ASAHW5

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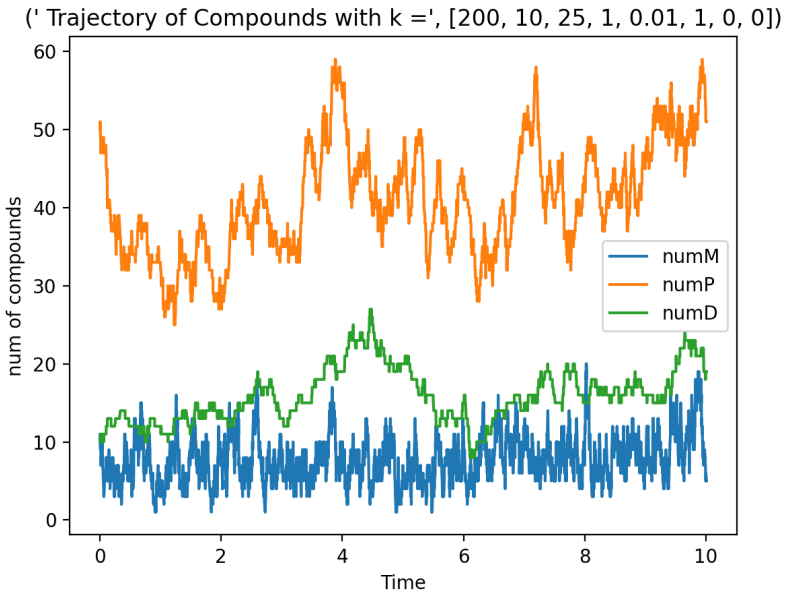
Since I programmed Gillespie's algorithm first. All of the explanations on the reactions are in section 2. Other two algorithms follow the same reason.

1 The Next Reaction

1.1 $\kappa = (200, 10, 25, 1, 0.01, 1, 0, 0)$

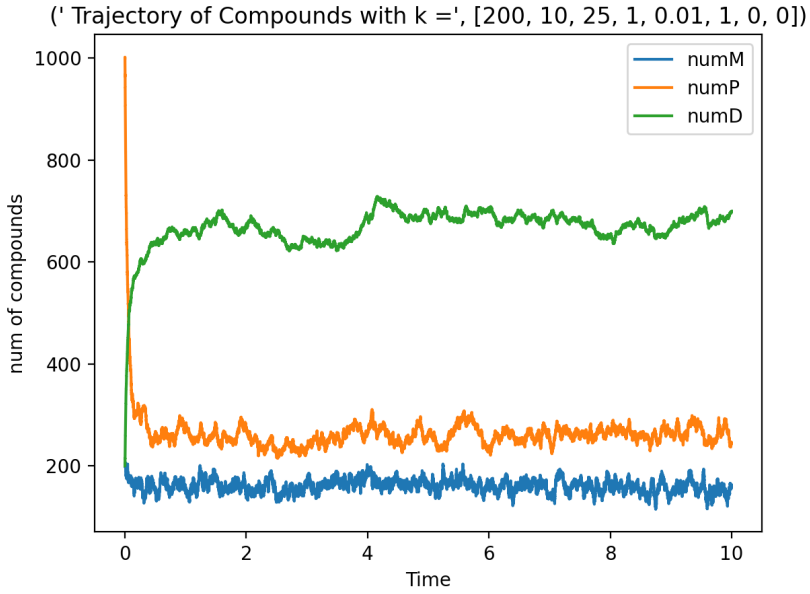
1.1.1 $X^{(0)} = (1, 10, 50, 10, 0)$

The final state is $X^{(T)} = (1, 7, 41, 18, 0)$.



