Homework5.1

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1 "Naive" stochastic simulation

Here we set $n_0 = 1000, k = 2, \Delta t = 0.001$. We stimulate it 4 times and get the following result.

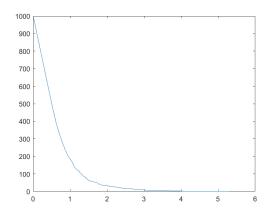


Figure 1: Simulation1

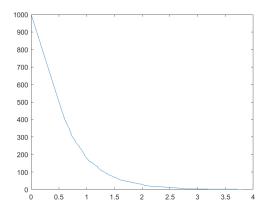


Figure 3: Simulation3

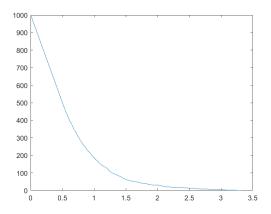


Figure 2: Simulation2

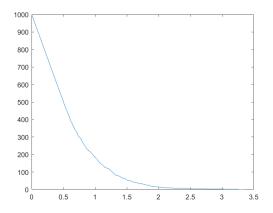


Figure 4: Simulation4

2 Gillespie stochastic simulation algorithm

Here we set $n_0 = 100, k = 2$. We simulation it 10 times and print the deterministic function on the same plot. Then we print the mean.

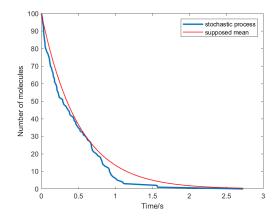


Figure 5: Simulation1

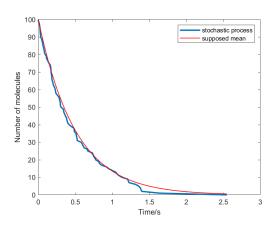


Figure 7: Simulation3

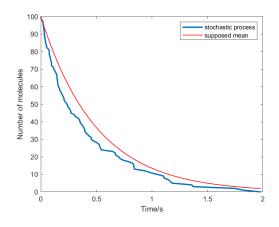


Figure 6: Simulation2

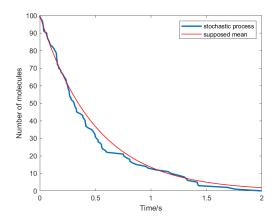


Figure 8: Simulation4

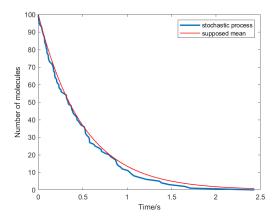


Figure 9: Simulation5

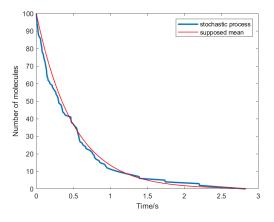


Figure 11: Simulation7

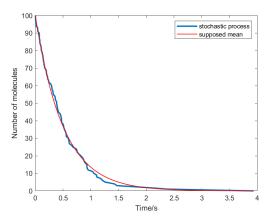


Figure 13: Simulation9

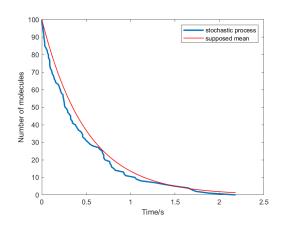


Figure 10: Simulation6

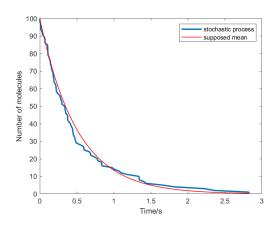


Figure 12: Simulation8

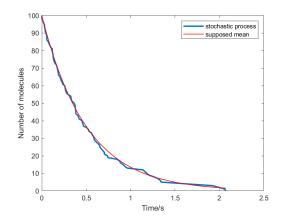


Figure 14: Simulation10

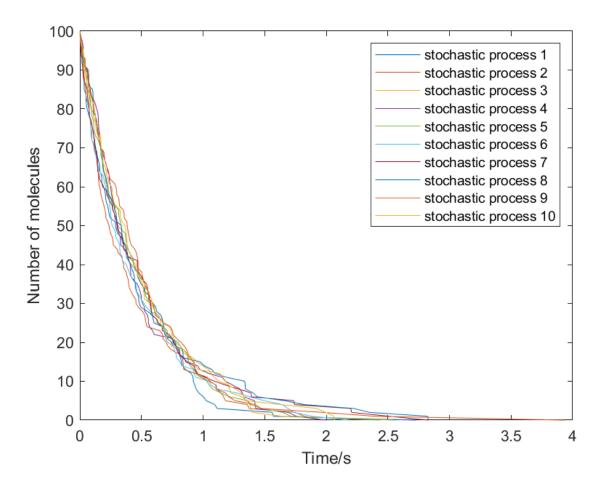


Figure 15: mean

3 Gillespie SSA for 2 reactions

First, we compute the deterministic function and get:

$$a = \frac{k_2}{k_1} + \frac{N_0 - \frac{k_2}{k_1}}{\exp^{k_1} t} \tag{1}$$

Then we set $n_0 = 100, k_1 = 2, k_2 = 4$. We simulation it 10 times and print the deterministic function on the same plot. Then we print the mean.

