Lecture 8

Real Program Simulation: Drug Concentration

Course: Medical Simulation and Modeling

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1 Simulation in Medicine (Motivation)

Simulation is a powerful tool in medicine. Instead of experimenting directly on real patients which can be expensive, slow, or even dangerous we build a *mathematical model* of the system and run the experiment on a computer.

- In **pharmacokinetics**, simulation helps us study how a drug moves through the body (absorption, distribution, metabolism, and elimination).
- We can predict drug concentration in the blood, decide safe and effective doses, and understand what happens if the patient forgets a dose or takes an overdose.
- Simulation allows us to test many scenarios quickly before clinical trials.

In this lecture we focus on a simple but very important example: **decay of drug concentration in the blood after taking a pill**. We will

1. Describe the medical problem.
2. Build a mathematical model (continuous and discrete).
3. Implement the model in Python and visualize the result.

2 Problem Statement

A patient takes a pill at time $t = 0$. After swallowing the pill, the drug reaches the blood stream. We will assume the following:

- Initial drug concentration in blood at $t = 0$ is $C(0) = 100$ mg/L.
- The drug is eliminated by the body over time.
- Every hour, the concentration decreases by about 20%.

Goal: Build a mathematical and computational model to describe and simulate how the concentration $C(t)$ decreases over time.

3 Continuous-Time Mathematical Model

A common model for drug elimination assumes that the rate of change of concentration is proportional to the current concentration:

$$\frac{dC}{dt} = -k\,C(t), \tag{1}$$

where $k > 0$ is the elimination rate constant.

Solving the Differential Equation (Continuous Method)

Starting from (1):

$$\frac{dC}{dt} = -kC(t).$$

Separate the variables:

$$\frac{1}{C(t)}\,dC = -k\,dt.$$

Integrate both sides:

$$\int \frac{1}{C(t)}\,dC = -k\int dt.$$

This gives

$$\ln(C(t)) + c_1 = -kt + c_2.$$

We can combine the constants:

$$\ln(C(t)) = -kt + C',$$

where $C' = c_2 - c_1$.

Using the initial condition $t = 0$ and $C(0)$:

$$\ln(C(0)) = -k \cdot 0 + C' \quad \Rightarrow \quad C' = \ln(C(0)).$$

So

$$\ln(C(t)) = -kt + \ln(C(0)).$$

Apply the exponential function to both sides:

$$C(t) = \exp(\ln(C(t))) = \exp(-kt + \ln(C(0))) = C(0)\,e^{-kt}.$$

Thus the continuous solution is

$$C(t) = C(0)\,e^{-kt}. \tag{2}$$

This formula gives the concentration at any continuous time $t \geq 0$.

4 Discrete-Time Model (Simulation Friendly)

For computer simulation we often work with discrete time steps Δt. Assume $\Delta t = 1$ hour. Starting again from (1):

$$\frac{dC}{dt} = -kC(t).$$

Using a simple forward difference approximation:

$$\frac{C(t+\Delta t) - C(t)}{\Delta t} \approx -kC(t).$$

For $\Delta t = 1$ hour this becomes

$$C(t+1) - C(t) = -kC(t).$$

Hence

$$C(t+1) = C(t)(1-k).$$

If we know that the drug decreases by 20% each hour, then

$$1 - k = 0.8 \quad \Rightarrow \quad k = 0.2.$$

So the discrete model becomes

$$C(t+1) = 0.8\, C(t), \tag{3}$$

with initial condition $C(0) = 100$ mg/L.

Manual Computation (First Few Hours)

$$\begin{aligned}
&C(0) = 100.00 \text{ mg/L},\\
&C(1) = 0.8 \times 100.00 = 80.00 \text{ mg/L},\\
&C(2) = 0.8 \times 80.00 = 64.00 \text{ mg/L},\\
&C(3) = 0.8 \times 64.00 = 51.20 \text{ mg/L},\\
&C(4) = 0.8 \times 51.20 = 40.96 \text{ mg/L},\\
&C(5) = 0.8 \times 40.96 = 32.77 \text{ mg/L (approx.)}.
\end{aligned}$$

Simulation Table

This table shows exactly what the computer will compute in the Python simulation.

Table 1: Discrete simulation of drug concentration over time.

Time (hours)	Concentration (mg/L)
0	100.00
1	80.00
2	64.00
3	51.20
4	40.96
5	32.77

5 Python Code (Discrete Simulation)

We now translate the discrete model (3) into Python code and visualize the concentration over time.

Listing 1: Python code for discrete drug concentration simulation.

```
import numpy as np
import matplotlib.pyplot as plt

# Time steps: 0, 1, 2, 3, 4, 5 hours
time = np.arange(0, 6, 1)

# Initial concentration C(0) = 100 mg/L
C = [100.0]

# Discrete model: C(t+1) = 0.8 * C(t)
for t in range(1, len(time)):
    C.append(0.8 * C[-1])

# Plot the result
plt.plot(time, C,
         marker='o',
         linestyle='-',
         label='Drug Concentration')

plt.xlabel('Time (hours)')
plt.ylabel('Concentration (mg/L)')
plt.title('Simple Drug Concentration Decay Over Time')
plt.grid(True)
plt.legend()
plt.tight_layout()
plt.savefig('fig.png', dpi=300)  # save the figure
plt.show()
```

The script computes the concentration at each integer hour and plots it. The saved plot is shown in Figure 1.

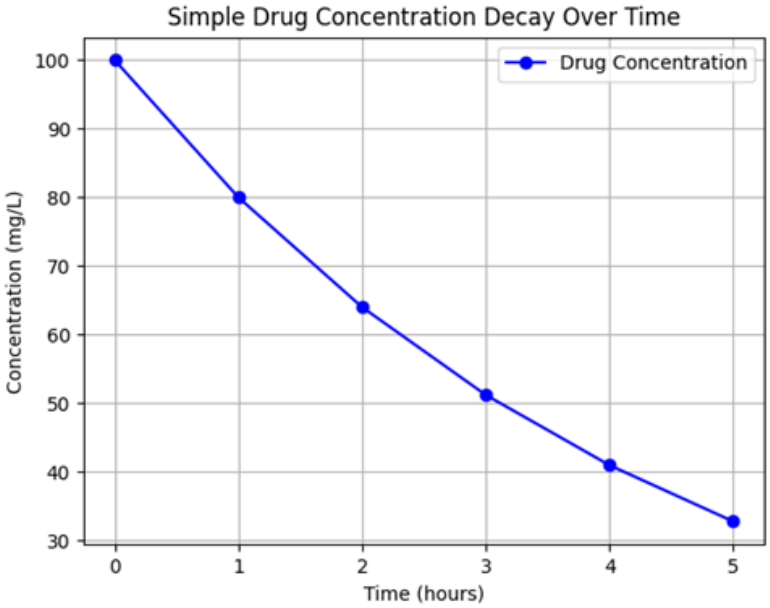

Figure 1: Simple drug concentration decay over time (discrete simulation).

6 Discussion and Medical Interpretation

From the simulation and Figure 1 we observe:

- The drug concentration decreases exponentially with time.
- After 5 hours, the concentration is roughly one third of the initial value.
- If there is a *therapeutic window* (safe and effective range), such a model helps clinicians decide the correct dosing interval.

This simple example illustrates the full workflow of medical simulation:

1. Start from a real medical problem (drug elimination in a patient).
2. Build a mathematical model (differential equation).
3. Derive a computationally convenient discrete form.
4. Implement the model in Python and visualize the results.

More advanced models can include absorption, multiple compartments, patient-specific parameters, or random variability (stochastic models), but the fundamental idea of simulation remains the same.