1.1.2 $X^{(0)} = (20, 200, 1000, 200, 0)$

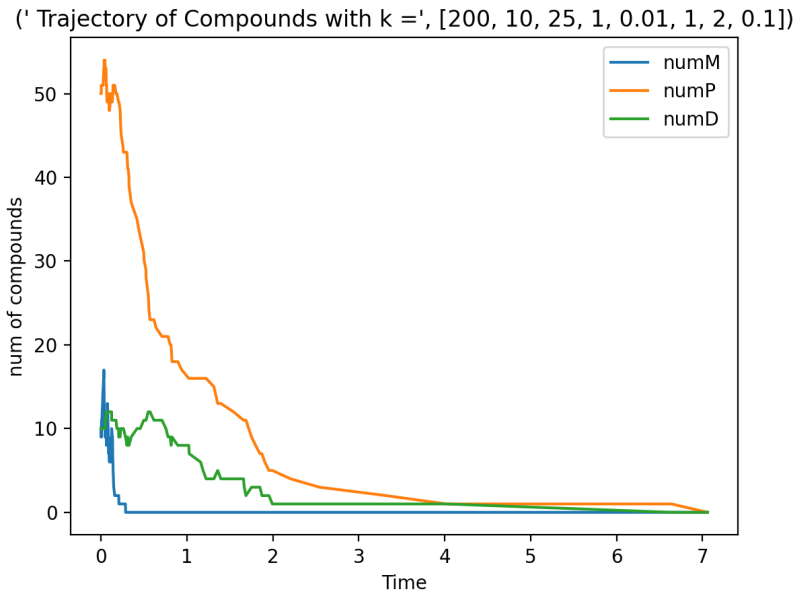
The final state is $X^{(T)} = (20, 144, 255, 644, 0)$.


(' Trajectory of Compounds with k =', [200, 10, 25, 1, 0.01, 1, 0, 0])
numM
numP
numD
num of compounds
Time
1000
800
600
400
200
0
2
4
6
8
10

1.2 $\kappa = (200, 10, 25, 1, 0.01, 1, 2, 0.1)$

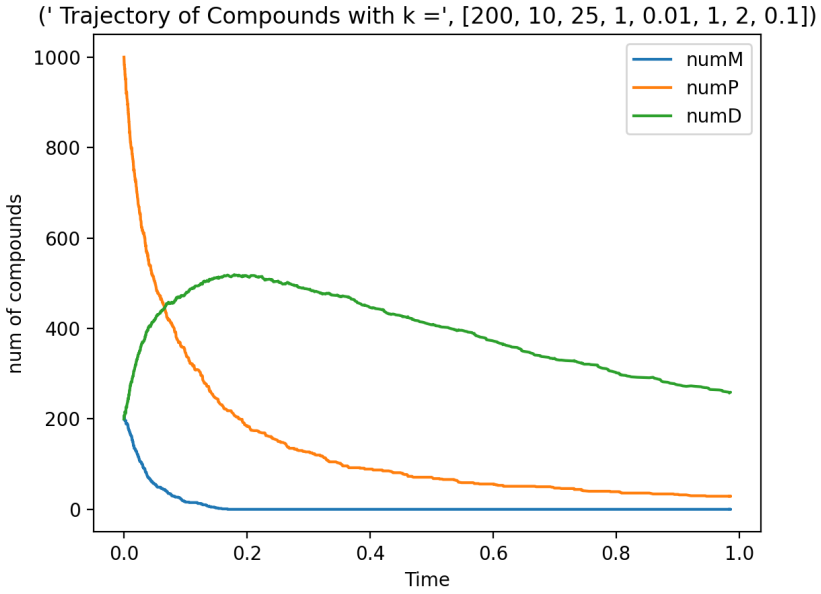
1.2.1 $X^{(0)} = (1, 10, 50, 10, 0)$

The final state is $X^{(T)} = (0, 1, 0, 1, 1)$.



1.2.2 $X^{(0)} = (20, 200, 1000, 200, 0)$

The final state is $X^{(T)} = (0, 2, 8, 73, 20)$. Since in this part, the final time $T = 1.0$, the process is similar to the earlier path of Gillespie and Tau Leaping.


