

Fourth-Order Approximation of the Fundamental Matrix of a Linear System of Differential Equations

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تقريب من الدرجة الرابعة للمصفوفة الأساسية لمنظومة معادلات تفاضلية خطية

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خلاصة - هذا البحث يقدم صيغة تقريبية جديدة من الرتبة الرابعة على شكل مصفوفة أسية تمثل مصفوفة الحل الأساسية لمعادلات تفاضلية خطية. تحسب قيمة المصفوفة الأسية من خلال تجزأة مدى التفاضل إلى مناطق جزئية واستخدام تقريب «ببدي» مع مبدأ «التوليف والتربيع». يمكن استخدام الصيغة الجديدة المقترحة لحل مسائل القيمة الابتدائية أو مسائل القيمة المحدودة ذات القيم الحدودية المخططة. كذلك يمكن استخدام المصفوفة التقريبية المقترحة كإداة تكامل لطرق الحل التي تتطلب معلومات عن القيم على مدى التكامل. يتعرض البحث لمثال عن استخدام التقريب المقترح لحل إحدى مسائل القيمة المحدودة ذات القيم الحدودية المخططة.

ABSTRACT: A fourth-order approximation to the fundamental matrix of a system of linear differential equations is presented in closed form as a matrix exponential. The matrix exponential is then discretized over the interval of integration. Pade approximation together with the method of scaling and squaring (Moler *et al.*, 1978) is used to evaluate the matrix exponential. This approach is suitable for solving both initial and boundary value problems with mixed boundary conditions. The approximating matrix can also be used as an integrating operator for methods which require information about the solution along the discretized subintervals. An example of a boundary value problem with mixed boundary conditions is presented.

The problem being considered is governed by the following set of linear differential equations

$$y'(x) = A(x)y(x), \quad x \in [a, b] \quad (1)$$

where y is a vector-valued function with n components, A is an $n \times n$ coefficients matrix. The motivation to study problem (1) comes from the fact that it includes various practical problems, including those arising in optimal control theory. The problem of obtaining a closed-form analytical representation of the fundamental matrix, has been extensively studied with limited success. However, if A is commutative then the fundamental matrix can be written in closed-form as a matrix exponential function, (Zhu *et al.* 1992). Shridharan *et al.* (1995) developed the existence-uniqueness as well as constructive theory for the solution of systems of nonlinear boundary value problems when only approximations of the fundamental matrix of the associated homogeneous linear differential systems are known. Roberts (1979) reported a method that directly uses the fundamental matrix to solve two-point boundary value problems with implicit boundary conditions. That method is based on the Alspaugh-Kagiwada-Kalaba method (Alspaugh *et al.* 1970) of invariant imbedding, where the fundamental matrix and its partitions are related to the Riccati equation.

The solution of equation (1) is given by

$$y(x) = \Phi(x, a)y(a)$$

where $\Phi(x, a)$ is the fundamental matrix, satisfying $\Phi(a, a) = I$, and I is the $n \times n$ identity matrix. One way of evaluating $\Phi(x, a)$ is by finding successive approximations to the solution in the form of the infinite series, (Coddington *et al.*, 1955)

$$\begin{aligned} \Phi(x, a) = & I + \int_a^x A(s_0) ds_0 + \int_a^x A(x_0) \int_a^{s_0} A(s_1) ds_1 ds_0 \\ & + \int_a^x A(s_0) \int_a^{s_0} A(s_1) \int_a^{s_1} A(s_2) ds_2 ds_1 ds_0 + \dots \end{aligned}$$

However, this requires the evaluation of multiple integrals of increasing complexity if accurate answers are to be found. Asfar *et al.* (1989a) suggested the division of the interval $[a, b]$ into a number of subintervals $[x_j, x_{j+1}]$, $j = 0, 1, \dots, (L-1)$, where $x_0 = a$ and $x_L = b$. The matrix $A(x)$ is then approximated by a constant matrix A_j over each subinterval $[x_j, x_{j+1}]$, and $\exp((x - x_j) A_j)$ was used to approximate $\Phi(x, x_j)$ in that subinterval. In that approach $\exp((x - x_j) A_j)$ is a first-order approximation to $\Phi(x, a)$, and was used

successfully by Asfar *et al* (1989b) and by Hussein (1994). In this work, higher order approximations to the matrix exponential are presented.

The fundamental matrix $\Phi(x, a)$ satisfies the equation

$$\Phi'(x, a) = A(x)\Phi(x, a), \tag{2}$$

so that expanding $\Phi(x, a)$ about $x = a$ in powers of $x - a$ and substituting in equation (2) gives

$$\Phi(x, a) = \sum_{j=0}^{\infty} \frac{(x-a)^j}{j!} \Phi^{(j)}(a, a) \tag{3}$$

where $\Phi^{(j)}(a, a)$ is the j th derivative of $\Phi(x, a)$ with respect to x , evaluated at $x = a$. Differentiating equation (2) repeatedly give the matrices $\Phi^{(j)}(a, a)$ as follows

$$\begin{aligned} \Phi(a, a) &= I \\ \Phi'(a, a) &= A_0 \\ \Phi''(a, a) &= A_0^2 + A_0' \\ \Phi'''(a, a) &= A_0^3 + A_0'A_0' + 2A_0'A_0 + A_0'' \end{aligned}$$

and so on, where $A_0 = A(a)$, $A_0' = A_0'(a)$, $A_0'' = A_0''(a)$, ... etc.

