Project for Math 224

Phase Plane Analysis on a Reaction System

Phase plane analysis is a very useful tool to understand the qualitative behavior of solutions of systems of first order autononous systems:

$$(1)\qquad \begin{cases} \dfrac{dx}{dt} = f(x,y), \\ \dfrac{dy}{dt} = g(x,y). \end{cases}$$

Such systems frequently arise in physics, chemistry and mathematical biology. On the other hand, there is rich and beautiful mathematics behind these systems. The text book gives a good introduction on this and the purpose of this project is to, through a concrete reaction model, further introduce various mathematical ideas and tools in phase plane analysis.

The reaction model. Consider a reaction mechanism

$$A \xrightarrow{k_1} X \xrightarrow{k_2} B,\ C \xrightarrow{k_3} Y,\ X + X + Y \xrightarrow{k_4} 3X,$$

where "$A \xrightarrow{k_1} X$" means that the chemical A decays into the chemical X at a rate proportional to the amount of A present, with proportionality constant k_1; similarly, "$X + X + Y \xrightarrow{k_4} 3X$" means that two X molecules and one Y molecule combine to form three X molecules at a rate proportional to the product of present amount of Y and the square of the present amount of X, with proportionality constant k_4. We measure the amount of a chemical by concentration in, say, mols/liter.

(**a**) Let $x(t)$ and $y(t)$ be the amounts of X and Y chemicals at time t, respectively. Using the Law of conservation of Mass (net rate of change = rate in - rate out), show that $x(t)$ and $y(t)$ satisfy the following system of 1st order ODE's:

$$(2)\qquad \begin{cases} \dfrac{dx}{dt} = k_1 a - k_2 x + k_4 x^2 y, \\ \dfrac{dy}{dt} = k_3 c - k_4 x^2 y, \end{cases}$$

where a and c are the amount of chemicals A and C, respectively.

From now on, assume that chemicals A and C are supplied so that a and c are kept constant. To beautify the system (2), introduce new dependent variables:

$$u(t) = c_1 x(c_2 t),\ \ v(t) = c_3 y(c_2 t),$$

where c_1, c_2, c_3 are positive constants.

(**b**) Choose c_1, c_2, c_3 suitably so that the new unknowns $u(t)$ and $v(t)$ satisfy the beautified system

$$(3) \qquad \begin{cases} \dfrac{du(t)}{dt} = m - u + u^2 v, \\ \dfrac{dv(t)}{dt} = n - u^2 v, \end{cases}$$

where m and n are some positive constant multiple of a and b. (This procedure is called *rescaling* or *non-dimensionalization* of (2).)

The starting point of phase plane analysis is always to find equilibrium point(s) and the nullclines, because they are deterministic to the phase portrait.

(**c**) Find the nullclines and the equilibrium point of (3). The nullclines devide the first quadrant of uv-plane into four regions (since both u and $v \geq 0$ by physical considerations, we focus on the 1st quadrant). In each of these regions, draw an arrow indicating the direction of orbits.

Denote the equilibrium point found in (**c**) by (u_o, v_o). The next thing to do is to study the behavior of orbits near the equilibrium point: we want to know if the equilibrium point is a sink, a source, a saddle or a center, etc. These properties of the equilibrium point are local in nature, i.e., they concern what happens in a *small* neighborhood of the point. By using the tangent plane approximation for the right hands of (3) (denoted by $f(u, v)$ and $g(u, v)$ respectively) near (u_o, v_o), we obtain the linearized system

$$(4) \qquad \begin{cases} \dfrac{dx}{dt} = \dfrac{\partial f}{\partial u}(u_0, v_0)x + \dfrac{\partial f}{\partial v}(u_0, v_0)y \\ \dfrac{dy}{dt} = \dfrac{\partial g}{\partial u}(u_0, v_0)x + \dfrac{\partial g}{\partial v}(u_0, v_0)y \end{cases}$$

Notice that $(0, 0)$ is an equilibrium point of (4) and it corresponds to the equilibrium point (u_0, v_0) of (3). We expect that the orbits of (4) near the origin resemble those of (3) near (u_0, v_0). For examples, if the orbits of (4) spirals towards $(0, 0)$, so do the orbits of (3) near (u_0, v_0). However, if the orbits of (4) are cycles (closed curves), the orbits of (3) near (u_0, v_0) may be cycles, or spirals (inward or outward). Our expectation is half right and half wrong. In class, you already learned when this expectation can go wrong. We state the following "positive" result that applies to the general system (1) with nice f and g.

Theorem 1. Consider system (1). Assume all the second partial derivatives of $f(x, y)$ and $g(x, y)$ be continuous. Let (x_0, y_0) be an equilibrium point of (1). If the equilibrium point $(0, 0)$ of the linearized system is a sink, spiral sink, a source, a spiral source, or a saddle, so is the equilibrium point (x_0, y_0) of (1), respectively.

Definition. When an equilibrium point is a sink or spiral sink, it is said to be *asymptotically stable*; when it is a source or a spiral source or a saddle, it is said to be *unstable*.

You already know that for linear homogeneous systems,

$$\frac{d\vec{y}}{dt} = A\vec{y} \tag{5}$$

where

$$\vec{y} = \begin{pmatrix} x \\ y \end{pmatrix}, \ A = \begin{pmatrix} a, & b \\ c, & d \end{pmatrix}, \ a - d \ constants,$$

the signs of the real parts of the eigenvalues of matrix A determine the type of the equilibrium point $(0, 0)$. They obviously depend on (m, n). Presumably, there are several regions on the first quadrant of the $m - n$ plane, on each of which the equilibrium point $(x, y) = (0, 0)$ (and hence $(u, v) = (u_0, v_0)$) is of one type (say, spiral sink). However, it would be hard for you if we want to distinguish sinks(with straight-line solutions) from the spiral sinks, sources from spiral sources: if we know that the real parts of all two eigenvalues are negative, then we know for sure that the equilirium point is either a sink or a spiral sink and hence asymptotically stable, and the similar thing can be said for sources and spiral sources(that is, when the point is unstable).

