Modelling and Mathematical Methods in Process and Chemical Engineering

Some useful theorems

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1 Fundamental stability theorem

Theorem 1.1. (Stability of linear systems)[1]

Given the linear system with constant coefficients

$$\frac{d\mathbf{x}}{dt} = \mathbf{A}\mathbf{x} \tag{1.1}$$

The origin is

(a) asymptotically stable if $Re\{\lambda_j\} < 0$, $\forall \lambda_j$.

(b) marginally stable if there exists at least one eigenvalue with $Re\{\lambda_j\} = 0$.

(c) unstable if there exists at least one eigenvalue with $Re\{\lambda_j\} > 0$.

Theorem 1.2. (Stability of nonlinear systems)[2]

Given the autonomous nonlinear system

$$\frac{d\mathbf{y}}{dt} = \mathbf{f}(\mathbf{y}) \tag{1.2}$$

a steady state $\mathbf{y}_s$ that is obtained from $\mathbf{f}(\mathbf{y}_s) = 0$ is

(a) asymptotically stable if the corresponding linearized systems is asymptotically stable

(b) unstable if the corresponding linearized system is unstable.

(c) No conclusion can be derived about the nature of the steady state if the corresponding linearized system is marginally stable.

[1] Varma A., Morbidelli M., *Mathematical Methods in Chemical Engineering,* Oxford University Press 1997, section 2.11

[2] Section 2.13

2 Hopf bifurcation theorem

Theorem 2.1. (Hopf Bifurcation)[3]

Consider the n-dimensional autonomous system

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}, \mu) \tag{2.1}$$

which depends upon a parameter μ.

(i) Let $\mathbf{f}(\mathbf{x}_0, \mu_0) = 0$, so that $\mathbf{x}_0$ is the steady state corresponding to the parameter value μ_0.

(ii) Furthermore, let the Jacobian $\mathbf{J}(\mathbf{x}_0, \mu_0)$ have a simple pair of purely imaginary eigenvalues $\lambda(\mu_0) = \pm i\omega_0$ with the remaining eigenvalues having strictly negative real parts.

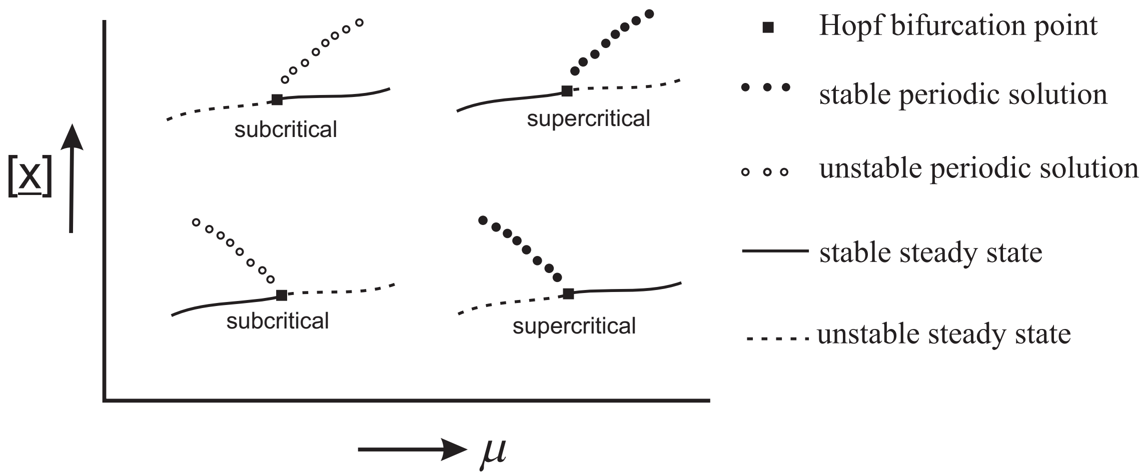
(iii) Finally, let the real part of λ indeed pass through zero as μ crosses μ_0. That is,

$$\left.\frac{d}{d\mu} Re\,(\lambda)\right|_{\mu_0} \neq 0$$

In case all three conditions hold there is a birth of periodic solutions as μ crosses μ_0 (emergence in one direction of crossing and disappearance in the opposite direction).

Remarks

- The period of the oscillatory solution at birth (i.e., a zero-amplitude oscillation) is $2\pi/\omega_0$.
- The stability of the periodic solutions is related to the direction of bifurcation. Possible situations are that near μ_0 either unstable periodic solutions surround stable steady states (*subcritical bifurcation*) or stable periodic solutions surround unstable steady states (*supercritical bifurcation*).



