Chapter 1
Rate Equations

Many real-world systems can be described in terms of the evolution of *state variables* for various system properties, starting from given initial configurations. The simplest models for such problems are given by ordinary differential equations (ODE) describing the rates of change of the state variables as functions of time.
Applications include:

- Mechanics: motion of masses subjected to forces
- Modern physics: radioactive decay of materials
- Statistical systems: queues, games, multi-stage processes
- Chemistry/Biochemistry: chemical reactions
- Biology: epidemic models for diseases in populations
- Ecology: dynamics of populations of predator and prey species

While the dynamics in some of these applications may rest on discrete events, like the radioactive decay of an atom or the death of an individual in a population, when averaged over large populations, reliable mean-rates of activities can occur; this is the basis for writing ODE rate equations and other *continuous models*. ODEs cannot describe all of the details of the processes occurring in these systems, but they provide a good starting point for investigations, often yielding accurate predictions of various phenomena.

For a system involving n evolving properties, the governing mathematical problem is typically written in the form

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}, t), \qquad \mathbf{x}(0) = \mathbf{x}_0. \tag{1.1}$$

where the vector of state variables, $\mathbf{x}(t) = (x_1(t), x_2(t), \ldots, x_n(t)) \in \mathbb{R}^n$, describes n properties of interest in the system, evolving for times $t \geq 0$ and starting from a given initial state $\mathbf{x}(0) = \mathbf{x}_0$. The *rate functions* for the rates of change of each x_i, $dx_i/dt = f_i$, have similarly been collected in a vector, $\mathbf{f} = (f_1, f_2, \ldots, f_n)$, where each f_i can potentially depend on all of the state variables.

T. Witelski and M. Bowen, *Methods of Mathematical Modelling*,
Springer Undergraduate Mathematics Series, DOI 10.1007/978-3-319-23042-9_1

System (1.1), where the rate functions have an explicit dependence on time, is called *non-autonomous*. In such systems, the solutions depend on the particular details of externally imposed time-dependent influences. In this chapter, we will focus on *autonomous systems*,

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}), \qquad \mathbf{x}(0) = \mathbf{x}_0, \tag{1.2}$$

where the rates only depend on the current state of the solution. These systems describe "natural" or unforced behaviour innate to the system and are the traditional starting points for studying new classes of problems. In later chapters we will return to the influence of inhomogeneous forcing with applications such as control theory and driven systems.

Problems that can be stated in the form (1.2) are called *dynamical systems*, where the independent variable t usually represents time, but may also represent other properties depending on the context of the system. The most fundamental issues to be addressed for a given dynamical system are

- Dynamics: What is the behaviour of the solution for $t > 0$ starting from given initial conditions $\mathbf{x}_0$? (i.e. Will the solution be oscillatory, or monotone increasing, or exponentially decaying? Do solutions of certain types exist for any $\mathbf{x}_0$? Does a unique solution exist?....)
- Stability: Can the system's behaviour be predicted starting from broad sets of initial conditions? (i.e. Do the solutions starting from other initial conditions follow the behaviour of the solution starting from $\mathbf{x}_0$?)

In the simplest cases (in dimensions $n = 1$ and $n = 2$), the complete behaviour of systems can be understood from local properties of the rate functions and geometric descriptions of the set of solutions. This can yield a complete characterisation of the dynamics without the need to attempt to explicitly construct the solutions. For $n = 2$, this geometric approach is called *phase plane analysis* and forms the basis of (general) *dynamical systems theory*.

1.1 The Motion of Particles

A classic example of a dynamical system from mechanics is the system for motion of a particle, where the unknowns describing the state of the particle are its position, **X**, and momentum, **P**. The rate of change of position is the velocity, and from Newton's second law [67, 91], the rate of change of momentum is given by the net applied force, **F**, so we can write

$$\frac{d\mathbf{X}}{dt} = \mathbf{V}, \qquad \frac{d\mathbf{P}}{dt} = \mathbf{F}, \tag{1.3}$$

where $\mathbf{P} = m\mathbf{V}$ and the applied forces could depend on position and momentum. If the mass is constant, then these equations can be combined to give the familiar law of motion linking mass times acceleration to the net applied force,

$$m\frac{d^2\mathbf{X}}{dt^2} = \mathbf{F}. \tag{1.4}$$

Note that every nth order autonomous differential equation can always be re-expressed in the form of a system of n (first-order) rate equations. Defining $\mathbf{x} = (X_1, X_2, X_3, P_1, P_2, P_3)$, system (1.3) can be put in form (1.2) as

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}) \qquad \text{with} \qquad \mathbf{f} = \begin{pmatrix} \mathbf{P}/m \\ \mathbf{F}(\mathbf{X}, \mathbf{P}) \end{pmatrix} \in \mathbb{R}^6. \tag{1.5}$$

Newton's laws give a well-defined procedure for constructing the dynamical system for a mechanics problem.[1] For other fields, different principles provide guidance; we will review how to set up rate equations for problems in chemistry and biology.

1.2 Chemical Reaction Kinetics

For chemical systems [6], the fundamental principle for translating chemical reactions into corresponding sets of rate equations is given by the *law of mass action*.

In "simple" (or *elementary*) reactions, generically of the form

$$\text{reactants} \overset{k}{\to} \text{products}, \tag{1.6}$$

the rate of creation of products depends on the concentrations of available reactants and is also characterised by a *rate constant* k. The rate of consumption of reactants also follows from this relation.

We will denote the concentration of chemical 'A' by $A(t) \geq 0$, and the total rate of production of A will have contributions from its creation and/or consumption due to each chemical reaction involving A,

$$\frac{dA}{dt} = +\sum_{n=1}^{N} (\text{creation rate})_n - \sum_{n=1}^{N} (\text{consumption rate})_n. \tag{1.7}$$

The rate equations form a system of first-order equations, one for each chemical in the set of reactions, $\{A, B, C, \ldots\}$, and the rate functions will be polynomials in terms of products of concentrations of the reactant chemicals.

