Mathematics and Computational Methods for Complex Systems

Assignment 2

Analytical Work

1.

$$[A] + [B] = N$$

$$\therefore [A] = N - [B]$$

$$[\dot{B}] = \beta \frac{[B]}{N}[A] - \gamma[B]$$

$$\therefore [\dot{\boldsymbol{B}}] = \boldsymbol{\beta} \frac{[\boldsymbol{B}]}{\boldsymbol{N}}(\boldsymbol{N} - [\boldsymbol{B}]) - \boldsymbol{\gamma}[\boldsymbol{B}]$$

2.

$$[\dot{B}] = \beta \frac{[B]}{N}(N - [B]) - \gamma[B] = 0$$

Rearrange to make [B] the subject

$$[B] = N - N\frac{\gamma}{\beta}$$

Therefore stationary point where:

$$[\boldsymbol{B}] = \boldsymbol{N} - \frac{\boldsymbol{N}}{\boldsymbol{R_0}} = \boldsymbol{B}^*$$

$$[\dot{A}] = \beta \frac{N - [A]}{N} A - \gamma(N - A) = 0$$

Rearrange to make [A] the subject

$$[A] = N\frac{\gamma}{\beta}$$

and where:

$$[\boldsymbol{A}] = \frac{\boldsymbol{N}}{\boldsymbol{R_0}} = \boldsymbol{A}^*$$

We know this is a valid point at which system is in equilibrium, as it continues to satisfy ***[A]* + [B]* = N***, and both classes have a rate of change of 0 at this same point.

There also exists a stationary point where **[B] = 0, [A] = N**, and where**[A] and [B]** (and N) **= 0**. Therefore, in all cases where $N > 0$, there only exist 2 stationary points.

$$\frac{\partial[\dot{B}]}{\partial[B]} = \beta\frac{[A]}{N} - \gamma \qquad \frac{\partial[\dot{B}]}{\partial[A]} = \beta\frac{[B]}{N}$$

$$\frac{\partial[\dot{A}]}{\partial[B]} = -\beta\frac{[A]}{N} + \gamma \qquad \frac{\partial[\dot{A}]}{\partial[A]} = -\beta\frac{[B]}{N}$$

$$J = \begin{pmatrix} \beta\frac{[A]}{N} - \gamma & \beta\frac{[B]}{N} \\ -\beta\frac{[A]}{N} + \gamma & -\beta\frac{[B]}{N} \end{pmatrix}$$

Note: I have used σ to denote the eigenvalues as opposed to the conventional γ

$$J(0,0) = \begin{pmatrix} -\gamma & 0 \\ \gamma & 0 \end{pmatrix} \qquad \begin{vmatrix} -\gamma - \sigma & 0 \\ \gamma & -\sigma \end{vmatrix} = 0 \qquad \therefore \boldsymbol{\sigma = 0 \; or \; -\gamma}$$

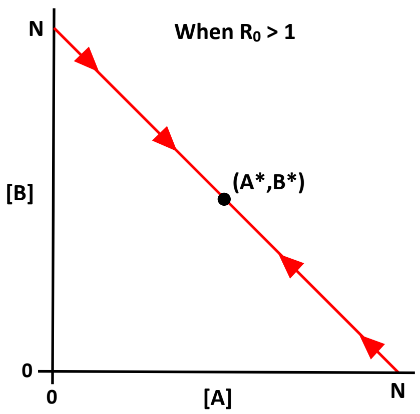
This is a stable equilibrium where [A] and [B] = 0, as γ is a positive real number resulting in a negative eigenvalue. Note this can only occur in the case that N = 0, so this should come as no surprise.

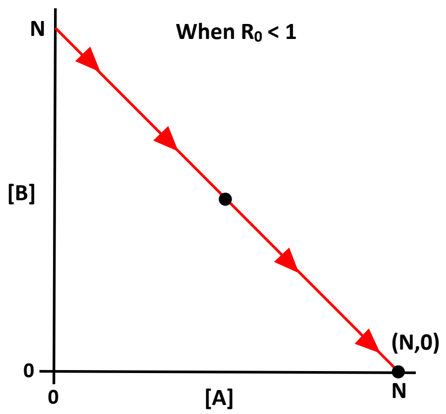
$$J(0,N) = \begin{pmatrix} \beta - \gamma & 0 \\ \gamma - \beta & 0 \end{pmatrix} \qquad \begin{vmatrix} \beta - \gamma - \sigma & 0 \\ \gamma - \beta & -\sigma \end{vmatrix} = 0 \qquad \therefore \boldsymbol{\sigma = 0 \; or \; \beta - \gamma}$$