(' Trajectory of Compounds with k =', [200, 10, 25, 1, 0.01, 1, 2, 0.1])
numM
numP
numD
num of compounds
Time
0
200
400
600
800
1000
0.0
0.2
0.4
0.6
0.8
1.0

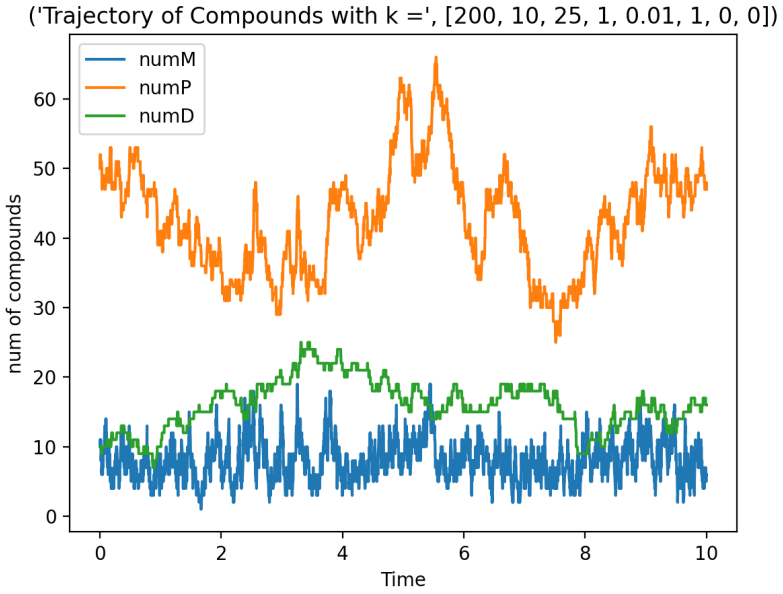
2 Gillespie Algorithm

2.1 $\kappa = (200, 10, 25, 1, 0.01, 1, 0, 0)$

2.1.1 $X^{(0)} = (1, 10, 50, 10, 0)$

With the reaction rate $\kappa = (200, 10, 25, 1, 0.01, 0, 0)$ and initial condition $X^{(0)} = (1, 10, 50, 10, 0)$, we simulate one realization of $X^{(t)}$ up to time $T = 100$ since $T = 10$ does not show the tendency obviously. Then, we have the final state

$$X^T = (1, 6, 48, 16, 0)$$



This is a reasonable result.

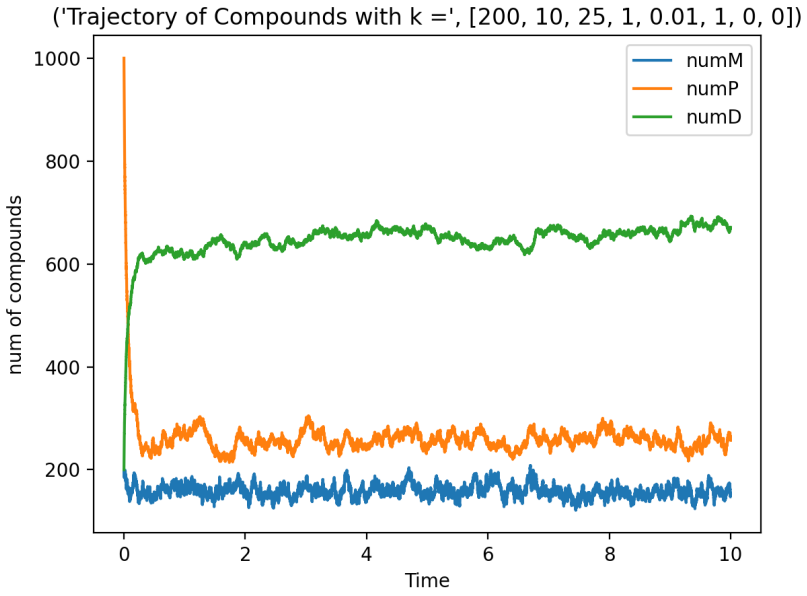
- **G $\rightarrow$ M $\rightarrow$ P**
  Since reaction 7 and 8 do not happen at all, the number of G stays the same in reaction 1. Also, reaction 1 creates more M and then triggers reaction 2. So, P is produced in this way.

- **P produces D**
  At the same time, since there is a large number of P, the reaction 5 is likely to be triggered; thus, D is produced. P is dissipated by reaction 4 and 5. As a result, we see the decreasing number of P and increasing number of D. G and M stay at almost the same level.

