1 Problem 1

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

$$\mathrm{X} \xrightarrow{\beta} \mathrm{X} + \mathrm{X}$$

$$\mathrm{X} \xrightarrow{\gamma} \emptyset$$

$$\mathrm{X} + \mathrm{X} \xrightarrow{\delta[n]} \mathrm{X}$$

where the first reaction accounts for reproduction of X-particles at rate β, the second, for spontaneous removal of X-particles at rate γ, 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, $p(n,t)$.

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

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

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

$$\boxed{\begin{aligned} \frac{\partial P(n,t)}{\partial t} = {} & \beta(n-1)P(n-1,t) + (n+1)(\gamma + \delta n)P(n+1,t) + \\ & -n(\beta + \gamma + \delta(n-1))P(n,t) \end{aligned}}$$

- 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., $\langle n(t \to \infty)\rangle$, and its stability depend on β, γ, and δ?

$$\langle n(t)\rangle = \sum_{n=0}^{\infty} n P(n,t) \Rightarrow \frac{d}{dt}\langle n(t)\rangle = \frac{d}{dt}\sum_{n=0}^{\infty} n P(n,t) =$$

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

$$-\sum_{n=0}^{\infty} n^2\left(\beta+\gamma+\delta(n-1)\right)P(n,t).$$

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

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

$$\therefore \frac{d}{dt}\langle n(t)\rangle = \sum_{n=0}^{\infty} nP(n,t)\left[\beta-\gamma-\delta(n-1)\right] =$$

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

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

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

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

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

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

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

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

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

We can even get the analytical solution for this equation.

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

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

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

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

$$Aa = 1 \Rightarrow A = \frac{1}{a} \Rightarrow B = \frac{b}{a}$$

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

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

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

$$* \; x(0) = x_0 = \frac{ae^{-c}}{1+be^{-c}} \Rightarrow ae^{-c} = x_0\left(1+be^{-c}\right) \Rightarrow e^{-c}(a-bx_0) = x_0 \Rightarrow$$

$$\Rightarrow e^{-c} = \frac{x_0}{a-bx_0}$$

$$\boxed{\therefore \; x(t) = \frac{\frac{ax_0}{a-bx_0}e^{at}}{1+\frac{bx_0}{a-bx_0}e^{at}} = \frac{ax_0e^{at}}{a-bx_0(1-e^{at})}}$$

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

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

$$* \; a<0: \; \lim_{t\to\infty} x(t) = \frac{0}{1+0} = \boxed{0}.$$

- 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 $\langle n(t \to \infty) \rangle$ 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 $\langle n(t) \rangle$:

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

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

We know that $\frac{d}{dt}\langle n^2(t)\rangle = \sum_{\ell} \langle \ell(\ell-2n)\Omega_{n\to n-\ell}\rangle =$

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

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

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

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

$$\therefore \frac{d}{dt}\langle n^2(t)\rangle = (\beta+\gamma-\delta)\langle n(t)\rangle + (2\beta-2\gamma+3\delta)\langle n^2(t)\rangle +$$
$$+4\delta\langle n(t)\rangle^3 - 6\delta\langle n(t)\rangle\langle n^2(t)\rangle$$

Now we have our closed system of equations:

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

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

Let's find it's fixed points:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Let's check it's stability:

- $\left.\dfrac{\partial f}{\partial x}\right|_{x=y=0} = \beta-\gamma+\delta$; - $\left.\dfrac{\partial f}{\partial y}\right|_{x=y=0} = -\delta$;

- $\left.\dfrac{\partial g}{\partial x}\right|_{x=y=0} = \beta+\gamma-\delta$; $\left.\dfrac{\partial g}{\partial y}\right|_{x=y=0} = 2\beta-2\gamma+3\delta$

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

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

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

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

$TrM > 0 \iff m_1, m_2 > 0$, $TrM < 0 \iff m_1, m_2 < 0$.

Therfore, $x = y = 0$ will be stable if $m_1, m_2 < 0 \Rightarrow TrM < 0 \Rightarrow$
$\Rightarrow 3\beta - 3\gamma + 4\delta < 0$.

* 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 it's 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 $\sqrt{(\beta^2 - \gamma + \delta)^2 - 8\beta\delta} < |\beta - \gamma + \delta|$, so:

$x_\pm > 0 \iff \beta - \gamma + \delta > 0$. 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 $TrM < 0$, 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 $\delta > \dfrac{15\beta + 3\gamma}{2}$.

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 δ ($\delta = 10^{-1}$, 10^{-2}, 10^{-3}), the analytical predictions you obtained for $\langle n(t \to \infty)\rangle$ with numerical simulations of the stochastic process using Gillespie's algorithm. For each value of δ, produce a figure that shows the number of particles as a function of time. Make sure that you some 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.