We briefly summarise the basic forms of elementary chemical reactions and the corresponding rate equations that follow from the law of mass action:

[1] In Chap. 3 we will consider a different approach.

(0) **Constant supply**: compound A is pumped into the system at a constant rate k

$$\text{(source)} \xrightarrow{k} A \qquad \Longrightarrow \qquad \frac{dA}{dt} = k. \tag{1.8}$$

This is called a zeroth-order reaction since the rate does not depend on the concentration of any reactants, $k = k \cdot 1 = kA^0$.

(i) **Decay**: substance A transforms into waste at rate k (i.e. A decomposes and is removed from the system)

$$A \xrightarrow{k} \text{(waste)} \qquad \Longrightarrow \qquad \frac{dA}{dt} = -kA. \tag{1.9}$$

This is called a first-order reaction since the reaction rate depends linearly on the concentration of a single reactant.

(ii) **Transformation**: A is consumed with B being produced from A

$$A \xrightarrow{k} B \qquad \Longrightarrow \qquad \frac{dA}{dt} = -kA, \qquad \frac{dB}{dt} = +kA. \tag{1.10}$$

This is the simplest reaction "system", having two distinct concentrations evolving due to a single reaction.

(iii) **Reversible transformation**: A transforms into B and vice versa. Such reactions should be explicitly expanded into separate forward and reverse reactions.

$$A \underset{k_2}{\overset{k_1}{\rightleftharpoons}} B \qquad = \qquad \{\, A \xrightarrow{k_1} B \quad \text{and} \quad A \xleftarrow{k_2} B \,\}$$

$$\Longrightarrow \qquad \frac{dA}{dt} = -k_1 A + k_2 B, \qquad \frac{dB}{dt} = k_1 A - k_2 B. \tag{1.11}$$

In this system, the net rate of production of each substance is obtained by summing the reaction rate from the reaction producing it minus the rate from the reaction consuming it, as in (1.7).

(iv) **Compound formation**: A and B combine to form C

$$A + B \xrightarrow{k} C \qquad \Longrightarrow$$

$$\frac{dA}{dt} = -kAB, \qquad \frac{dB}{dt} = -kAB, \qquad \frac{dC}{dt} = kAB. \tag{1.12}$$

The production rate of C being proportional to the product of the reactant concentrations follows from a probabilistic description of the collision of independent molecules [6]. The probability of forming a molecule of C increases when either of the concentrations of A, B increases (and clearly the reaction will not proceed if either is absent, $A = 0$ or $B = 0$).

However, suppose A and B are the same chemical, then from (1.12)

$$A + A \xrightarrow{k} C \quad = \quad 2A \xrightarrow{k} C \quad \Longrightarrow$$
$$\frac{dC}{dt} = +kA^2 \qquad \left(\text{but} \;\; \frac{dA}{dt} \neq -kA^2 \;\; (?)\right) \tag{1.13}$$

The equation for the rate of consumption of A cannot be correct because it implies that A, C have equal but opposite rates of change, while we know that formation of each molecule of C should consume *two* molecules of A. This is an issue with "double-counting" that points to the need for a more precise definition of the "reaction rate," as will be addressed in the final type of elementary reaction.

(v) **Multiple products**: n molecules of A and m molecules of B react to produce p molecules of C and q molecules of D:

$$n\ A + m\ B \xrightarrow{k} p\ C + q\ D \tag{1.14a}$$

The problem associated with (1.13) is resolved by defining the reaction rate to be

$$\begin{aligned} \text{Reaction Rate} &= -\text{rate of consuming one unit of reactant} \\ &= +\text{rate of creating one unit of product.} \end{aligned}$$

Then for (1.14a) we get

$$\text{Rate} = \frac{1}{p}\frac{dC}{dt} = \frac{1}{q}\frac{dD}{dt} = -\frac{1}{n}\frac{dA}{dt} = -\frac{1}{m}\frac{dB}{dt} = kA^nB^m$$

and can write the rate equations as

$$\text{reactants:} \quad \frac{dA}{dt} = -nkA^nB^m \qquad \frac{dB}{dt} = -mkA^nB^m \tag{1.14b}$$

$$\text{products:} \quad \frac{dC}{dt} = pkA^nB^m \qquad \frac{dD}{dt} = qkA^nB^m \tag{1.14c}$$

Consequently, the rate equation for A for the reaction (1.13) is now correctly given by

$$\frac{dA}{dt} = -2kA^2. \tag{1.15}$$

For systems without losses or sources of chemicals, as in the case of (1.10) or (1.11), physical expectations based on the conservation of mass suggest that $A+B =$ constant, which is validated by evaluating $\frac{d}{dt}(A+B)$ using the rate equations. This is called a *conservation law* linking the products and reactants. Typically, the value for the constant is set by the summed initial concentrations and can be used to express one concentration in terms of the other. For example, if $A + B =$ constant, then

$B(t) = (A_0 + B_0) - A(t)$, allowing us to reduce the number of unknowns in the system. In some cases there may be various combinations of reactants/products that can be used to write a conservation law. For example, for (1.14a), one possible form of mass balance is given by

$$\frac{d}{dt}\left(\frac{1}{n}A + \frac{1}{p}C\right) = 0.$$

1.3 Ecological and Biological Models

Rate equations are also widely used for predicting population growth and the spread of epidemics (namely, the growth of the population of diseased individuals) [18, 74].