2.1.2 $X^{(0)} = (20, 200, 1000, 200, 0)$

With the same reaction rate and $X^{(0)} = (20, 200, 1000, 200, 0)$, we plot the trajectory of 5 compounds. The final state is

$$X^{(T)} = (20, 152, 257, 671, 0)$$



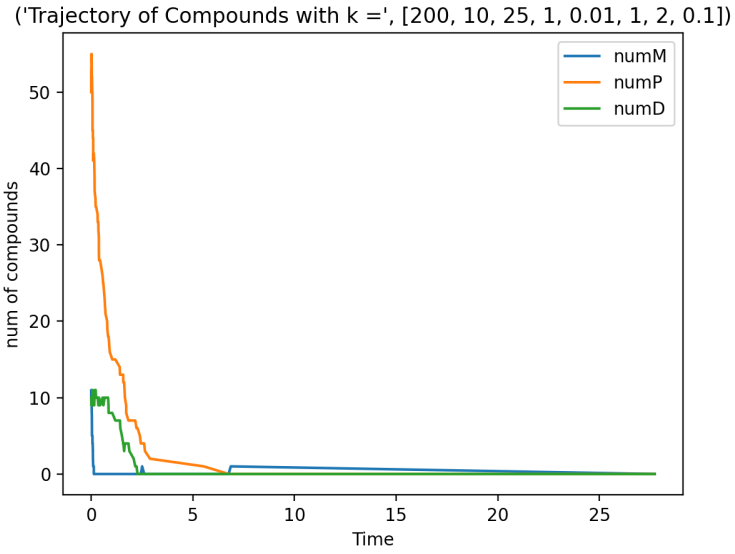
- **P $\rightarrow$ D**
  Starting off, we see that there is a large amount of P with reaction rate of reaction 5 being $\kappa_3 x_3(x_3 - 1)$. Thus, reaction 5 is highly likely to be triggered and causes the number of D increasing. Indeed, according to the output of the program, at the beginning of the experiments, most are reaction 5.

2.2 $\kappa = (200, 10, 25, 1, 0.01, 1, 2, 0.1)$

2.2.1 $X^{(0)} = (1, 10, 50, 10, 0)$

In this part, we also set $T = 100$. The final state is

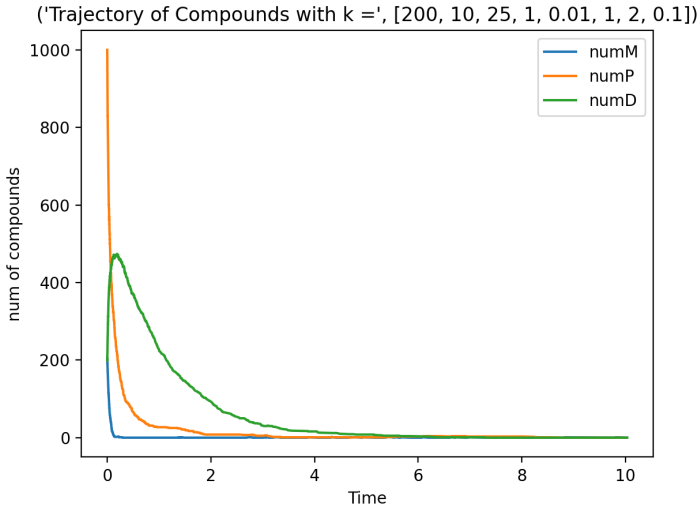
$$X^{(T)} = (0, 1, 0, 0, 1)$$



- **Reaction 7: G and B**
  In this set up, we should expect that the total number of G + B is a constant since in order to produce B, one G must be consumed. However, there is no reaction can produce G. Indeed, one G turns into one B in the above result.

2.3 $X^{(0)} = (20, 200, 1000, 200, 0)$

The final state at is $X^{(T)} = (0, 1, 3, 0, 20)$



- **G and B**
  For the same reason as above, $G^t + B^t = G^0 + B^0 = 0 + 20 = 20 + 0$, as expected.

3 tau-leaping

First, we set $T = 10$ and $h = 0.0001$. We will demonstrate the order of accuracy in section 3.2.

