Part IV

Multivariate functions and applications

Chapter 20

The gradient vector

In this chapter we consider functions of more than one variable, for example $f(x, y)$, and start to develop a technique for identification of points x_0, y_0 where $f(x, y)$ is locally maximum or minimum. To do this we introduce the valuable concept of the **gradient** of a multivariate function.

20.1 Directional derivatives

Consider a function $f(x, y)$, and a (vector) displacement $\mathbf{ds} = (dx, dy)$ as shown schematically in figure 20.1. The change in $f(x, y)$ during that displacement is given straightforwardly by the chain rule:

$$\begin{aligned} df &= \frac{\partial f}{\partial x}dx + \frac{\partial f}{\partial y}dy, \\ &= (dx, dy).\left(\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}\right)^T = \mathbf{ds}.\boldsymbol{\nabla} f. \end{aligned}$$

$\boldsymbol{\nabla} f$ is the **gradient** of f, also called grad$f$. In cartesian coordinates in two dimensions

$$\boldsymbol{\nabla} f = \left(\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}\right).$$

We can write the displacement $\mathbf{ds} = ds\hat{\mathbf{s}}$, where $|\hat{\mathbf{s}}| = 1$. Then

$$\frac{df}{ds} = \hat{\mathbf{s}}.\boldsymbol{\nabla} f. \qquad (20.1)$$

the left hand side of (20.1) is the **directional derivative** of f in the direction $\hat{\mathbf{s}}$.

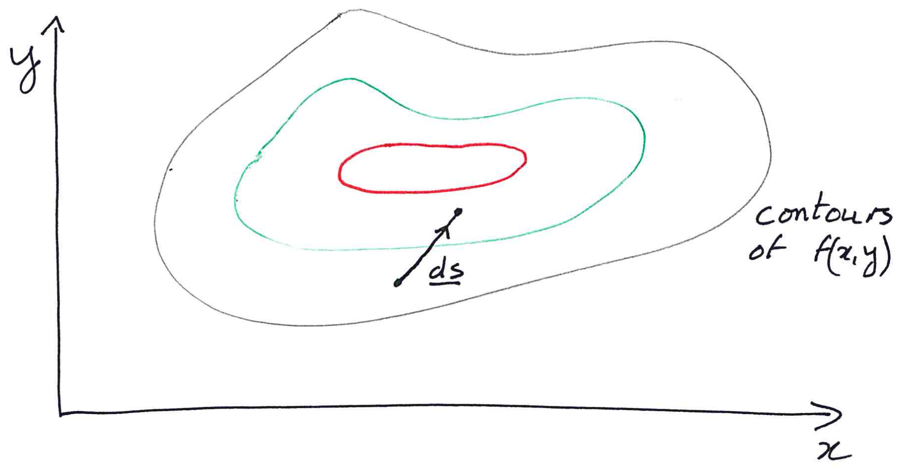

Figure 20.1: Schematic representation of a displacement $\mathbf{ds} = (dx, dy)$ in the domain of definition of a bivariate function $f(x, y)$. Contours of $f(x, y)$ are also sketched.

Definition

The **gradient** vector of $f(x, y)$, written as $\text{grad}f = \boldsymbol{\nabla}f$ is defined by (20.1). It is a **vector**, as shown schematically in figure 20.2, and has the following properties.

- As shown in figure (20.2):

$$\left|\frac{df}{ds}\right| = |\boldsymbol{\nabla}f| \cos\theta.$$

- Therefore:

$$\max_{\theta}\left(\frac{df}{ds}\right) = |\boldsymbol{\nabla}f| \,.$$

- $\boldsymbol{\nabla}f$ has magnitude equal to the maximum rate of change of $f(x, y)$ with distance in the $x - y$ plane.
- $\boldsymbol{\nabla}f$ points in the direction in which f increases most rapidly.
- If $\hat{\mathbf{s}}$ points along a contour, then f does not vary in that direction and so

$$\frac{df}{ds} = 0 \rightarrow \hat{\mathbf{s}}.\boldsymbol{\nabla}f = 0.$$

  Therefore $\boldsymbol{\nabla}f$ is everywhere orthogonal to contours (or **level curves** or **isolines**) of f.

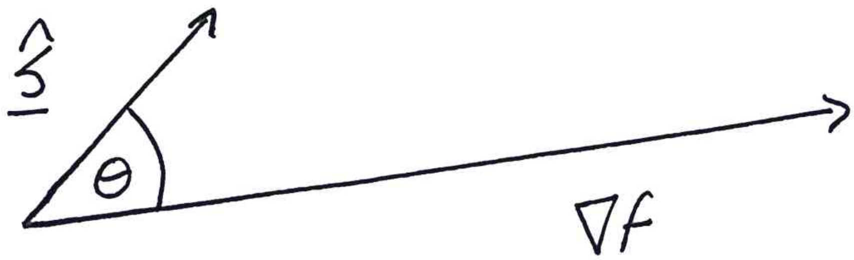

Figure 20.2: Schematic representation of the gradient vector $\boldsymbol{\nabla} f$.