The simplest model of population growth, called Malthus' law, describes a growth rate proportional to the current population, and generates exponential growth,

$$\frac{dA}{dt} = kA \qquad \Longrightarrow \qquad A(t) = A_0 e^{kt}. \tag{1.16}$$

In analogy with the description of chemical reactions, using (1.14a) the growth of the population would be due to additions by births, with the parent remaining in the population,

$$A \xrightarrow{\beta} A + A \qquad \Longrightarrow \qquad \frac{dA}{dt} = -\beta A + 2\beta A = \beta A. \tag{1.17}$$

We note that the rate constant β would incorporate the time needed for the birth process (the gestation period) as well as the fraction of the total population who choose to become parents. More generally, the net rate of population growth would be the difference between the birth rate β and the death (decay) rate δ, $k = \beta - \delta$.

The weakness of Malthus' law with respect to predicting unlimited growth of populations lead to an improved model developed by Pierre Verhulst (1804–1849), usually called the *logistic equation*,

$$\frac{dA}{dt} = (\beta - \delta)A - \gamma A^2 = (k - \gamma A)A, \tag{1.18}$$

where the coefficient γ scales the influence of competition effects in decreasing the birth rate (and/or increasing the death rate) in growing populations. Here, the effective growth rate, $\tilde{k}(A) = k - \gamma A$, depends on the population size and changes the dynamics from growth ($\tilde{k} > 0$) for small populations to decay ($\tilde{k} < 0$) for large populations. The borderline between these two cases defines a critical population size, $A_* = k/\gamma$, called the carrying capacity, which allow (1.18) to be written as

$$\frac{dA}{dt} = k\left(1 - \frac{A}{A_*}\right)A. \tag{1.19}$$

The logistic equation is the simplest model that makes progress in capturing the influence of limited external resources (e.g. food) on growth of the population.

A more detailed way to describe the coupling of populations to their use of resources is to introduce additional rate equations to also describe the growth/decay of the resources. Consider a population of rabbits whose number evolves according to the logistic equation (1.18). Let that population of rabbits, $A(t)$, also serve as the food supply (prey) for a population of foxes (predators), $B(t)$. Let the foxes have a constant death rate and reproduce only when food available, analogous to a chemical reaction of the form, $A + B \to B + B$. The influence of the consumption of prey by predators is called *predation* and generates an additional loss term in the logistic equation (1.19) for the rabbit population. Along with the rate equation for the fox population, this yields a Lotka-Volterra predator-prey system [45, 74],

$$\frac{dA}{dt} = (\beta - \delta)A - \gamma A^2 - \rho AB, \qquad \frac{dB}{dt} = -\kappa B + \sigma AB. \tag{1.20}$$

In the context of the spread of diseases [18], simple models of epidemics divide the total population into sub-groups depending on whether individuals are infected ($I(t)$), susceptible to the disease ($S(t)$) or recovering from the disease ($R(t)$). The transitions between these states can be interpreted as reactions

$$I + S \to I + I, \qquad I \to R,$$

yielding a basic version of what are generally called SIR models

$$\frac{dS}{dt} = -kSI, \qquad \frac{dI}{dt} = kSI - \gamma I, \qquad \frac{dR}{dt} = \gamma I. \tag{1.21}$$

This particular system conserves the total population, $N = S + I + R$, but other formulations can allow for growing or declining overall populations. Diseases for which immunity is not achievable can be described by reversible transitions between susceptible and infected states, analogous to (1.11),

$$S \underset{k_2}{\overset{k_1}{\rightleftharpoons}} I \qquad \Longrightarrow \qquad \frac{dS}{dt} = -k_1 S + k_2 I, \qquad \frac{dI}{dt} = k_1 S - k_2 I, \tag{1.22}$$

and are generally called SIS models. Many further extensions are possible, including, for example, subdividing the infected population into individuals that are in an earlier, exposed phase, $E(t)$, versus a later infectious phase, $I(t)$, called *SEIR* models [19].

1.4 One-Dimensional Phase-Line Dynamics

The simplest applications described above were expressed as initial value problems for a single autonomous ODE (e.g. (1.15), (1.19)),

$$\frac{dx}{dt} = f(x), \qquad x(0) = x_0. \tag{1.23}$$

If the rate function $f(x)$ is linear or a polynomial function of x, then various methods, such as separation of variables can be used to determine the exact solution. However, we will see that many problems will yield more complicated rate functions where the solution cannot be explicitly calculated. For this reason, it is very useful to have a general theory that provides an understanding of all solutions of (1.23) without having to find explicit solutions. Further, even when a solution can be written out, it may be complicated to analyse. In contrast, there is a qualitative approach that can be easier to calculate and to interpret.

The dynamics of the solutions of (1.23) can be described by a one-dimensional[2] "phase line" in terms of the graph of the function $f(x)$ (see Fig. 1.1 (left)). Assuming that $f(x)$ is a nice function[3] the behaviour of all solutions, $x(t)$, can be described qualitatively in relation to the properties of $f(x)$ at its zeroes. The values $x = x_*$ where $f(x_*) = 0$ are called *equilibrium points* of (1.23). The values x_* define steady state solutions since where $dx/dt = 0$, solutions starting at x_* remain there forever. The behaviour of solutions starting from within a small neighbourhood around x_* can be analysed by approximating $f(x)$ by its Taylor series about $x = x_*$,

$$f(x) \approx f(x_*) + f'(x_*)(x - x_*) + \tfrac{1}{2} f''(x_*)(x - x_*)^2. \tag{1.24}$$

Writing the separation from the equilibrium point as $u(t) = x(t) - x_*$, (1.24) becomes

$$f(x) \approx 0 + au + bu^2 + cu^3 + \cdots \qquad \text{as } u \to 0, \tag{1.25}$$

where $a = f'(x_*)$. If $a \neq 0$, then as $u \to 0$ (corresponding to $x \to x_*$), (1.23) can be approximated by the linearised equation,

$$\frac{du}{dt} = au \qquad \Rightarrow \qquad u(t) = Ce^{at}, \tag{1.26}$$

and hence yields $x(t) \approx x_* + Ce^{at}$ with $C \neq 0$ for any solution not starting exactly at the equilibrium point. For $a > 0$ the equilibrium is locally 'repelling' since the separation from the equilibrium point increases with time, while conversely for $a < 0$ the separation decreases with time and the equilibrium is locally 'attracting'. More generally, if *any* solution starting near an equilibrium point leaves the neighbourhood

[2] Here one-dimensional indicates that the dynamics of solutions can be understood in terms of a single variable, x.

