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3/29/2023

MATH5131

HW 5

2)

```
clear;
close;

%%First part a so Gillespie is done then ode is done later
% Parameters
k1 = 0.001;
k2 = 0.01;
k3 = 1.2;
k4 = 1 ;
NumA = 0;
NumB = 0;
t = 0;
reactions = 100000;

% Arrays
A = zeros(1,reactions);
B = zeros(1,reactions);
T = zeros(1,reactions);

% Gillespie
for i = 1:reactions
eq1 = k1 * (NumA) * (NumA-1);
eq2 = k2 * NumA * NumB;
eq3 = k3;
eq4 = k4;
eq0 = eq1 + eq2 + eq3 + eq4;

r = rand(1,2);
tau = log(1/r(1))/eq0;
t = t + tau;
T(i) = t;

if (0 < r(2)) && (r(2) < eq1/eq0)
NumA = NumA-2;
NumB = NumB;
elseif (eq1/eq0 <= r(2)) && (r(2) < (eq1+eq2)/eq0)
NumA = NumA - 1;
NumB = NumB - 1;
elseif ((eq1+eq2)/eq0 <= r(2)) && (r(2) < (eq1+eq2+eq3)/eq0)
NumB = NumB;
NumA = NumA + 1;
elseif ((eq1+eq2+eq3)/eq0 <= r(2)) && (r(2) < 1)
NumA = NumA;
NumB = NumB + 1;
end
```

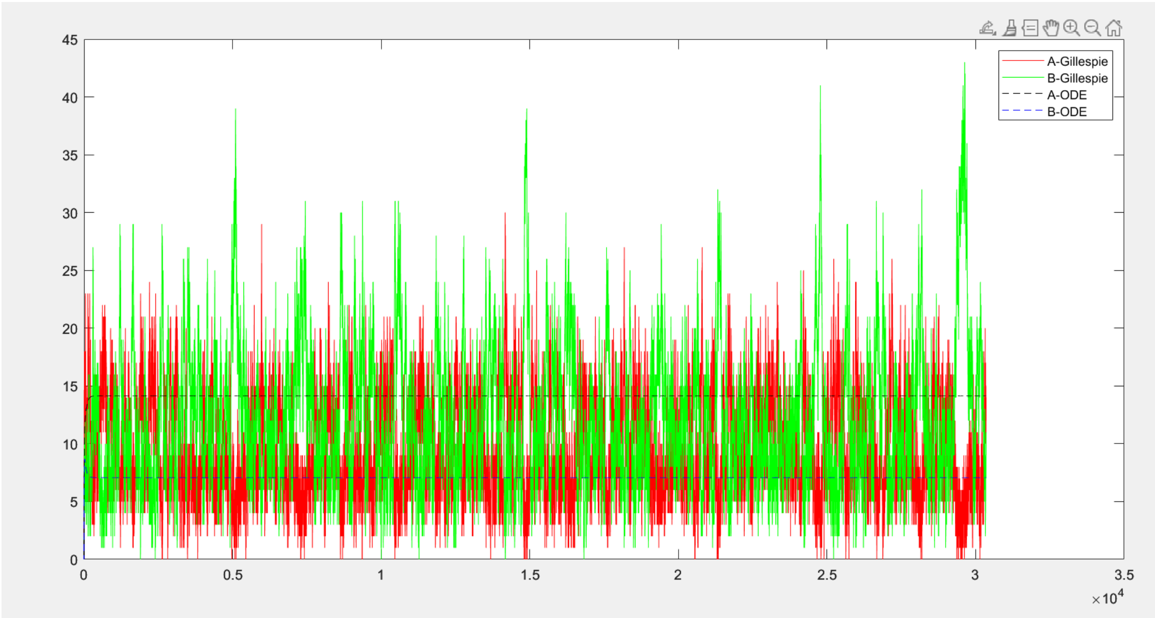
```
A(i) = NumA;
B(i) = NumB;
end

% ODE parameters
k1 = 1e-3;
k2 = 1e-2;
k3 = 1.2;
k4 = 1;
tspan = [T(1) T(end)];
y0 = [0 0];

% ODE
[t,Y] = ode45(@(t,y) ode_fun(t,y,k1,k2,k3,k4), tspan, y0);

% Plot
figure(1)
plot(T,A,'-r'),hold on
plot(T,B,'-g')
plot(t,Y(:,1),'--k')
plot(t,Y(:,2),'--b')
hold off
legend('A-Gillespie','B-Gillespie','A-ODE','B-ODE')

% Function for ODEs
function dydt = ode_fun(t,y,k1,k2,k3,k4)
    dydt = zeros(2,1);
    dydt(1) = -k1*y(1)*y(1) - k2*y(1)*y(2) + k3;
    dydt(2) = -k2*y(1)*y(2) + k4;
end
```



