The centre manifold of the exciplex mechanism

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We had previously reduced the exciplex mechanism to the following set of dimensionless ODEs:

$$\dot{a} = -2\beta a^2 + c(2\beta + 1), \tag{1a}$$
$$\dot{c} = \beta a^2 - c(\beta + 1). \tag{1b}$$

(I renamed the parameter α to β to make the visual distinction between a and the parameter a bit easier to see.) This system has a single equilibrium point at $(a^*, c^*) = (0, 0)$. The Jacobian evaluated at this point is

$$\mathbf{J}^* = \begin{bmatrix} 0 & 2\beta + 1 \\ 0 & -(\beta + 1) \end{bmatrix}$$

The two eigenvalues of this matrix are $\lambda = 0$ and $\lambda = -(\beta + 1)$. The zero eigenvalue combined with the negative eigenvalue means that we can't determine the local stability of the equilibrium point from the linear stability analysis alone. However, we know that, at least near the equilibrium point, trajectories will move towards a centre manifold along the eigenvector corresponding to the negative eigenvalue. To complete the stability analysis, we therefore need to figure out what happens on the centre manifold.

The first step is to figure out the orientation of the centre manifold near the equilibrium point, which is given by the eigenvector associated with the zero eigenvalue. It is also helpful, in order to have a complete picture of the dynamics, to also determine the stable eigenvector. Eigenvectors satisfy

$$\mathbf{J}^*\mathbf{v} = \lambda\mathbf{v}$$

or

$$(\mathbf{J}^* - \lambda\mathbf{I})\mathbf{v} = \mathbf{0}.$$

For the stable eigenvector, we have

$$\left(\begin{bmatrix} 0 & 2\beta+1 \\ 0 & -(\beta+1) \end{bmatrix} - \begin{bmatrix} -(\beta+1) & 0 \\ 0 & -(\beta+1) \end{bmatrix}\right)\begin{bmatrix} v_1^{(-)} \\ v_2^{(-)} \end{bmatrix} = \mathbf{0}.$$

$$\therefore \begin{bmatrix} \beta+1 & 2\beta+1 \\ 0 & 0 \end{bmatrix}\begin{bmatrix} v_1^{(-)} \\ v_2^{(-)} \end{bmatrix} = \mathbf{0}$$

$$\therefore (\beta+1)v_1^{(-)} + (2\beta+1)v_2^{(-)} = 0.$$

$$\therefore \frac{v_2^{(-)}}{v_1^{(-)}} = -\frac{\beta+1}{2\beta+1}.$$

This is the slope of the stable eigenvector.

We proceed similarly for the centre eigenvector:

$$(\mathbf{J}^* - \lambda\mathbf{I})\mathbf{v} = \mathbf{J}^*\mathbf{v}.$$

$$\therefore \begin{bmatrix} 0 & 2\beta+1 \\ 0 & -(\beta+1) \end{bmatrix}\begin{bmatrix} v_1^{(0)} \\ v_2^{(0)} \end{bmatrix} = \mathbf{0}.$$

$$\therefore (2\beta+1)v_2^{(0)} = -(\beta+1)v_2^{(0)} = 0.$$

The centre eigenvector is therefore $(1, 0)$, i.e. it lies along the a axis or, equivalently, has a slope of zero. As noted in the textbook, this is not always the case, although it happens quite often in irreversible chemical systems with a centre manifold.