We will content ourselves with the following: find the regions on the first quadrant of the $m - n$ plane on each of which the equilirium point $(u, v) = (u_0, v_0)$ of (3) is either asymptotically stable or unstable.

As said above, the signs of the real parts of the eigenvalues are crucial for stability and instablity. To study them directly for the present problem, you will sink into morass of nasty calculations. The following two results are elegant and can keep dry.

(**d**) Let λ_1 and λ_2 be the eigenvalues of A. Show that

$$\lambda_1 + \lambda_2 = a + d, \quad \lambda_1 \lambda_2 = \begin{vmatrix} a, & b \\ c, & d \end{vmatrix}. \tag{6}$$

($a + d$ is called the *trace* of A and is denoted by TrA).

(**e**) Show now that if $detA > 0$ and $TrA >$, then the real parts of λ_1 and λ_2 are positive; if $detA > 0$ and $TrA < 0$, then the real parts are negative. What if $detA < 0$?

Now you can tackle the stability question of the equilibrium point (u_0, v_0) of the reaction system (3).

(**f**) Show that if

$$n - m > (m + n)^3 \tag{7}$$

then the equilibrium point (u_0, v_0) of (3) is unstable.

(**g**) Show that if

$$n - m < (m + n)^3, \tag{8}$$

then the equilibrium point (u_0, v_0) of (3) is asymptotically stable.

(**h**) Now we realize that the equation

$$n - m = (m + n)^3 \tag{9}$$

is the borderline condition for stability and instability. Sketch the curve represented by (9) in the first quadrant of the $m - n$ plane. Indicate the region of instability, i.e., the region represented by the inequality (8).

Now we know that if (m, n) is outside that region of instability all orbits of (3) nearby (u_0, v_0) converge to (u_0, v_0) as $t \to \infty$, and if (m, n) is inside the region, all these orbits move away from (u_0, v_0). A natural and interesting question arises: in the latter case, where do these orbits go in the long run? It turns out that these orbits will spiral towards a cycle, called *limiting cycle*:

(**i**) Sketch on $t - u$ or $t - v$ plane the curves of $u(t)$ and $v(t)$ which correspond to the orbit drawn above. (Your curves should be oscillatory because the orbit converges to a limiting cycle.)

Terminology: When the parameters (m, n) move from the region of stability into the region of instablity, the type of the equilibrium changes and thus a bifurcation occurs. In fact, a limiting cycle suddenly emerges when (m, n) crosses into the region of instability. In this scenario, we say a Hopf bifurcation occurs.

Now let's see why when (m, n) is in the region of instability, orbits of (3) near (u_0, v_0) converge to a limiting cycle. To this end, we need the following beautiful

Poincaré-Bendixson Theorem. Consider system (1) where $f(x, y)$ and $g(x, y)$ are nice in the sense that all their 1st order partials are continuous. Suppose (1) has only one equilibrium point (x_0, y_0). Then any bounded orbit (that is, the orbit is always inside a square of fixed size), either converges to (x_0, y_0) or spirals towards a limiting cycle as $t \to \infty$, or the orbit itself is a cycle.

A very important condition in the above theorem is the boundedness of the orbit. To verify this condition, we use a simple and yet powerful device, called *invariant region*. An invariant region of system (1) is a region in $x - y$ plane on whose boundary the vector $(f(x,y), g(x,y))$ always points into the region:

Any orbit that starts inside an invariant region will be confined in it forever: it will never cross the boundary because there the tangent vector $(\frac{dx}{dt}, \frac{dy}{dt})$ of the orbit points into the region.

(**j**) For our system (3), show that the following shaded rectangular region (infinite long) is an invariant region.

(**k**) Show that any orbit of (3) that starts inside the 1st quadrant is bounded. Hint: (Adjust the height of the invariant region discussed in (l) so that it contains $(u(0), v(0))$. Then the orbit will be confined in the region. So the only way for the orbit to be unbouned is to go far away to the right in the region. This can't happen. Here is why: adding the two equations in (3) we get

$$\frac{d(u+v)}{dt} = (m+n) - u.$$

so if $u > m + n$, $(u + v)(t)$ is decreasing. So ....)

Now we are ready to apply the Poincaré-Bendixson Theorem to

(**l**) Show when (m, n) is in the region of instability, i.e. when m and n satisfy (12), every orbit of (3) near (u_0, v_0) spirals towards a limiting cycle.

Hint:By virtue of Poincaré-Bendixson, you only need to rule out the case that the orbit converge to (u_0, v_0) as t goes to ∞ and the case that the orbit is a cycle.

(**m**) **Computer simulations**: Use Matlab to draw the phase portraits of (3) in each of the following cases:

(i) $n = 0.5,\ m = 0.5$;

(ii) $n = 0.5,\ m = 0.05$.

Use the portraits to illustrate the above results of stability, instability and the presence of limiting cycles (as discussed in parts (**f**), (**g**) and (**l**)). When using Matlab, you should adjust the ranges for x and y so that your portraits show the relevant phenomena *clearly*.

For (m, n) inside the region of stability, try to find two sets of values for (m, n) so that the equilirium point is a sink with straight-line solutions, and a spiral sink, respectively.