^{-5}	8.17007×10^{-5}
$\left\|e^{At}-P(2/1,3/1)^{[0,1]}_{e^A}(t)\right\|_\infty$	1.87527×10^{-4}	4.95199×10^{-7}	1.55864×10^{-5}
$\left\|e^{At}-P(3/1)^{[0,1]}_{e^A}(t)\right\|_\infty$	1.40313×10^{-5}	4.95199×10^{-7}	1.55864×10^{-5}

It is obvious to see that these approximants are equal to e^{At} at the interpolation nodes. Some errors of these approximants for the $\infty-$norm in the interval [0, 1] are given in Table 2. From Table 2, it is known that the accuracy of the constructed approximants for e^{At} increases as the order or the node increases.

To provide some indication of the accuracy of the constructed approximants, we compute the matrix Padé-type approximants $(2/1)_{e^A}(t)$ and $(3/1)_{e^A}(t)$ by Theorem 4.3 in [5],

$$(2/1)_{e^A}(t)=\frac{\begin{bmatrix}10/3t+5 & -5/3t^2+5t\\ 0 & 10/3t^2-20/3t+5\end{bmatrix}}{10/3t+5},$$

$$(3/1)_{e^A}(t)=\frac{\begin{bmatrix}t+2 & 1/3t^3-t^2+2t\\ 0 & -2/3t^3+2t^2-3t+2\end{bmatrix}}{t+2}.$$

In Table 3, we give the maximum errors of the constructed approximation and the matrix Padé-type approximation for the $\infty-$norm in the interval [0, 1/2] and [1/2, 1].

Table 3. The maximum errors of the approximants for the $\infty-$norm in [0, 1]

m	t	$\max_t\left\|e^{At}-P(m/1)^{[0,1]}_{e^A}(t)\right\|_\infty$	$\max_t\left\|e^{At}-(m/1)_{e^A}(t)\right\|_\infty$
2	$t\in[0,1/2]$	3.79007×10^{-4}	7.12056×10^{-3}
2	$t\in[1/2,1]$	1.39429×10^{-4}	6.46647×10^{-2}
3	$t\in[0,1/2]$	5.71361×10^{-5}	1.21277×10^{-3}
3	$t\in[1/2,1]$	2.10192×10^{-5}	2.42242×10^{-2}

It is clear that the constructed method is a better method than the matrix Padé-type method for the same order to approximate the exponential function in the interval [0, 1].

5. Conclusions

In this paper, a piecewise modified matrix Padé-type approximation of hybrid order in the interval [0, 1] has been presented. This approximation has two advantages: highly accurate and locally controllable. We can improve the accuracy of the i th approximant of the piecewise modified matrix Padé-type approximation of hybrid order by increasing the order.

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