Chemistry 4010 Lecture 5: Andronov-Hopf bifurcations

Marc R. Roussel

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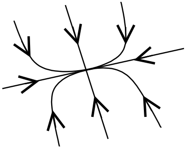
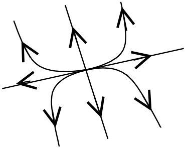
- If all the eigenvalues at an equilibrium point are real and of the same sign, we call that point a node.
- Two possibilities:



eigenvalues negative
stable node

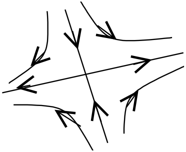


eigenvalues positive
unstable node

Nodes, saddles, foci

Saddle points

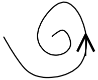
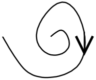
- If there is a mixture of real positive and negative eigenvalues, we have a saddle point



Nodes, saddles, foci

Stable and unstable foci

- In two dimensions, if the eigenvalues are a complex-conjugate pair, the equilibrium point is a focus.
- If there are complex-conjugate eigenvalues in higher dimensions, the classification is sometimes a bit more complex.
- Two possibilities:

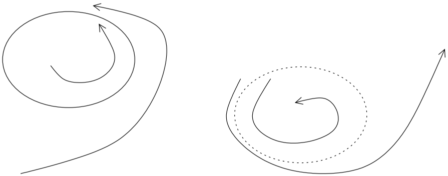
		
real parts of the eigenvalues	negative	positive
	stable focus	unstable focus

Andronov-Hopf bifurcations

- Suppose that we have a parameter in our model that changes the sign of a pair of complex-conjugate eigenvalues from negative to positive, all of the other eigenvalues being real and negative.
- This clearly destabilizes the equilibrium point.
- The change in stability of a focus has another remarkable consequence: it creates a periodic solution called a limit cycle.

Limit cycles

- A limit cycle is a periodic orbit.
- The size, shape and position of the limit cycle in phase space are fixed by the parameters, i.e. the limit cycle is the same for any initial conditions within the cycle's basin of attraction (for stable cycles).
- Two possibilities (in two dimensions, but these are common in higher dimensions as well):

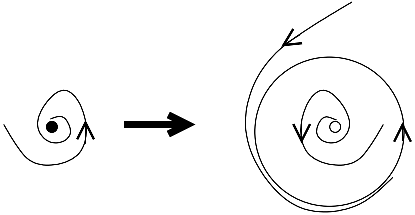


stable limit cycle   unstable limit cycle

Supercritical Andronov-Hopf bifurcation

- When the real part of a complex-conjugate pair of eigenvalues changes sign, there is always an associated bifurcation creating a limit cycle.
- These bifurcations come in two varieties.
- If, as we vary a parameter, the real part of a pair of complex-conjugate eigenvalues of a stable equilibrium point passes cleanly through zero from negative to positive, we often see the "birth" of a stable limit cycle surrounding the equilibrium.
- The limit cycle has zero amplitude at the bifurcation point, and grows as the parameter moves away from the bifurcation.
- This is called a supercritical Hopf bifurcation.

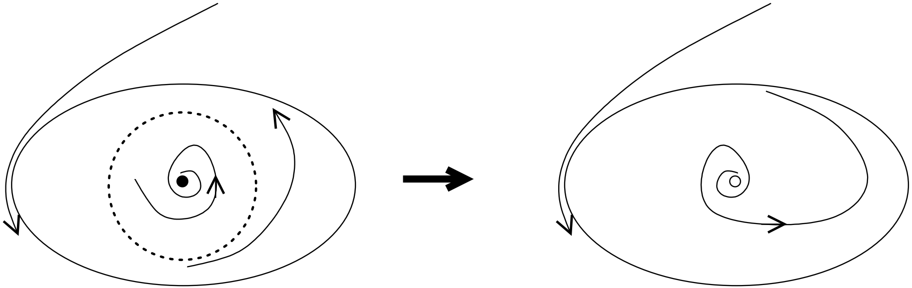
Supercritical Andronov-Hopf bifurcation



Subcritical Andronov-Hopf bifurcation

- The other possibility is that an unstable limit cycle shrinks into the equilibrium point, destabilizing it.
- The eigenvalues of the equilibrium point have the same behavior as before: the real part of a complex conjugate pair crosses cleanly through zero.
- This is called a subcritical Andronov-Hopf bifurcation.
- Such systems often have a stable limit cycle as a second attractor, so the loss of stability of the equilibrium point leaves the limit cycle as the only attractor.
- In this (common) case, if the system is initially operating at the equilibrium point, destabilization results in the sudden onset of large-amplitude oscillations.

Subcritical Andronov-Hopf bifurcation



Note: Catastrophes and hysteresis can result from a subcritical Andronov-Hopf bifurcation.

Distinguishing supercritical and subcritical Andronov-Hopf bifurcations

Supercritical AH: A limit cycle, initially of very small amplitude, grows out of the equilibrium point following the destabilization of the equilibrium.

- The bifurcation is reversible without hysteresis.

