



Digital version

CS226 Math Modeling Applications - Homework 1

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Problem 1 (15 points).

We start with N bacteria in a controlled environment with infinite food to grow. Each small time step Δt there is a small probability $\gamma \Delta t$ for each bacteria to double (assume that each doubling is an independent process)

- (a) Derive the discrete time master equation of exponential growth. (5 points)

$$w_{M-1 \rightarrow M} = \mathcal{P}(M|M-1; \Delta t) = (M-1)\gamma \Delta t$$

$$P_M(t + \Delta t) = P_M(t) \cdot (1 - M\gamma \Delta t) + (P_{M-1}(t) \cdot (M-1)\gamma \Delta t - P_{M+1}(t) \cdot 0)$$

$$\therefore P_M(t + \Delta t) = P_M(t) \cdot (1 - M\gamma \Delta t) + P_{M-1}(t) \cdot (M-1)\gamma \Delta t$$

- (b) Derive the continuous time master equation of exponential growth. (5 points)

$$P_M(t + \Delta t) - P_M(t) = P_M(t) \cdot (-M\gamma \Delta t) + P_{M-1}(t) \cdot (M-1)\gamma \Delta t$$

$$\frac{P_M(t + \Delta t) - P_M(t)}{\Delta t} = P_M(t) \cdot (-M\gamma) + P_{M-1}(t) \cdot (M-1)\gamma$$

$$\therefore \dot{P}_M(t) = -M\gamma P_M(t) + (M-1)\gamma P_{M-1}(t)$$

- (c) What is the equation of the average number of bacteria depending on time? (5 points)

$$n(t) = \sum_{M=N}^{\infty} M P_M(t)$$

$$\dot{n}(t) = \sum_{M=N}^{\infty} M \dot{P}_M(t) = \sum_{M=N}^{\infty} M(-M\gamma P_M(t) + (M-1)\gamma P_{M-1}(t))$$

$$= \sum_{M=N}^{\infty} M((M-1)\gamma P_{M-1}(t) - M\gamma P_M(t)) = \gamma \sum_{M=N}^{\infty} (M-1)M P_{M-1}(t) - M^2 P_M(t)$$

$$= \gamma \left(\sum_{M=N-1}^{\infty} M(M+1)P_M(t) - \sum_{M=N}^{\infty} M^2 P_M(t) \right) = \gamma \sum_{M=N}^{\infty} M P_M(t) = \gamma n(t)$$

$$n(t) = \alpha e^{\gamma t}, \alpha \in \mathbb{R}$$

Problem 2 (30 points).

Change from the previous problem the probability for each bacteria to double. Instead of $\gamma\Delta t$ take $\gamma(1 - \beta M)\Delta t$ where M is the amount of bacteria currently in the system.

- (a) Derive the discrete time master equation (5 points)

Same as last problem, except take the probability of doubling as $\gamma(1 - \beta M)$, where M is the current number of bacteria.

$$\therefore P_M(t + \Delta t) = P_M(t) \cdot (1 - M\gamma(1 - \beta M)\Delta t) + P_{M-1}(t) \cdot (M-1)\gamma(1 - \beta(M-1))\Delta t$$

- (b) Derive the continuous time master equation (5 points)

Same as last problem, except take $\gamma = (1 - \beta M)$.

$$\therefore \dot{P}_M(t) = -M\gamma(1 - \beta M)P_M(t) + (M-1)\gamma(1 - \beta(M-1))P_{M-1}(t)$$

- (c) Derive the equation of the average number of bacteria depending on time (10 points)

Now this one is not that simple, we need to open the brackets and see what happens.

$$\begin{aligned} n(t) &= \sum_{M=N}^{\infty} MP_M(t) \\ \dot{n}(t) &= \sum_{M=N}^{\infty} M\dot{P}_M(t) = \sum_{M=N}^{\infty} M(-M\gamma(1 - \beta M)P_M(t) + (M-1)\gamma(1 - \beta(M-1))P_{M-1}(t)) \\ &= \gamma \sum_{M=N}^{\infty} M(M-1)(1 - \beta(M-1))P_{M-1}(t) - M^2(1 - \beta M)P_M(t) \\ &= \gamma \sum_{M=N}^{\infty} M(M-1)P_{M-1}(t) - M^2P_M(t) + \beta M^3P_M(t) - \beta M(M-1)^2P_{M-1}(t) \\ &= \gamma \left(\sum_{M=N}^{\infty} (M+1)(M)P_M(t) - \sum_{M=N}^{\infty} M^2P_M(t) + \sum_{M=N}^{\infty} \beta M^3P_M(t) - \sum_{M=N}^{\infty} \beta(M+1)M^2P_M(t) \right) \\ &= \gamma \left(\sum_{M=N}^{\infty} MP_M(t) - \sum_{M=N}^{\infty} \beta M^2P_M(t) \right) \\ &= \gamma (n(t) - \beta(\text{Var}(M)(t) + (n(t))^2)) \end{aligned}$$

- (d) Is detailed balance possible in this system? If so, what is the solution of detailed balance? (10 points)

The equation of equilibrium:

$$\sum_j \bar{P}_j w_{j \rightarrow i} = \bar{P}_i \sum_j w_{i \rightarrow j} \implies \dot{P}_M(t) w_{M \rightarrow M-1} = \dot{P}_{M+1}(t) w_{M-1 \rightarrow M}$$

The rate from going from $M + 1$ to M is always zero, because our system only models doubling of bacteria. Hence:

$$\begin{aligned}\dot{P}_{M-1}(t)w_{M-1 \rightarrow M} &= 0 \\ (-M\gamma(1 - \beta M)P_M(t) + (M - 1)\gamma(1 - \beta(M - 1))P_{M-1}(t)) \cdot (M - 1)\gamma(1 - \beta(M - 1)) &= 0 \\ \therefore 1 - \beta(M - 1) &= 0 \implies M = \frac{1}{\beta} + 1\end{aligned}$$

Problem 3 (15 points).

