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Power law approximations for radioactive decay chains

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ABSTRACT

Consider a radioactive decay chain $X_1 \to \cdots \to X_n \to$ and let $N_n(t)$ be the amount of X_n at time t. This paper establishes error bounds for small and intermediate time approximations to $N_n(t)$ including the power-law approximation $N_n(t) \approx Ct^{m-1}$ for $\tau_{m+1} << t << \tau_m$ where τ_j is the j^{th} largest half-life. The approximations shed light on the qualitative behavior of $N_n(t)$ and are useful for reducing the roundoff error when computing $N_n(t)$ for small t which is a problem with the usual formula. The error bounds allow one to find the range of t for which these approximations can be used with a given degree of precision.

1. Introduction

This paper is concerned with radioactive decay chains $X_1 \to X_2 \to \cdots \to X_n \to$ where a fraction b_j of the nuclide X_j decays into X_{j+1} with decay constant λ_j and half-life $T_j = ln(2)/\lambda_j$. The remaining fraction $1 - b_j$ of X_j decays with the same decay constant λ_j into a nuclide other than X_{j+1}. If X_n is stable then $\lambda_n = 0$. Let $N_j(t)$ be that portion of the amount of X_j present at time t that has been produced by decays following the chain. The $N_j(t)$ satisfy the radioactive decay equations [1, p. 172]:

$$\begin{aligned} dN_1/dt &= -\lambda_1 N_1 \\ dN_j/dt &= b_{j-1}\lambda_{j-1}N_{j-1} - \lambda_j N_j \text{ for } j \geqslant 2 \end{aligned} \tag{1}$$

If $N_j(0) = 0$ for $j \geqslant 2$ then $N_n(t)$ is given by

$$N_n(t) = N_1(0)a_n E_n(t; \lambda_1, \ldots, \lambda_n) \tag{2}$$

where

$$a_n = b_1 b_2 \cdots b_{n-1}\lambda_1\lambda_2\cdots\lambda_{n-1} \tag{3}$$

and the function $E_r(t; \alpha_1, \ldots, \alpha_r)$ is the convolution of exponential functions $e^{-\alpha_j t}$, i.e.

$$E_r(t; \alpha_1, \ldots, \alpha_r) = e^{-\alpha_1 t} * \cdots * e^{-\alpha_r t} \tag{4}$$

Here $*$ denotes convolution, i.e. $g(t) * h(t) = \int_0^t g(s)h(t-s)ds$ for $t \geqslant 0$. $E_r(t; \alpha_1, \ldots, \alpha_r)$ is a symmetric function of the α_j since convolution is commutative and associative. If the α_j are distinct, one has

$$E_r(t; \alpha_1, \ldots, \alpha_r) = \sum_{j=1}^{r} C_j e^{-\alpha_j t} \tag{5}$$

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$$C_j = \prod_{\substack{i=1 \\ i \neq j}}^{r} (\alpha_i - \alpha_j)^{-1} \tag{6}$$

The formula (2) coupled with (5) was originally established by Bateman [2] using Laplace transforms. Since then a number of other interesting derivations of (2) have been given [3–9]. When some of the α_j are equal, (5) is more complicated [10–12].

The approximations in this paper address two problems with (5). First, it is hard to see the behavior of $N_n(t)$ from (5) except for times on the order of the largest half-life. Second, round-off errors can be encountered when (5) is used to compute $N_n(t)$ for times t that are small compared to the largest half-life.

We begin by describing how the approximations in this paper fill in missing knowledge about $N_n(t)$. In doing this we look at three previously known properties of $N_n(t)$. The first of these is that $N_n(t)$ is a log-concave function, i.e. $\ln[N_n(t)]$ is a concave function. This is because the convolution of log-concave functions is again log-concave [13]. In particular, if $\lambda_n > 0$ then $N_n(t)$ increases from zero to a maximum and then decreases back down to zero as t goes from zero to infinity.