[3] Varma A., Morbidelli M., *Mathematical Methods in Chemical Engineering,* Oxford University Press 1997, section 2.20

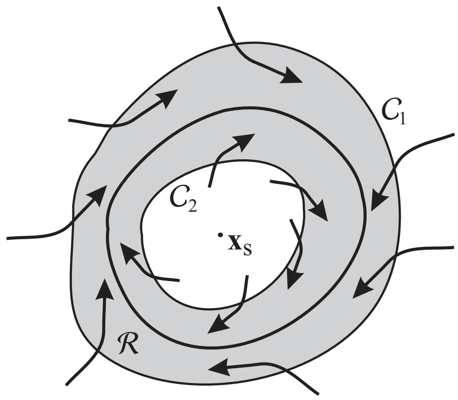
- the Hopf bifurcation theorem is a strictly local result. It provides information only near the bifurcation point, as the parameter μ crosses μ_0.

3 Poincaré-Bendixon theorem

Theorem 3.1. (Poincaré-Bendixon)[4]
Consider the 2-dimensional autonomous system

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}) \tag{3.1}$$

in $\mathbb{R}^2$. If there exists a closed annular region $\mathcal{R}$ bounded by two closed curves $\mathcal{C}_1$ and $\mathcal{C}_2$, with $\mathcal{C}_2$ inside $\mathcal{C}_1$, such that all trajectories crossing $\mathcal{C}_1$ and $\mathcal{C}_2$ enter the annular region $\mathcal{R}$ between them, and if $\mathcal{R}$ has no steady state in it, then there exists at least one limit cycle in $\mathcal{R}$ that attracts all trajectories as $t \to \infty$.



Remarks

- Having a closed curve $\mathcal{C}_2$ from which all trajectories are escaping requires the region enclosed by $\mathcal{C}_2$ to have an unstable steady state (node or focus) $\mathbf{x}_s$ in it. The construction of the curve $\mathcal{C}_2$ is then trivial.

- The closed curve $\mathcal{C}_1$ describes a *confined set* enclosing $\mathbf{x}_s$. The requirement that all trajectories crossing $\mathcal{C}_1$ enter the confined set is expressed through the scalar product,

  $$\mathbf{f}(\mathbf{x}) \cdot \mathbf{n}(\mathbf{x}) < 0$$

  where $\mathbf{x} \in \mathcal{C}_1$ and where $\mathbf{n}(\mathbf{x})$ is the normal pointing outward of $\mathcal{C}_1$.

- The Poincaré-Bendixon theorem applies also to an unstable limit cycle when all trajectories crossing $\mathcal{C}_1$ and $\mathcal{C}_2$ escape from the annular region $\mathcal{R}$.

Theorem 3.2. (Bendixon criterion)[5]
Consider the 2-dimensional autonomous system

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}) \tag{3.2}$$

[4] Jordan D.W., Smith P., *Nonlinear Ordinary Differential Equations, 4th edition,* Oxford University Press 2007
[5] Verhulst F., *Nonlinear Differential Equations and Dynamical Systems, 2nd edition,* Springer 1996

in $D \subset \mathbb{R}^2$ where D is simply conected (there are no "holes" or "separate parts"), that is, $\mathbf{f}(\mathbf{x})$ is continuously differentiable in D. Then, (3.2) can only have periodic solutions in D if $\nabla \cdot \mathbf{f}$ changes sign in D, or $\nabla \cdot \mathbf{f} = 0$ in D.

Remarks

- The theorem says only whether periodic solutions can exist; having $\nabla \cdot \mathbf{f}$ not changing sign in D proves only the non-existence of limit cycles.

4 An example: The Brusselator

The Brusselator describes a hypothetical oscillating chemical reaction. In dimensionless form, the equations read as

$$\begin{cases} \dot{x} = 1 - (1+b)x + ax^2 y \\ \dot{y} = bx - ax^2 y \end{cases} \tag{4.1}$$

where $x, y > 0$ are dimensionless concentrations and $a, b > 0$ are parameters (the rate constants). The analysis of (4.1) proceeds as follows:

1. **Steady States.** The system (4.1) has a single steady state:

$$\mathbf{x}_s = (x_s, y_s) = (1,\ b/a) \tag{4.2}$$

2. **Stability.** Linearizing (4.1) leads to the Jacobian,

$$\mathbf{J} = \begin{bmatrix} -(1+b)+2axy & ax^2 \\ bx-2axy & -ax^2 \end{bmatrix} \tag{4.3}$$