Substituting the above values of Φ and their derivatives in equation (3) and grouping equal powers of $x - a$, gives

$$\begin{aligned} \Phi(x, a) &= \exp((x-a)A_0) + \frac{(x-a)^2}{2!}A_0' + \frac{(x-a)^3}{3!}[A_0'A_0' \\ &+ 2A_0'A_0 + A_0''] + \frac{(x-a)^4}{4!}[A_0^2A_0' + 2A_0'A_0'A_0 \\ &+ A_0'A_0'' + 3A_0'A_0^2 + 3A_0'A_0' + 3A_0''A_0 + A_0'''] + \dots \end{aligned} \tag{4}$$

In equation (4), the expression $\exp((x-a)A_0)$ is a first-order approximation to $\Phi(x, a)$. Higher order approximations to the solution can be obtained, using the approximation

$$\Psi(x, a) = \exp\left(t \sum_{j=1}^r \alpha_j A(\alpha + \beta_j t)\right), \tag{5}$$

for $\Phi(x, a)$ where $t = x - a$ and $r = 2$. Expanding $A(\alpha + \beta_j t)$ in powers of t , substituting in equation (5) and grouping equal powers of t , give

$$\Psi(x, a) = \exp\left(\sum_{j=0}^{\infty} u_j \frac{t^j}{j!} A_0^{(j)}\right), \quad u_j = \sum_{i=1}^r \alpha_i \beta_i^j \tag{6}$$

Expanding the exponential function in equation (6), and grouping equal powers of t , give

$$\begin{aligned} \Psi(x, a) &= \exp((x-a)u_0 A_0) + \frac{2u_1}{2!}(x-a)^2 A_0' \\ &+ \frac{(x-a)^3}{3!}[3u_0 u_1 (A_0'A_0' + A_0'A_0) + 3u_2 A_0''] + \dots \end{aligned}$$

If $u_0 = 1$ and $u_1 = 1/2$, then the difference $\mathcal{E}(x, a)$ between $\Phi(x, a)$ and $\Psi(x, a)$ is

$$\begin{aligned} \mathcal{E}(x, a) &= \Phi(x, a) - \Psi(x, a) \\ &= \frac{(x-a)^3}{12} [A_0'A_0' - A_0'A_0 + 6(\frac{1}{3} - u_2)A_0''] \\ &+ O((x-a)^4). \end{aligned}$$

With $u_0 = 1$ and $u_1 = 1/2$, the parameters $\alpha_1, \alpha_2, \beta_1$ and β_2 satisfy the following equations

$$\alpha_1 + \alpha_2 = 1 \tag{7}$$

$$\alpha_1 \beta_1 + \alpha_2 \beta_2 = 1/2. \tag{8}$$

The equations (7) and (8) can be used to generate a second-order family of approximations to $\Phi(x, a)$ with two free parameters, say α_1 and β_1 . In order to keep the number of matrix $A(x)$ evaluations to a minimum, (by evaluating $A(x)$ only on the discretized points) the values of the free parameters are taken to be $\alpha_1 = 1/2, \beta_1 = 0$, so that $\alpha_2 = 1/2$ and $\beta_2 = 1$. Thus

$$\Psi(x, a) = \exp((x-a)\{A(a) + A(x)\}/2) \tag{9}$$

and

$$\begin{aligned} \mathcal{E}(x, a) &= \frac{(x-a)^3}{12} [A(a)A(a) - A(a)A'(a) - A''(a)] \\ &+ O((x-a)^4). \end{aligned} \tag{10}$$

Also one can take $\alpha_1 = 0$, so that $\alpha_2 = 1$ and $\beta_2 = 1/2$ and

$$\Psi(x, a) = \exp\left((x-a)A\left(\frac{a+x}{2}\right)\right) \tag{11}$$

with

$$\mathcal{E}(x, a) = \frac{(x-a)^3}{12} [A'(a)A(a) + \frac{1}{2}A''(a)] + O((x-a)^4). \tag{12}$$

FOURTH-ORDER APPROXIMATION OF THE FUNDAMENTAL MATRIX

The $\Psi(x, a)$ matrix given in equations (9) and (11) is a second-order approximation to the fundamental matrix $\Phi(x, a)$, with the error $\mathcal{E}(x, a)$ given by equations (10) and (12), respectively.

