Modeling Drug Concentrations

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Introduction The dosage and frequency are key parameters to select to safely and effectively administer a given drug. Given values for these two parameters, I have created two different implementations of an exponential-decay based simulation which models the concentrations of a particular drug remaining in a person's system.

Differences in two implementations Both of the two implementations I used involve analytic solutions for exponential decay. However, one implementation requires the step between the addition of each pill to be computed separately. The other implementation follows a formula to produce a sum of decays, one for the amount remaining in each pill, after a given amount of time. This implementation makes the assumption that the amount of each pill remaining in the body can be modeled separately.

Summation method Let Q be the concentration of a pill left in the body after a given amount of time t, k be the rate constant, and Q_0 be the initial concentration in the body. The formula that gives the decay of a single pill is then simply modeled by exponential decay

$$Q(t) = Q_0 \mathrm{e}^{-kt}$$

After a given amount of time, interval length I, a second pill will be added to the system, such that we have the concentration of drug in the body modeled the concentration left of the first pill plus that left of the second pill.

$$\begin{aligned} Q(t) &= Q_0 \mathrm{e}^{-kt} + Q_0 \mathrm{e}^{-k(t-I)} \\ &= Q_0 \mathrm{e}^{-kt}(1 + e^{kI}) \end{aligned}$$

One pill is added at $t = 0$ and an additional pill is added after every I length of time. So, let $N = \text{floor}(\frac{t}{I} + 1)$ be the total number of pills added after t time. Then, after an arbitrary amount of time, we have the following sum

$$\begin{aligned} Q(t) &= Q_0 \mathrm{e}^{-kt} + Q_0 \mathrm{e}^{-k(t-I)} + ... + Q_0 \mathrm{e}^{-k(t-nI)} \\ &= Q_0 \mathrm{e}^{-kt}(1 + \mathrm{e}^{kI} + ... + \mathrm{e}^{knI}) \\ &= Q_0 \mathrm{e}^{-kt} \sum_{n=0}^{N-1} \mathrm{e}^{knI} \end{aligned}$$

Given that t is finite, this sum may be simplified to the following expression

$$\begin{aligned} & Q_0 \mathrm{e}^{-kt} \sum_{n=0}^{N-1} \mathrm{e}^{knI} \\ = Q_0 \mathrm{e}^{-kt} & \frac{\mathrm{e}^{kIN} - 1}{\mathrm{e}^{kI} - 1} \end{aligned}$$

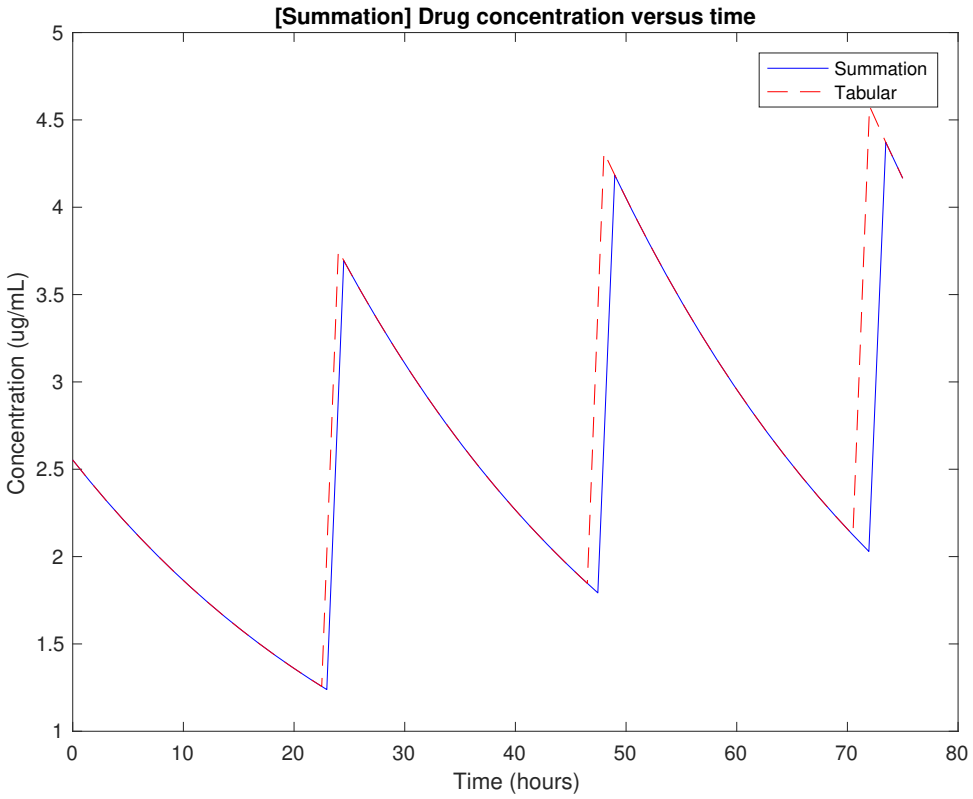

Figure 1: Comparison of two implementations with plotted with 50 points, with an interval of 24 hours, over a 75 hour period. The error on the discretized function builds as time goes on.

Tabular method The tabular method differs in that instead of having an explicit formula to give the concentration of drug remaining after t hours and after N pills have been added, we use a discretized method that relies on computing the amount remaining in steps that at largest must be smaller than the time interval after which each pill is added.

We use a piece-wise function to determine whether to add the concentration of another pill

$$f(t) = \begin{cases} 0 & t \mod I = 0 \\ 1 & \text{else} \end{cases}$$

Our formula is then

$$Q(t + \Delta t) = f(t + \Delta t)Q_0 + Q(t)\mathrm{e}^{-k\Delta t}$$

Comparison

	Summation method	Tabular method
Accuracy	precise	approximation
Exponent size	larger magnitude	smaller magnitude
Comp. time (graph)	O(n)	O(n)
Comp. time (point)	O(1)	O(n)
Comp. space	O(1)	O(n)
Restrictions on ΔT	none	$I \mod \Delta t = 0$