Chemistry 4010 Lecture 4: Saddle-node and transcritical bifurcations

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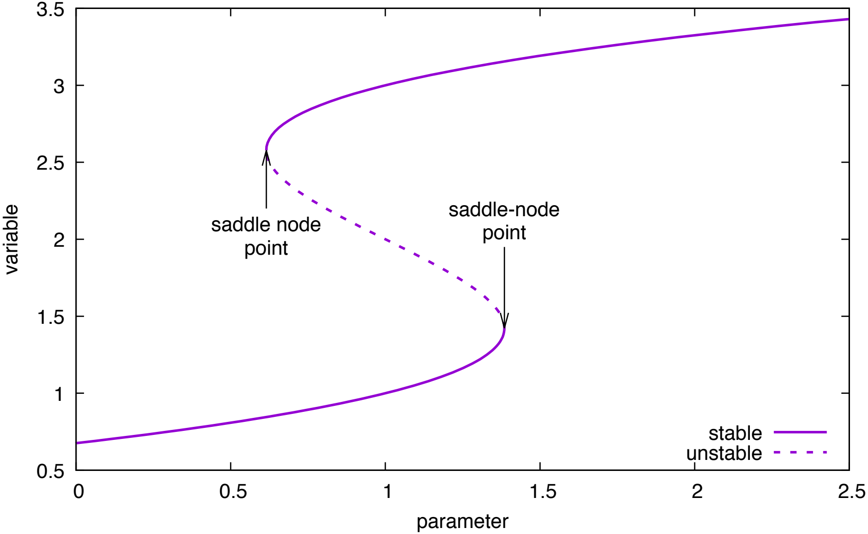
What is a bifurcation?

- Interesting dynamical systems typically have at least one attractor, i.e. some kind of structure in phase space that is reached from almost all points inside a basin of attraction.
- The only type of attractor we have considered so far are equilibrium points.
- A bifurcation is a change in the qualitative behavior of the system that can be observed by scanning the parameters.
- Changes in behavior can include
  - A change in the stability of an attractor
  - A change in the number of attractors
  - A change in the types of attractors
  - Often, several of the above at the same time

Bifurcation diagrams

- A bifurcation diagram shows how the attractors change as we change a parameter.

Saddle-node bifurcation



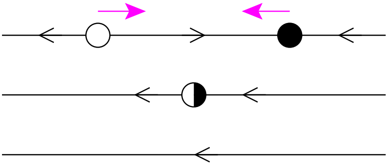
Saddle-node bifurcation

- The name of these bifurcations comes from their appearance in two- and higher-dimensional systems, but they are really a bifurcation in one-dimensional dynamics.
- "Snapshots" of the dynamics:

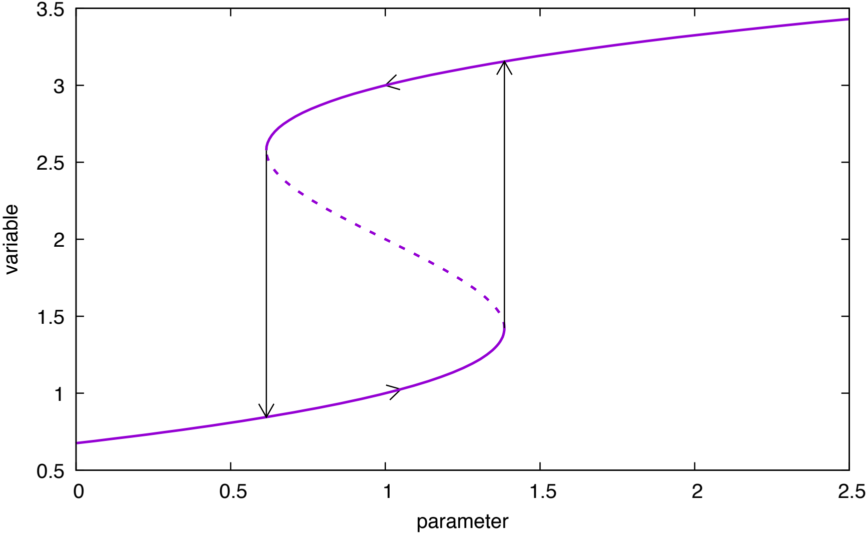
Two steady states:

At bifurcation:

After the bifurcation:

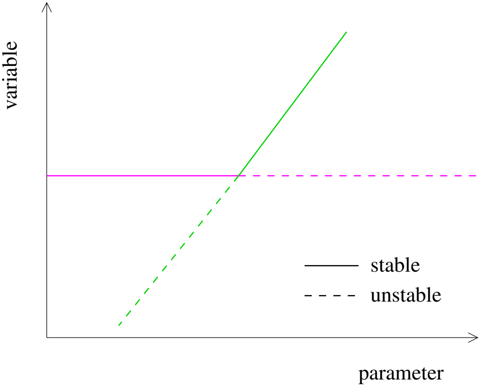


Hysteresis and catastrophes



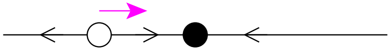
Transcritical bifurcation

- There is one other possibility when a stable and an unstable equilibrium point collide, which is that they pass through each other, exchanging stability as this happens:

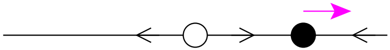


Transcritical bifurcation

- "Snapshots" of the dynamics:

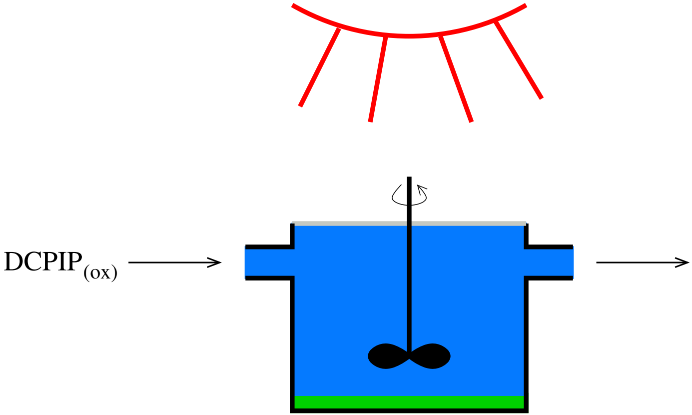
Before the bifurcation: 

At bifurcation: 

After the bifurcation: 

Example 1: a photoactivated enzyme-catalyzed reaction

- Experimental setup:



Hervagault et al., in *Dynamics of Biochemical Systems* (Ricard and Cornish-Bowden, Eds.), Plenum: New York, 1984, pp. 157–169.

Example 1 (continued)

Stirred tank reactors

- The device is a continuous stirred tank reactor (CSTR), with fresh reactant solution pumped in at a rate f (perhaps measured in L/h).
- If the concentration of DCPIP in the inflow is S_0, then the change in concentration of DCPIP due to the inflow is $+fS_0/V$.
- Because of the vigorous stirring, the concentration of DCPIP in the tank is uniform, with value S. The change in concentration of DCPIP due to outflow is $-fS/V$.

Example 1 (continued)

- The thylakoid membrane preparation at the bottom of the reactor needs light to reduce DCPIP.
- The reaction rate is therefore proportional both to the rate of enzyme catalysis (treated in the Michaelis-Menten approximation) and to the intensity of the light that reaches the membrane (I).
- DCPIP absorbs red light strongly, so I depends on S.

Example 1 (continued)

- Overall rate equation:

$$\frac{dS}{dt} = \frac{f}{V}(S_0 - S) - I(S)\frac{\mathfrak{v}_{\max} S}{S + K_M}$$

- Now we just need to figure out $I(S)$ using the Beer-Lambert law:

$$A = \log_{10}\left(\frac{I_0}{I(S)}\right) = \varepsilon LS$$

$$\therefore I(S) = I_0 10^{-\varepsilon SL}$$

- Dimensionless equation:

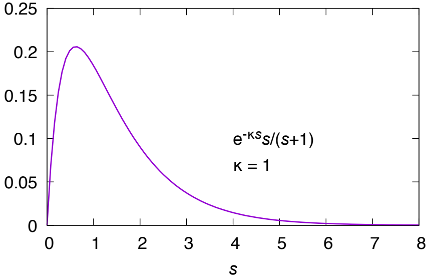
$$\boxed{\dot{s} = s_0 - s - \lambda e^{-\kappa s}\frac{s}{s+1}}$$

Example 1 (continued)

- Equilibrium points satisfy

$$\frac{1}{\lambda}(s_0 - s) = e^{-\kappa s}\frac{s}{s+1}$$

- The left-hand size is a straight line with negative slope.
- Right-hand side:



Example 2: A model for a fatal infectious disease

- There is a fairly standard mass-action formulation for infectious diseases known as "SIR models", originally due to Kermack and McKendrick.

  S: Susceptible
  I: Infected
  R: Recovered

- We're going to look at a very simple model without an R class, so an SI model.
- We're going to assume (for now) 100% mortality in the infected class.

Example 2 (continued)

- Assume the following dynamical equations:

$$\frac{dS}{dt} = rS\left(1 - \frac{S}{K}\right) - cIS$$
$$\frac{dI}{dt} = cIS - mI$$

- c is a transmission coefficient for the infection.