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Numerical determination of the transition matrix

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SEZIONE II

(Fisica, chimica, geologia, paleontologia e mineralogia)

Fisica. — *Numerical determination of the transition matrix.* Nota di MAURELIO BOARI e PAOLO TOTH (*), presentata (**) dal Socio G. EVANGELISTI.

RIASSUNTO. — Vengono esaminati alcuni metodi per la soluzione numerica dell'equazione differenziale matriciale

$$\frac{dX(t)}{dt} = P(t)\,X(t)$$

con condizioni iniziali note, associate al sistema di equazioni differenziali lineari con coefficienti variabili

$$\frac{d\overline{X}(t)}{dt} = P(t)\,\overline{X}(t) + \overline{F}(t).$$

Si dimostra dapprima come i metodi di integrazione numerica passo passo normalmente usati, risultino in alcuni casi poco convenienti sia riguardo la precisione conseguibile sia rispetto al tempo di calcolo; in tali casi risulta particolarmente vantaggioso avere a disposizione per $X(t)$ una espressione analitica, ottenuta ad esempio mediante opportuno sviluppo in serie di potenze.

Vengono quindi messi in evidenza gli aspetti computazionali di un algoritmo che, determinati mediante formule di tipo ricorrente i coefficienti dello sviluppo in serie di $X(t)$, consente la determinazione della matrice di transizione con una maggiore precisione e un minore tempo di calcolo.

Si eseguono infine confronti numerici tra il metodo proposto e il metodo di integrazione di Runge-Kutta a 4 punti onde mettere in evidenza i vantaggi conseguibili.

INTRODUCTION.

A typical problem in the analysis of linear systems is met with in determining the solution of the matrix differential equation with given initial conditions

$$\frac{dX(t)}{dt} = P(t)\cdot X(t);$$

this solution may be obtained numerically by adopting one of the classical step-by-step integration methods. However, their application is often complicated and cumbersome; this inconvenience is particularly felt when, as often happens, the transition matrix must be calculated only in relation to

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some values of the independent variable. The above-mentioned inconveniences can, of course, be avoided but there should be an analytical expression available for $X(t)$. For this purpose, when it exists, a suitable power series expansion may, be utilized such as is already known in the field of pure mathematics.

Since, indeed, the expansion coefficients are known, it is possible to determine within the desired precision, the transition matrix corresponding to each value of the independent variable.

The purpose of this paper is to bring out the computational aspects of an algorithm which, based on this concept, has not been proposed until now.

In the first part, the algorithm for determining the coefficients of the series expansion is developed and the analytical expressions are deduced from it. In the second part, a comparison is made with traditional numerical integration methods thus emphasizing the advantages obtainable both as precision and as regards duration of the calculation. The above-mentioned characteristics are shown by means of an example of numerical elaboration.

Transition matrix of linear systems.

Let us consider a system of N differential linear equations of the first order of the following type:

$$\frac{dx_k(t)}{dt} = \sum_{s=1}^{N} p_{k,s}(t)\, x_s(t) + f_k(t) \tag{1}$$

with: $k = 1, 2, \cdots, N$ and: $a \leq t \leq b$.

Writing equation (1) in vectorial form, we get:

$$\frac{d\bar{x}(t)}{dt} = P(t)\,\bar{x}(t) + \bar{F}(t) \tag{2}$$

where:

$$\bar{x}(t) = [x_1(t), x_2(t), \cdots, x_N(t)]$$

is the vector column of the unknown functions, $P(t)$ is the square matrix of order N, whose elements $P_{k,s}(t)$, $(k = 1, 2, \cdots, N; s = 1, 2, \cdots, N)$ are continuous functions in the interval defined above,

$$\bar{F}(t) = [f_1(t), f_2(t), \cdots, f_N(t)]$$

is the vector column of the force functions supposed continuous in the interval (a, b).

As is well known, the solution of the system (2) can be expressed by formula

$$\bar{x}(t) = X(t)\,\bar{C} + \int_a^t X(t)\,[(X(\tau)]^{-1}\,\bar{F}(\tau)\,d\tau \tag{3}$$

where $\bar{C}$ represents the vector column $x(a)$ of the initial conditions, and $X(t)$ is the solution of the matrix linear homogeneous differential equation:

$$\frac{dX(t)}{dt} = P(t)\, X(t). \tag{4}$$

The integral matrix $X(t)$ is uniquely determined if we assign the value $X(t_0) = X_0$ (where X_0 is a non singular square matrix of order N) in correspondence to a value $t = t_0$, in the interval of definition. In the particular case, where $X_0 = I$, with I a unitary matrix of order N, the integral matrix $X(t)$ is normalized and is often called the matrizant of the system (4).