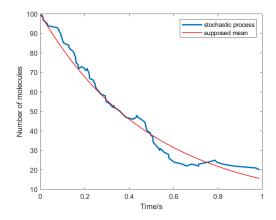


Figure 16: Simulation1

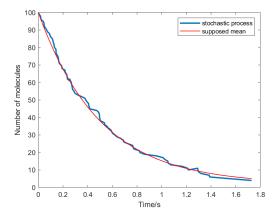


Figure 18: Simulation3

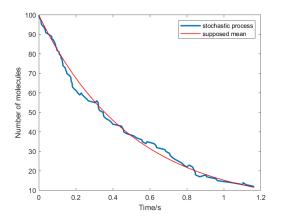


Figure 17: Simulation2

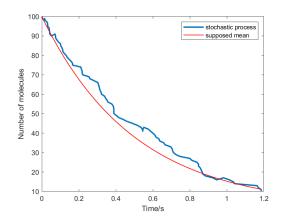


Figure 19: Simulation4

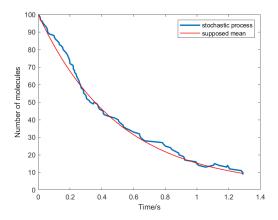


Figure 20: Simulation5

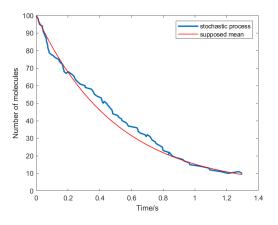


Figure 22: Simulation7

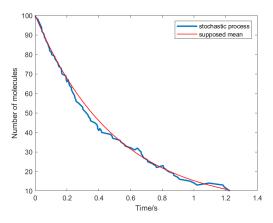


Figure 24: Simulation9

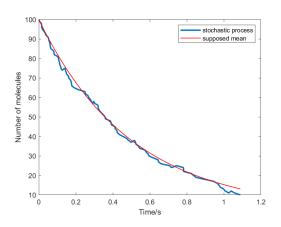


Figure 21: Simulation6

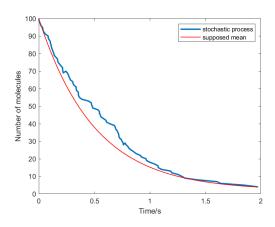


Figure 23: Simulation8

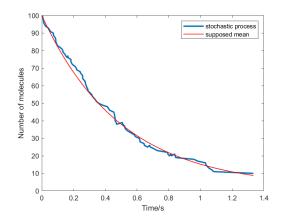


Figure 25: Simulation10

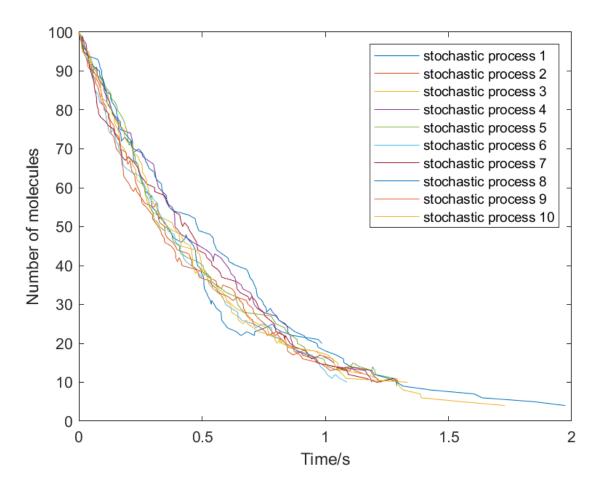


Figure 26: mean

4 code

4.1 "Naive" stochastic simulation

```
k=2;
   deltat = 0.001;
   n0 = 1000;
   naivess1 (k, deltat, n0);
   function naivess1(k, deltat, n0)
   A=n0:
   a=n0:
   while a>0
        r=rand;
        if r<a*k*deltat
10
             a = a - 1;
11
        end
        A=vertcat(A,a);
13
   end
14
   [m, n] = size(A);
15
   x=linspace (deltat, m*deltat, m);
   plot(x,A);
17
   end
```