20.2 Stationary points

There is always one direction in which $df/ds = 0$, i.e. tangent to the local contour of f. **Local** maxima and minima have $df/ds = 0$ for all directions. Therefore

$$\hat{\mathbf{s}}.\boldsymbol{\nabla} f = 0 \ \forall \ \hat{\mathbf{s}} \rightarrow \boldsymbol{\nabla} f = \mathbf{0} \rightarrow \frac{\partial f}{\partial x} = \frac{\partial f}{\partial y} = 0, \tag{20.2}$$

in a cartesian coordinate system.

Both a local maximum (upper panels) and a local minimum (lower panels) are shown in figure 20.3. Note that the gradient vector points towards a maximum and away from a minimum, and in both situations the contours (right panels) are locally elliptical.

However $\boldsymbol{\nabla} f = 0$ also at a **saddle point**, as shown schematically in figure 20.4. Contours are locally hyperbolic at a saddle, and in general contours can only cross at a saddle. There is clearly a need to distinguish mathematically between the different kinds of **stationary points** where $\boldsymbol{\nabla} f = \mathbf{0}$, i.e. between saddles, minima and maxima.

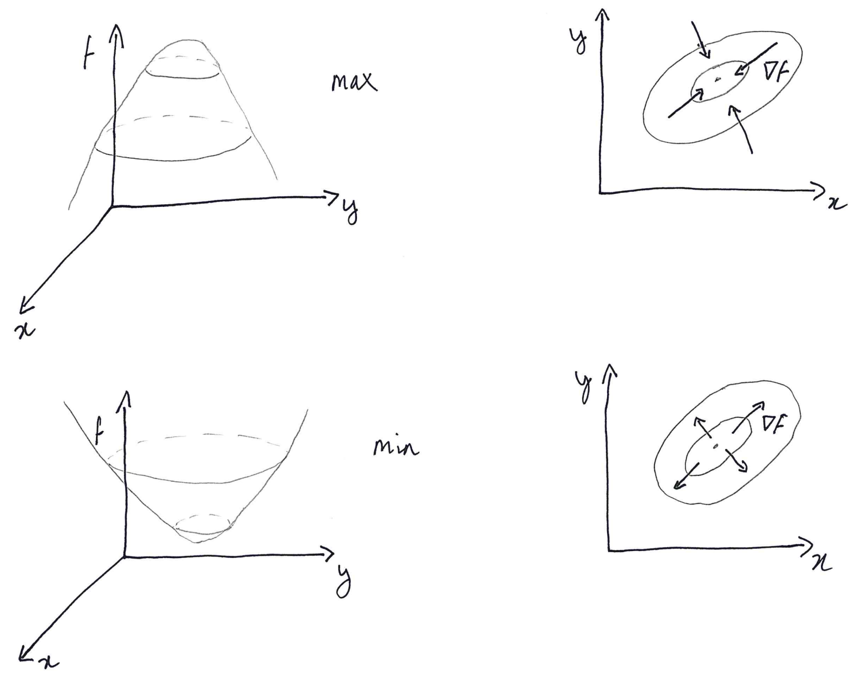

Figure 20.3: Schematic representation of a local maximum (upper panels) and a local minimum (lower panels). Note that the contours are locally elliptical.

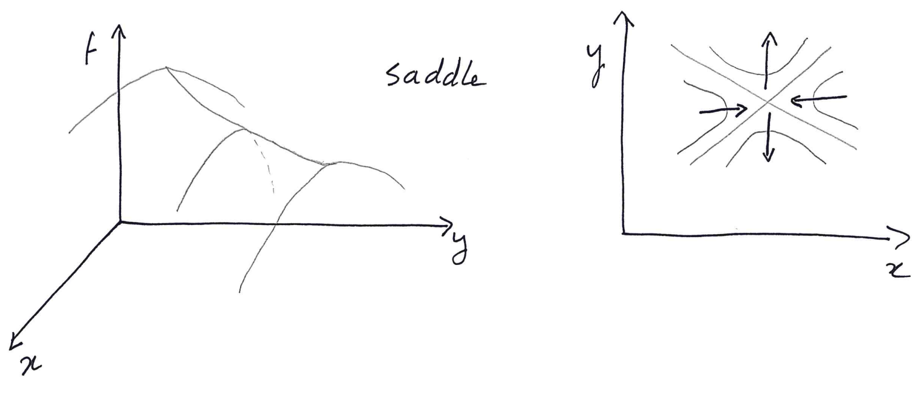

Figure 20.4: Schematic representation of a saddle. Note that the contours are locally hyperbolic.

Chapter 21

Stationary point classification

In this chapter we describe how to distinguish mathematically between different kinds of stationary points.