Evaluated at $\mathbf{x}_s = (1,\ b/a)$ gives

$$\mathbf{J}_{(1,b/a)} = \begin{bmatrix} b-1 & a \\ -b & -a \end{bmatrix} \tag{4.4}$$

which admits

$$\det \mathbf{J}_{(1,b/a)} = a > 0, \qquad \mathrm{tr}\ \mathbf{J}_{(1,b/a)} = b - 1 - a \tag{4.5}$$

Having a positive determinant implies that the steady state $\mathbf{x}_s$ cannot be a saddle and it is either a stable or an unstable node or focus, depending on the value of the trace. It follows that

$$\begin{cases} b < a+1 & \Rightarrow \text{stable node or focus (negative trace)} \\ b > a+1 & \Rightarrow \text{unstable node or focus (positive trace)} \end{cases} \tag{4.6}$$

3. **Nullclines.** The nullclines follow from equating the right hand side of (4.1) to zero. From the first of (4.1) we get the $\dot{x}$-nullcline:

$$y = \frac{(1+b)x - 1}{ax^2}, \tag{4.7}$$

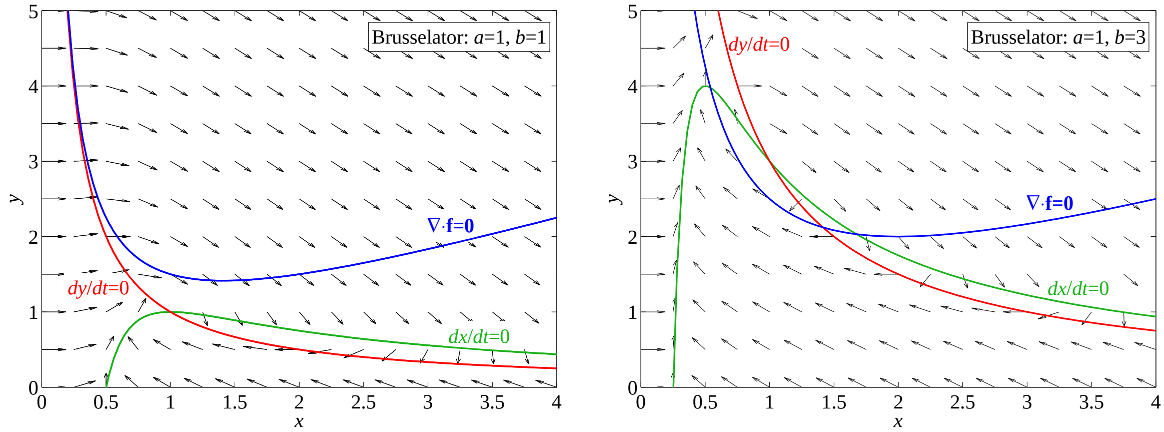
whereas from the second of (4.1) we get the (two) $\dot{y}$-nullclines:

$$x = 0, \qquad y = \frac{b}{ax}. \tag{4.8}$$

Fig. 1ab shows the nullclines for a stable and an unstable case, respectively. Note that the vector field does not allow for drawing any conclusion of a limit cycle. Therefore, to prove the existence of a limit cycle, we apply our two theorems.

4. **Divergence of the flux (Bendixon criterion)**. The divergence $\nabla \cdot \mathbf{f}(x, y)$ equates from (4.1) to

$$\nabla \cdot \mathbf{f}(x, y) = \frac{\partial f_1}{\partial x} + \frac{\partial f_2}{\partial y} = -(1+b) + 2axy - ax^2 \tag{4.9}$$



(a) (b)

Figure 1: Nullclines, (4.7) and (4.8), and the isoline of the divergence (4.9) for the case of a stable (a) and an unstable (b) steady state. Note that the vector field is normalized, i.e., the length of the vectors does not correspond to the local velocity.

which is obviously equal to the trace of the Jacobian (4.3). Solving (4.9) for $\nabla \cdot \mathbf{f} = 0$ gives

$$y = \frac{(1+b) + ax^2}{2ax} \tag{4.10}$$

which describes the line where the divergence vanishes; above this line the divergence is positive whereas below this line it is negative. Fig. 1 shows this line. Notably, for both the stable and the unstable case the divergence changes sign in the domain of (4.1). Thus, *limit cycles are possible in both cases.*

5. **Confined Set (Poincaré-Bendixon).** The confined set (i.e., the curve $\mathcal{C}_1$) describes a closed curve where all crossing trajectories are pointing inwards (outwards) in case of a stable (unstable) limit cycle, respectively. The construction of a confined set is in general a rather cumbersome task. For the present example where (4.1) is confined in the first quadrant $(x, y > 0)$ we suggest to construct $\mathcal{C}_1$ as a *polygon*, where we start the construction of the polygon by considering a segment lying on the x-axis.

