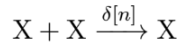
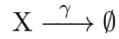
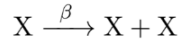


## 1 Problem 1

Consider a reproduction-death process defined by the following set of stochastic reactions:



where the first reaction accounts for reproduction of  $X$ -particles at rate  $\beta$ , the second, for spontaneous removal of  $X$ -particles at rate  $\gamma$ , and the third reaction represents the destruction of one of the particles upon the encounter between two particles.

- Define the random variable,  $\hat{n}$  that gives the number of particles in the system. Write the master equation for the probability of having  $n$  particles at time  $t$ ,  $p(n, t)$ .

$$\frac{\partial P(n, t)}{\partial t} = \sum_{\ell} (E^{\ell} - 1) \left[ \Omega_{n \rightarrow n-\ell} P(n, t) \right].$$

$$* \Omega_{n \rightarrow n-\ell} = \begin{cases} \beta n, & \ell = -1 \\ \gamma n + \delta n(n-1), & \ell = 1 \\ 0, & \text{else} \end{cases}$$

$$\therefore \frac{\partial P(n, t)}{\partial t} = (E^{-1} - 1) [\beta n P(n, t)] + (E - 1) [\gamma n P(n, t) + \delta n(n-1) P(n, t)] = >$$

$$\frac{\partial P(n, t)}{\partial t} = \beta(n-1)P(n-1, t) + (n+1)(\gamma + \delta n)P(n+1, t) + \\ -n(\beta + \gamma + \delta(n-1))P(n, t)$$

- Analyze the mean value of particles as a function of time using a mean field approximation. How does the mean number of particles in the stationary state, i.e.,  $\langle n(t \rightarrow \infty) \rangle$ , and its stability depend on  $\beta$ ,  $\gamma$ , and  $\delta$ ?

$$\begin{aligned} \langle n(t) \rangle &= \sum_{n=0}^{\infty} n P(n, t) \Rightarrow \frac{d}{dt} \langle n(t) \rangle = \frac{d}{dt} \sum_{n=0}^{\infty} n P(n, t) = \\ &= \sum_{n=0}^{\infty} n \frac{dP(n, t)}{dt} = \sum_{n=0}^{\infty} n \beta (n-1) P(n-1, t) + \sum_{n=0}^{\infty} n (n+1) (\gamma + \delta n) P(n+1, t) + \\ &\quad - \sum_{n=0}^{\infty} n^2 (\beta + \gamma + \delta (n-1)) P(n, t). \end{aligned}$$

$$* \sum_{n=0}^{\infty} n \beta (n-1) P(n-1, t) = \sum_{n=0}^{\infty} \beta n (n+1) P(n, t);$$

$$* \sum_{n=0}^{\infty} n (n+1) (\gamma + \delta n) P(n+1, t) = \sum_{n=0}^{\infty} n (n-1) (\gamma + \delta (n-1)) P(n, t)$$

$$\begin{aligned} \therefore \frac{d}{dt} \langle n(t) \rangle &= \sum_{n=0}^{\infty} n P(n, t) [\beta - \gamma - \delta (n-1)] = \\ &= (\beta + \delta - \gamma) \langle n(t) \rangle - \delta \langle n^2(t) \rangle. \end{aligned}$$

$$* \text{M.F.A.: } \langle (n(t) - \langle n(t) \rangle)^2 \rangle = \langle n^2(t) \rangle - \langle n(t) \rangle^2 = 0$$

$$\therefore \frac{d}{dt} \langle n(t) \rangle = (\beta + \delta - \gamma) \langle n(t) \rangle - \delta \langle n(t) \rangle^2$$

$$\cdot \text{Steady state: } \frac{d}{dt} \langle n(t) \rangle = 0 \Rightarrow (\beta + \delta - \gamma) \langle n(t) \rangle - \delta \langle n(t) \rangle^2 = 0 \Rightarrow$$

$$\Rightarrow \langle n(t) \rangle = 0 \quad \text{or} \quad \langle n(t) \rangle = \frac{\beta + \delta - \gamma}{\delta}$$

$$F(x) = (\beta + \delta - \gamma)x - \delta x^2 \Rightarrow F'(x) = \beta + \delta - \gamma - 2\delta x.$$

$$\hookrightarrow F'(0) = \beta + \delta - \gamma \Rightarrow \underline{\langle n(t) \rangle = 0 \text{ is stable if } \beta + \delta - \gamma < 0 \Rightarrow \gamma > \beta + \delta}$$

$$\hookrightarrow F'\left(\frac{\beta + \delta - \gamma}{\delta}\right) = \beta + \delta - \gamma - 2(\beta + \delta - \gamma) = \gamma - \beta - \delta \Rightarrow$$

$$\Rightarrow \underline{\langle n(t) \rangle = \frac{\beta + \delta - \gamma}{\delta} \text{ is stable if } \beta + \delta - \gamma > 0 \Rightarrow \gamma < \beta + \delta}$$

We can even get the analytical solution for this equation.