[3] With f being bounded and sufficiently smooth.

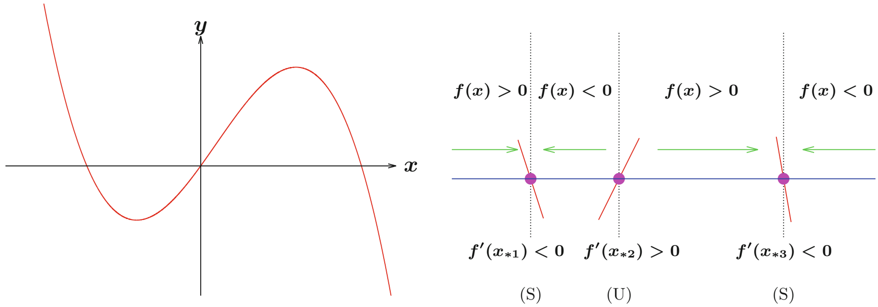

Fig. 1.1 (*Left*) A smooth rate function $f(x)$ with three equilibrium points, (*Right*) corresponding dynamics on the phase line for (1.23) obtained from local properties of f at its equilibrium points

of x_* as $t \to \infty$, then x_* is called *asymptotically unstable*, while if *all* solutions starting within the neighbourhood approach x_* as $t \to \infty$ then the equilibrium is called *asymptotically stable*. The characterisation of the dynamics of the solutions near x_* based on the linearised equation (1.26) is commonly called *linear stability analysis*.

In graphical terms, x_* is stable if the slope $f'(x_*)$ is negative ($a < 0$) and unstable if the slope is positive ($a > 0$). If we consider $x(t)$ to be the position of a point moving along the x-axis in Fig. 1.1 (the phase line) then this follows from f's role as the velocity, or rate of change of position x. If x starts to the right of x_{*3} ($x_0 > x_{*3}$) where $f(x) < 0$ then $x(t)$ will decrease (move to the left, $dx/dt < 0$) back towards x_{*3}. In contrast if $x_0 > x_{*2}$ where $f(x) > 0$ then $x(t)$ would increase with time ($dx/dt > 0$), moving away from x_{*2}.

Linear stability results provide guidance to understanding the global dynamics (not limited to small neighbourhoods of the x_*'s). Since f changes sign only at its zeroes (where we have assumed $f'(x_*)$ to be non-zero), solutions starting at x_0 within intervals between zeroes will either be monotone increasing (moving to the right on the phase line) or decreasing (moving to the left on the phase line) depending on the sign of f. This is consistent with the results of the local stability analysis at each x_* being controlled by the sign of $f'(x_*)$.

The case where $a = f'(x_*) = 0$ is called a degenerate equilibrium point; the local analysis for $u \to 0$ is still addressed using the Taylor series (1.25), but now the first nontrivial term in the expansion is (at least) quadratic and so the rates of growth or decay will be algebraic rather than exponential. If $f''(x_*) \neq 0$, then the ODE

$$\frac{du}{dt} = bu^2 \tag{1.27}$$

can be used to show that a degenerate equilibrium point x_* is unstable for any $b \neq 0$. Similarly, for the case with $f'(x_*) = f''(x_*) = 0$, but $f'''(x_*) \neq 0$ yielding

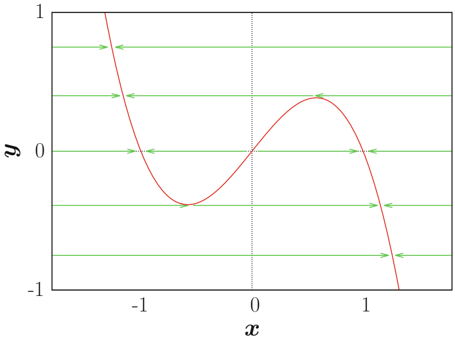

Fig. 1.2 The graph of $y = f(x) = h(x) - k$ for (1.29), giving the dynamics for $x(t)$ on different phase lines, graphically parametrised by $y = k$

$$\frac{du}{dt} = cu^3, \tag{1.28}$$

a third-order degenerate equilibrium point can be shown to be stable if $f'''(x_*) < 0$.

The dependence of solutions on parameters in the system will be an important aspect of many problems. Consider the ODE

$$\frac{dx}{dt} = h(x) - k \qquad \text{where } h(x) = x - x^3, \tag{1.29}$$

where k is a parameter. Matching to (1.23), we identify the rate function as $f(x) = h(x) - k$. Plotting $f(x)$ in Fig. 1.2, we illustrate how the family of problems (1.29) parametrised by k can be understood from this graph. Observe that for different values of the constant k, the horizontal lines $y = k$ form a "stacked" set of phase lines cutting through the curve $y = h(x)$ at the equilibrium points, $f(x_*) = 0$, corresponding to that value of k. The positions of the equilibrium are functions of k, but more significantly, the number and type of the equilibrium points change for different ranges of k, such qualitative changes in the structure of sets of solutions are called *bifurcations*. For (1.29), the dynamics for all times is restricted to a single phase line, with $y = k$ fixed, in the next section we'll review systems with coupling to a second rate equation for $y(t)$ yielding general motion in the xy plane. Despite its restricted form, we will see that problems like (1.29) occur as pseudo-two-dimensional phase plane structures in reductions of more complicated systems in Chap. 10.