21.1 Multivariate Taylor series

Consider a finite displacement $\boldsymbol{\delta}\mathbf{s}$ along a straight line in the $x - y$ plane, as shown schematically in figure 21.1. Then,

$$\delta s \frac{d}{ds} = \boldsymbol{\delta}\mathbf{s}.\boldsymbol{\nabla}.$$

The Taylor series along the line is:

$$\begin{aligned}
f(\mathbf{s}) &= f(\mathbf{s}_0 + \boldsymbol{\delta}\mathbf{s});\ \mathbf{s} = (x, y);\ \mathbf{s}_0 = (x_0, y_0), \\
&= f(\mathbf{s}_0) + \delta s \frac{df}{ds} + \frac{1}{2} (\delta s)^2 \frac{d^2 f}{ds^2} + \ldots \\
&= f(\mathbf{s}_0) + \boldsymbol{\delta}\mathbf{s}.\boldsymbol{\nabla} f + \frac{1}{2} (\delta s)^2 (\hat{\mathbf{s}}.\boldsymbol{\nabla}) (\hat{\mathbf{s}}.\boldsymbol{\nabla}) f + \ldots
\end{aligned}$$

Here

$$\boldsymbol{\delta}\mathbf{s}.\boldsymbol{\nabla} f = \delta x \frac{\partial f}{\partial x} + \delta y \frac{\partial f}{\partial y} = (x - x_0) \frac{\partial f}{\partial x} + (y - y_0) \frac{\partial f}{\partial y},$$

and

$$\begin{aligned}
(\delta s)^2 (\hat{\mathbf{s}}.\boldsymbol{\nabla}) (\hat{\mathbf{s}}.\boldsymbol{\nabla}) f &= (\delta s)^2 \left[\hat{s}_x \frac{\partial}{\partial x} + \hat{s}_y \frac{\partial}{\partial y} \right] \left[\hat{s}_x \frac{\partial f}{\partial x} + \hat{s}_y \frac{\partial f}{\partial y} \right], \\
&= (\delta x)^2 \frac{\partial^2 f}{\partial x^2} + (\delta x \delta y) \frac{\partial^2 f}{\partial y \partial x} \\
&\quad + (\delta y \delta x) \frac{\partial^2 f}{\partial x \partial y} + (\delta y)^2 \frac{\partial^2 f}{\partial y^2},
\end{aligned}$$

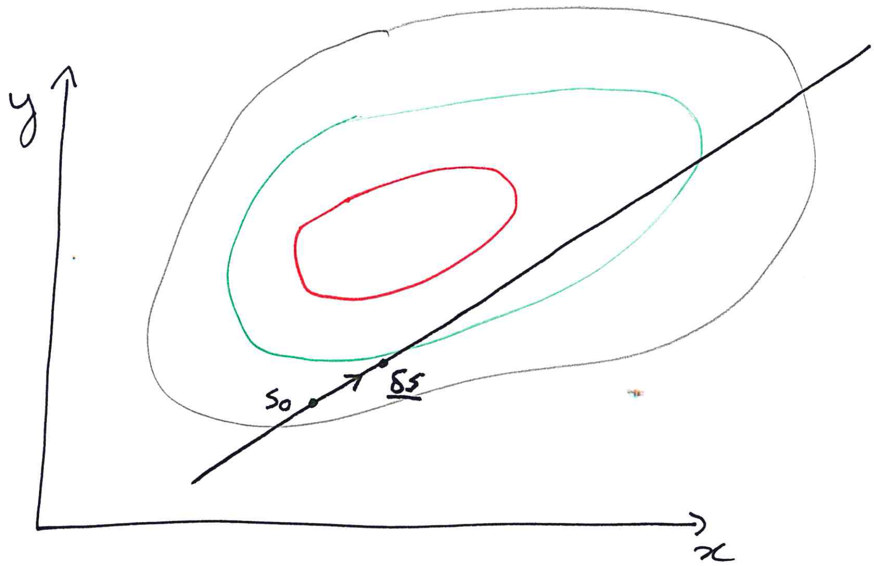

Figure 21.1: Schematic representation of a finite displacement $\boldsymbol{\delta}\mathbf{s}$.

using the fact that

$$\boldsymbol{\delta}\mathbf{s} = \delta s \hat{\mathbf{s}} = ([\delta s]\hat{s}_x, [\delta s]\hat{s}_y) = (\delta x, \delta y).$$

This last expression can be written in matrix form since

$$(\hat{\mathbf{s}}.\boldsymbol{\nabla})(\hat{\mathbf{s}}.\boldsymbol{\nabla}) f = (\delta x, \delta y) \begin{pmatrix} f_{xx} & f_{xy} \\ f_{yx} & f_{yy} \end{pmatrix} \begin{pmatrix} \delta x \\ \delta y \end{pmatrix},$$

where the matrix

$$[\boldsymbol{\nabla}\boldsymbol{\nabla} f] = \begin{pmatrix} f_{xx} & f_{xy} \\ f_{yx} & f_{yy} \end{pmatrix} = \mathsf{H}$$

is the **Hessian** matrix.

21.1.1 Taylor series in 2D cartesian coordinates

Therefore, the leading order terms of a Taylor series expansion in 2D cartesian coordinates about the point $\mathbf{x}_0 = (x_0, y_0)$ for a function with continuous second derivatives at $\mathbf{x}_0$ are

$$\begin{aligned} f(x,y) &= f(x_0,y_0) + (x-x_0)f_x + (y-y_0)f_y \\ &\quad + \frac{1}{2}\left[(x-x_0)^2 f_{xx} + 2(x-x_0)(y-y_0)f_{xy} + (y-y_0)^2 f_{yy}\right] + \ldots, \end{aligned}$$

where all derivatives are evaluated at $\mathbf{x}_0 = (x_0, y_0)$. This is the cartesian representation of the general coordinate-free form:

$$f(\mathbf{x}) = f(\mathbf{x}_0) + \boldsymbol{\delta}\mathbf{x}^T.\boldsymbol{\nabla} f(\mathbf{x}_0) + \frac{1}{2}\boldsymbol{\delta}\mathbf{x}^T.\left[\boldsymbol{\nabla}\boldsymbol{\nabla} f(\mathbf{x}_0)\right].\boldsymbol{\delta}\mathbf{x} + \dots$$

where $\mathbf{x} = \mathbf{x}_0 + \boldsymbol{\delta}\mathbf{x}$, and the superscript T denotes transpose.