The solution of the system of differential equations (1) is, in this manner, related to the solution of the matrix differential equation (4) with initial conditions $X(a) = I$.

NUMERICAL SOLUTION OF THE TRANSITION MATRIX AND ITS POWER SERIES EXPANSION.

The solution of the matrix differential equation (4) can be obtained numerically with a step-by-step integration method.

In fact, we can substitute for equation (4) the equivalent system of linear differential equations of the first order:

$$\frac{dX_{i,j}(t)}{dt} = \sum_{l=1}^{N} P_{i,l}(t)\, X_{l,j}(t) \tag{5}$$

with $i = 1, 2, \cdots, N$; $j = 1, 2, \cdots, N$; where $X_{i,j}(t)$ is the generic component of the integral matrix $X(t)$ and where the initial conditions are expressed by:

$$X_{i,j}(a) = 1 \qquad \text{for} \quad i = j$$

$$X_{i,j}(a) = 0 \qquad \text{for} \quad i \neq j$$

There are some cases for which, in order to determine the integral matrix $X(t)$, we have to adopt very laborious formulas of numerical integration, or, at least, to assume a sufficiently small integration step. In both cases the resulting calculation time is particularly high. This disadvantage becomes particularly manifest, when the knowledge of the integral matrix $X(t)$ is not required in the whole interval of definition, but only for some values of t.

It is possible to avoid these disadvantages if the integral matrix $X(t)$ is expressed in a proper analytical form, for example by means of a suitable power series expansion.

To make this possible it is necessary for the matrix of the coefficients $P(t)$ in its turn to be expandable in power series. This condition is almost always true in the study of problems of practical interest.

That is:

$$P(t) = P_0 + P_1(t-a) + P_2(t-a)^2 + \cdots + P_k(t-a)^k + \cdots = \sum_{k=0}^{\infty} P_k(t-a)^k \tag{6}$$

for: $a \leq t \leq b$.

Expanding the integral matrix $X(t)$ in a power series, we obtain:

$$X(t) = A_0 + A_1(t-a) + A_2(t-a)^2 + \cdots + A_l(t-a)^l + \cdots = \sum_{l=0}^{\infty} A_l(t-a)^l \tag{7}$$

with: $A_0 = I$ for: $a \leq t \leq b$.

The convergence of the series (7) is assured by the existence of a dominating series converging in the interval considered (1).

DESCRIPTION AND DISCUSSION OF THE CALCULUS ALGORITHM SUGGESTED.

Differentiating equation (7), we obtain:

$$\frac{dX(t)}{dt} = A_1 + 2A_2(t-a) + \cdots + lA_l(t-a)^{l-1} + \cdots = \sum_{l=1}^{\infty} lA_l(t-a)^{l-1}. \tag{8}$$

The matrix differential equation:

$$\frac{dX(t)}{dt} = P(t)\,X(t)$$

upon substituting for $P(t)$, $X(t)$ and $\frac{dX(t)}{dt}$ respectively from equations (6), (7) and (8), becomes:

$$\begin{aligned} A_1 + 2A_2(t-a) + \cdots + lA_l(t-a)^{l-1} + \cdots = \\ = (P_0 + P_1(t-a) + \cdots + P_k(t-a)^k + \cdots) \\ (A_0 + A_1(t-a) + A_2(t-a)^2 + \cdots + A_l(t-a)^l + \cdots) \end{aligned} \tag{9}$$

from which, we obtain:

$$\begin{aligned} A_1 + 2A_2(t-a) + \cdots + lA_l(t-a)^{l-1} + \cdots = P_0A_0 + \\ + (P_0A_1 + P_1A_0)(t-a) + (P_0A_2 + P_1A_1 + P_2A_0)(t-a)^2 + \\ + \cdots + (P_0A_l + P_1A_{l-1} + \cdots + P_lA_0)(t-a)^l + \cdots \end{aligned} \tag{10}$$

From equation (10) we have:

$$\left\{\begin{aligned} A_1 &= P_0A_0 \\ A_2 &= \frac{1}{2}(P_0A_1 + P_1A_0) \\ A_3 &= \frac{1}{3}(P_0A_2 + P_1A_1 + P_2A_0) \\ &\cdots\cdots\cdots \\ A_l &= \frac{1}{l}(P_0A_{l-1} + P_1A_{l-2} + \cdots + P_{l-1}A_0). \\ &\cdots\cdots\cdots \end{aligned}\right. \tag{11}$$

(1) A demonstration of the existence and convergence of the dominating series is given, for instance, in F. R. GANTMACHER, *Applications of the theory of matrices*.