Subcritical AH: Following destabilization of the equilibrium point, a large-amplitude motion suddenly appears (e.g. a large-amplitude limit cycle).

- Hysteresis is observed.

Example 1: simplified Sel'kov model

Example 2: Salnikov model for a non-isothermal reactor

- Suppose that we have a chemical reactor to which a fresh supply of a reactant A is continually added, followed by a first-order reaction of A:

$$\xrightarrow{k_0} \mathrm{A} \xrightarrow{k_1} \mathrm{P}$$

- k_0 depends on the pumping rate and on the concentration of A in an external reservoir, so it is externally controlled.
- k_1 depends on T:

$$k_1(T) = Ae^{-E_a/RT}$$

- We therefore have the differential equation

$$\frac{dA}{dt} = k_0 - k_1(T)A$$

Example 2: Salnikov model (continued)

- Suppose that the reaction is exothermic. The heat produced by the reaction will warm the reaction mixture. Thermostating will remove the excess heat, but this is not an instantaneous process.
- In a small interval of time dt, the heat stored in the reactor will increase due to the reaction by

  $$dq_r = -\Delta_r HV \, d\xi$$

  $d\xi = k_1(T)A \, dt$ is the reaction progress (mol/L of A reacted in time dt)
- Heat is also exchanged with the surroundings (thermostatting fluid) at temperature T_0.

  $$dq_e = S\chi(T_0 - T)dt$$

  S is the surface area of the reactor in contact with the thermostatting fluid, and χ is the coefficient of heat transfer.

Example 2: Salnikov model (continued)

- The heat is connected to the change in temperature by

$$dq_r + dq_e = C\,dT$$

  C is the heat capacity of the reactor.

- Thus,

$$C\frac{dT}{dt} = -\Delta_r HVk_1(T)A + S\chi(T_0 - T)$$

  and

$$\frac{dA}{dt} = k_0 - k_1(T)A$$

Example 2: Arrhenius term of the Salnikov model

- From the Arrhenius equation,

$$\begin{aligned}\frac{k_1(T)}{k_1(T_0)} &= \frac{e^{-E_a/RT}}{e^{-E_a/RT_0}}\\ &= \exp\left[\frac{E_a}{R}\left(\frac{1}{T_0}-\frac{1}{T}\right)\right]\\ &= \exp\left[\frac{E_a}{R}\left(\frac{T-T_0}{TT_0}\right)\right]\\ &= \exp\left[\frac{E_a}{RT_0}\left(\frac{T-T_0}{T}\right)\right]\end{aligned}$$

Example 2: Arrhenius term of the Salnikov model

- Dimensionless temperature:

$$\theta = E_a(T - T_0)/RT_0^2$$
$$\therefore T - T_0 = RT_0^2\theta/E_a$$
$$\therefore T = T_0 + RT_0^2\theta/E_a$$
$$\therefore k_1(T) = k_1(T_0)\exp\left(\frac{\theta}{1 + (RT_0/E_a)\theta}\right)$$

- Define $\epsilon = RT_0/E_a$.

$$\therefore k_1(T) = k_1(T_0)f(\theta)$$

with

$$f(\theta) = \exp\left(\frac{\theta}{1 + \epsilon\theta}\right)$$

Gray, Kay and Scott, Proc. R. Soc. Lond. A **416**, 321 (1988)

Example 2: Salnikov model (continued)

- $$\frac{dT}{dt} = -\frac{\Delta_r HV}{C} k_1(T_0)Af(\theta) - \frac{S\chi RT_0^2}{CE_a}\theta$$
- $dT = (RT_0^2/E_a)d\theta$
$$\frac{d\theta}{dt} = -\frac{\Delta_r HVE_a}{CRT_0^2} k_1(T_0)Af(\theta) - \frac{S\chi}{C}\theta$$
- Choose $\tau = S\chi t/C$.
$$\frac{d\theta}{d\tau} = -\frac{\Delta_r HVE_a}{S\chi RT_0^2} k_1(T_0)Af(\theta) - \theta$$

Gray, Kay and Scott, Proc. R. Soc. Lond. A **416**, 321 (1988)

Example 2: Salnikov model (continued)

- Define

$$a = -\frac{\Delta_r HVE_a}{S\chi RT_0^2} k_1(T_0)A$$
$$\therefore \dot{\theta} = af(\theta) - \theta$$

and

$$\dot{a} = \mu - \kappa af(\theta)$$

with

$$\mu = \frac{-\Delta_r HCE_a Vk_1(T_0)}{S^2\chi^2 RT_0^2} k_0$$
$$\kappa = \frac{Ck_1(T_0)}{S\chi}$$

Gray, Kay and Scott, Proc. R. Soc. Lond. A **416**, 321 (1988)

Example 2: Salnikov model (continued)

- Final system of equations:

$$\dot{\theta} = af(\theta) - \theta$$

$$\dot{a} = \mu - \kappa af(\theta)$$

$$f(\theta) = \exp\left(\frac{\theta}{1 + \epsilon\theta}\right)$$

Gray, Kay and Scott, Proc. R. Soc. Lond. A **416**, 321 (1988)