   ① The first segment is taken as a segment lying on the x-axis (Fig. 2), i.e., $y = 0$. The flux vector on this segment reads as

$$\mathbf{f}_{(y=0)} = (1 - (1+b)x,\ bx)^T. \tag{4.11}$$

   The unit normal orthogonal to the first segment pointing *away* from the steady state is $\mathbf{n} = (0,\ -1)^T$. Hence, $\mathbf{f} \cdot \mathbf{n} = -bx < 0$ which holds for $x > 0$. Thus, along the positive x-axis the flux is pointing *inwards*.

   ② Next, we consider a segment parallel to the y-axis left hand side to the steady state (Fig. 2), say $x = x_L < x_s$. The flux on this segment reads as

$$\mathbf{f}_{(x=x_L)} = \begin{pmatrix} 1 - (1+b)x_L + ax_L^2 y \\ bx_L - ax_L^2 y \end{pmatrix} \tag{4.12}$$

The unit normal orthogonal to this second segment pointing *away* from the steady state is $\mathbf{n} = (-1,\ 0)^T$. Hence, $\mathbf{f} \cdot \mathbf{n} = -1 + (1+b)x_L - ax_L^2 y < 0$. This condition is fulfilled when y lies above the $\dot{x}$-nullcline (4.7), which translates into a condition for x_L:

$$0 < x_L < \frac{1}{1+b} \tag{4.13}$$

③ We continue by considering a segment parallel to the x-axis that lies above the steady state, say $y = y_U > y_s$ (Fig. 2). The flux on this segment reads as,

$$\mathbf{f}_{(y=y_U)} = \begin{pmatrix} 1 - (1+b)x + ax^2 y_U \\ bx - ax^2 y_L \end{pmatrix} \tag{4.14}$$

The unit normal orhogonal to this segment is pointing *away* from the steady state is $\mathbf{n} = (0,\ 1)^T$. Hence, $\mathbf{f} \cdot \mathbf{n} = bx - ax^2 y_U < 0$ from which it follows that y_u must lie above the $\dot{y}$-nullcline (4.8)

$$y_U > \frac{b}{ax_L} \tag{4.15}$$

④ Next, we were to consider a segment parallel to the y-axis right hand side to the steady state, $x = x_R > x_s$, say. The flux along this segment reads as

$$\mathbf{f}_{(x=x_R)} = \begin{pmatrix} 1 - (1+b)x_R + ax_R^2 y \\ bx_R - ax_R^2 y \end{pmatrix} \tag{4.16}$$

Further, $\mathbf{n} = (1,\ 0)^T$ and $\mathbf{f} \cdot \mathbf{n} = 1 - (1+b)x_R + ax_R y < 0$. From this it follows that this fourth segment has only a flux pointing *inwards* for y lying below the $\dot{x}$-nullcline.

This means that the confined set with inward flux cannot be constructed as rectangle.

⑤ Inevitably, we need a fifth segment connecting the third and the forth segment. Here, we propose this fifth segment to be a straight line of negative slope m, say $y = q - mx$, where $m > 0$ and $q > \max(y_s + mx_s,\ y_U + mx_L)$ such that the line lies above the steady state, and it intersects the third segment (Fig. 2). The unit normal to this segment pointing away from the steady state is $\mathbf{n} = (m,\ 1)^T$. The flux along this line equates to

$$\mathbf{f}_{(y=q-mx)} = \begin{pmatrix} 1 - (1+b)x + ax^2(q - mx) \\ bx - ax^2(q - mx) \end{pmatrix} \tag{4.17}$$

The scalar product is

$$\mathbf{f} \cdot \mathbf{n} = m\Big(1 - (1+b)x + ax^2(q - mx)\Big) + bx - ax^2(q - mx) < 0$$

which is quadratic in m. Analytical treatment of this inequality is cumbersome. Therefore we arbitrary choose a value for m and see if the inequality is valid. Inspecting the vector field hints that $m = 1$ might be a promising candidate: Setting $m = 1$ simplifies the above equation to

$$\mathbf{f} \cdot \mathbf{n} = 1 - x < 0$$

which holds for $x > 1$. Hence, a straight line with a negative slope $m = 1$ that intersects with