Take, for conciseness:  $\beta + \delta - \gamma \rightarrow a$ ,  $\delta \rightarrow b$ ,  $\langle n(t) \rangle \rightarrow x(t)$ :

$$\frac{dx}{dt} = ax - bx^2, \quad a, b > 0. \quad \text{Let's solve this:}$$

$$\Rightarrow \int dt = \int \frac{dx}{x(a - bx)}, \quad x \neq 0, \quad x \neq a/b$$

$$* \frac{1}{x(a - bx)} = \frac{A}{x} + \frac{B}{a - bx} \Rightarrow 1 = A(a - bx) + Bx \Rightarrow Ab = B, \\ Aa = 1 \Rightarrow A = \frac{1}{a} \Rightarrow B = \frac{b}{a}$$

$$\therefore t = \int dx \left( \frac{1}{ax} + \frac{b}{a(a - bx)} \right) = \frac{1}{a} \ln(ax) + \frac{b}{ab} \ln(a^2 - abx) + C$$

$$= \frac{1}{a} \ln\left(\frac{x}{a - bx}\right) + C \Rightarrow \frac{x}{a - bx} = e^{at - C} \Rightarrow x = e^{at - C}(a - bx) \Rightarrow$$

$$\Rightarrow x(1+be^{at-c}) = ae^{at-c} \Rightarrow x(t) = \frac{ae^{at-c}}{1+be^{at-c}}$$

$$* X(0) = X_0 = \frac{ae^{-c}}{1+b\bar{e}^{-c}} \Rightarrow ae^{-c} = X_0(1+b\bar{e}^{-c}) \Rightarrow \bar{e}^{-c}(a-bx_0) = X_0 \Rightarrow$$

$$\Rightarrow \bar{e}^{-c} = \frac{X_0}{a-bx_0}$$

$$\therefore X(t) = \frac{\frac{ax_0}{a-bx_0} e^{at}}{1 + \frac{bx_0}{a-bx_0} e^{at}} = \frac{ax_0 e^{at}}{a-bx_0(1-e^{at})}$$

Taking the limit  $t \rightarrow \infty$ , we should expect to recover our equilibrium points  $X=0$  and  $X=\frac{b}{a}$ . And that's exactly what we get:

$$* a > 0: \lim_{t \rightarrow \infty} X(t) = \lim_{t \rightarrow \infty} \frac{\frac{ax_0}{a-bx_0}}{\cancel{e^{-at}} + \frac{bx_0}{a-bx_0}} = \boxed{\frac{a}{b}}$$

$$* a < 0: \lim_{t \rightarrow \infty} X(t) = \frac{0}{1+0} = \boxed{0}$$

- How do the results you obtained in the previous point change when you introduce the effect of fluctuations (i.e., you use a Gaussian approximation instead of a mean-field one)? Does  $\langle n(t \rightarrow \infty) \rangle$  change? If so, how does the new correction factor relate to the value you obtained using a mean-field approximation?

We already have the equation for the average  $\langle n(t) \rangle$ :

$$\frac{d}{dt} \langle n(t) \rangle = (\beta + \gamma - \delta) \langle n(t) \rangle - \delta \langle n^2(t) \rangle,$$

but what about  $\langle n^2(t) \rangle$ ?

$$\text{We know that } \frac{d}{dt} \langle n^2(t) \rangle = \sum_l \langle l(l-2n) R_{n \rightarrow n-l} \rangle =$$

$$= \langle -1(-1-2n) \beta n \rangle + \langle 1 \cdot (1-2n) (\gamma n + \delta n(n-1)) \rangle =$$

$$= \beta \langle n(t) \rangle + 2\beta \langle n^2(t) \rangle + \gamma \langle n(t) \rangle - 2\gamma \langle n^2(t) \rangle + \delta \langle n(t)(n(t)-1) \rangle +$$

$$- 2\delta \langle n^2(t)(n(t)-1) \rangle =$$

$$= (\beta + \gamma - \delta) \langle n(t) \rangle + 2\left(\beta - \gamma + \frac{3}{2} \delta\right) \langle n^2(t) \rangle - 2\delta \langle n^3(t) \rangle$$

$$* \text{G.A.: } \langle n^3(t) \rangle = 3 \langle n(t) \rangle \langle n^2(t) \rangle - 2 \langle n(t) \rangle^3$$

$$\therefore \frac{d}{dt} \langle n^2(t) \rangle = (\beta + \gamma - \delta) \langle n(t) \rangle + (2\beta - 2\gamma + 3\delta) \langle n^2(t) \rangle +$$

$$+ 4\delta \langle n(t) \rangle^3 - 6\delta \langle n(t) \rangle \langle n^2(t) \rangle$$