Problem for this algorithm

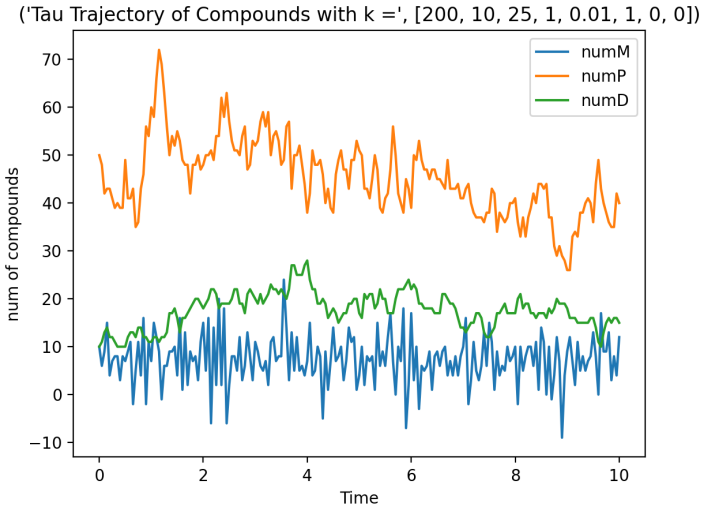
Since this an approximation algorithm, for larger h, it might happen that the jump for the current interval is to big so that $X^{(kh)}$ contains negative values. We use the two brute ways to deal with this issue.

- We want h to be smaller enough so that this does not happen frequently.
- If $X^{(kh)}$ does contain negative values, then we will just let the negative values to be zero. However, the conservation in the reaction is broken. For example, if we examine the $G + D$, it is not always conservative if h is large, say $h = 0.05$.

3.1 $\kappa = (200, 10, 25, 1, 0.01, 1, 0, 0)$

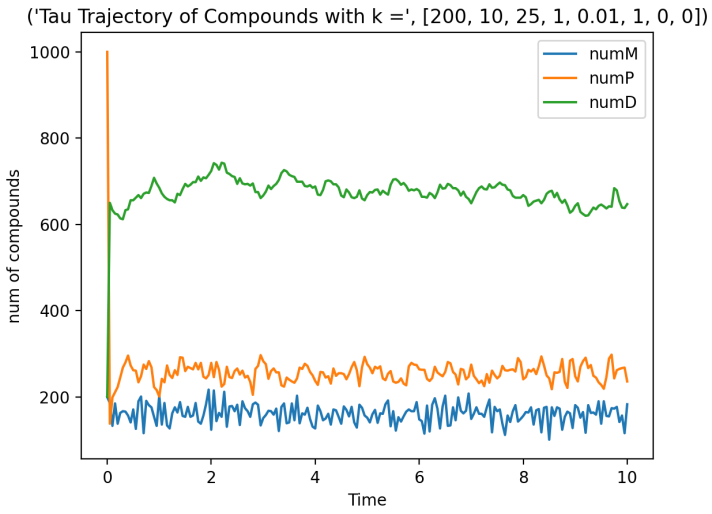
3.1.1 $X^{(0)} = (1, 10, 50, 10, 0)$

The final state is $X^{(T)} = (1, 12, 40, 15, 0)$



3.1.2 $X^{(0)} = (20, 200, 1000, 200, 0)$

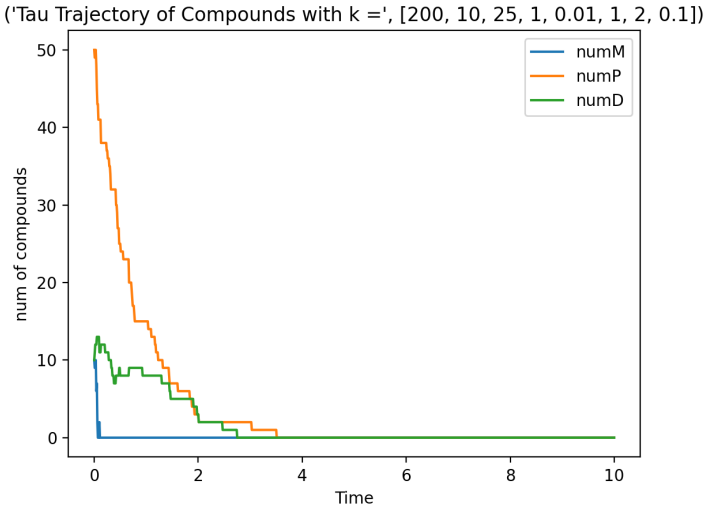
The final state is $X^{(T)} = (20, 183, 236, 647, 0)$