21.2 Stationary point classification

Therefore, near a stationary point, where $\boldsymbol{\nabla} f = \mathbf{0}$ by construction:

$$f(\mathbf{x}) = f(\mathbf{x}_0) + \frac{1}{2}\boldsymbol{\delta}\mathbf{x}^T.\left[\boldsymbol{\nabla}\boldsymbol{\nabla} f(\mathbf{x}_0)\right].\boldsymbol{\delta}\mathbf{x} + \dots = f(\mathbf{x}_0) + \frac{1}{2}\boldsymbol{\delta}\mathbf{x}^T.\mathsf{H}.\boldsymbol{\delta}\mathbf{x} + \dots, \tag{21.1}$$

where $\mathsf{H} = \boldsymbol{\nabla}\boldsymbol{\nabla} f(\mathbf{x}_0)$ is the Hessian matrix evaluated at $\mathbf{x}_0$, and $\mathbf{x} = \mathbf{x}_0 + \boldsymbol{\delta}\mathbf{x}$.

Minima

We say that H is **positive definite** if

$$\boldsymbol{\delta}\mathbf{x}^T.\mathsf{H}.\boldsymbol{\delta}\mathbf{x} > 0 \ \forall\ \boldsymbol{\delta}\mathbf{x} \neq \mathbf{0}.$$

If H is positive definite at a stationary point, then that stationary point is a **minimum**.

Maxima

We say that H is **negative definite** if

$$\boldsymbol{\delta}\mathbf{x}^T.\mathsf{H}.\boldsymbol{\delta}\mathbf{x} < 0 \ \forall\ \boldsymbol{\delta}\mathbf{x} \neq \mathbf{0}.$$

If H is negative definite at a stationary point, then that stationary point is a **maximum**.

Saddles

If there exists a $\boldsymbol{\delta}\mathbf{x}_1$ and a $\boldsymbol{\delta}\mathbf{x}_2$ such that

$$\boldsymbol{\delta}\mathbf{x}_1^T.\mathsf{H}.\boldsymbol{\delta}\mathbf{x}_1 < 0;\ \ \boldsymbol{\delta}\mathbf{x}_2^T.\mathsf{H}.\boldsymbol{\delta}\mathbf{x}_2 > 0,$$

then H is **indefinite**. If H is indefinite at a stationary point, then that stationary point is a **saddle**.

21.3 Determination of definiteness

H is a symmetric matrix. In the 2D cartesian case, $f_{xy} = f_{yx}$ which can be naturally generalised to higher dimensions. Since H is symmetric it can be diagonalized. Therefore, for a function $f(\mathbf{x})$ dependent on n independent variables $\mathbf{x} = (x_1, x_2, \ldots x_n)$, with respect to principal axes (remember V & M), it is possible to write

$$\begin{aligned}\boldsymbol{\delta}\mathbf{x}^T.\mathsf{H}.\boldsymbol{\delta}\mathbf{x} &= (\delta x_1, \delta x_2, \ldots \delta x_n)\begin{pmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \ddots & \\ & & & \lambda_n \end{pmatrix}\begin{pmatrix} \delta x_1 \\ \delta x_2 \\ \vdots \\ \delta x_n \end{pmatrix}, \\ &= \lambda_1 \delta x_1^2 + \lambda_2 \delta x_2^2 + \cdots + \lambda_n \delta x_n^2.\end{aligned}$$

Therefore, H being positive definite (remember that is a condition for all $\boldsymbol{\delta}\mathbf{x}$) is equivalent to **all** the eigenvalues being positive. Similarly, H being negative definite is equivalent to **all** the eigenvalues being negative.

21.3.1 The signature of the Hessian

The **signature** of H is the pattern of signs of the ordered subdeterminants of the principal minors, i.e.

$$\begin{aligned}|\mathsf{H}_1| &= |f_{x_1x_1}|, \\ |\mathsf{H}_2| &= \begin{vmatrix} f_{x_1x_1} & f_{x_1x_2} \\ f_{x_2x_1} & f_{x_2x_2} \end{vmatrix}, \\ |\mathsf{H}_n| = |\mathsf{H}| &= \begin{vmatrix} f_{x_1x_1} & f_{x_1x_2} & \cdots & f_{x_1x_n} \\ f_{x_2x_1} & f_{x_2x_2} & \cdots & f_{x_2x_n} \\ \vdots & \vdots & \ddots & \vdots \\ f_{x_nx_1} & f_{x_nx_2} & \cdots & f_{x_nx_n} \end{vmatrix}.\end{aligned}$$

If H is positive definite, and equivalently the stationary point is a minimum, then each of the sub Hessians i.e. H_1, H_2, $\ldots \mathsf{H}_n$ is also positive definite, since the stationary point must also be a minimum in any subspace that includes it, and its determinant (i.e. the product of the eigenvalues) is positive. Therefore, in terms of the signature:

- H being positive definite is equivalent to the signature being $+ + \cdots +$ (this is also known as **Sylvester's criterion**);
- H being negative definite is equivalent to the signature being $- + - \ldots (-1)^n$, i.e. the sub Hessians with an odd number of rows and

columns have negative determinants, while the sub Hessians with an even number of rows and columns have positive determinants;

- If neither of these conditions apply, and yet there is both + and − in the signature, H is indefinite.