Writing this in summation notation we have:

$$A_l = \frac{1}{l} \sum_{m=0}^{l-1} P_m A_{(l-1)-m} \tag{12}$$

for: $l \geq 1$ and with: $A_0 = I$.

The formula (12) of recurrent type allows one to obtain the coefficients of the series expansion (7), which represents an analytical solution of the matrix differential equation for each value of the independent variable in the interval (a, b).

From a computational point of view, the application of the above-mentioned method obliges one to define a criterion according to which the series expansions (6) and (7) can be terminated.

This criterion is determined according to the desired precision during the calculation.

If we denote as M and L, respectively, the number of terms of the series so obtained (equations (6) and (7)), we have:

$$P(t) = \sum_{k=0}^{M} P_k (t-a)^k \tag{13}$$

$$X(t) = \sum_{l=0}^{L} A_l (t-a)^l . \tag{14}$$

Consequently, the formula (12) becomes:

$$A_0 = I$$

$$A_l = \frac{1}{l} \sum_{m=0}^{l-1} P_m A_{(l-1)-m} \qquad \text{for: } 1 \leq l \leq M+1$$

$$A_l = \frac{1}{l} \sum_{m=0}^{M} P_m A_{(l-1)-m} \qquad \text{for: } l \geq M+1$$

because:

$$P_m = 0 \qquad \text{for: } m > M$$

The advantages of this method of solution are manifest either concerning the attainable precision in the determination of $X(t)$, or concerning the calculation time.

With regard to the precision we must say that it is higher with the proposed method of solution, because it lacks the inherent error involved in the numerical integration methods and because, in the series expansion of the integral matrix $X(t)$, it is possible, as already said, to determine the number of terms, according to the desired accuracy.

With regard to the calculation time the advantages of the proposed method are particularly evident, if the integral matrix $X(t)$ has to be calculated only in correspondence with specific values of the independent variable.

In fact, if a value of t is defined in the interval (a, b), the corresponding value of the integral matrix $X(t)$ can be directly obtained from equation (14) as soon as the coefficients of the series expansion are known.

The advantages of the suggested algorithm are still more evident if the matrix elements of the coefficients $P(t)$ are of the polynomial type.

If the type of the matrix differential equation (4) and the size of the interval of integration (a, b) need the calculation of a high number of terms of the series (14), the convergence of this series can be accelerated, dividing the interval of integration into K subintervals and calculating the integral matrix $X(t)$ for each of them.

In fact, for a well-known property of the matrizant, we obtain:

$$X_a(t) = X_{t_0}(t)\, X_a(t_0)$$

where $X_a(t)$ and $X_{t_0}(t)$ represent the integral matrices calculated in t with respectively initial conditions:

$$X_a(a) = I \quad \text{and} \quad X_{t_0}(t_0) = I.$$

Numerical example.

Let us consider the matrix differential equation:

$$\frac{dX(t)}{dt} = P(t)\, X(t) \tag{16}$$

with: $0 \leq t \leq 2$ and $X(0) = I$
where:

$$P(t) = \begin{bmatrix} 2t^2 & \sin 3t & -\cos 2t \\ -t^3 & 2 + t^4 & -\sin 3t + \cos 2t \\ 1 & 2t & 3t^2 \end{bmatrix}. \tag{17}$$

Using a numerical integration method the equation (16) is transformed, as already seen into the system:

$$\frac{dX_{i,j}(t)}{dt} = \sum_{l=1}^{3} P_{i,l}(t)\, X_{l,j}(t) \tag{18}$$

with: $i = 1, 2, 3$; $j = 1, 2, 3$

$$\begin{cases} \dfrac{dX_{1,j}(t)}{dt} = 2t^2 X_{1,j}(t) + \sin 3t\, X_{2,j}(t) - \cos 2t\, X_{3,j}(t) \\ \dfrac{dX_{2,j}(t)}{dt} = -t^3 X_{1,j}(t) + (2 + t^4)\, X_{2,j}(t) - (\sin 3t - \cos 2t)\, X_{3,j}(t) \\ \dfrac{dX_{3,j}(t)}{dt} = X_{1,j}(t) + 2t\, X_{2,j}(t) + 3t^2 X_{3,j}(t) \end{cases} \tag{19}$$

with: $j = 1, 2, 3$.