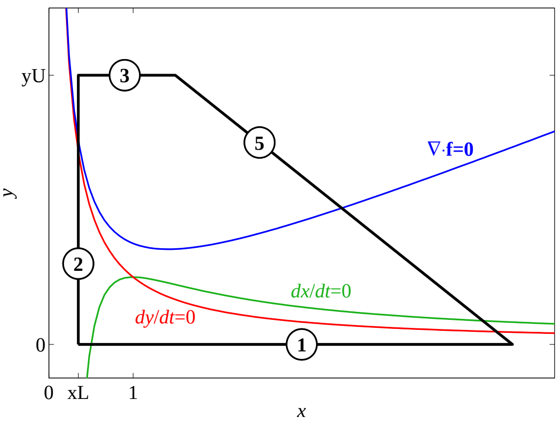
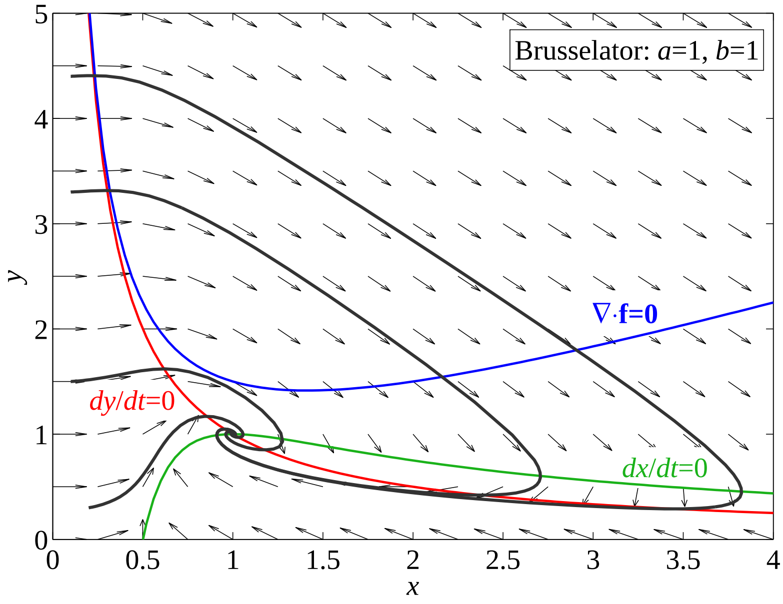


Figure 2: Confined set.

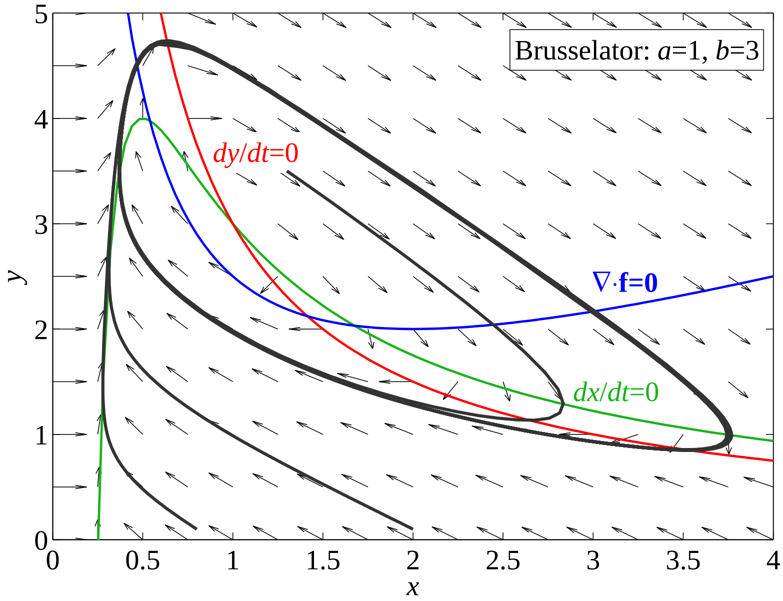
the third segment at $x > 1$ (that is, right to the steady state) has everywhere a flux that is pointing inwards. Note that this finding makes the forth segment dispensable.

Remarks.

- A confined set, i.e., a curve $\mathcal{C}_1$, is found in both cases when the steady state is stable and unstable. However, only in the case of an unstable steady state we can find a curve $\mathcal{C}_2$ encompassing the steady state on which all crossing trajectories are flowing outwards. Hence, according to theorem 2 only the case where the steady state is unstable admits a limit cycle. This is confirmed by solving (4.1) numerically. Solution for a set of different ICs is shown in Fig. 3.
- There are many ways to construct a confined set.



(a)



(b)

Figure 3: Trajectories for various ICs. In (a) the steady state $(1, b/a)$ is stable whereas in (b) it is unstable. The latter case admits a stable limit cycle.