Note if $\det \mathsf{H} = 0$, and $\lambda_j \geq 0$ for all j, or $\lambda_j \leq 0$ for all j, then the stationary point is said to be **degenerate**, and other techniques (e.g. more terms in the Taylor series) typically need to be used to determine the character of the stationary point.

21.4 Contours of $f(x, y)$

Let $\mathbf{x}_0$ be a stationary point. We define our coordinate system relative to the principal axes of H, and so

$$\mathsf{H} = \left(\begin{array}{cc} \lambda_1 & 0 \\ 0 & \lambda_2 \end{array} \right); (\mathbf{x} - \mathbf{x}_0) = (\xi, \eta) = \boldsymbol{\delta}\mathbf{x}.$$

Therefore

$$f = C \to \boldsymbol{\delta}\mathbf{x}^T.\mathsf{H}.\boldsymbol{\delta}\mathbf{x} = C \text{ locally} \to \lambda_1 \xi^2 + \lambda_2 \eta^2 = C,$$

where C is a constant. At a maximum or minimum, since λ_1 and λ_2 have the same sign, the contours are ellipses, while at a saddle, λ_1 and λ_2 have opposite signs, and so the contours are hyperbolae. As ever, let us try and fix ideas by considering an example.

Example

Consider the function

$$f(x, y) = 4x^3 - 12xy + y^2 + 10y + 6. \tag{21.2}$$

For this function:

$$\begin{array}{rr} f_x = 12x^2 - 12y, & f_y = -12x + 2y + 10, \\ f_{xx} = 24x, & f_{yx} = -12, \\ f_{xy} = -12, & f_{yy} = 2. \end{array}$$

At stationary points, $f_x = f_y = 0$ and so we require simultaneously that

$$12x^2 - 12y = 0 \to y = x^2,$$

and

$$-12x + 2y + 10 = 0 \to -6x + x^2 + 5 = 0 \to (x-5)(x-1) = 0.$$

Therefore, $x = 1, 5$ implying that $y = 1, 25$ respectively, and so there are two stationary points $(1, 1)$ and $(5, 25)$.

Let us consider the two stationary points in turn. Firstly, at $(1, 1)$,

$$\mathsf{H} = \boldsymbol{\nabla}\boldsymbol{\nabla} f = \begin{pmatrix} 24 & -12 \\ -12 & 2 \end{pmatrix}.$$

Therefore $|\mathsf{H}_1| = 24 > 0$, while $|\mathsf{H}_2| = |\mathsf{H}| = 48 - 144 < 0$. This signature is neither of the form associated with a positive definite Hessian, nor of the form associated with a negative definite Hessian, and so H is indefinite, and the stationary point is a saddle.

From (21.1), defining $\boldsymbol{\delta}\mathbf{x} = (\xi, \eta)$, we see that

$$\begin{aligned} f(\mathbf{x}) &= f(1,1) + \frac{1}{2}\left(f_{xx}\xi^2 + 2f_{xy}\xi\eta + f_{yy}\eta^2\right), \\ &= 9 + \frac{1}{2}\left(24\xi^2 + 2(-12)\xi\eta + 2\eta^2\right) \\ &= 9 + 12\xi^2 - 12\xi\eta + \eta^2. \end{aligned}$$

Therefore, the equation (locally) for the two intersecting contours is

$$\eta^2 - 12\xi\eta + 12\xi^2 = 0 \to \eta = \left(6 \pm 2\sqrt{6}\right)\xi.$$

On the other hand, at $(5, 25)$,

$$\mathsf{H} = \boldsymbol{\nabla}\boldsymbol{\nabla} f = \begin{pmatrix} 120 & -12 \\ -12 & 2 \end{pmatrix}.$$

Therefore $|\mathsf{H}_1| = 120 > 0$, and also $|\mathsf{H}_2| = |\mathsf{H}| = 240 - 144 > 0$. This signature is of the form associated with a positive definite Hessian, and so the stationary point is a minimum, and we expect the contours in the vicinity of this point to be ellipses. We sketch (rather badly) the contours of $f(x, y)$ in figure 21.2, showing the direction of $\boldsymbol{\nabla} f$ in some places. Note the (expected) local shape of the contours in the vicinities of the fixed points.