Equs. (19) represent a system of 9 differential equations, which was solved with the Runge-Kutta 4 point method and with integration step $\Delta t = 0.005$.

The values of the components of the integral matrix X (t) in correspondence with $t = 0.5$; 1.0; 1.5 and 2.0 are shown in Table I.

Using the proposed method of solution, we first have to expand the matrix of coefficients P (t) according to:

$$(20)\quad P(t)=P_0+P_1(t-t_0)+P_2(t-t_0)^2+\cdots+P_k(t-t_0)^k+\cdots=\sum_{k=0}^{M} P_k(t-t_0)^k .$$

The calculation was executed dividing the interval of integration (0, 2) into two sub-intervals (0, 1) and (1, 2).

Denoting generically as t_0 the initial value of each of the two sub-intervals, we obtain:

$$P_0 = \begin{bmatrix} 2t_0^2 & \sin 3t_0 & -\cos 2t_0 \\ -t_0^3 & 2+t_0^4 & -\sin 3t_0+\cos 2t_0 \\ 1 & 2t_0 & 3t_0^2 \end{bmatrix}$$

$$P_1 = \begin{bmatrix} 4t_0 & 3\cos 3t_0 & 2\sin 2t_0 \\ -3t_0^2 & 4t_0^3 & -3\cos 3t_0-2\sin 2t_0 \\ 0 & 2 & 6t_0 \end{bmatrix}$$

$$P_2 = \begin{bmatrix} 2 & -4.5\sin 3t_0 & 2\cos 2t_0 \\ -3t_0 & 6t_0^2 & 4.5\sin 3t_0-2\cos 2t_0 \\ 0 & 0 & 3 \end{bmatrix}$$

$$P_3 = \begin{bmatrix} 0 & -4.5\cos 3t_0 & -\frac{4}{3}\sin 2t_0 \\ -1 & 4t_0 & 4.5\cos 3t_0+\frac{4}{3}\sin 2t_0 \\ 0 & 0 & 0 \end{bmatrix}$$

$$P_4 = \begin{bmatrix} 0 & \frac{27}{8}\sin 3t_0 & -\frac{2}{3}\cos 2t_0 \\ 0 & 1 & -\frac{27}{8}\sin 3t_0+\frac{2}{3}\cos 2t_0 \\ 0 & 0 & 0 \end{bmatrix}$$

For $l \geq 5$, we get:

$$\left.\begin{aligned} P_{li,j} = 0 \text{ except: } P_{l1,2} &= \frac{3^l}{l!}\sin 3t_0(-1)^{l/2} \\ P_{l1,3} &= -\frac{2^l}{l!}\cos 2t_0(-1)^{l/2} \end{aligned}\right\} \text{for } l \text{ even}$$

$$\left.\begin{aligned} P_{l1,2} &= \frac{3^l}{l!}\cos 3t_0(-1)^{(l-1)/2} \\ P_{l1,3} &= \frac{2^l}{l!}\sin 2t_0(-1)^{(l-1)/2} \end{aligned}\right\} \text{for } l \text{ odd}$$

$$P_{l2,3} = -P_{l1,2} - P_{l1,3} .$$

Imposing that, for the values $t = 1$ and $t = 2$, the series expansion of $P(t)$ is calculated correct to seven decimal places we obtain: $M = 15$.

Then, we calculate the coefficients A_l with the:

$$(21) \quad \begin{cases} A_0 = I \\ A_l = \frac{1}{l} \sum_{m=0}^{l-1} P_m A_{(l-1)-m} & \text{for} \quad 1 \leq l \leq 16 \\ A_l = \frac{1}{l} \sum_{m=0}^{15} P_m A_{(l-1)-m} & \text{for} \quad l \geq 16 \end{cases}$$

The coefficients A_l are calculated respectively in the intervals $(0, 1)$ and $(1, 2)$, so that the integral matrix $X(t)$ can be obtained correct to six decimal places.

The values of $X(t)$ corresponding to: $t = 0.5$; 1.0; 1.5 and 2.0 are shown in Table I.

The necessary calculation time to obtain the coefficients A_l with the imposed precision, and to calculate the matrix $X(t)$ in correspondence with the above-noted values of t, is about a quarter of the time employed to solve the (19) differential equations system, using the 4 point R.K. method and an integration step $\Delta t = 0.005$.