In the case that [B] = 0 and [A] = N, its stability depends on the relative sizes of β and γ, in the case that β is larger, $R_0 > 1$ and the system is unstable. If γ is larger, $R_0 < 1$, and it is stable. In the case that they are equal ($R_0 = 1$), we get a centre subspace, specifically a slow manifold, the stability of which we can't be certain.

$$J(B^*, A^*) = \begin{pmatrix} 0 & \beta - \gamma \\ 0 & \gamma - \beta \end{pmatrix} \qquad \begin{vmatrix} -\sigma & \beta - \gamma \\ 0 & \gamma - \beta - \sigma \end{vmatrix} = 0 \qquad \therefore \boldsymbol{\sigma = 0 \; or \; \gamma - \beta}$$

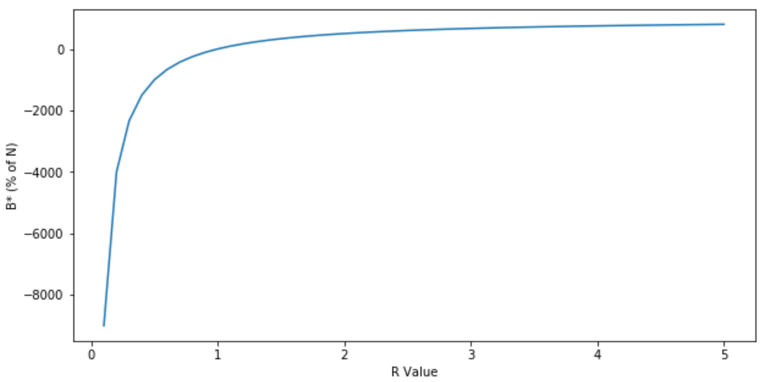
n the case that [B] = $N - \frac{N}{R_0}$ and [A] = $\frac{N}{R_0}$, its stability depends on the relative sizes of β and γ, in the case that β is larger, $R_0 > 1$ and the system is stable. If γ is larger, $R_0 < 1$, it is unstable. In the case that they are equal ($R_0 = 1$), we once again get a centre subspace, specifically a slow manifold, the stability of which is uncertain.





3)

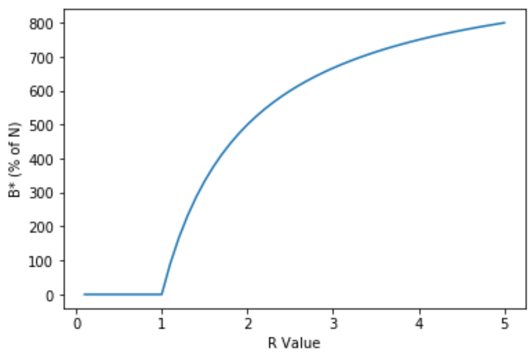
Figure 1: Graph to Show How Varying R Impacts B*



Please refer to the included .ipynb file for the associated code to produce the above. Note how when $R_0 = 1$, B* = 0, this corroborates our findings in the previous section. When R > 1, the equilibrium extends above 0, tending towards N in a logarithmic manner. As soon as R_0 is reduced below 1, the value of B* is made exponentially more negative – in practice the value of B won't be able to go below 0, but regardless this is exemplary of the stable equilibrium where A = N and B = 0.

On the right is an identical plot, except values of B* have been restricted to those that are strictly positive as per the problem description. And as such I anticipate it to be the more valuable metric to draw comparison with should such a comparison be necessary.

Figure 2 – Bifurcation with restricted range



4. a)

$$[\dot{B}] = \beta\frac{[B]}{N}(N-[B]) - \gamma[B]$$

Rearrange

$$[\dot{B}] = \frac{\beta[B]N}{N} - \frac{\beta[B]^2}{N} - \gamma[B]$$

$$[\dot{B}] = \beta[B] - \gamma[B] - [B]^2\frac{\beta}{N}$$

$$[\dot{B}] = [B](\beta-\gamma) - [B]^2\frac{\beta}{N}$$

Divide both sides by $[B]^2$

$$\frac{\mathbf{1}}{[\boldsymbol{B}]^2}[\dot{\boldsymbol{B}}] = \frac{\mathbf{1}}{[\boldsymbol{B}]}(\boldsymbol{\beta} - \boldsymbol{\gamma}) - \frac{\boldsymbol{\beta}}{\boldsymbol{N}}$$

b)