Fourth-order approximation

Taking $r = 3$ in equation (5) gives,

$$\mathcal{E}(x, a) = \frac{(x-a)^3}{12} [A'(a)A(a) - A(a)A'(a)] + 2(1-3u_2)A''(a) + O((x-a)^4)$$

where $u_0 = 1$ and $u_1 = \frac{1}{2}$. Thus increasing the value of r in equation (5) does not increase the order of approximation. However we could use the approximation $\Omega(x, a) = \exp(t B_1 + t^2 B_2)$, where $t = x - a$,

$$B_1 = \sum_{j=1}^3 \alpha_j A(a + \beta_j t), \quad B_2 = \sum_{j=1}^3 \gamma_j A(a + \delta_j t).$$

Expanding A in powers of t and grouping equal powers, gives

$$\begin{aligned} \mathcal{F}(x, a) &= \Phi(x, a) - \Omega(x, a) = e^{(x-a)A_0} - e^{u_0(x-a)A_0} \\ &+ \frac{(x-a)^2}{2!} [(1-2u_1)A_0' - 2(\gamma_1 + \gamma_2)A_0] \\ &+ \frac{(x-a)^3}{3!} [(1-3u_2)A_0'' + \{2-3u_0u_1 - 6(\gamma_1\delta_1 + \gamma_2\delta_3)\}A_0'A_0 \\ &+ \{1-3u_0u_1 - 6(\gamma_1\delta_2 + \gamma_2\delta_4)\}A_0A_0' - 6u_0(\gamma_1 + \gamma_2)A_0^3] \\ &+ \frac{(x-a)^4}{4!} [\{1-4u_0^2u_1 - 12u_1(\gamma_1 + \gamma_2 - 12u_0(\gamma_1\delta_2 + \gamma_2\delta_4)\}A_0^2A_0' \\ &+ \{3-4u_0^2u_1 - 12(\gamma_1 + \gamma_2) - 12u_0(\gamma_1 + \gamma_2\delta_3)\}A_0'A_0^2 \\ &+ \{1-4u_3\}A_0''' - 12\{(\gamma_1 + \gamma_2)^2 + u_0^2(\gamma_1 + \gamma_2)\}A_0^4 \\ &+ \{2-12u_0(\gamma_1\delta_1 + \gamma_2\delta_3) - 12u_0(\gamma_1\delta_2 + \gamma_2\delta_4) - 4u_0^2u_1\}A_0'A_0'A_0 \\ &+ \{1-6u_0u_2 - 12(\gamma_1\delta_2^2 + \gamma_2\delta_4^4)\}A_0A_0'' \\ &+ \{3-6u_0u_2 - 12(\gamma_1\delta_1^2 + \gamma_2\delta_3^2)\}A_0''A_0 \\ &+ \{3-12u_1^2 - 24(\gamma_1\delta_1\delta_2 + \gamma_2\delta_3\delta_4)\}A_0 \\ &+ O((x-a)^5). \end{aligned}$$

If

$$u_0 = 1, \quad u_1 = \frac{1}{2}, \quad u_2 = \frac{1}{3}, \quad u_3 = \frac{1}{4}. \quad (13)$$

$$\gamma_1 + \gamma_2 = 0, \quad \gamma_1\delta_1 + \gamma_2\delta_3 = \frac{1}{12}, \quad \gamma_1\delta_2 + \gamma_2\delta_4 = \frac{-1}{12}. \quad (14)$$

$$\begin{aligned} \gamma_1\delta_1^2 + \gamma_2\delta_3^2 &= \frac{1}{12}, \quad \gamma_1\delta_2^2 + \gamma_2\delta_4^2 = \frac{-1}{12}, \\ \gamma_1\delta_1\delta_2 + \gamma_2\delta_3\delta_4 &= 0. \end{aligned} \quad (15)$$

then $\mathcal{F}(x, a) = O((x-a)^5)$. The parameter values given in equations (14) and (15) result in the following relations

$$\delta_1 = \frac{12\gamma_1 + 1}{24\gamma_1} = \delta_4, \quad \delta_2 = \frac{12\gamma_1 - 1}{24\gamma_1} = \delta_3.$$

The conditions given in equation (13) give the following system of four non-linear algebraic equations, in terms of the parameters $\alpha_1, \alpha_2, \alpha_3, \beta_1, \beta_2,$ and β_3 .

$$\sum_{j=1}^3 \alpha_j \beta_j^i = \frac{1}{i+1}, \quad i = 0, 1, 2, 3.$$

In order to keep the number of the coefficient matrix A evaluations to a minimum, the following values are taken for $\beta_1, \beta_2, \beta_3$ and γ_1 :

$$\beta_1 = 0, \quad \beta_2 = \frac{1}{2}, \quad \beta_3 = 1, \quad \gamma_2 = \frac{-1}{12},$$

and the other parameters are

$$\delta_1 = 0, \quad \delta_2 = 1, \quad \delta_3 = 1, \quad \delta_4 = 0,$$

$$\alpha_1 = \frac{1}{6}, \quad \alpha_2 = \frac{4}{6}, \quad \alpha_3 = \frac{1}{6}, \quad \gamma_1 = \frac{1}{12}.$$

