Computer Physics Communications ▮ (▮▮▮▮) ▮▮▮–▮▮▮

Contents lists available at ScienceDirect

Computer Physics Communications

journal homepage: www.elsevier.com/locate/cpc

Decay chain differential equations: Solutions through matrix analysis

Edmond Levy

Stanmore, Middlesex, UK

ARTICLE INFO

Article history:
Received 9 March 2018
Accepted 16 July 2018
Available online xxxx

Keywords:
Radioactivity
Decay chain equations
Matrix exponential
Triangular matrix
Divided differences

ABSTRACT

This paper demonstrates how the solutions to conventional radioactive decay equations can be derived using results from matrix analysis. In particular, we draw on results for the matrix exponential function when the matrix is triangular. By applying key theorems, the paper explains how the solutions to these equations can be presented in algorithmic form and in terms of divided differences of the exponential function. Furthermore, with little additional effort, the approach yields solutions to more general variations of these equations.

1. Introduction

The production rates of a network of nuclides undergoing spontaneous decay is described by the simultaneous linear differential equation system introduced by Bateman [1]. When nuclear reactions are induced in a neutron flux, Rubinson [2] provided a modification to include transformation by neutron absorption in addition to spontaneous decay. Although this model and its solution are well known through applying the methods of Laplace transforms, integrating factors or matrix algebra, this paper shows that there is much to be gained by taking an alternative, and perhaps more natural, approach using the matrix exponential function.

Following a description of the decay chain differential equations we introduce the matrix exponential function. The subsequent sections demonstrate the easy discovery of the Bateman solution and how important extensions to the basic model may be evaluated using this approach.

2. The decay chain equations

We begin with the description of the basic model as presented by Amaku et al. [3]. A serial decay chain of n nuclides is one where the ith nuclide of the chain decays to the $(i+1)$th nuclide of the chain. We denote the quantity of the ith nuclide at time t by $N_i(t)$ and its decay constant by λ_i (sec^{-1}). If we allow for nuclei immersed in a constant neutron flux ϕ (neutrons cm^{-2} sec^{-1}) and total neutron reaction cross section σ_i (cm^2) for the ith nuclide, then the differential equation system may be written as

$$
\begin{aligned}
N_1'(t) &= -\kappa_1 N_1(t)\\
N_2'(t) &= \lambda_1 N_1(t) - \kappa_2 N_2(t)\\
N_3'(t) &= \lambda_2 N_2(t) - \kappa_3 N_3(t)\\
&\ \ \vdots\\
N_n'(t) &= \lambda_{n-1} N_{n-1}(t) - \kappa_n N_n(t),
\end{aligned}
\tag{1}
$$

where $N_i'(t) = dN_i(t)/dt$ and $\kappa_i = \lambda_i + \phi\sigma_i$ being the ith modified decay constant. The initial conditions at $t = 0$ are $N_i(0) = N_{i0}$ for $i = 1, \dots, n$. If we define branching ratios, r_{ij}, from the jth nuclide to the ith nuclide (for $j = 1, \dots, n-1$ and $i = j+1, \dots, n$) and denote partial decay constants by $b_{ij} = r_{ij}\lambda_j$ (with $\sum_{i=j+1}^{n} r_{ij} = 1$), the system (1) is then extended as

$$
\begin{aligned}
N_1'(t) &= -\kappa_1 N_1(t)\\
N_2'(t) &= b_{21} N_1(t) - \kappa_2 N_2(t)\\
N_3'(t) &= b_{31} N_1(t) + b_{32} N_2(t) - \kappa_3 N_3(t)\\
&\ \ \vdots\\
N_n'(t) &= b_{n1} N_1(t) + b_{n2} N_2(t) + \cdots + b_{n,n-1} N_{n-1}(t) - \kappa_n N_n(t).
\end{aligned}
\tag{2}
$$

In matrix form, the equations in (2) can be written as

$$
\begin{bmatrix} N_1'(t)\\ N_2'(t)\\ N_3'(t)\\ \vdots\\ N_n'(t) \end{bmatrix}
=
\begin{bmatrix}
-\kappa_1 & 0 & 0 & \dots & 0\\
b_{21} & -\kappa_2 & 0 & \dots & 0\\
b_{31} & b_{32} & -\kappa_3 & & 0\\
\vdots & \vdots & & & \\
b_{n1} & b_{n2} & b_{n3} & \dots b_{n,n-1} & -\kappa_n
\end{bmatrix}
$$

E-mail address: e_levy@sky.com.

https://doi.org/10.1016/j.cpc.2018.07.011

$$\times \begin{bmatrix} N_1(t) \\ N_2(t) \\ N_3(t) \\ \vdots \\ N_n(t) \end{bmatrix}$$

or, with obvious notation, the differential equation system

$$\mathbf{N}'(t) = \mathbf{A}\mathbf{N}(t). \tag{3}$$

We denote the system's initial conditions at $t = 0$ by $\mathbf{N}_0 = (N_{10}, N_{20}, \ldots, N_{n0})^T$. (Throughout this paper, $\mathbf{x}^T$ denotes the transpose of $\mathbf{x}$).

