Cubic-matrix splines and second-order matrix models

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Abstract
We discuss the direct use of cubic-matrix splines to obtain continuous approxima-
tions to the unique solution of matrix models of the type $Y''(x) = f(x, Y(x))$.
For numerical illustration, an estimation of the approximation error, an algorithm
for its implementation, and an example are given.

1 Introduction.
Matrix initial value problems of the form:

\[
\begin{align*}
Y''(x) &= f(x, Y(x)) \\
Y(a) &= Y_0, \quad Y'(a) = Y_1
\end{align*}
\]

are frequently encountered in different fields of physics and engineering (see e.g. [Zha02]).
In the scalar case, numerical methods for the calculation of approximate solutions of
(1) can be found in [Col93]. For matrix problems, linear multi-step matrix methods
with constant steps have been studied in [Jod93]. Although in this case there exist
\textit{a priori} error bounds for these methods (expressed as function of the data problem),
these error bounds are given in terms of an exponential which depends on the integra-
tion step $h$. Therefore, in practice, $h$ will take too small values. Problems of the type
(1) can be written as an extended first-order matrix problem. Such a standard approach,
however, involves an increase of the computational cost caused by the increase of the
problem dimension. Recently, cubic-matrix splines were used in the resolution of first-
order matrix differential systems [Def06], obtaining approximations that, among other
advantages, were of class $C^1$ in the interval $[a, b]$, and easy to compute producing an
approximation error $O(h^4)$. The present work extends this powerful scheme to the so-
lution of matrix problems of type (1). Throughout this work, we will adopt the notation
for norms and matrix cubic splines as in [Def06] and common in matrix calculus. The
paper is organized as follows. Section 2 develops the proposed method. Finally, in
Section 3, an example is presented.
2 Construction of the method.

Let us consider the initial value problem
\[
\begin{aligned}
Y''(x) &= f(x, Y(x)) \quad a \leq x \leq b, \\
Y(a) &= Y_0, \quad Y'(a) = Y_1
\end{aligned}
\]
(2)
where \(Y_0, Y_1, Y(t) \in \mathbb{C}^{r \times q}, f : [a, b] \times \mathbb{C}^{r \times q} \times \mathbb{C} \rightarrow \mathbb{C}^{r \times q}, f \in \mathcal{C}^0(T),\) with
\[
T = \{ (x, Y) : a \leq x \leq b, Y \in \mathbb{C}^{r \times q} \},
\]
and \(f\) fulfills the global Lipschitz's condition
\[
\| f(x, Y_1) - f(x, Y_2) \| \leq L \| Y_1 - Y_2 \|, \quad a \leq x \leq b, Y_1, Y_2 \in \mathbb{C}^{r \times q}.
\]
(3)

Let us also use the partition of the interval \([a, b]\) defined by
\[
\Delta_{[a,b]} = \{ a = x_0 < x_1 < \ldots < x_n = b \}, \quad x_k = a + kh, \quad k = 0, 1, \ldots, n,
\]
(5)
where \(h = (b - a)/n, n\) being a positive integer. We will construct in each subinterval \([a + kh, a + (k + 1)h]\) a matrix-cubic spline approximating the solution of problem (2).

For the first interval \([a, a + h]\), we consider that the matrix-cubic spline is given by
\[
S_{[a,a+h]}(x) = Y(a) + Y'(a)(x-a) + \frac{1}{2!}Y''(a)(x-a)^2 + \frac{1}{3!}A_0(x-a)^3,
\]
(6)
where \(A_0 \in \mathbb{C}^{r \times q}\) is a matrix parameter to be determined. It is straightforward to check:
\[
S_{[a,a+h]}(a) = Y(a), \quad S'_{[a,a+h]}(a) = Y'(a), \quad S''_{[a,a+h]}(a) = Y''(a) = f(a, S_{[a,a+h]}(a)).
\]
Thus, (6) satisfies the equations of problem (2) at point \(x = a\). To fully construct the matrix-cubic spline, we must still determine \(A_0\). By imposing that (6) is a solution of problem (2) in \(x = a + h\), we have:
\[
S''_{[a,a+h]}(a + h) = f(a + h, S_{[a,a+h]}(a + h)),
\]
(7)
and obtain from (7) the matrix equation with only one unknown matrix \(A_0\):
\[
A_0 = \frac{1}{h} \left[ f \left( a + h, Y(a) + Y'(a)h + \frac{1}{2}Y''(a)h^2 + \frac{1}{6}A_0h^3 \right) - Y''(a) \right].
\]
(8)
Assuming that the matrix equation (8) has only one solution \(A_0\), the matrix-cubic spline is totally determined in the interval \([a, a + h]\). Now, in the next interval \([a + h, a + 2h]\), the matrix-cubic spline is defined by:
\[
S_{[a+h,a+2h]}(x) = S_{[a,a+h]}(a + h) + S'_{[a,a+h]}(a + h)(x - (a + h)) + \frac{1}{2!}S''_{[a,a+h]}(a + h)(x - (a + h))^2 + \frac{1}{3!}A_1(x - (a + h))^3,
\]
(9)
so that $S(x)$ is of class $C^2([a, a + h] \cup [a + h, a + 2h])$, and all of the coefficients of matrix-cubic spline $S_{\lfloor [a+h,a+2h]\rfloor}(x)$ are determined with the exception of $A_1 \in \mathbb{C}^{r \times q}$.