Now we have our closed system of equations:

$$\frac{d}{dt} \langle n(t) \rangle = (\beta + \delta - \gamma) \langle n(t) \rangle - \delta \langle n^2(t) \rangle = F(\langle n(t) \rangle, \langle n^2(t) \rangle)$$

$$\begin{aligned} \frac{d}{dt} \langle n^2(t) \rangle &= (\beta + \gamma - \delta) \langle n(t) \rangle + (2\beta - 2\gamma + 3\delta) \langle n^2(t) \rangle + \\ &\quad + 4\delta \langle n(t) \rangle^3 - 6\delta \langle n(t) \rangle \langle n^2(t) \rangle = g(\langle n(t) \rangle, \langle n^2(t) \rangle) \end{aligned}$$

Let's find it's Fixed Points:

Take  $\langle n(t) \rangle \rightarrow x, \langle n^2(t) \rangle \rightarrow y$ :

$$* \frac{dx}{dt} = 0 \Rightarrow (\beta + \delta - \gamma)x - \delta y = 0 \Rightarrow y = \frac{\beta + \delta - \gamma}{\delta} x$$

$$* \frac{dy}{dt} = 0 \Rightarrow (\beta + \gamma - \delta)x + (2\beta - 2\gamma + 3\delta)y + 4\delta x^3 - 6\delta xy = 0$$

$$\Rightarrow (\beta + \gamma - \delta)x + (2\beta - 2\gamma + 3\delta)(\beta - \gamma + \delta) \frac{x}{\delta} + 4\delta x^3 - 6(\beta - \gamma + \delta)x^2 = 0.$$

$1^{st} \text{ solution: } x=0 \Rightarrow y=0$

$$\Rightarrow 4\delta x^2 - 6(\beta - \gamma + \delta)x + \beta + \gamma - \delta + \frac{1}{\delta}(2\beta - 2\gamma + 3\delta)(\beta - \gamma + \delta) = 0 \Rightarrow$$

$$ax^2 + bx + c = 0, \quad a = 4\delta, \quad b = -6(\beta - \gamma + \delta),$$

$$c = \beta + \gamma - \delta + \frac{1}{\delta}(2\beta - 2\gamma + 3\delta)(\beta - \gamma + \delta).$$

$$\Rightarrow x_{\pm} = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}, \quad y_{\pm} = \frac{\beta - \gamma + \delta}{\delta} x_{\pm}.$$

$$\text{But } x_{\pm} \in \mathbb{R} \Leftrightarrow b^2 - 4ac \geq 0 \Rightarrow$$

$$\Rightarrow 36(\beta^2 + \gamma^2 + \delta^2 - 2\beta\gamma + 2\beta\delta - 2\gamma\delta) - 16[\beta\delta + \gamma\delta - \delta^2 + 2\beta^2 + 2\gamma^2 + 3\delta^2 - 4\beta\gamma + 5\beta\delta - 5\gamma\delta] \geq 0 \Rightarrow$$

$$\Rightarrow 4(\beta^2 + \gamma^2 + \delta^2) - 8\beta\gamma - 24\beta\delta - 8\gamma\delta \geq 0 \Rightarrow \beta^2 + \gamma^2 + \delta^2 - 2\beta\gamma - 6\beta\delta - 2\gamma\delta \geq 0 \Rightarrow$$

$$\Rightarrow (\beta - \gamma + \delta)^2 - 8\beta\delta \geq 0$$

\* If  $(\beta - \gamma + \delta)^2 < 8\beta\delta$ , the only fixed point is  $x = y = 0$ .

Let's check it's stability:

$$\cdot \frac{\partial F}{\partial x} \Big|_{x=y=0} = \beta - \gamma + \delta ; \quad \cdot \frac{\partial F}{\partial y} \Big|_{x=y=0} = -\delta ;$$

$$\cdot \frac{\partial g}{\partial x} \Big|_{x=y=0} = \beta + \gamma - \delta ; \quad \frac{\partial g}{\partial y} \Big|_{x=y=0} = 2\beta - 2\gamma + 3\delta$$

$$M = \begin{pmatrix} \beta - \gamma + \delta & -\delta \\ \beta + \gamma - \delta & 2\beta - 2\gamma + 3\delta \end{pmatrix}$$

$$\text{Tr } M = 3\beta - 3\gamma + 4\delta$$

$$\det M = 2\beta^2 + 2\gamma^2 + 2\delta^2 - 4\beta\gamma + 6\beta\delta - 4\gamma\delta = 2[(\beta - \gamma + \delta)^2 + \beta\delta] > 0$$

If  $m_1$  and  $m_2$  are the eigenvalues of  $M$ , having  $\det M > 0$  means  $m_1$  and  $m_2$  have the same sign, if  $m_1, m_2 \in \mathbb{R}$ .