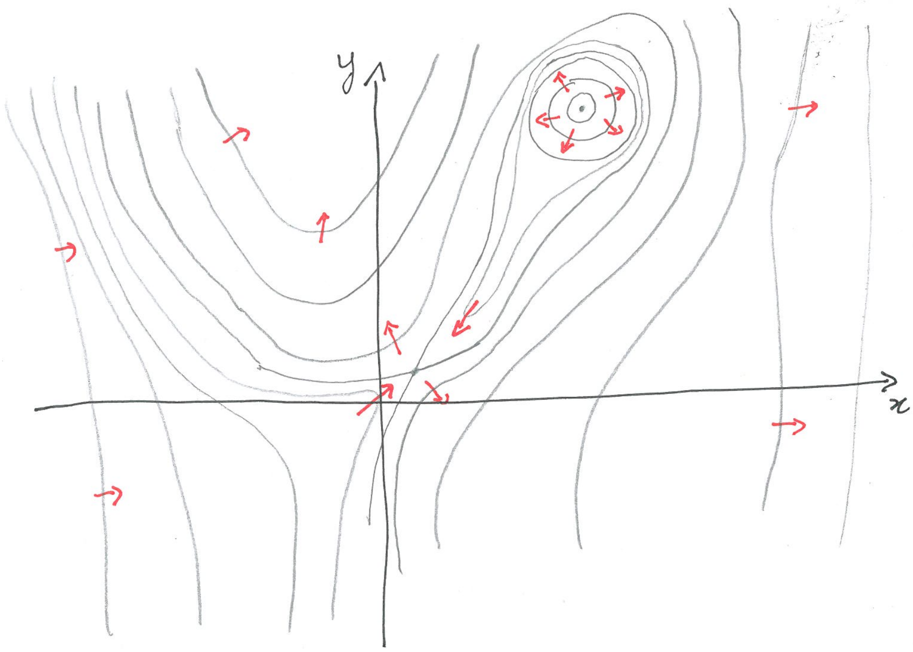

Figure 21.2: Schematic representation of the contours of $f(x, y)$ as defined in (21.2). Note the local shape of the contours in the vicinity of the two stationary points. Some directions of the gradient of f are also marked.

Chapter 22

Systems of linear equations

In this chapter we consider the behaviour of **systems** of first order linear differential equations of multiple independent variables coupled to each other.

22.1 Equivalence of systems

Consider two dependent variables which satisfy coupled first order differential equations:

$$\dot{y}_1 = ay_1 + by_2 + f_1(t), \tag{22.1}$$
$$\dot{y}_2 = cy_1 + dy_2 + f_2(t). \tag{22.2}$$

Therefore

$$\dot{\mathbf{Y}} = \mathsf{M}\mathbf{Y} + \mathbf{F}; \mathbf{Y} = \begin{pmatrix} y_1 \\ y_2 \end{pmatrix}; \; \mathsf{M} = \begin{pmatrix} a & b \\ c & d \end{pmatrix}; \; \mathbf{F} = \begin{pmatrix} f_1 \\ f_2 \end{pmatrix}.$$

Differentiating (22.1), we obtain

$$\ddot{y}_1 = a\dot{y}_1 + b\dot{y}_2 + \dot{f}_1.$$

Equation (22.2) can be used to eliminate $\dot{y}_2$ to obtain

$$\ddot{y}_1 = a\dot{y}_1 + bcy_1 + dby_2 + bf_2 + \dot{f}_1.$$

Equation (22.1) can be re-arranged to express y_2 in terms of y_1, $\dot{y}_1$ and f_1 to obtain:

$$\ddot{y}_1 - (a+d)\dot{y}_1 + (ad - bc)y_1 = bf_2 - df_1 + \dot{f}_1,$$

which is of the form

$$\ddot{y}_1 + A\dot{y}_1 + By_1 = F,$$

i.e. the system of equations can be transformed into a second order differential equation. Note that for the equation to be nontrivially second order $B \neq 0$, which is equivalent to the matrix M having a non-zero determinant, and hence being invertible.

Conversely, if

$$\ddot{y} + \alpha\dot{y} + \beta y = f,$$

if we write $y_1 = y$, and $y_2 = \dot{y}$ then we can obtain the equivalent system of equations

$$\dot{y}_1 = y_2;\ \dot{y}_2 = f - \alpha y_2 - \beta y_1.$$

This system can be posed in matrix form:

$$\dot{\mathbf{Y}} = \mathsf{M}\mathbf{Y} + \mathbf{F}; \mathbf{Y} = \begin{pmatrix} y_1 \\ y_2 \end{pmatrix};\ \mathsf{M} = \begin{pmatrix} 0 & 1 \\ -\beta & -\alpha \end{pmatrix};\ \mathbf{F} = \begin{pmatrix} 0 \\ f \end{pmatrix}.$$

Observe again that the requirement that the matrix is invertible is that $\beta \neq 0$, which is consistent with the requirement that the original differential equation is non-trivially second order. Indeed, any n^{th} order differential equation can be written as a system of N first order differential equations.

22.2 Methods of solution

Now consider methods of solution of the general system of equations:

$$\dot{\mathbf{Y}} = \mathsf{M}\mathbf{Y} + \mathbf{F} \leftrightarrow \dot{\mathbf{Y}} - \mathsf{M}\mathbf{Y} = \mathbf{F}. \tag{22.3}$$

where M has all constant elements. As in Part III of the course, we solve such an inhomogeneous system in two stages:

1. We find the general complementary function $\mathbf{Y}_c$ as a solution of the **homogeneous** system of equations:

$$\dot{\mathbf{Y}} - \mathsf{M}\mathbf{Y} = \mathbf{0}.$$

2. We then find a particular integral $\mathbf{Y}_p$ as a solution of the full (forced) system of equations (22.3) with non-trivial forcing $\mathbf{F} \neq \mathbf{0}$.