By construction, matrix-cubic spline (9) satisfies the differential equation (2) in $x = a + h$. We can obtain $A_1$ by requiring that the differential equation (2) holds at point $x = a + 2h$:

$$S''_{\lfloor [a+h,a+2h]\rfloor}(a + 2h) = f\left(a + 2h, S_{\lfloor [a+h,a+2h]\rfloor}(a + 2h)\right).$$

Expanding, we obtain the matrix equation with only one unknown matrix $A_1$:

$$A_1 = \frac{1}{h} \left[ f \left(a + 2h, S_{\lfloor [a+h,a+2h]\rfloor}(a + h) + S'_{\lfloor [a+h,a+2h]\rfloor}(a + h)h + \frac{1}{2} S''_{\lfloor [a+h,a+2h]\rfloor}(a + h)h^2 + \frac{1}{6} A_1 h^3 \right) - S''_{\lfloor [a+h,a+2h]\rfloor}(a + h) \right].$$

(10)

Let us assume that the matrix equation (10) has only one solution $A_1$. This way the spline is now totally determined in the interval $[a + h, a + 2h]$. Iterating this process, let us construct the matrix-cubic spline taking $[a + (k - 1)h, a + kh]$ as the last subinterval. For the next subinterval $[a + kh, a + (k + 1)h]$, we define the corresponding matrix-cubic spline as

$$S_{\lfloor [a+kh,a+(k+1)h]\rfloor}(x) = \beta_k(x) + \frac{1}{3!} A_k (x - (a + kh))^3,$$

where

$$\beta_k(x) = \sum_{l=0}^{2} \frac{1}{l!} S_{\lfloor [a+(h-k)h,a+kh]\rfloor}^{(l)}(a + kh)(x - (a + kh))^l.$$

(11)

With this definition, it is $S(x) \in C^2\left( \bigcup_{j=0}^{k} [a + jh, a + (j + 1)h] \right)$ which fulfills the differential equation (2) at point $x = a + kh$. As an additional requirement, we assume that $S(x)$ satisfies the differential equation (2) at the point $x = a + (k + 1)h$, i.e.

$$S''_{\lfloor [a+kh,a+(k+1)h]\rfloor}(a + (k + 1)h) = f\left(a + (k+1)h, S_{\lfloor [a+kh,a+(k+1)h]\rfloor}(a + (k + 1)h)\right).$$

Subsequent expansion of this equation with the unknown matrix $A_k$ yields

$$A_k = \frac{1}{h} \left[ f \left(a + (k+1)h, \beta_k(a + (k + 1)h) + \frac{1}{6} A_k h^3 \right) - \beta'''_k(a + (k + 1)h) \right].$$

(12)

Note that this matrix equation (12) is analogous to equations (8) and (10), when $k = 0$ and $k = 1$, respectively. For a fixed $h$, we will consider the matrix function of matrix variable $g : \mathbb{C}^{r \times q} \mapsto \mathbb{C}^{r \times q}$ defined by

$$g(T) = \frac{1}{h} \left[ f \left(a + (k+1)h, \beta_k(a + (k + 1)h) + \frac{1}{6} Th^3 \right) - \beta'''_k(a + (k + 1)h) \right].$$
Relation (12) holds if and only if $A_k = g(A_k)$, that is, if $A_k$ is a fixed point for function $g(T)$. Applying the global Lipschitz’s conditions (4), it follows that

$$\|g(T_1) - g(T_2)\| \leq \frac{Lh^2}{6} \|T_1 - T_2\|.$$ 

Taking $h < \sqrt{\frac{6}{L}}$, $g(T)$ yields a contractive matrix function, which guarantees that equation (12) has unique solutions $A_k$ for $k = 0, 1, \ldots, n - 1$. Hence, the matrix-cubic spline is now fully determined. Taking into account [Los67, Theorem 5], the following result has been established:

**Theorem 2.1** If $h < \sqrt{\frac{6}{L}}$, then the matrix-cubic spline $S(x)$ exists in each subinterval $[a + kh, a + (k + 1)h]$, $k = 0, 1, \ldots, n - 1$, as defined by the previous construction. Furthermore, if $f \in C^1(T)$, then $\|Y(x) - S(x)\| = O(h^3) \forall x \in [a, b]$, where $Y(x)$ is the theoretical solution of system (2).

Depending on the function $f$, matrix equations (8) and (12) can be solved explicitly or by using some iterative method [Ort72]. Summarizing, we have the following algorithm:

- Take $n > \frac{(b - a)\sqrt{T}}{\sqrt{6}}$, $h = (b - a)/n$ and $\Delta_{[a, b]}$ defined by (5).
- Solve (8) and determine $S|_{[a, a+h]}(x)$ defined by (6).
- For $k = 1$ to $n - 1$, solve (12). Determine $S|_{[a+kh, a+(k+1)h]}(x)$ defined by (11).

### 3 Example

The problem

$$Y''(t) + AY(t) = 0,$$ 

with $Y(0) = Y_0$, $Y'(0) = Y_1$, has the exact solution

$$Y(t) = \cos (\sqrt{A}t) Y_0 + (\sqrt{A})^{-1} \sin (\sqrt{A}t) Y_1,$$

where $\sqrt{A}$ denotes any square root of a non-singular matrix $A$, [Har05]. The principal drawback of this formal solution is the difficult computation of $\sqrt{A}$, $\cos (\sqrt{A}t)$ and $\sin (\sqrt{A}t)$. The proposed method avoids this drawback. We consider problem (13) where $A = \begin{pmatrix} 1 & 0 \\ 2 & 1 \end{pmatrix}$, $Y_0 = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$, $Y_1 = \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix}$, $t \in [0, 1]$, whose exact solution is $Y(t) = \sin \begin{pmatrix} \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix} t \end{pmatrix} = \begin{pmatrix} \sin (t) & 0 \\ t \cos (t) & \sin (t) \end{pmatrix}$. In this case $L \approx 2.82843$. By Theorem 2.1, we need to take $h < 1.45647$, so we choose $h = 0.1$ for example. The results are summarized in the following table, where the numerical estimates have been rounded to the fourth relevant digit. In each subinterval, we evaluated the difference between the estimates of our numerical approach and the exact solution. The maximum of these errors are indicated in the third column.
| Interval | Approximation | Max Error |
|----------|--------------|-----------|
| [0, 0.1] | \[ x - 0.1664z^2 \] | 1.0072 × 10^{-6} |
| [0.1, 0.2] | \[ 1.00005z - 0.0005z^2 - 0.164z^3 \] | 6.3032 × 10^{-6} |
| [0.2, 0.3] | \[ 1.00005z - 0.0005z^2 - 0.164z^3 \] | 2.0059 × 10^{-5} |
| [0.3, 0.4] | \[ -0.0002 + 1.0018z - 0.0009z^2 - 0.156z^3 \] | 4.6213 × 10^{-5} |
| [0.4, 0.5] | \[ -0.0002 + 1.0018z - 0.0009z^2 - 0.156z^3 \] | 8.8359 × 10^{-5} |
| [0.5, 0.6] | \[ -0.0002 + 1.0018z - 0.0009z^2 - 0.156z^3 \] | 1.4964 × 10^{-4} |
| [0.6, 0.7] | \[ -0.0002 + 1.0018z - 0.0009z^2 - 0.156z^3 \] | 3.2267 × 10^{-4} |
| [0.7, 0.8] | \[ -0.0002 + 1.0018z - 0.0009z^2 - 0.156z^3 \] | 3.3941 × 10^{-4} |
| [0.8, 0.9] | \[ -0.0002 + 1.0018z - 0.0009z^2 - 0.156z^3 \] | 4.7114 × 10^{-4} |
| [0.9, 1] | \[ -0.0002 + 1.0018z - 0.0009z^2 - 0.156z^3 \] | 6.2838 × 10^{-4} |

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