Hence

$$\Omega(x, a) = \exp((x-a)B_1 + (x-a)^2B_2) \quad (16)$$

where

$$B_1 = \frac{1}{6} [A(a) + 4A\left(\frac{a+x}{2}\right) + A(x)],$$

$$B_2 = \frac{1}{12} [A(x)A(a) - A(a)A(x)],$$

and

$$\begin{aligned} \mathcal{F}(x, a) = & \frac{(x-a)^5}{5!} \left[\frac{-1}{24} A_0^{(4)} + \frac{1}{6} \{A_0^3 A_0' - A_0' A_0^3 \right. \\ & + A_0 A_0''' - A_0''' A_0 + A_0^2 A_0'' - 2 A_0'' A_0 + A_0'' A_0^2 \} \\ & \left. + \frac{1}{2} \{A_0' A_0' A_0^2 - A_0^2 A_0' A_0' + A_0' A_0' A_0' - 2 A_0' A_0' A_0' \right. \\ & \left. + A_0' A_0' A_0' \} \right] + O((x-a)^6) \end{aligned}$$

which shows that $\Omega(x, a)$ is a fourth-order approximation to $\Phi(x, a)$. In approximating the fundamental matrix $\Phi(x, a)$ over the interval $[a, b]$, we discretize the second-order approximation $\Psi(x, a)$ or the fourth-order approximation $\Omega(x, a)$ over L subintervals $[x_0, x_1], [x_1, x_2], \dots, [x_{L-1}, x_L]$ where $x_0 = a, x_L = b$ and $x_{j+1} = x_j + h_{j+1}, j = 0, 1, 2, \dots, (L-1)$. The approximating matrix is then given, over each subinterval, in closed form.

Computation of the matrix exponential

The matrix exponential $\exp(hQ)$ can be approximated by many methods, but the method of scaling and squaring (Moler et al, 1978) is appropriate especially when $h\|Q\|$ is very large, where the norm is taken to be the Euclidean norm. The method is based on the property of the matrix exponential

$$\exp(hQ) = [\exp(hQ/m)]^m \tag{17}$$

where $m = 2^j$. When $h\|Q\|$ is very large, the roundoff error difficulties can be controlled by using a suitable value of j for which $\exp(hQ/m)$ can be reliably and efficiently computed, and then to form $\exp(hQ)$ by repeated squaring of $\exp(hQ/m)$. The matrix $\exp(hQ/m)$ can be satisfactorily computed by the following Padé approximation:

$$\exp(hQ) \approx R_{qq}(hQ) = [D_{qq}(hQ)]^{-1} N_{qq}(hQ), \tag{18}$$

where

$$N_{qq}(hQ) = \sum_{j=0}^q P_j(hQ), \quad D_{qq}(hQ) = \sum_{j=0}^q (-1)^j P_j(hQ)$$

and

$$P_j(hQ) = \frac{(2q-j)!q!}{(2q)!j!(q-j)!} (hQ)^j.$$

A rather extensive treatment of Padé approximation can be found in Ralston et al (1978). If $\exp(hQ/m)$ is to be approximated by $R_{qq}(hQ/m)$, where $m = 2^j$, then the values of j and q have to be chosen. Moler et al (1978) reported that if

$$h\|Q\| \leq 2^{j-1}$$

then

$$[R_{qq}(hQ/m)]^m = \exp(hQ + Z)$$

where

$$\frac{\|Z\|}{h\|Q\|} \leq 8 \left(\frac{h\|Q\|}{2^j} \right)^{2q} \left(\frac{(q!)^2}{(2q)!(2q+1)!} \right) \tag{19}$$

The value of j can be calculated from equation (17), and if

$$\frac{\|Z\|}{h\|Q\|} \leq \epsilon$$

then equation (19) can be used to calculate the value of q , as reported in table (1) below, (Moler et al 1978) which gives the optimum values of (q, j) associated with $[R_{qq}(hQ/m)]^m$ for a given ϵ and $h\|Q\|$.

Applications to systems of differential equations

The second-order approximation $\Psi(x, a)$, given in equations (9) or (11), and the fourth-order approximation $\Omega(x, a)$, given in equation (16), can be used to approximate the solution of a linear system of differential equations, with initial or mixed boundary conditions. In the case of an initial value problem, one of the following equations

$$y(x) = \Psi(x, a) y(a)$$

or

$$y(x) = \Omega(x, a) y(a)$$

can be used to approximate step by step the solution along the interval of interest. In the case of a boundary value problem, the interval $[a, b]$ of interest is divided into L subintervals $[x_j, x_{j+1}], j = 0, 1, 2, \dots, (L-1)$; and then the solutions

$$y_{j+1}(x) = \exp((x-x_j)G_{j+1}(x, x_j)) y_{j+1}(x_j) \tag{20}$$

are matched at the mid points. In equation (20) above, $G_{j+1}(x, x_j)$ is taken to be

$$G_{j+1}(x, x_j) = \frac{1}{2} \{A(x_j) + A(x)\}$$

for the second-order approximation, and

FOURTH-ORDER APPROXIMATION OF THE FUNDAMENTAL MATRIX

$$G_{j+1}(x, x_j) = \frac{1}{6} \left[A(x_j) + 4A\left(\frac{x_j+x}{2}\right) + A(x) \right] + \frac{(x-x_j)}{12} [A(x)A(x_j) - A(x_j)A(x)]$$

$$\begin{pmatrix} u(T) \\ v(T) \end{pmatrix} = y_L(t_L) = e^{hG_L(t_L, t_{L-1})} y_{L-1}(t_{L-1}). \quad (27)$$

for the fourth-order approximation. The matched equations together with the boundary conditions, give a system of linear algebraic equations, with band structure which can easily be solved by Gaussian elimination.