22.2.1 Complementary functions

Unsurprisingly, an appropriate form for the complementary function is

$$\mathbf{Y}_c = \mathbf{v}e^{\lambda t},$$

where $\mathbf{v}$ is a constant vector. Therefore,

$$\lambda \mathbf{v} - \mathsf{M}\mathbf{v} = \mathbf{0} \to \mathsf{M}\mathbf{v} = \lambda \mathbf{v},$$

and so λ is an eigenvalue and $\mathbf{v}$ is its associated eigenvector.

Identification of λ and $\mathbf{v}$ is then straightforward. Since

$$(\mathsf{M} - \lambda \mathsf{I})\mathbf{v} = \mathbf{0} \to |\mathsf{M} - \lambda \mathsf{I}| = 0.$$

The requirement that this determinant is zero yields the characteristic equation for λ. Roots of this equation are the eigenvalues, for each of which it is straightforward to identify the associated eigenvectors. As usual, let us fix ideas by considering an example.

Example

Consider the system

$$\dot{\mathbf{Y}} - \begin{pmatrix} -4 & 24 \\ 1 & -2 \end{pmatrix} \mathbf{Y} = \begin{pmatrix} 4 \\ 1 \end{pmatrix} e^t. \tag{22.4}$$

For the complementary function $\mathbf{Y}_c = \mathbf{v}\exp(\lambda t)$, we obtain

$$\begin{vmatrix} -4-\lambda & 24 \\ 1 & -2-\lambda \end{vmatrix} = 0 \to 8 + 6\lambda + \lambda^2 - 24 = 0 = (\lambda+8)(\lambda-2),$$

and so the eigenvalues are $\lambda = 2$ and $\lambda = -8$.

$\lambda = 2$

For $\lambda = 2$, the associated eigenvector must satisfy

$$\begin{pmatrix} -6 & 24 \\ 1 & -4 \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = \mathbf{0} \to \mathbf{v} = \begin{pmatrix} 4 \\ 1 \end{pmatrix}.$$

$\lambda = -8$

Similarly, for $\lambda = -8$, the associated eigenvector must satisfy

$$\begin{pmatrix} 4 & 24 \\ 1 & 6 \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = \mathbf{0} \to \mathbf{v} = \begin{pmatrix} -6 \\ 1 \end{pmatrix}.$$

Therefore, the general complementary function is

$$\mathbf{Y} = A \begin{pmatrix} 4 \\ 1 \end{pmatrix} e^{2t} + B \begin{pmatrix} -6 \\ 1 \end{pmatrix} e^{-8t}, \tag{22.5}$$

for arbitrary constants A and B. Phase space trajectories are sketched in figure 22.1.

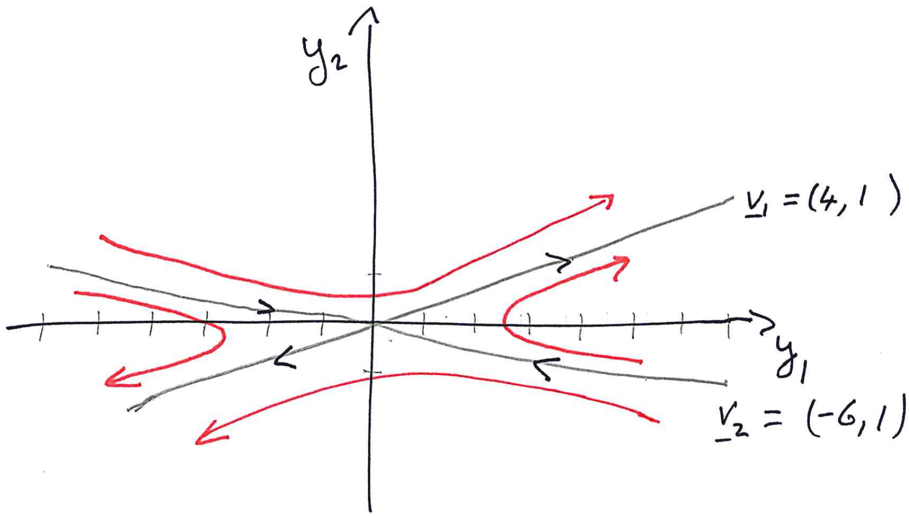

Figure 22.1: Schematic representation of the phase space trajectory for the complementary functions defined by (22.5).

Particular integral

For the particular integral, we assume a form inspired by the right hand side of (22.4), and so we try $\mathbf{Y}_p = \mathbf{u}e^t$ for some constant vector $\mathbf{u}$. Therefore

$$\begin{aligned}
\begin{pmatrix} u_1 \\ u_2 \end{pmatrix} - \begin{pmatrix} -4 & 24 \\ 1 & -2 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} &= \begin{pmatrix} 4 \\ 1 \end{pmatrix}, \\
\rightarrow \begin{pmatrix} 5 & -24 \\ -1 & 3 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} &= \begin{pmatrix} 4 \\ 1 \end{pmatrix}, \\
\rightarrow \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = \frac{-1}{9} \begin{pmatrix} 3 & 24 \\ 1 & 5 \end{pmatrix} \begin{pmatrix} 4 \\ 1 \end{pmatrix} &= \begin{pmatrix} -4 \\ -1 \end{pmatrix},
\end{aligned}$$

if we remember how to invert a matrix properly (unlike in the lecture ...)