1.5 Two-Dimensional Phase Plane Analysis

For systems of two coupled autonomous rate equations (called *phase plane systems*) the approach of the previous section can be extended to similarly give a qualitative understanding of all solutions from just local properties of the rate functions.

For $n = 2$ with $\mathbf{x}(t) = (x(t), y(t))$, Eq. (1.2) can be written as

$$\frac{dx}{dt} = f(x, y), \qquad \frac{dy}{dt} = g(x, y), \tag{1.30a}$$

with initial conditions at $t = 0$,

$$x(0) = x_0, \qquad y(0) = y_0. \tag{1.30b}$$

Interpreting variable t as time, this problem can be interpreted as describing the motion of a point in the xy "phase plane" starting from position $\mathbf{x}_0 = (x_0, y_0)$ subject to a position-dependent velocity $\mathbf{v} = (f, g)$. The solution of (1.30a, 1.30b) is a parametric curve (or *trajectory*) passing through the point $\mathbf{x}_0$.

Using the chain rule to eliminate t from $y(x) = y(x(t))$, (1.30a) leads to the *associated ODE* (also called the *slope field equation*),

$$\frac{dy}{dx} = \frac{g(x, y)}{f(x, y)}. \tag{1.31}$$

Solving this first order ODE for $y(x)$ yields a family of *implicit solutions* called the *integral curves* that trace out the same paths in the plane as the trajectories. The implicit solutions give only the shape of the curves while parametric solutions also give the direction of motion on the curves with respect to increasing t.

Analogous to the analysis of the phase line, equilibrium points (x_*, y_*) are defined by positions where both rate functions vanish,

$$f(x_*, y_*) = 0, \qquad g(x_*, y_*) = 0. \tag{1.32}$$

With the exception of equilibrium points, results on uniqueness of solutions ensure that each point $\mathbf{x}_0$ has a single solution curve passing through it and that those curves cannot cross. Consequently, assuming f and g are smooth, the solutions are smooth curves everywhere in the phase plane except at the equilibrium points. Observe from (1.31) that at an equilibrium point the slope dy/dx is indeterminate (formally $dy/dx =$'0/0') and requires more careful analysis to describe the local structure of solutions.

Near an equilibrium point, define $\mathbf{u}(t) = (x(t) - x_*, y(t) - y_*)$ satisfying $d\mathbf{u}/dt = \mathbf{f}(\mathbf{u} + \mathbf{x}_*)$, and using a multi-variable Taylor series approximation of $\mathbf{f}$ for $|\mathbf{u}| \to 0$ yields the linearised system

$$\frac{d\mathbf{u}}{dt} = \mathbf{A}\mathbf{u}, \tag{1.33}$$

where the matrix $\mathbf{A}$ is the *Jacobian* (or gradient $\nabla\mathbf{f}$), evaluated at (x_*, y_*),

$$\mathbf{A} = \mathbf{J}(x_*, y_*) \equiv \begin{pmatrix} \partial_x f(x_*, y_*) & \partial_y f(x_*, y_*) \\ \partial_x g(x_*, y_*) & \partial_y g(x_*, y_*) \end{pmatrix}. \tag{1.34}$$

Seeking solutions of the form $\mathbf{u}(t) = \mathbf{v}e^{\lambda t}$ then reduces (1.33) to the matrix eigenvalue problem,

$$\mathbf{A}\mathbf{v} = \lambda\mathbf{v}.$$

At each equilibrium point, linear algebra yields the eigenvalues as the roots of the characteristic polynomial obtained from the setting the determinant to zero,

$$|\mathbf{A} - \lambda\mathbf{I}| = 0.$$

Subsequently, for each eigenvalue, the eigenvectors can be obtained by row-reductions as the nontrivial nullvector of $(\mathbf{A} - \lambda_k\mathbf{I})\mathbf{v}_k = \mathbf{0}$. The general solution of the linearised system is then given by the linear combination of the eigenmodes,

$$\mathbf{x}(t) \approx \mathbf{x}_* + c_1\mathbf{v}_1 e^{\lambda_1 t} + c_2\mathbf{v}_2 e^{\lambda_2 t} \qquad \text{for } |\mathbf{x} - \mathbf{x}_*| \to 0. \tag{1.35}$$

If $\mathbf{A}$ does not have a complete set of eigenvectors (a possibility with repeated eigenvalues) then this form must be modified.

Extending the discussion of asymptotic stability from Sect. 1.4 in terms of all solutions approaching $\mathbf{x}_*$ or any diverging from it, the stability of solutions starting near $\mathbf{x}_*$ can be understood in terms of the eigenvalues, see Table 1.1. Problems having $\text{Re}(\lambda) = 0$ fall into a degenerate case, called a centre manifold, and must be studied more carefully, somewhat like (1.27, 1.28).

While for the phase line case the behaviour of solutions could be inferred directly from the slope of the rate function, $\lambda = a = f'(x_*)$, the geometry for the phase plane case is more complicated. The stability properties are still set by the derivatives of the rate functions at $\mathbf{x}_*$ but now the different cases are most conveniently expressed in terms of the eigenvalues of $\mathbf{A}$, (1.35). The local geometry of the integral curves near non-degenerate $\mathbf{x}_*$ is then given by the cases outlined in Table 1.2, where the

Table 1.1 Asymptotic stability of equilibrium point $\mathbf{x}_*$ in terms of eigenvalues from the linear stability analysis

λ's	Stability	$t \to \infty$
Both $\text{Re}(\lambda) < 0$	Stable	$\lvert\mathbf{u}(t)\rvert \to 0$
Either $\text{Re}(\lambda) > 0$	Unstable	$\lvert\mathbf{u}(t)\rvert \to \infty$

Table 1.2 Geometry of trajectories near equilibrium point $\mathbf{x}_*$ in terms of the eigenvalues

λ's	Name	Geometry	Stability
λ_1, λ_2 same sign	Node	Rays	$\text{Re}(\lambda)$
λ_1, λ_2 opp. signs	Saddle	Hyperbolas	Unstable
$\lambda = \pm i\beta$	Centre	Circles	Neutral
$\lambda = \alpha \pm i\beta$	Spiral	Spirals	$\text{Re}(\lambda)$

eigenvectors set the orientation of the geometry (most notably the directions of the stable and unstable axes of a saddle point).