Example:

In this example we consider the following two-point boundary value problem with oscillatory coefficients over the interval $[0, T]$:

$$y'(t) = A(t) y(t), \quad (21)$$

where

$$A(t) = \begin{pmatrix} \sin(kt) & \cos(kt) \\ \cos(kt) & -\sin(kt) \end{pmatrix}, \quad y(t) = \begin{pmatrix} u(t) \\ v(t) \end{pmatrix},$$

and $T = s\pi/k$, the interval width T can be changed, by changing the value of s . The boundary conditions are

$$u(0) - v(0) = 1 \quad (22)$$

$$v(T) = 0. \quad (23)$$

If we divide the interval $[0, T]$ into L subintervals, then the solution along each subinterval $[t_j, t_{j+1}]$ is given by the following set of equations

$$y_{j+1}(t) = \exp((t-t_j) G_{j+1}(t, t_j)) y_{j+1}(t_j), \quad j = 0, 1, 2, \dots, (L-1) \quad (24)$$

The solutions from two adjacent subintervals are equal at the middle point, then equations (24) can be written as

$$y_{j+1}(t_{j+1}) = \exp(hG_{j+1}(t_{j+1}, t_j)) y_j(t_j), \quad j = 1, 2, 3, \dots, (L-2) \quad (25)$$

with the solution at the end points

$$y_1(t_1) = e^{hG_1(t_1, t_0)} y_1(t_0) = e^{hG_1(t_1, t_0)} \begin{pmatrix} u(0) \\ v(0) \end{pmatrix} \quad (26)$$

and

Using the approximation in equation (18), the above three equations (25) - (27) become

$$N_1 \begin{pmatrix} u(0) \\ v(0) \end{pmatrix} = D_1 y_1(t_1)$$

$$N_{j+1} y_j(t_j) = D_{j+1} y_{j+1}(t_{j+1}), j = 1, 2, 3, \dots, (L-2)$$

$$N_L y_{L-1}(t_{L-1}) = D_L \begin{pmatrix} v(T) \\ v(T) \end{pmatrix}.$$

Adapting the notation $u(t) = u_j$ and $v(t) = v_j$, for $j = 0, 1, 2, \dots, L$ together with the boundary conditions given in equations (26) and (27), a system of $2L \times 2L$ linear algebraic equations with the unknowns $\{u_0, u_1, v_1, u_2, v_2, \dots, u_{L-1}, v_{L-1}, u_L\}$ is formed. In this example, (2,2)-Padé approximation ($q = 2$) was used together with $j = 0$, to approximate the matrix exponential. Table (2) below shows, the number of subintervals needed to solve problem (21) using either the second-order approximation, or the fourth-order approximation for both $s = k = 10$ and $s = k = 40$. Figures (1) - (4) represent, respectively the $u(t)$ and $v(t)$ components of the solution $y(t)$ for the two sets of s and k .

TABLE 1

The optimum values of (q, j) .

ϵ $h Q $	10^{-3}	10^{-6}	10^{-9}	10^{-12}	10^{-15}
10^2	(1,0)	(1,0)	(2,0)	(3,0)	(3,0)
10^1	(1,0)	(2,0)	(2,0)	(4,0)	(4,0)
1	(2,1)	(3,1)	(3,0)	(5,1)	(6,1)
10	(2,5)	(3,5)	(4,1)	(5,5)	(6,5)
10^2	(2,8)	(3,8)	(4,5)	(5,8)	(6,8)
10^3	(2,11)	(3,11)	(4,11)	(5,11)	(6,11)
10^4	(2,15)	(3,15)	(4,15)	(5,15)	(6,15)
10^5	(2,18)	(3,18)	(4,18)	(5,18)	(6,18)
10^6	(2,21)	(3,21)	(4,21)	(5,21)	(6,21)