We now know that the centre manifold has a Taylor expansion around the equilibrium point of the following form:

$$c_{\mathrm{CM}}(a) = \gamma_2 a^2 + \gamma_3 a^3 + \ldots. \tag{2}$$

The constant term is zero because the equilibrium point passes through the origin, i.e. $c_{\mathrm{CM}}(a^*) = c^*$, and both a^* and c^* are zero. The linear term is zero because the slope of the centre manifold (centre eigenvector) at the equilibrium point is zero. To find the behavior on the centre manifold, we can substitute c_{CM} into equation (1a). This will give us the evolution equation for a on the centre manifold. If we try this, we get

$$\dot{a} = -2\beta a^2 + (2\beta + 1)\left(\gamma_2 a^2 + \gamma_3 a^3 + O(a^4)\right). \tag{3}$$

Our objective from here is to determine the behavior of this differential equation to lowest order in a, since this will in turn determine the behavior near the equilibrium point. This means that we need to figure out (at least) the value of γ_2. To do this, we use the **invariance equation**. The centre manifold is an invariant manifold, i.e. a trajectory, written in the form $c = c_t extCM(a)$. differentiating this equation with respect to time and using the chain rule, we get

$$\frac{dc}{dt} = \frac{dc_{\mathrm{CM}}}{da}\frac{da}{dt}.$$

Every trajectory is a solution of the invariance equation. However, by using what we already know about the centre manifold, namely that its first two Taylor coefficients vanish, we specialize our result to this manifold.

Substituting equation (2) into the invariance equation, we get

$$\begin{aligned}&\beta a^2 - (\beta + 1)\left(\gamma_2 a^2 + \gamma_3 a^3 + O(a^4)\right)\\ &\quad = \left(2\gamma_2 a + 3\gamma_3 a^2 + O(a^3)\right)\left[-2\beta a^2 + (2\beta + 1)\left(\gamma_2 a^2 + \gamma_3 a^3 + O(a^4)\right)\right].\end{aligned}$$

The trick now is to collect all the terms in a^i for each i starting with 2. Since we are only interested in the behavior near equilibrium, we will stop as soon as we are able to determine this behavior, i.e. as soon as we get a nonzero term in equation (3). First, we collect terms in a^2:

$$\beta - (\beta + 1)\gamma_2 = 0.$$
$$\therefore \gamma_2 = \frac{\beta}{\beta + 1}.$$

If we substitute this value of γ_2 into equation (3), we get

$$\begin{aligned}\dot{a} &= a^2\left(-2\beta + \frac{\beta(2\beta + 1)}{\beta + 1}\right) + (2\beta + 1)\left(\gamma_3 a^3 + O(a^4)\right)\\ &\approx -\frac{\beta}{\beta + 1}a^2.\end{aligned}$$

We now have what we want, namely an equation for the evolution on the centre manifold near the equilibrium point. This equation is itself a one-dimensional dynamical system, with a semi-stable equilibrium point at $a = 0$.

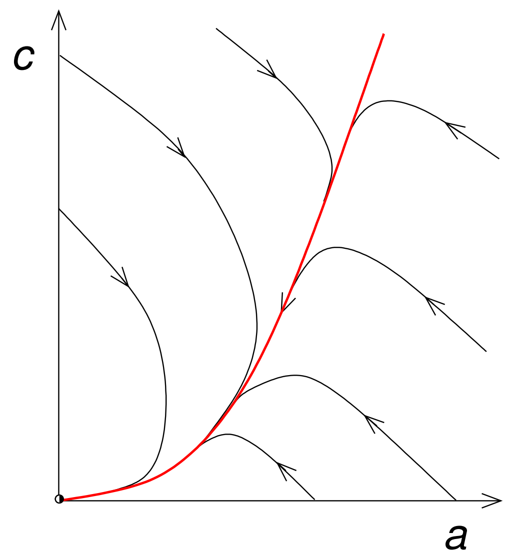

Figure 1: Flow near equilibrium. The centre manifold, which is quadratic near the equilibrium point, is shown in red. The equilibrium point is semi-stable, i.e. only stable when approached from positive values of a.

Thus, for any positive initial conditions near the equilibrium point, after the system has relaxed to the centre manifold, trajectories will approach the equilibrium point. The equilibrium point is therefore an attractor for initial conditions sufficiently close to the equilibrium point. We have to use other techniques (phase-plane analysis, Lyapunov functions) to determine what happens for initial conditions far from equilibrium. Figure 1 summarizes our conclusions.