4.2 Gillespie stochastic simulation algorithm

```
k=2;
    deltat = 0.01;
    n0 = 100;
   T1=gillespie (k, deltat, n0, 'b1.png');
    T2=gillespie(k,deltat,n0,'b2.png');
    T3=gillespie (k, deltat, n0, 'b3.png');
    T4=gillespie(k, deltat, n0, 'b4.png');
    T5=gillespie (k, deltat, n0, 'b5.png');
    T6=gillespie (k, deltat, n0, 'b6.png');
    T7=gillespie (k, deltat, n0, 'b7.png');
10
    T8=gillespie(k, deltat, n0, 'b8.png');
    T9=gillespie(k, deltat, n0, 'b9.png');
    T10=gillespie(k, deltat, n0, 'b10.png');
13
    x = linspace (n0, 0, n0+1);
14
    plot(T1,x, 'DisplayName', 'stochastic_process_1'); hold on
    plot (T2,x, 'DisplayName', 'stochastic process 2');
plot (T3,x, 'DisplayName', 'stochastic process 3');
17
    plot (T4,x, 'DisplayName', 'stochastic_process_4');
    plot (T4,x, DisplayName', stochastic process 4),
plot (T5,x, 'DisplayName', 'stochastic process 5');
plot (T6,x, 'DisplayName', 'stochastic process 6');
plot (T7,x, 'DisplayName', 'stochastic process 7');
plot (T8,x, 'DisplayName', 'stochastic process 8');
21
    plot (T9, x, 'DisplayName', 'stochastic process 9');
    plot (T10, x, 'DisplayName', 'stochastic process 10');
    legend()
    ylabel ('Number of molecules')
    xlabel('Time/s')
    hold off
28
    saveas(gcf, 'mean1.png');
    function T=gillespie (k, deltat, n0, name)
```

```
T = linspace(0, n0, n0+1);
   t = 0:
   a=n0;
33
   for i = 2:n0+1
34
        r=rand;
        t=t+\log(1/r)/(a*k);
36
        a=a-1;
37
       T(i)=t;
38
   end
   x = linspace (n0, 0, n0+1);
40
   plot (T,x, 'LineWidth', 2, 'DisplayName', 'stochastic process'); hold on
41
   T2=linspace(0,T(n0+1),1000);
   Y=n0*exp(-k*T2);
   plot (T2,Y, 'r', 'LineWidth', 1, 'DisplayName', 'supposed_mean');
44
   hold off
45
   legend()
   ylabel ('Number of molecules')
   xlabel ('Time/s')
   saveas (gcf, name);
   end
```

4.3 Gillespie SSA for 2 reactions

```
k1 = 2:
    k2 = 4;
    n0 = 100;
     [T1, A1] = gillespie2(k1, k2, n0, 'c1.png');
     [T2, A2] = gillespie2(k1, k2, n0, 'c2.png');
      [T3, A3] = gillespie2 (k1, k2, n0, 'c3.png');
      [T4, A4] = gillespie2(k1, k2, n0, 'c4.png');
      T5, A5] = gillespie 2 (k1, k2, n0, 'c5.png');
      T6, A6 = gillespie 2 (k1, k2, n0, 'c6.png');
      T7,A7 = gillespie2(k1,k2,n0,'c7.png');
10
      [T8, A8] = gillespie2(k1, k2, n0, 'c8.png');
11
      [T9, A9] = gillespie2(k1, k2, n0, 'c9.png');
12
     [T10, A10] = gillespie2(k1, k2, n0, 'c10.png');
13
     \begin{array}{l} \textbf{plot}\left(T1,A1,\text{'DisplayName','stochastic}_{\square}\textbf{process}_{\square}1\text{'}\right); \textbf{hold} \ \ \textbf{on} \\ \textbf{plot}\left(T2,A2,\text{'DisplayName','stochastic}_{\square}\textbf{process}_{\square}2\text{'}\right); \\ \textbf{plot}\left(T3,A3,\text{'DisplayName','stochastic}_{\square}\textbf{process}_{\square}3\text{'}\right); \\ \end{array} 
15
     plot\left(T4,A4,\,'DisplayName\,'\,,\,'stochastic_{\,\sqcup\,}process_{\,\sqcup\,}4\,'\right);
     plot (T5, A5, 'DisplayName', 'stochastic process 5');
     plot (T6, A6, 'DisplayName', 'stochastic_process_6');
    plot (T7, A7, 'DisplayName', 'stochastic process 7');
    plot (T8, A8, 'DisplayName', 'stochastic process 8');
plot (T9, A9, 'DisplayName', 'stochastic process 9');
     plot (T10, A10, 'DisplayName', 'stochastic process 10');
23
    legend()
24
     ylabel ('Number of molecules')
    xlabel('Time/s')
    hold off
27
    saveas(gcf, 'mean2.png');
    function [T,A]=gillespie2(k1,k2,n0,name)
    T = linspace(0, 100, 101);
    A=linspace(0,101,101);
    t = 0:
```

```
A(1)=n0;
   a=n0;
   for i = 2:101
35
        r1=rand;
        r2=rand;
        alpha=a*k1+k2;
38
        t=t+\log(1/r1)/(alpha);
39
        if r2 < k2/alpha
40
             a=a+1;
        else
42
             a=a-1;
43
        \quad \text{end} \quad
        A(i)=a;
        T(i)=t;
46
   end
47
   plot\left(T,A, \text{ 'LineWidth', 2, 'DisplayName', 'stochastic} \sqcup process'\right); \\ hold \text{ on }
   T2=linspace(0,T(101),1000);
   Y=k2/k1+(n0-k2/k1)*exp(-k1*T2);
   plot (T2,Y, 'r', 'LineWidth', 1, 'DisplayName', 'supposed mean');
   hold off
   legend()
   ylabel('Number⊥of⊥molecules')
54
   xlabel('Time/s')
   saveas(gcf, name);
   end
```