We start with $N = 1000$ particles of Uranium that decays into Thorium.

- (a) Take the probability of decay $\gamma = 0.001$ (5 points)

Write a function *simulate()* that will use an N sized array to store integers 0 and 1 representing *Th* and *U* to loop over the array and with γ probability of change from 1 to 0 while skipping over the zeroes. This loop should be done $K = 100$ times. The function should return a K sized array of the amount of Uranium after each step.

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

N = 1000
K = 100
gamma = 0.001

def simulate():
    uraniums = np.full(K,N)

    atoms = np.ones(N)
    for i in range(K):
        if i != 0:
            uraniums[i] = uraniums[i-1]
        for j in range(N):
            if atoms[j] == 0:
                continue

            if random.random() < gamma:
                atoms[j] = 0
                uraniums[i]-=1
    return uraniums
```

(b) Take $\beta = 0.0001$ (5 points)

Now write a new function *simulate_square()* where the only difference is that the probability of change is $\gamma(1 - \beta M)$ where M is the amount of Uranium on the previous step.

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

N = 1000
K = 100
gamma = 0.001

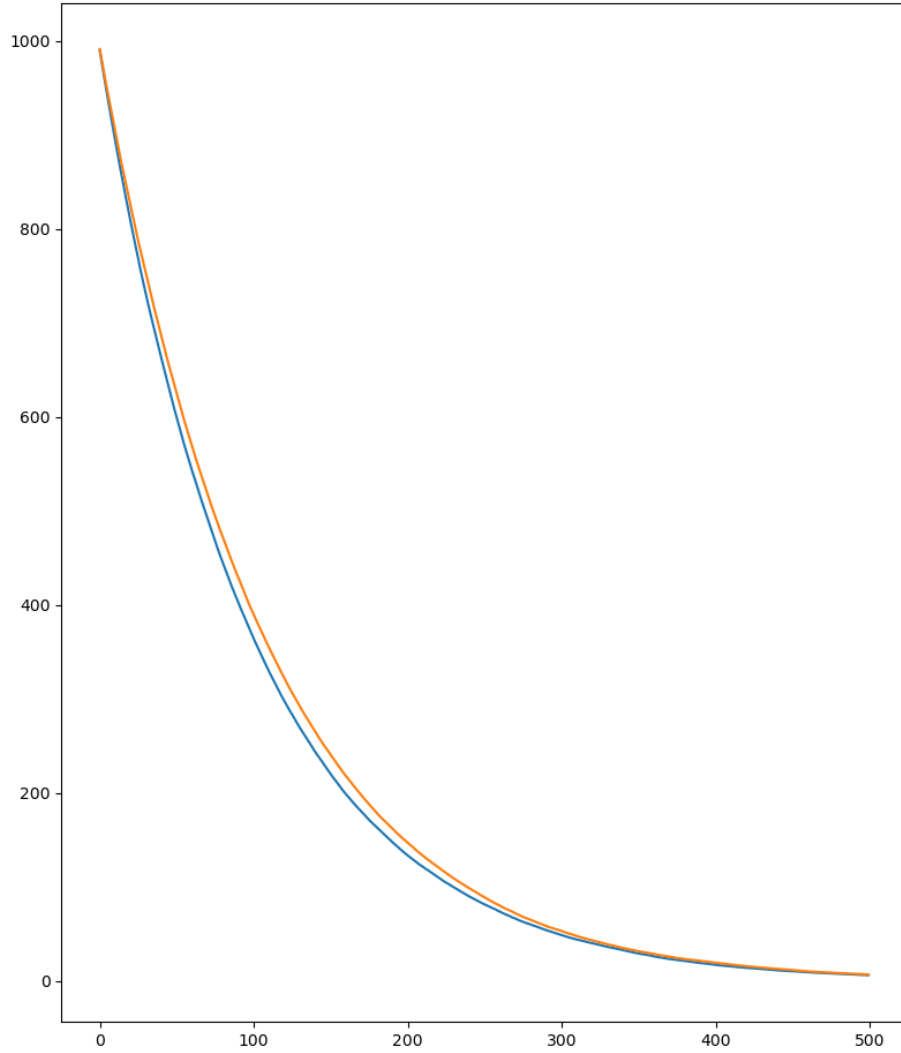
beta = 0.0001

def simulate_square():
    uraniums = np.full(K,N)

    atoms = np.ones(N)
    for i in range(K):
        if i != 0:
            uraniums[i] = uraniums[i-1]
        u0 = uraniums[i]
        for j in range(N):
            if atoms[j] == 0:
                continue

            if random.random() < gamma*(1-beta*u0):
                atoms[j] = 0
                uraniums[i]-=1
    return uraniums
```

(c) Repeat these simulations many times and take their respective averages. After that plot them and discuss the differences and their reasons. (5 points)



The calculations were ran with $K = 500$ and $\gamma = 0.01$, to make the exponential decay more visible. At first, our initial model decays faster than the second model, but with less Uranium atoms left, the second model started to decay faster than the initial model. This can be concluded from the probabilities, as $\gamma(1 - \beta M)$ means that the less Uranium atoms are left, the higher the probability of a decay.