45
40
35
30
25
20
15
10
5
0
0
0.5
1
1.5
2
2.5
3
3.5
$\times 10^4$
A-Gillespie
B-Gillespie
A-ODE
B-ODE

b)

$$\frac{da}{dt} = -2k_1 a^2 - k_2 ab + k_3$$

$$\frac{db}{dt} = -k_2 ab + k_4$$

$$\frac{da}{dt} = 0, \quad \frac{db}{dt} = 0$$

$$0 = -2k_1 a^2 - k_2 ab + k_3 \qquad 0 = -k_2 ab + k_4$$

$$k_2 ab = k_4$$

$$k_1 = 0.001 \qquad k_4 = 1 \qquad ab = \frac{k_4}{k_2}$$

$$k_2 = 0.01$$

$$k_3 = 1.2$$

$$ab = \frac{1}{0.01} = 100$$

$$0 = -2k_1 a^2 - 100 k_2 + k_3$$

$$0 = -2(0.001)a^2 - 100(0.01) + 1.2$$

$$0 = -0.002a^2 - 1 + 1.2$$

$$0 = -0.002a^2 + 0.2$$

$$0.002a^2 = 0.2$$

$$a^2 = \frac{0.2}{0.002} = 100$$

$$a^2 = 100$$

$$a = \pm 10$$

$$b = \pm 10$$

Code

```
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k3 = 1.2;
k4 = 1 ;
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NumB = 0;
t = 0;
reactions = 100000;

% Arrays
A = zeros(1,reactions);
B = zeros(1,reactions);
T = zeros(1,reactions);

% Gillespie
for i = 1:reactions
eq1 = k1 * (NumA) * (NumA-1);
eq2 = k2 * NumA * NumB;
eq3 = k3;
eq4 = k4;
eq0 = eq1 + eq2 + eq3 + eq4;

r = rand(1,2);
tau = log(1/r(1))/eq0;
t = t + tau;
T(i) = t;

if (0 < r(2)) && (r(2) < eq1/eq0)
NumA = NumA-2;
NumB = NumB;
elseif (eq1/eq0 <= r(2)) && (r(2) < (eq1+eq2)/eq0)
NumA = NumA - 1;
NumB = NumB - 1;
elseif ((eq1+eq2)/eq0 <= r(2)) && (r(2) < (eq1+eq2+eq3)/eq0)
NumB = NumB;
NumA = NumA + 1;
elseif ((eq1+eq2+eq3)/eq0 <= r(2)) && (r(2) < 1)
NumA = NumA;
NumB = NumB + 1;
end

A(i) = NumA;
B(i) = NumB;
end

% ODE parameters
k1 = 1e-3;
k2 = 1e-2;
```

```
k3 = 1.2;
k4 = 1;
tspan = [T(1) T(end)];
y0 = [0 0];

% ODE
[t,Y] = ode45(@(t,y) ode_fun(t,y,k1,k2,k3,k4), tspan, y0);

% Plot
figure(1)
plot(T,A,'-r'),hold on
plot(T,B,'-g')
plot(t,Y(:,1),'--k')
plot(t,Y(:,2),'--b')
hold off
legend('A-Gillespie','B-Gillespie','A-ODE','B-ODE')

% Function for ODEs
function dydt = ode_fun(t,y,k1,k2,k3,k4)
    dydt = zeros(2,1);
    dydt(1) = -k1*y(1)*y(1) - k2*y(1)*y(2) + k3;
    dydt(2) = -k2*y(1)*y(2) + k4;
end
```