Networks and Complexity

Exercise Sheet 17: Coarse-graining

This is an exercise sheet from the forthcoming book Networks and Complexity. Find more exercises and solutions at https://github.com/NC-Book/NCB

Ex 17.1: Simple change of variables [1]
Consider the system

$$\begin{aligned}\dot{x} &= 2x - 3y \\ \dot{y} &= xy\end{aligned}$$

Rewrite the system in terms of x and the new variable $s = x + y$

Ex 17.2: Simple timescale renormalization [1]
In the system

$$\dot{x} = k(x - x^2)$$

renormalize the timescale to make the parameter k disappear. (Hint: If you are not sure how to do it, renomalise time by a factor a and then decide how you need to chose this factor.)

Ex 17.3: Fast prey [2]
Consider the predator-prey system

$$\begin{aligned}\dot{X} &= rX - aXY - X^2 \\ \dot{Y} &= caXY - dY\end{aligned}$$

a) Look at the system and decide who is the predator.
b) Assume that the dynamics of the predator is much slower than the dynamics of the prey, while the predator still inflicts significant losses on the prey losses on the prey. Which parameter have to be small for this to be the case?
c) Now use time-scale separation coarse-graining to remove the fast prey variable from the system. (There are two cases to consider)

Ex 17.4: Slow-Fast [3]
Analyze the following system

$$\begin{aligned}\dot{x} &= -x^3 + x + y \\ \dot{y} &= -\alpha x\end{aligned}$$

where again $\alpha \ll 1$. What happens in this system in the long run? (Hint: Make sure to check the stability of the slow manifold, the result may be surprising)

Ex 17.5: Michaelis-Menten kinetics [3]
The Holling type-II functional response in ecology has an equivalent in biochemistry that is called the Michaelis-Menten kinetics: In both cases reaction rates involve the factor

$$\frac{Ax}{B + x}$$

where x is a variable. This is the so-called At first glance the appearance of these terms is surprising because they are not mass action terms and neither do such fractions commonly appear in physical laws. So where do they come from?

Let's consider a chemical reaction where an enzyme binds to a substrate to turn it into a product. We will call the substrate X, the product Y , the enzymes that are not bound to substrate E and the complex that is formed if the enzyme is bound to the reactant C. The dynamics are then described by the following reaction system:

$$\begin{aligned} \mathrm{E} + \mathrm{X} &\overset{r}{\to} \mathrm{C} \\ \mathrm{C} &\overset{s}{\to} \mathrm{Y} \end{aligned}$$

In a big biochemical reaction system both X and Y will participate in many other chemical reactions, however the binding and unbinding of the enzyme is a very fast process.

a) Denote the concentrations of X, C, Y, and E by the variables x, c, y, e, respectively. Write ODEs for these variables using mass action. In the ODEs for X and Y include addtional terms $o_x(x)$ and $o_y(y)$ as a placeholder for other reactions that X and Y may be involved in.

b) The equations contain a conservation law. What is the conserved quantity? Call the conserved quantity a, state the conservation law mathematically and prove it by showing $\dot{a} = 0$.

c) We now consider the fast subsystem. In these systems the concentrations of the enzyme are many magnitudes smaller than the concentration of substrate or product. Every enzyme needs to bind to and process many substrate molecules before a there is a significant percentage change in x or y. This justifies considering the variables c and e in isolation for a moment.

   Consider only the ODEs for c and e and find their steady state value e^* of e. Use the conservation law to eliminate all instances of c. (Hint: x is a constant in the fast system, so the solution should be a function $e^*(x, s, r, a)$)

d) Show that in the fast system the steady state e^* is stable. (hint: all you need to consider is a one-dimensional ODE)

e) We have now shown that the slow manifold is stable is unconditionally stable, which means the system will just collapse to the slow manifold. So to understand the dynamics of the bigger reaction system that we would normally be interested in we only need to consider the dynamics on the slow manifold.

   Rewrite your differential equation system from part a. Use your insights on the slow manifold to eliminate e and c from the equations for x and y such that these equations only depend on a, r, s and the placeholders $o_x(x)$ and $o_y(y)$. Because c and e no longer appear, you can drop the corresponding equations, so that the result is a 2-dimensional ODE. Show that the Michaelis-Menten kinetics appears and express the parameters A and B of the general form in terms of our parameters a, r, s.

Ex 17.6: Timescale separation in the SIS model [5]

Use timescale separation coarse-graining to find better moment expansions/closures for the SIS model or the adaptive voter model.