If  $m_1, m_2$  are complex,  $\det M > 0$ ,  $\text{Re}(m_1) = \text{Re}(m_2) > 0$ . We can then determine the sign of both eigenvalues by  $\text{Tr } M$ .

$$\text{Tr } M > 0 \Leftrightarrow m_1, m_2 > 0, \quad \text{Tr } M < 0 \Leftrightarrow m_1, m_2 < 0.$$

Therefore,  $x=y=0$  will be stable if  $m_1, m_2 < 0 \Rightarrow \text{Tr } M < 0 \Rightarrow$   
 $\Rightarrow 3\beta - 3\gamma + 4\delta < 0$ .

\* Now, let's consider  $(\beta - \gamma + \delta)^2 \geq 8\beta\delta$ . In this case we also have the equilibrium point  $x=y=0$ , and its stability will be the same as before, i.e. stable if  $3\beta - 3\gamma + 4\delta < 0$ .

The other two equilibrium points are

$$x_{\pm} = \frac{6(\beta - \gamma + \delta) \pm \sqrt{(\beta - \gamma + \delta)^2 - 8\beta\delta}}{8\delta}.$$

Notice that  $\sqrt{(\beta - \gamma + \delta)^2 - 8\beta\delta} < |\beta - \gamma + \delta|$ , so:

$x_{\pm} > 0 \Leftrightarrow \beta - \gamma + \delta > 0$ . On the contrary, we can discard  $x_{\pm}$ .

So let's consider  $\beta - \gamma + \delta > 0$ , and find stability conditions for  $x_+$  and  $x_-$ . Calculations will get messy, so let's use Mathematica

(Problem1.nb File), obtaining that  $x_-$  is never stable, and  $x_+$  is stable if  $\det M > 0$  and  $\text{Tr } M < 0$ , which happens if:

•  $\beta > \gamma$  and  $\left( \delta < 3\beta + \gamma - 2\sqrt{2}\sqrt{\beta^2 + \beta\gamma} \text{ or } \delta > 3\beta + \gamma + 2\sqrt{2}\sqrt{\beta^2 + \beta\gamma} \right)$ ; or

•  $\beta \leq \gamma \leq 7\beta$  and  $\delta > 3\beta + \gamma + 2\sqrt{2}\sqrt{\beta^2 + \beta\gamma}$ ; or

•  $\gamma > 7\beta$  and  $\delta > \frac{15\beta + 3\gamma}{2}$ .



We conclude that in the Gaussian Approximation we have a different Fixed Point, stable (in G.A.) in specific shown settings. Let's compare it to the nontrivial fixed point of the mean field approximation:

$$\Delta = \frac{3(\beta - \gamma + \delta) + \sqrt{(\beta - \gamma + \delta)^2 - 8\beta\delta}}{4\delta} - \frac{\beta - \gamma + \delta}{\delta} =$$

$$= \frac{-(\beta - \gamma + \delta) + \sqrt{(\beta - \gamma + \delta)^2 - 8\beta\delta}}{4\delta} < 0, \text{ given } (\beta - \gamma + \delta)^2 > 8\beta\delta.$$

We see that M.F.A. predicts a higher value than G.A., but the difference will depend on the system's parameters:

$$\beta = 2, \gamma = 1 \Rightarrow \frac{-(1 + \delta) + \sqrt{(1 + \delta)^2 - 16\delta}}{4\delta} = \frac{-1 - \delta + \sqrt{1 + \delta^2 - 14\delta}}{4\delta}$$

- Fix  $\beta = 2$  and  $\gamma = 1$ . Compare, for three different values of  $\delta$  ( $\delta = 10^{-1}, 10^{-2}, 10^{-3}$ ), the analytical predictions you obtained for  $\langle n(t \rightarrow \infty) \rangle$  with numerical simulations of the stochastic process using Gillespie's algorithm. For each value of  $\delta$ , produce a figure that shows the number of particles as a function of time. Make sure that you choose a time interval long enough so the system reaches the stationary state. In each figure include: 5 realizations of the stochastic dynamics  $n(t)$ , the mean value that you calculate by averaging over 100 individual realizations, and the analytical approximations obtained with the mean-field and the Gaussian approximation. Discuss your results.

Code in Problem1.ipynb file.