If $f(x, y)$ and $g(x, y)$ are linear functions, then there will be a single equilibrium point and the above analysis describes the form of the entire phase plane. Otherwise, this gives a description in a neighbourhood surrounding each $\mathbf{x}_*$. However, using the results on uniqueness of trajectories (i.e. curves may cross only at equilibrium points), trajectories can be smoothly extended and a global structure can be sketched by piecing-together the local linearised geometries around each of the equilibrium points.

In addition to systems of rate equations, phase plane analysis can also be applied to second-order autonomous ODEs for $x(t)$, such as

$$\frac{d^2x}{dt^2} - g\left(x, \frac{dx}{dt}\right) = 0, \tag{1.36}$$

which can be written as an equivalent system by defining an intermediate variable $y(t)$:

$$\frac{dx}{dt} = y, \qquad \frac{dy}{dt} = g(x, y). \tag{1.37}$$

In this system, the relationship $x' = y$ defines the direction of trajectories as follows:

- $x' > 0 : x(t)$ increasing $(\rightarrow)$ for $y > 0$ (upper half xy plane)
- $x' < 0 : x(t)$ decreasing $(\leftarrow)$ for $y < 0$ (lower half xy plane)

This choice for the intermediate variable is not unique but has a nice physical interpretation in term of $(x, y) =$ (position, velocity) with the x-axis being states at rest (zero velocity). An example of a different choice for $y(t)$ will be given in a later chapter.

As an example, consider the pendulum equation for the angular position of a suspended mass swinging under the influence of gravity [7],

$$\frac{d^2\theta}{dt^2} + \sin\theta = 0. \tag{1.38}$$

Letting $x(t) = \theta(t)$ and following (1.37), we arrive at the phase plane system,

$$\frac{dx}{dt} = y, \qquad \frac{dy}{dt} = -\sin x. \tag{1.39}$$

Applying (1.32), the equilibrium points are given by $y_* = 0$ with $x_* = n\pi$ for $n = 0, \pm 1, \pm 2, \ldots$. From (1.34) the Jacobian matrix at any (x, y) is

$$\mathbf{J}(x, y) = \begin{pmatrix} 0 & 1 \\ -\cos x & 0 \end{pmatrix}.$$

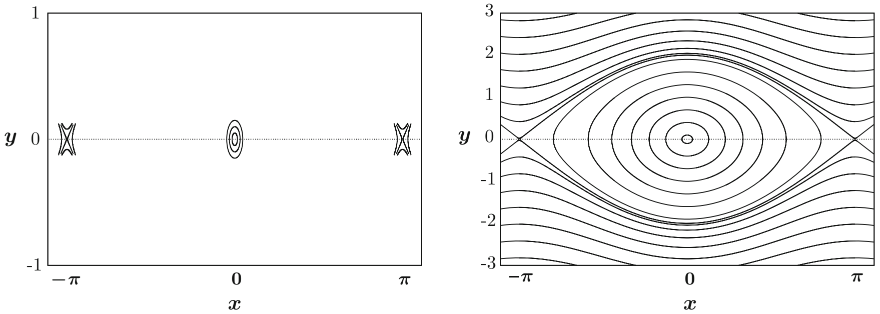

Fig. 1.3 The phase plane for the pendulum (1.39): (*Left*) Sketch of linearised behaviours in neighbourhoods of the equilibrium points and (*Right*) a computed plot of the full phase plane

Evaluating the Jacobian at the equilibrium point (0, 0) yields

$$\mathbf{A} = \mathbf{J}(0,0) = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \quad \Longrightarrow \quad \lambda^2 + 1 = 0, \quad \lambda = \pm i \quad \text{(a centre)},$$

while the equilibrium point $(\pi, 0)$ yields

$$\mathbf{A} = \mathbf{J}(\pi,0) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \Longrightarrow \quad \lambda^2 - 1 = 0, \quad \lambda = \pm 1 \quad \text{(a saddle point)},$$

with eigenvectors $(1, -1)$ and $(1, 1)$. These vectors define the asymptotes of the family of hyperbolas centred at this equilibrium point, called the stable manifold (for $\lambda < 0$) and unstable manifold (for $\lambda > 0$), $y = \pm(x - \pi)$, see Fig. 1.3 (left). Other equilibrium points at $([2k + 1]\pi, 0)$ also have exactly the same form by the periodic nature of $g(x)$. Figure 1.3 shows that the full phase plane smoothly extends the local behaviours at the equilibria to cover all possible solutions. It is notable that trajectories connecting the saddles (called *heteroclinic orbits*) separate small-amplitude periodic oscillations abound $\theta = 0$ (the continuous family of closed curves) from high-speed "spinning" solutions, where the angle increases (or decreases) monotonically for all time.

1.5.1 Nullclines

Nullclines are curves in the xy plane that can provide further understanding of systems by dividing the phase plane into regions with different behaviours. The nullclines are *not* solutions of the system, but they do yield valuable insight on the properties of solution trajectories that pass through the nullcline curves (or lie on one side or the other).