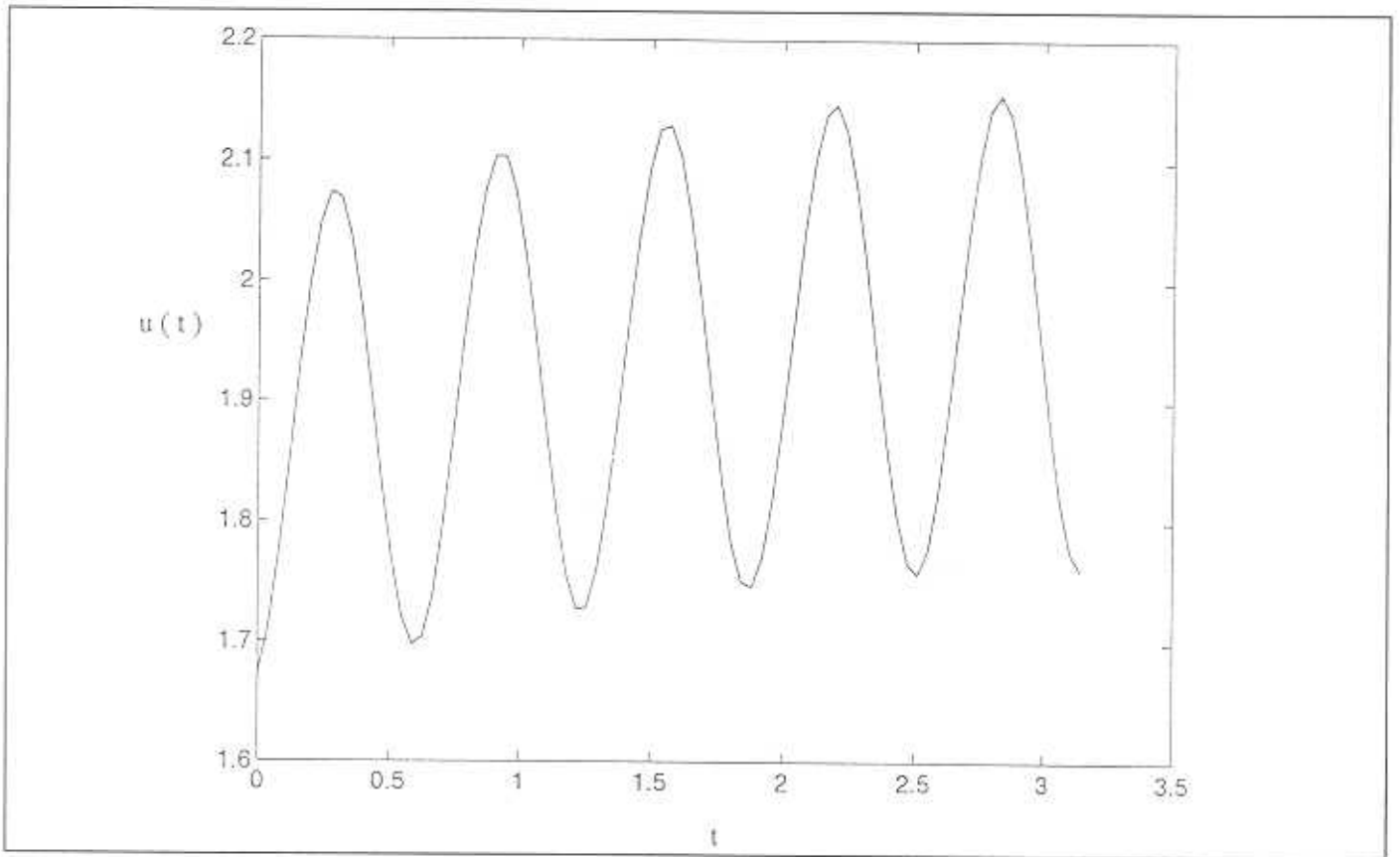


Figure 1. $u(t)$ for $s = 10$ & $K = 10$.