$$y = \frac{1}{[B]} \qquad \therefore\ \dot{y} = -\frac{1}{[B]^2} = -y^2$$

$$y^2[\dot{B}] = y(\beta - \gamma) - \frac{\beta}{N}$$

$$-\dot{y}[\dot{B}] = y(\beta - \gamma) - \frac{\beta}{N}$$

$$\dot{y} = \frac{dy}{d[B]}$$

$$-\dot{y}[\dot{B}] = -\frac{dy}{d[B]}\frac{d[B]}{dt} = -\frac{dy}{dt}$$

$$\therefore \frac{\boldsymbol{dy}}{\boldsymbol{dt}} = \boldsymbol{y}(\boldsymbol{\gamma} - \boldsymbol{\beta}) + \frac{\boldsymbol{\beta}}{\boldsymbol{N}}$$

c)

$$\frac{dy}{dt} = -\lambda\, y(t) + I$$

$$\lambda = (\beta - \lambda) \qquad I = -\frac{\beta}{N}$$

$$y(t) = \left(\frac{I}{kc\lambda}e^{\lambda t} + c\right)ke^{-\lambda t}$$

$$y(t) = kce^{-\lambda t} + \frac{I}{\lambda}$$

$$\boldsymbol{y}(\boldsymbol{t}) = \boldsymbol{kce}^{(\boldsymbol{\gamma} - \boldsymbol{\beta})\boldsymbol{t}} + \frac{\boldsymbol{\beta}}{\boldsymbol{N}(\boldsymbol{\beta} - \boldsymbol{\gamma})}$$

d)

$$[B](t) = \frac{1}{y(t)}$$

$$[B](t) = \left(kce^{(\gamma-\beta)t} + \frac{\beta}{N(\beta-\gamma)}\right)^{-1}$$

$[B] = B_0$ when t=0,

$$B_0 = \left(kc + \frac{\beta}{N(\beta-\gamma)}\right)^{-1}$$

$$\therefore kc = \frac{1}{B_0} - \frac{\beta}{N(\beta-\gamma)}$$

Sub in to [B](t) and rearrange

$$[B](t) = \left(\left(\frac{1}{B_0} - \frac{\beta}{N(\beta-\gamma)}\right)e^{(\gamma-\beta)t} + \frac{\beta}{N(\beta-\gamma)}\right)^{-1}$$

$$[B](t) = \left(\left(\frac{1}{B_0} - \frac{1}{B^*}\right)e^{(\gamma-\beta)t} + \frac{1}{B^*}\right)^{-1}$$

$$[B](t) = \frac{1}{\left(\frac{1}{B_0} - \frac{1}{B^*}\right)e^{(\gamma-\beta)t} + \frac{1}{B^*}}$$

$$\boldsymbol{[B](t) = \frac{B^*}{\left(\frac{B^*}{B_0} - 1\right)e^{(\gamma-\beta)t} + 1}}$$

5)

Figure 3.1 – How B(t) varies with R

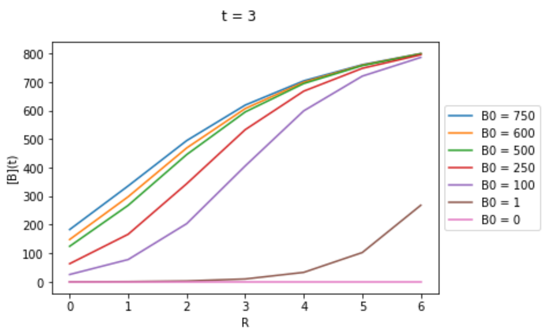
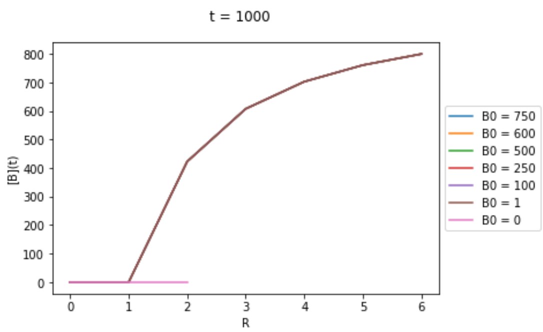


Figure 3.2 – How B(t) varies with R



When [B] = 0, we find ourselves at a stable equilibrium we discovered earlier, and so in the case that $B_0 = 0$, the system will remain as such. Above you can see the value of B(t) versus R_0, for various different initial B values, both when t = 3 and when t = 1000. With the exception of when B_0

= 0, all lines do indeed converge to B* given a large enough value for T. Although it may not seem apparent when looking at our initial bifurcation plot from section 3, that is simply due to the extended range shown, as soon as we restrict the value of B* to being strictly positive, the two look almost identical.