3.2 $\kappa = (200, 10, 25, 1, 0.01, 1, 2, 0.1)$

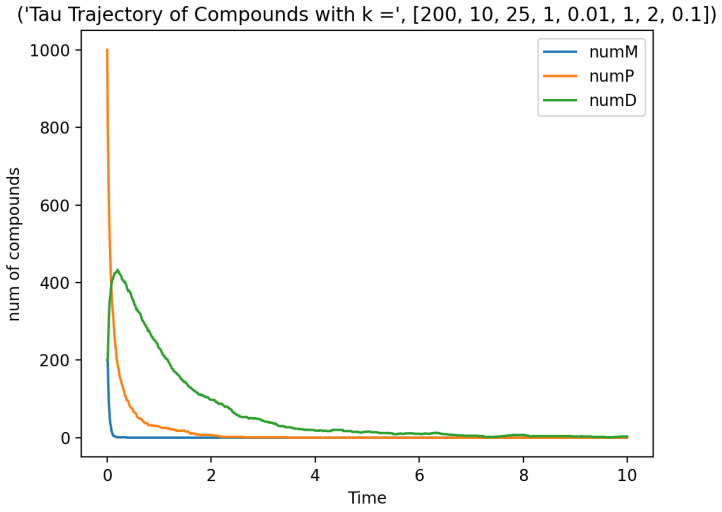
3.2.1 $X^{(0)} = (1, 10, 50, 10, 0)$

The final state is $X^{(T)} = (0, 0, 0, 0, 1)$



3.2.2 $X^{(0)} = (20, 200, 1000, 200, 0)$

The final state is $X^{(T)} = (1, 8, 11, 4, 19)$



3.3 Weak Order of Accuracy

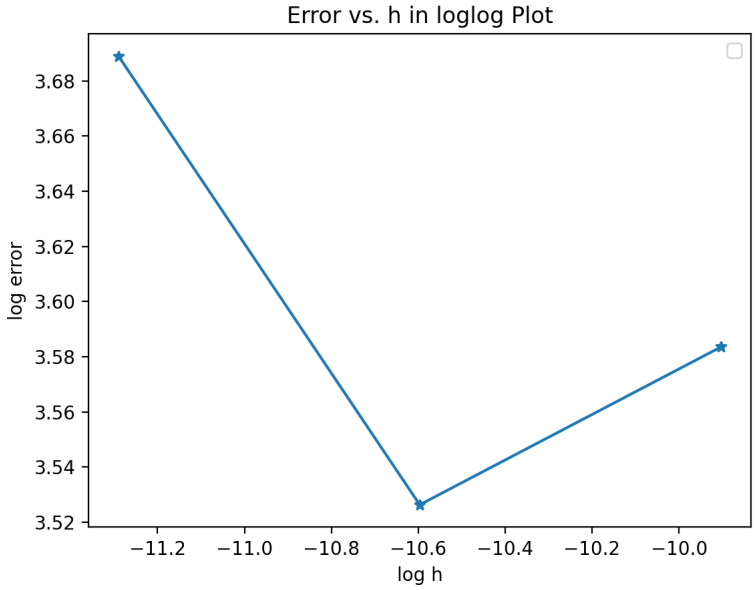
Tau leaping is proved to have weak order of accuracy 1 and strong order 1/2 according to [Li07][1]. We should pick t so that $|X_t^{(h)} - X_t^{true}|$ is maximized, according to the definition.
In practical, we pick $t = 0 : 0.25 : T$. Compute the the max error

$$max_{0 \le t \le T} E(h) = |X_t^{(h)} - X_t^{true}|$$

where X_t^{true} is generated by Gillespie's algorithm.
Then,

$$p = \frac{log(E(h_1) - E(h_2))}{log(h_1 - h_2)}$$

is expected to be 1 for weak order of accuracy. **loglog** plot of error vs. h is linear of slope 1. However, the output is not too accurate. Here is the **loglog**.



[1] http://citeseerx.ist.psu.edu/viewdoc/download?doi=10.1.1.333.32rep=rep1type=pdf