The *x-nullcline* is a curve in the phase plane on which $dx/dt = 0$. On this nullcline $x(t)$ instantaneously has zero rate of change, hence x is fixed while $y(t)$ changes with time, so a trajectory passing through the x-nullcline will have a *vertical* tangent. The x-nullcline is given by the implicitly defined curve $f(x, y) = 0$. The x-nullcline also separates solutions that have $x(t)$ increasing from those that have x decreasing with time,

$$\begin{array}{lll} \text{Region where } f(x, y) < 0: & \dfrac{dx}{dt} < 0 & x(t) \text{ decreasing } (\leftarrow) \\ \text{Region where } f(x, y) > 0: & \dfrac{dx}{dt} > 0 & x(t) \text{ increasing } (\rightarrow) \end{array}$$

Analogously, the *y-nullcline* is a curve on which $dy/dt = 0$. Here $y(t)$ instantaneously has zero rate of change and a trajectory passing through the y-nullcline will have a *horizontal* tangent. The y-nullcline is given by the implicitly defined curve $g(x, y) = 0$. The y-nullcline also separates solutions that have $y(t)$ increasing from those that have y decreasing with time,

$$\begin{array}{lll} \text{Region where } g(x, y) < 0: & \dfrac{dy}{dt} < 0 & y(t) \text{ decreasing } (\downarrow) \\ \text{Region where } g(x, y) > 0: & \dfrac{dy}{dt} > 0 & y(t) \text{ increasing } (\uparrow) \end{array}$$

Combining the information on horizontal and vertical components of motion from the x, y-nullclines respectively, yields very useful local qualitative information on the directions of trajectories that can be extended to understand the structure of the phase plane. In particular, note that the intersections of the nullclines are equilibrium points and the transitions in values of dx/dt and dy/dt can help identify the type of equilibrium point without doing the linear stability analysis.

As an example consider the system

$$\frac{dx}{dt} = y - \frac{x^2}{\sqrt{2}}, \qquad \frac{dy}{dt} = x^2 + y^2 - 4. \tag{1.40}$$

The first equation gives the x-nullcline as the parabola $y = x^2/\sqrt{2}$. Above the parabola $x(t)$ is increasing with time, while below the parabola $x(t)$ is monotone decreasing. On the parabola, trajectories have vertical tangents. The second equation in (1.40) gives the y-nullcline as the circle $x^2 + y^2 = 4$. Inside the circle $y(t)$ is decreasing, while outside the circle $y(t)$ is increasing. On the circle, trajectories have horizontal tangents.

The intersection of the nullclines makes the locations of the two equilibrium points immediately clear. These points could also be obtained analytically from (1.32) as $(x_*, y_*) = (\pm\sqrt{2}, \sqrt{2})$. Subsequently, the eigenvalues for the linear stability analysis at the equilibrium points can be obtained by solving

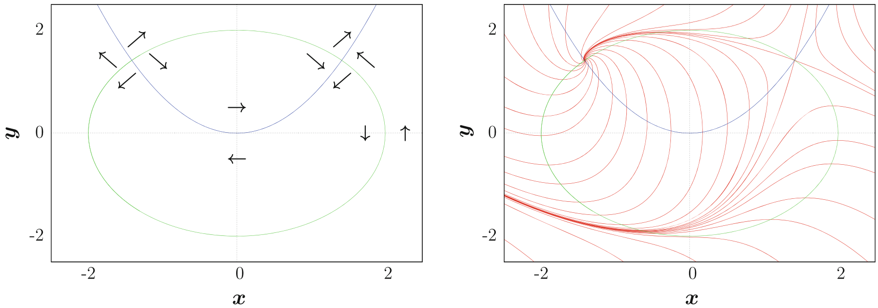

Fig. 1.4 Nullclines for system (1.40): (*Left*) directional information determined from the x- and y-nullclines and its application to local structure near the two equilibrium points, (*Right*) computed trajectories for the system

$$\begin{vmatrix} -\sqrt{2}x_* - \lambda & 1 \\ 2x_* & 2y_* - \lambda \end{vmatrix} = 0.$$

At (x_*^+, y_*) we get $\lambda_1 \approx 3.356$ and $\lambda_2 \approx -2.528$ yielding a saddle point. At (x_*^-, y_*) we get an unstable spiral with $\lambda_{1,2} \approx 2.414 \pm 1.630i$. The nature of these equilibria could be inferred from information provided by the nullclines without these slightly cumbersome algebraic calculations, see Fig. 1.4. The usefulness of nullclines becomes more significant in reducing more complicated systems and constructing proofs about properties of families of solutions.

1.6 Further Directions

The analysis of the linear stability of equilibrium points can be extended to dynamical systems in n-dimensions [70]. However, the phase plane is special because some geometric arguments do not extend in a simple way to curves in space $\mathbb{R}^n$ for $n \geq 3$. Consequently it is very helpful when higher-order systems can be reduced down to phase planes.

The material in this chapter gives only a very brief review of selected fundamental results. For more detailed background on phase planes and further coverage of bifurcations and dynamical systems theory, see, for example [43, 45, 54, 70, 94].

Comprehensive presentations of chemical reaction systems are found in most chemistry textbooks, for example [6]. More concise introductions are given in the applied mathematics books by Holmes [49] and Keener and Sneyd [57].

The models described here by systems of ODE are the simplest type of rate equations, sometimes also called state-space models, with the rates of evolution dependent on the current solution state. In *delay differential equations*, the current rate depends on the solution at an earlier time, $dx/dt = f(x(t-1))$ [35]. *Discrete-time maps*, also called *difference equations* are analogous algebraic equations describing evolving solutions at discrete times, say year-to-year, as in $x_{n+1} = f(x_n)$ [5]. *Stochastic differential equations* have randomly varying contributions to the rate functions and are sometimes used to represent the variations among the dynamics of individuals in a large population, improving on (1.2) which describes a uniform average behaviour [36]. More detailed models of populations, called *structured population models* divide up the population by age or size; if these are treated as continuous variables, then the rate equations yield partial differential equations. We will touch on some of these topics in later chapters. Haberman's book [45] also provides very accessible introductions to several of these types of models.