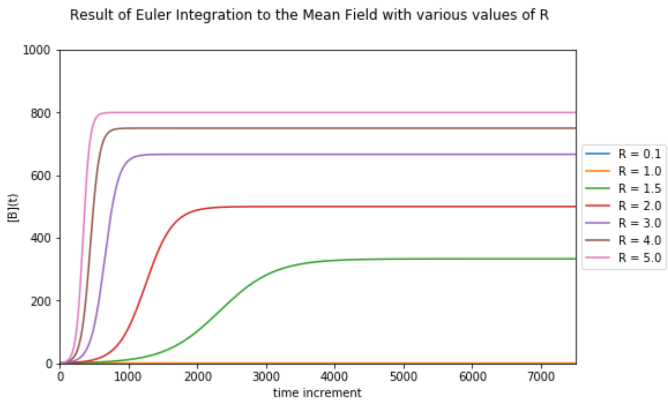


Figure 4 – How B(t) varies over time with different values of R_0

Above you can see our plotted Euler Integration results, initially they may not seem to agree visually, however this is simply because we have plotted for every value of *t* at certain increments of R, as opposed to the other way around. If you observe the value B(t) converges towards for a given R value, they are very consistent between plots, serving as the visual conformation we seek.

When R_0 = 1, the value of B* is 0, since $N - \frac{N}{1} = 0$ regardless of any other parameters. This is visually confirmed in these graphs, by the convergence towards B(t) = 0 seen in figures 3, in the domain R ≤ 1, as well as in figure 4 by the line R=1 plateauing where B(t) = 0.

When the value of gamma changes, under normal circumstances this would directly impact the value of R, with a larger gamma leading to a smaller R. However provided the value of beta is adjusted accordingly to maintain a consistent R value, varying gamma would bear no effect on the system, since it is only concerned with the ration between the two (R_0).

Simulation Work

For simulation work, please refer to the included Gillespie.ipynb file

Critical Thinking

1)

One real life system that this model could be representative of is that of a chemical reaction, where A and B represent the relative quantities of each reactant, and R a catalyst. If B is the fuel in this reaction, and R an anticatalyst or inhibitor, then the critical regime would be of interest as it identifies the critical value of R that is sufficient to sustain the reaction – too little and the reaction is accelerated, depleting B. Depending on the nature of the reaction, the equilibria (B*) could be indicative of the heat or energy output of the reaction. A specific reaction that seems applicable is that which occurs in a nuclear reactor, R may represent how deeply the control rods are inserted, and the equilibria the energy output. Note the dangerous spikes which would likely lead to combustion as soon as R drops below the critical regime. The issue I have with this idea is I struggle to specify exactly what A and B represent as states of an individual within a fixed population, in some cases they may be the charge of particles perhaps, although may limited chemistry knowledge prevents me from going in to any further depth here.

The alternative that seems potentially more fitting is modelling the spread of disease within a population, where B represents those who are infected, and A those who are not. In this case, β is a constant dictating how contagious the disease is, and γ is the rate at which people recover. The critical regime is now of interest is that is the ratio between the two that must be achieved for convergence towards a disease-free environment, anything greater than 1 and the infection rate will instead converge towards the non-zero equilibrium, the overall infection rate of the disease.

In both cases there are many experiments that could be carried out, however the costs and potential risks make them far better suited to be being carried out on a model such as this one. In the case of the second example in particular, I can see it being useful to predict pandemics and outbreaks, as well as learning how to combat them, perhaps with restrictions such as a limited amount of vaccines (provided the code was extended to support such modelling).

2)

If we assume that the system is modelled upon our second idea, it would of course be unrealistic to assume that all members of the population are in contact with each other. One primitive suggestion could be to introduce a constant to denote the amount of people that a given individual may come in to contact with, representative of the population density, and simply scale β with it through multiplication. Varying the new value would have the same effect as we have already seen in doing so with β, however it would allow the 'infectiousness' it denotes to be broken down in to the two separate components – the contagiousness of the disease, and how much contact an individual has with other members of the population.

A more thorough suggestion would be to perhaps assume that individuals only come in to contact with those physically near them and edit the selection operator within the Gillespie algorithm to function more akin to that of a spatial genetic algorithm. Both of these would however be making the assumption that all individuals come in to contact with the same amount of people (excluding the marginal boundary cases in special selection). I believe this could be negated by instead representing the population as a graph, with each vertex representing a member of the population. The degree of each vertex would then represent the amount of other nodes that individual would come in to contact with at each time increment, allowing for the modelling of individuals with varying levels of social connectivity. The selection operator would then have its choice limited to nodes that are adjacent to one that carries the 'infection', changing the state of each one from A to B with a probability proportional to β. This would mean that an individual with 10 interactions per unit of time, would be twice as likely to get infected as someone with 5.

After implementing this proposed change, I anticipate the 'infection' to struggle to bridge the gaps between more separate communities, particularly those that are more isolated (much as is the case in the real world), however those vertexes that are connected by edges with the highest betweenness scores will be the conduits for doing so.