Pressyanov [4] provides a good description of the Laplace transform approach to solving Eq. (1). Moral and Pacheco [5] and Amaku et al. [3] provide the steps needed to apply the conventional matrix algebra approach to solving, respectively, (1) and (3). In the following sections we apply instead the matrix exponential function and demonstrate how the approach lends itself to other specifications of this decay chain model.

3. The matrix exponential function

Apostol [6] provides a helpful introduction to the development of the matrix exponential function and its use in solving systems of differential equations with constant coefficients.

For a real number t and fixed $n \times n$ matrix $\mathbf{A}$, with typical element a_{ij}, let $\mathbf{S}_m(t)$ denote the partial sum

$$\mathbf{S}_m(t) = \mathbf{I} + \mathbf{A}t + \frac{1}{2!}\mathbf{A}^2t^2 + \frac{1}{3!}\mathbf{A}^3t^3 + \cdots + \frac{1}{m!}\mathbf{A}^mt^m.$$

Then, subject to a suitable definition for the *norm* of a matrix, e.g. $\|\mathbf{A}\| = \sum_{i,j}|a_{ij}|$, it can be shown (see [6], Sec. 7.5) that the sequence of matrices $\{\mathbf{S}_1(t), \mathbf{S}_2(t), \ldots\}$ has a limit for all t and all fixed $\mathbf{A}$. We define the limit of the sequence $\{\mathbf{S}_1(t), \mathbf{S}_2(t), \ldots\}$ to be $e^{\mathbf{A}t}$. That is:

$$e^{\mathbf{A}t} = \sum_{k=0}^{\infty} \frac{1}{k!}\mathbf{A}^kt^k. \tag{4}$$

We state a few properties and consequences which are easily established and will help with the exposition later in the paper:

- $e^{\mathbf{A}0} = \mathbf{I}$, since $\mathbf{A}0 = \mathbf{0}$.
- Differentiating (4) with respect to t (term by term), we have
$$\begin{aligned} \frac{de^{\mathbf{A}t}}{dt} &= \frac{d}{dt}\sum_{k=0}^{\infty}\frac{1}{k!}\mathbf{A}^kt^k = \sum_{k=1}^{\infty}\frac{1}{(k-1)!}\mathbf{A}^kt^{k-1} \\ &= \mathbf{A}\sum_{j=0}^{\infty}\frac{1}{j!}\mathbf{A}^jt^j = \mathbf{A}e^{\mathbf{A}t}. \end{aligned}$$
- If $\mathbf{A}$ is a lower triangular matrix then $\mathbf{A}^k$ must also be a lower triangular matrix (since the product of two lower triangular matrices is itself a lower triangular matrix) and it follows that $e^{\mathbf{A}t}$ will be lower triangular.
- If $\mathbf{A}$ is a lower triangular matrix with ith diagonal entry α_i then $\mathbf{A}^k$ has ith diagonal entry α_i^k and it follows that $e^{\mathbf{A}t}$ will have ith diagonal element $e^{\alpha_i t}$.
- Let $\mathbf{F} = e^{\mathbf{A}t}$, then $\mathbf{A}$ and $\mathbf{F}$ commute (i.e., $\mathbf{AF} = \mathbf{FA}$), since $\mathbf{A}^k$ and $\mathbf{A}$ commute.
- If matrices $\mathbf{A}$ and $\mathbf{B}$ (both of order n) commute then $e^{\mathbf{A}t}e^{\mathbf{B}t} = e^{(\mathbf{A}+\mathbf{B})t}$. To see this, expand both sides of this equation using (4) and equate terms in t^k. (See also [6], Sec. 7.8.)
- It follows, since $\mathbf{A}t$ and $\mathbf{A}s$ commute, that $e^{\mathbf{A}t}e^{\mathbf{A}s} = e^{\mathbf{A}(t+s)}$ and setting $s = -t$ we have $e^{\mathbf{A}t}e^{-\mathbf{A}t} = e^{\mathbf{A}0} = \mathbf{I}$ and so $e^{-\mathbf{A}t}$ is the inverse of $e^{\mathbf{A}t}$.

4. Solving the decay equations

In this section, we use the matrix exponential function to solve the system (3) and exploit its triangular form. We show how an explicit expression for the general solution can be derived in an economic manner. An earlier paper that applied this approach is Attaya [7].

As (3) is a homogeneous system with constant coefficients, we may write the unique solution to (3) as

$$\mathbf{N}(t) = e^{\mathbf{A}t}\mathbf{N}_0. \tag{5}$$

(See [6], Theorem 7.7.) Differentiating (5) with respect to t gives $\mathbf{N}'(t) = \mathbf{AN}(t)$ and noting (5) yields $\mathbf{N}(0) = \mathbf{N}_0$ at $t = 0$ confirms (5) as a solution to (3).