1.7 Exercises

1.1 Consider the problem of tracking the vertical position, $z(t)$, of a rocket whose mass changes as it consumes its fuel. If the rocket starts from rest at $z(0) = 0$ with initial mass $m(0) = m_0$ and obeys

$$\frac{d}{dt}\left(m(t)\frac{dz}{dt}\right) = -mg + \tau m, \qquad \frac{dm}{dt} = -m,$$

solve the ODEs to determine $z(t)$ and determine the condition on τ that is necessary for lift-off.

1.2 Use basic solution methods for first order ODEs to solve the elementary reactions (1.8–1.13) for $A(t)$, $B(t)$, $C(t)$ starting from initial conditions A_0, B_0, C_0 respectively.

1.3 Write the four rate equations for chemicals C, E, P, S governed by the reactions[4]

$$S + E \underset{k_2}{\overset{k_1}{\rightleftharpoons}} C \qquad C \xrightarrow{k_3} P + E.$$

1.4 Write the rate equations for $X(t)$, $Y(t)$, $Z(t)$ describing the reaction system

$$\text{(source)} \xrightarrow{A} X \qquad Y \underset{C}{\overset{B}{\rightleftharpoons}} X \qquad Z \underset{E}{\overset{D}{\rightleftharpoons}} Y \qquad 3Y \xrightarrow{G} Z \qquad Z \xrightarrow{H} \text{(waste)}.$$

1.5 Consider the dynamics of $x(t)$ satisfying the first order ODE,

$$\frac{dx}{dt} = x - x^3 - k \qquad x(0) = x_0,$$

for different values of the parameter k (see Fig. 1.2).

[4] We delay solving more complicated systems of reactions to Chap. 10. Here we only want to set up the rate equations.

(a) For $k = 0$, obtain the exact solutions starting from $x_0 = 1/2$ and $x_0 = -2$. Show that these solutions match the linearised results from (1.26) at the equilibrium points $x_* = \{-1, 0, 1\}$ for the long-time behaviour ($t \to \infty$), and the "pre-history" of the solution ($t \to -\infty$). Show that for all initial conditions with $x_0 \neq 0$, one of two final states are approached as $t \to \infty$.

(b) Determine the two values of k for which the ODE has only two distinct equilibrium points. Sometimes called *critical values* or *bifurcation points*, such parameter values determine special cases, where different analysis is needed to describe the system; in this case, this will involve second-order degenerate equilibrium points. Determine the coefficient b occurring in the equation for the local behaviour of solutions near the degenerate equilibrium points, $du/dt = bu^2$ with $u(t) = x(t) - x_*$.
Show that for this problem, these bifurcation values separate ranges of k where there are *global attractors* (unique final states approached by all initial conditions for $t \to \infty$) from cases where two stable equilibrium states co-exist (called *bi-stability*).

1.6 Consider the equations for local behaviour at second- and third-order degenerate equilibrium points, (1.27) and (1.28).

(a) Use separation of variables to solve the ODE analytically and subsequently describe the stability of the equilibrium point at $u = 0$ for both choices of the sign of b.

(b) Using only the sign of the velocity on the phase line consider solutions starting from initial conditions with $u_0 \gtrless 0$ to obtain the stability of the equilibrium point without the need for the ODE solutions.

(c) Repeat (a, b) for the dependence of (1.28) on c.

1.7 Consider the second order ODE for $x(t)$,

$$\frac{d^2x}{dt^2} = x - \tfrac{1}{2}x^2.$$

(a) Let $y = dx/dt$ and write the ODE as a phase plane system. Determine the linear stability properties of the two equilibrium points.

(b) Show that the solutions satisfy the equation

$$\tfrac{1}{2}(x')^2 - \tfrac{1}{2}x^2 + \tfrac{1}{6}x^3 = H,$$

where H is a constant of integration, sometimes called the *Hamiltonian*.

(c) For a range of values, $0 < x < M$, this problem has a continuous set of periodic solutions. Show that the maximum and minimum values of $x(t)$ of each periodic solution satisfy a polynomial equation involving H. Define the amplitude of the oscillations as $A = x_{\max} - x_{\min}$. Show that $A = 0$ corresponds to an equilibrium point. Show that the largest amplitude solution has $x_{\min} = 0$; determine its value for $x_{\max}(=M)$. What is the range of values for H?

(d) Use $t = \int dt = \int \frac{dx}{dx/dt}$ to show that the period of oscillation for these solutions is given by

$$P = 2 \int_{x_{\min}}^{x_{\max}} \frac{dx}{\sqrt{x^2 - \frac{1}{3}x^3 + 2H}}.$$

(e) Show that the simpler *piecewise-linear model*

$$\frac{d^2x}{dt^2} = f(x) \qquad \text{with} \quad f(x) = \begin{cases} x & x < 1 \\ 2 - x & x \geq 1 \end{cases}$$

has the same equilibrium points and the same linear stability properties at the equilibria.
Solve the two linear problems

$$\frac{d^2x_A}{dt^2} = x_A \qquad x_A(0) = x_{\min} \qquad x'_A(0) = 0$$
$$\frac{d^2x_B}{dt^2} = 2 - x_B \qquad x_B(P/2) = x_{\max} \qquad x'_B(P/2) = 0$$

and construct a periodic solution of the piecewise-linear model by enforcing smoothness, $x'_A = x'_B$ at $x_A = x_B = 1$.