As there is not an analytical expression for the matrix $X(t)$, we assume, as comparison values for the two methods, the results obtained using the series expansion method and making the calculation in double precision, correct to twelve decimal places.

In order to justify the validity of this double-precision solution, we use the identity of Jacobi, which allows one to obtain an analytical expression of the determinant associated with the matrix $X(t)$.

In fact, we have:

$$(22) \qquad |X(t)| = e^{\int_a^t t_r(P(s))\,ds}$$

where, as known:

$$(23) \qquad t_r(P(s)) = P_{1,1}(s) + P_{2,2}(s) + \cdots + P_{N,N}(s)$$

is the trace of the matrix $P(s)$.

In the said example, we have:

$$t_r(P(s)) = s^4 + 5s^2 + 2 .$$

The analytical expression of the determinant is:

$$(24) \qquad |X(t)| = e^{\int_0^t (s^4+5s^2+2)\,ds} = e^{\frac{s^5}{5} + \frac{5}{3}s^3 + 2s} .$$

The determinant values obtained from eqn. (24) correspond, up to the twelve decimal places, to those ones obtained with the double-precision solution.

TABLE I.

	T = 0.5				
	b	*a*	*c*	*b–c*	*a–c*
$X_{1,1}$	0.987212	0.987212	0.987212	0	0
$X_{1,2}$	0.573054	0.573053	0.573054	0	1
$X_{1,3}$	—0.377566	—0.377566	—0.377566	0	0
$X_{2,1}$	— .00995921	— .00995922	— .00995921	0	1
$X_{2,2}$	2.71327	2.71327	2.71327	0	0
$X_{2,3}$	0.302265	0.302265	0.302265	0	0
$X_{3,1}$	0.544867	0.544867	0.544867	0	0
$X_{3,2}$	0.628920	0.628919	0.628920	0	1
$X_{3,3}$	1.08096	1.08096	1.08096	0	0

	T = 1.0				
	b	*a*	*c*	*b–c*	*a–c*
$X_{1,1}$	1.64553	1.64553	1.64553	0	0
$X_{1,2}$	3.28498	3.28497	3.28498	0	1
$X_{1,3}$	—0.559714	—0.559713	—0.559714	0	1
$X_{2,1}$	—1.11198	—1.11198	—1.11198	0	0
$X_{2,2}$	6.70245	6.70247	6.70245	0	2
$X_{2,3}$	0.278916	0.278916	0.278916	0	0
$X_{3,1}$	1.89028	1.89028	1.89028	0	0
$X_{3,2}$	8.26981	8.26978	8.26981	0	3
$X_{3,3}$	2.56151	2.56150	2.56151	0	1

	T = 1.5				
	b	*a*	*c*	*b–c*	*a–c*
$X_{1,1}$	15.8443	15.8443	15.8443	0	0
$X_{1,2}$	46.3806	46.3803	46.3806	0	3
$X_{1,3}$	4.59114	4.59110	4.59114	0	4
$X_{2,1}$	—29.7642	—29.7641	—29.7642	0	1
$X_{2,2}$	13.7256	13.7256	13.7256	0	0
$X_{2,3}$	— 0.869120	— 0.869077	— 0.869120	0	43
$X_{3,1}$	3.25616	3.25614	3.25616	0	2
$X_{3,2}$	162.333	162.332	162.333	0	1
$X_{3,3}$	28.6089	28.6088	28.6089	0	1

	T = 2.0				
	b	*a*	*c*	*b–c*	*a–c*
$X_{1,1}$	608.326	608.322	608.326	0	4
$X_{1,2}$	5215.12	5215.08	5215.12	0	4
$X_{1,3}$	809.925	809.919	809.925	0	6
$X_{2,1}$	—18466.9	—18466.8	—18466.9	0	1
$X_{2,2}$	—31205.5	—31205.2	—31205.5	0	3
$X_{2,3}$	— 5366.64	— 5366.57	— 5366.64	0	7
$X_{3,1}$	—12431.7	—12431.6	—12431.7	0	1
$X_{3,2}$	4332.16	4332.17	4332.16	0	1
$X_{3,3}$	481.174	481.191	481.174	0	17

In Table I, we have listed with a, b, and c respectively, the values of $X(t)$ obtained with the R.K. method and with the series expansion in single and double precision.

We have also listed the differences $(a - c)$ and $(b - c)$ referred to six significant places.

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