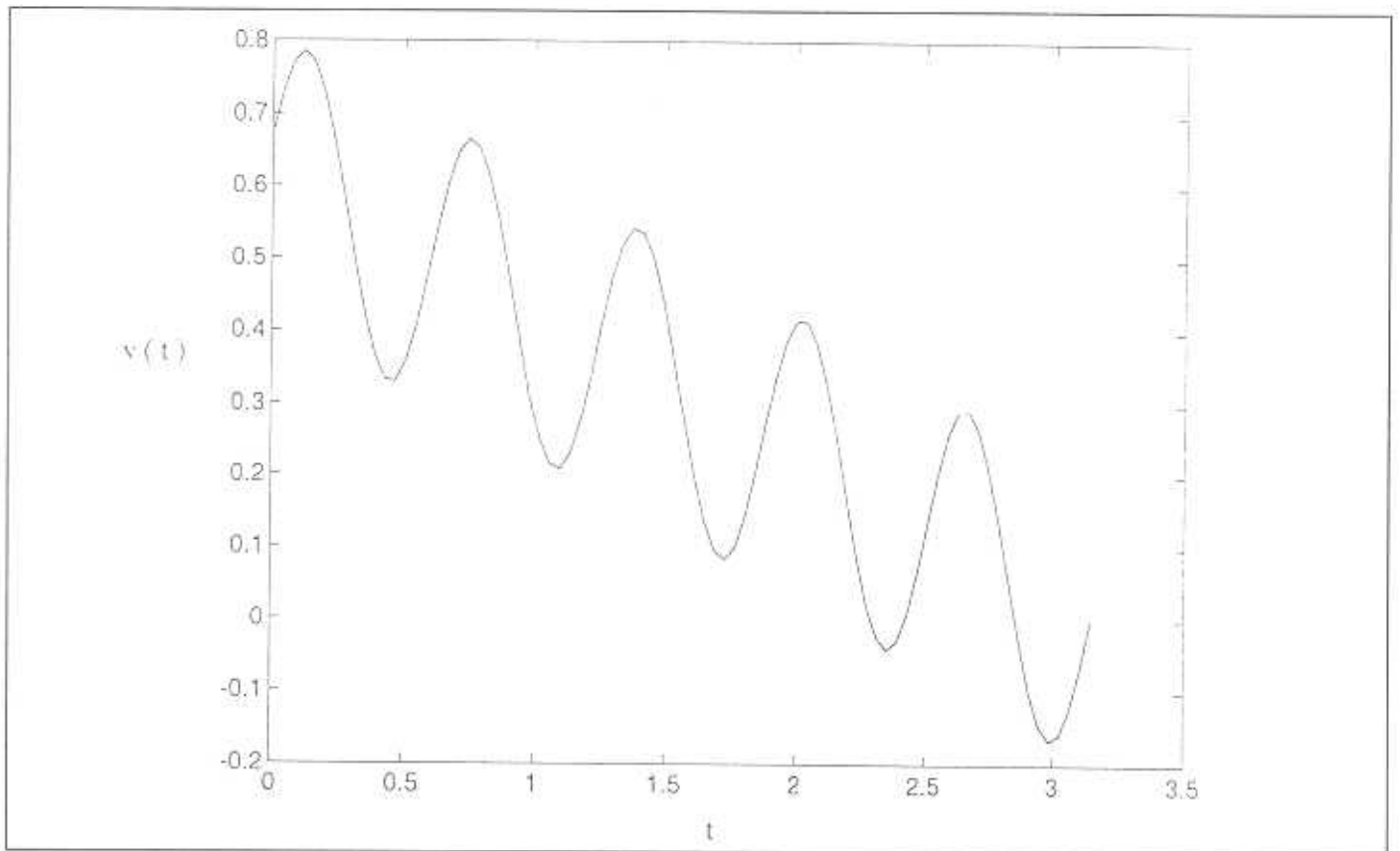


Figure 2. $v(t)$ for $s = 10$ & $K = 10$.

FOURTH-ORDER APPROXIMATION OF THE FUNDAMENTAL MATRIX

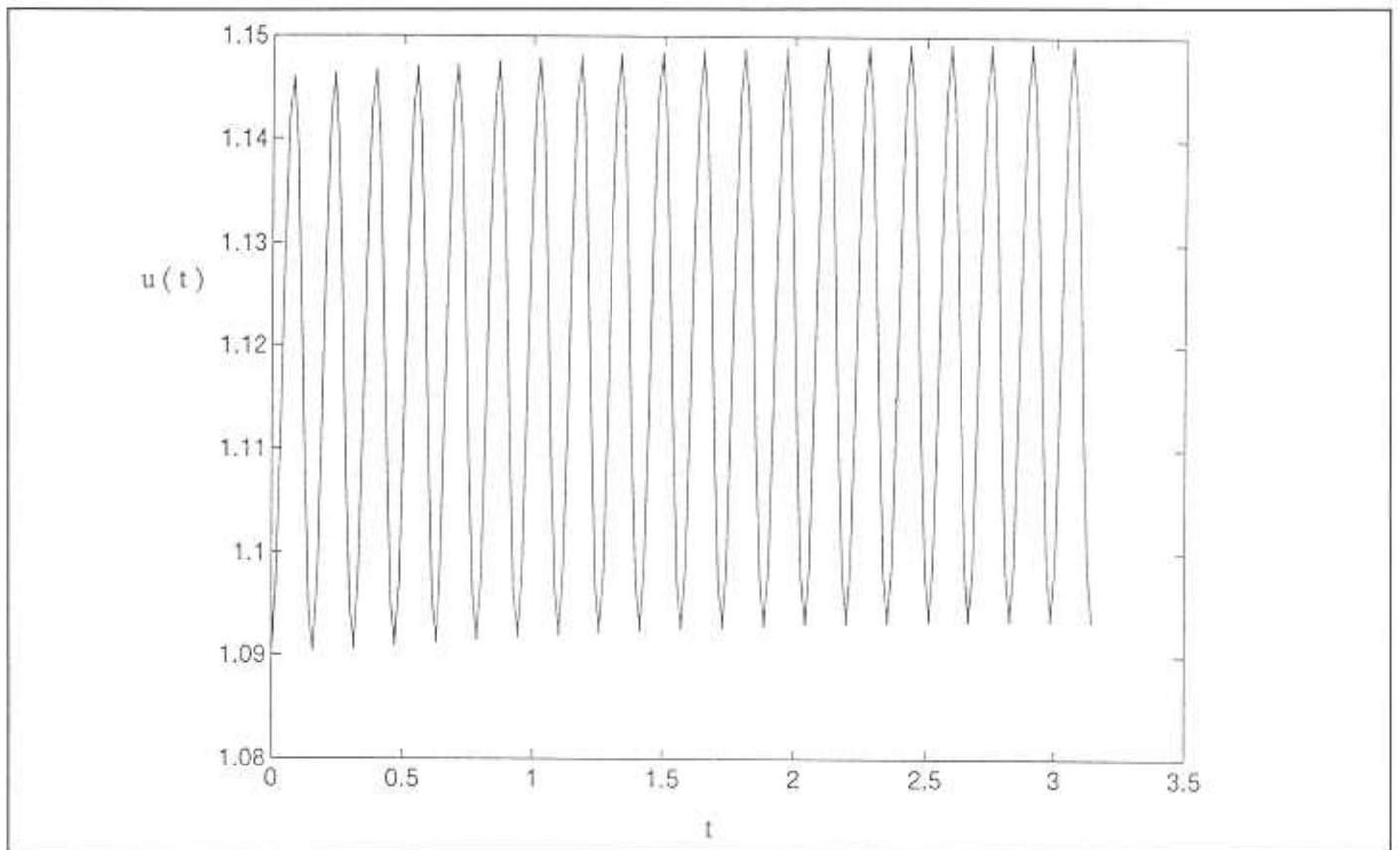


Figure 3. $u(t)$ for $s = 40$ & $K = 40$.