Although (5) provides an explicit formula, there still remains the problem of actually computing the entries for the exponential matrix $e^{\mathbf{A}t}$. Moler and Van Loan [8] assess the many approaches to performing this calculation for a general fixed matrix $\mathbf{A}$ and is an excellent review of the potential practical difficulties. Here, we will exploit the advantages provided by the triangular form of the matrix $\mathbf{A}$ in our case.

Denoting $\mathbf{F} = e^{\mathbf{A}t}$ and to have typical element f_{ij}, then we know, as $\mathbf{F}$ is lower triangular, $f_{ij} = 0$ for $i < j$. We can therefore represent the solution for (3) as:

$$\begin{bmatrix} N_1(t) \\ N_2(t) \\ N_3(t) \\ \vdots \\ N_n(t) \end{bmatrix} = \begin{bmatrix} f_{11} & 0 & 0 & \ldots & 0 & 0 \\ f_{21} & f_{22} & 0 & \ldots & 0 & 0 \\ f_{31} & f_{32} & f_{33} & & & 0 \\ \vdots & \vdots & \ddots & & \ddots & \\ f_{n1} & f_{n2} & f_{n3} & \ldots & f_{n,n-1} & f_{nn} \end{bmatrix} \begin{bmatrix} N_{10} \\ N_{20} \\ N_{30} \\ \vdots \\ N_{n0} \end{bmatrix}.$$

We have that $\{-\kappa_1, \ldots, -\kappa_n\}$ are the diagonal entries for $\mathbf{A}$. Consequently, the diagonal entries for $\mathbf{F}$ are $f_{ii} = e^{-\kappa_i t}$ for $i = 1, \ldots, n$. Furthermore, as $\mathbf{A}$ and $\mathbf{F}$ commute, $\mathbf{AF} = \mathbf{FA}$. This matrix equation provides us with sufficient information to solve for the remaining f_{ij} entries. For instance, the first subdiagonal entries of each side of $\mathbf{AF} = \mathbf{FA}$ give

$$b_{i,i-1}f_{i-1,i-1} - \kappa_i f_{i,i-1} = b_{i,i-1}f_{ii} - \kappa_{i-1}f_{i,i-1} \quad (i = 2, \ldots, n)$$

yielding

$$f_{i,i-1} = \frac{b_{i,i-1}(f_{ii} - f_{i-1,i-1})}{\kappa_{i-1} - \kappa_i} \quad (i = 2, \ldots, n).$$

Moving down to the next subdiagonal, we have

$$\begin{aligned} &b_{i,i-2}f_{i-2,i-2} + b_{i,i-1}f_{i-1,i-2} - \kappa_i f_{i,i-2} \\ &\quad = b_{i,i-2}f_{ii} + b_{i-1,i-2}f_{i,i-1} - \kappa_{i-2}f_{i,i-2} \quad (i = 3, \ldots, n) \end{aligned}$$

or

$$f_{i,i-2} = \frac{b_{i,i-2}(f_{ii} - f_{i-2,i-2})}{\kappa_{i-2} - \kappa_i} + \frac{f_{i,i-1}b_{i-1,i-2} - b_{i,i-1}f_{i-1,i-2}}{\kappa_{i-2} - \kappa_i}$$
$$(i = 3, \ldots, n).$$

Moving down once more, we have

$$\begin{aligned} &b_{i,i-3}f_{i-3,i-3} + b_{i,i-2}f_{i-2,i-3} + b_{i,i-1}f_{i-1,i-3} - \kappa_i f_{i,i-3} = \\ &\qquad b_{i-2,i-3}f_{i,i-2} + b_{i-1,i-3}f_{i,i-1} + b_{i,i-3}f_{ii} - \kappa_{i-3}f_{i,i-3} \\ &\qquad (i = 4, \ldots, n) \end{aligned}$$

or

$$\begin{aligned} f_{i,i-3} = &\frac{b_{i,i-3}(f_{ii} - f_{i-3,i-3})}{\kappa_{i-3} - \kappa_i} + \frac{f_{i,i-2}b_{i-2,i-3} - b_{i,i-2}f_{i-2,i-3}}{\kappa_{i-3} - \kappa_i} \\ &+ \frac{f_{i,i-1}b_{i-1,i-3} - b_{i,i-1}f_{i-1,i-3}}{\kappa_{i-3} - \kappa_i} \\ &(i = 4, \ldots, n) \end{aligned}$$

…and so on.

Please cite this article in press as: E. Levy, Decay chain differential equations: Solutions through matrix analysis, Computer Physics Communications (2018), https://doi.org/10.1016/j.cpc.2018.07.011.