The second known property of $N_n(t)$ is that if t is small compared to all the half-lives $T_j = \ln(2)/\lambda_j$, then

$$N_n(t) \approx N_1(0) a_n \frac{t^{n-1}}{(n-1)!} \tag{7}$$

This approximation is used both in applications to radioactivity (see [14, p. 24] and [15, pp. 83, 87]) and reliability (see [4, p. 291]). The relative error in (7) is less than $\bar{\lambda} t$ where $\bar{\lambda}$ is the mean of $\lambda_1, \ldots, \lambda_n$, i.e.

$$\left| N_n(t) - N_1(0) a_n \frac{t^{n-1}}{(n-1)!} \right| \leqslant \bar{\lambda} t N_1(0) a_n \frac{t^{n-1}}{(n-1)!} \tag{8}$$

This inequality follows from the following upper and lower bound for $E_n(t) = E_n(t; \lambda_1, \ldots, \lambda_n)$

$$(1 - \bar{\lambda} t) \frac{t^{n-1}}{(n-1)!} \leqslant E_n(t) \leqslant \frac{t^{n-1}}{(n-1)!} \tag{9}$$

which is proved in [4, pp. 289–290]. It assumes the λ_j are non-negative and it implies $| E_n(t) - t^{n-1}/(n-1)! | \leqslant \bar{\lambda} t^n/(n-1)!$. Multiplying by $N_1(0) a_n$ proves (8). Thus, the relative error in (7) will be less than ε if $t < \varepsilon/\bar{\lambda}$ and (7) will be good if t is small compared to the half-lives of all of $X_1, \ldots, X_n$. Another small time approximation that usually holds for a larger range of values of t than (7) is the following.

Approximation 1. If t is small, then

$$N_n(t) \approx N_1(0) a_n \frac{t^{n-1} e^{-\bar{\lambda} t}}{(n-1)!} \tag{10}$$

We have not seen precisely this approximation in the literature, but there are similar ones. For example, [4, p. 291] considers the case $\lambda_n = 0$ and uses the mean of $\lambda_1, \ldots, \lambda_{n-1}$ instead of $\bar{\lambda}$ in the exponent. In [16, p. 12] an example is considered where $n = 2$ and λ_1 and λ_2 are close to together and which uses λ_2 instead of $\bar{\lambda}$ in the exponent; see Example 2 in Section 6. Theorem 1 in Section 2 has an error bound for Approximation 1 that shows that the smaller the variance of the λ_j is the larger the interval $t < t^*$ is for which (10) holds with a given degree of precision.

The third known property of $N_n(t)$ is its large time behavior. If $T_p = \ln(2)/\lambda_p$ is the largest half-life (where p is between 1 and n) and if t is large compared to all the half-lives except T_p, then (5) implies $N_n(t) \approx N_1(0) a_n C_p e^{-\lambda_p t}$. In [17, Theorem 3] this is extended as follows. Let $T_q = \ln(2)/\lambda_q$ be the second largest half-life and $\theta = \prod_{j \in J} (\lambda_j - \lambda_p)^{-1}$ where $J = \{j : 1 \leqslant j \leqslant n$ and $j \neq p, q\}$. If t is large compared to the third largest half life, then $N_n(t) \approx N_1(0) a_n \theta^{-1} E_2(t; \lambda_p, \lambda_q)$ where $E_2(t; \lambda_p, \lambda_q) = (e^{-\lambda_p t} - e^{-\lambda_q t})/(\lambda_q - \lambda_p)$. Implicit in this approximation is the fact that the value τ_n of t where $N_n(t)$ is a maximum is close to the value $\tau_2 = \ln(\lambda_q/\lambda_p)/(\lambda_q - \lambda_p)$ of t where $E_2(t; \lambda_p, \lambda_q)$ is maximum, i.e. one has

Approximation 2. If $\mu_2 \ll \mu_3$ then $\tau_n \approx \tau_2$.

Theorem 2 in Section 2 gives an error bound for this approximation. This approximation, along with the others in this paper, is illustrated in Example 1 in Section 6.

To summarize, the behavior of $N_n(t)$ for "small" t and "large" t and its log-concavity is known. The remaining approximations in this paper shed light on the behavior of $N_n(t)$ for values of t between small t and large t. To state these approximations we sort the decay constants λ_j and half-lives T_j in order. Let

$$\left.\begin{array}{l} \mu_1 \leqslant \mu_2 \leqslant \cdots \leqslant \mu_n \text{ be the values } \lambda_1, \ldots, \lambda_n \text{ arranged in increasing order} \\ S_1 \geqslant S_2 \geqslant \cdots \geqslant S_n \text{ be the values } T_1, \ldots, T_n \text{ arranged in decreasing order} \\ a_m = \frac{b_1 b_2 \cdots b_{n-1} \mu_1 \mu_2 \cdots \mu_m}{\lambda_n} \text{ with } \frac{\mu_1}{\lambda_n} \text{ replaced by one if } \lambda_n = 0 \\ E_n(t) = E_n(t; \lambda_1, \ldots, \lambda_n) = E_n(t; \mu_1, \ldots, \mu_n) \end{array}\right\} \tag{11}$$