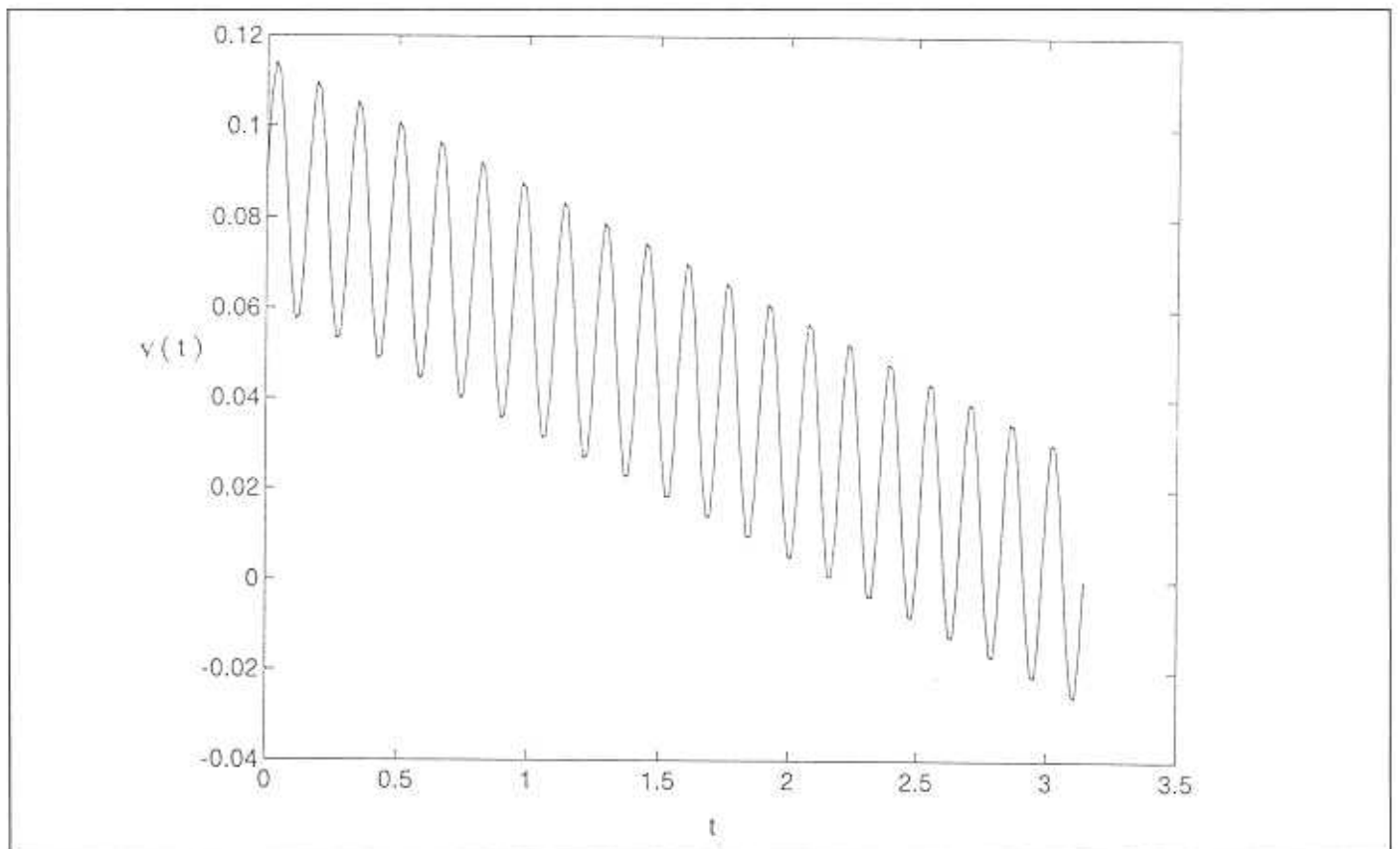


Figure 4. $v(t)$ for $s = 40$ & $K = 40$.

FOURTH-ORDER APPROXIMATION OF THE FUNDAMENTAL MATRIX

TABLE 2
The number of subintervals needed

s	k	2nd-order approximation <i>L</i> for equation (37)	4th-order approximation <i>L</i> for equation (38)
10	10	260	80
40	40	550	200

Conclusion

A fourth-order approximation to the fundamental matrix of a system of linear differential equations was derived in closed form. The derived approximation was successfully applied to a boundary value problem with mixed boundary conditions. The approximation can be easily applied to solve initial value problems as well. The approximation was in the form of a matrix exponential, which was evaluated using Padé approximation together with the method of scaling and squaring.

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