Therefore the general solution is

$$\mathbf{Y} = A \begin{pmatrix} 4 \\ 1 \end{pmatrix} e^{2t} + B \begin{pmatrix} -6 \\ 1 \end{pmatrix} e^{-8t} - \begin{pmatrix} 4 \\ 1 \end{pmatrix} e^{t}.$$

22.3 Non-degenerate phase portraits

In general, the solution to $\dot{\mathbf{Y}} = \mathsf{M}\mathbf{Y}$ is

$$\mathbf{Y} = \mathbf{v}_1 e^{\lambda_1} t + \mathbf{v}_2 e^{\lambda_2} t.$$

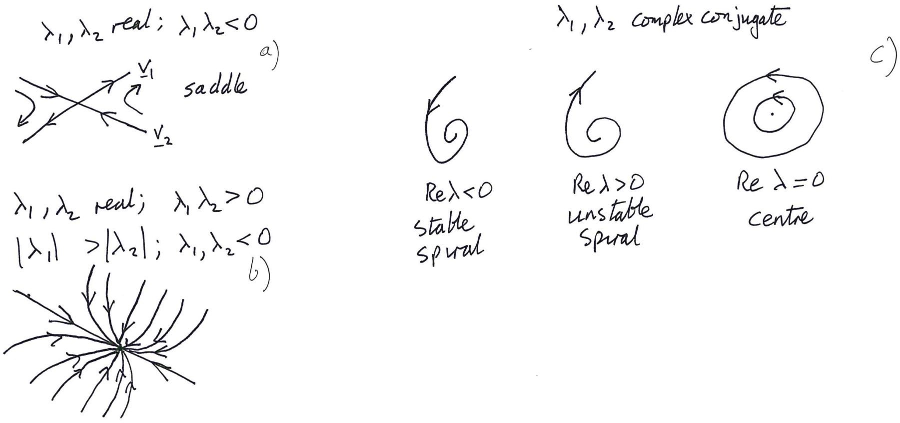

Figure 22.2: Schematic representation of different types of phase portraits associated with different types of non-degenerate fixed points: a) a saddle with two real eigenvalues λ_1 and λ_2 such that $\lambda_1\lambda_2 < 0$. In the figure, $\lambda_1 > 0$ and $\lambda_2 < 0$; b) a node with two real eigenvalues λ_1 and λ_2 such that $\lambda_1\lambda_2 > 0$. In the figure, $\lambda_1 < \lambda_2 < 0$ and so the node is stable. If $\lambda_1 > \lambda_2 > 0$ the picture looks the same just with the arrow heads reversed; c) the three different situations for complex conjugate distinct eigenvalues, $\lambda_1 = \lambda$, $\lambda_2 = \lambda^*$ leading to a stable spiral if $Re(\lambda) < 0$, an unstable spiral if $Re(\lambda) > 0$ and a centre if $Re(\lambda) = 0$ precisely.

In this course we will only consider **non-degenerate** cases, i.e. where $\lambda_1 \neq 0$, $\lambda_2 \neq 0$ and $\lambda_1 \neq \lambda_2$. These more funky flows (leading to **star nodes**, **defective nodes**, **combs**, **parallel lines** and even blank pages [?!]) will be discussed in other courses of course, in particular in Dynamical Systems in Part II.

Even restricting ourselves to non-degenerate characteristic equations, we have three different types of phase portrait behaviour in the vicinity of a fixed point as shown in figure 22.2 Each case is associated with different properties of the eigenvalues.

Case I

This case is shown in figure 22.2a. Here λ_1 and λ_2 are real such that $\lambda_1\lambda_2 < 0$. The stationary point is a **saddle**. In both figure 22.2a and figure 22.1, $\lambda_1 > 0$ and $\lambda_2 < 0$.

Case II

This case is shown in figure 22.2b. Here λ_1 and λ_2 are real such that $\lambda_1\lambda_2 > 0$. Without loss of generality, $|\lambda_1| > |\lambda_2|$. The case shown in the figure has $\lambda_1 < \lambda_2 < 0$, and so the stationary point is a **stable node**. If $\lambda_1 > \lambda_2 > 0$, the phase portrait would look the same, with the arrow direction reversed, and the stationary point would be an **unstable node**.

Case III

These cases are shown in figure 22.2c, and are associated with complex conjugate eigenvalues $\lambda_1 = \lambda_2^* = \lambda$. with non-zero imaginary part.

- If $Re(\lambda) < 0$, the phase portrait is a **stable spiral** and solutions spiral **into** the stationary point.
- If $Re(\lambda) > 0$, the phase portrait is an **unstable spiral** and solutions spiral **out from** the stationary point.
- If λ is purely imaginary, the stationary point is a **centre** and solutions loop around the stationary point on locally elliptical paths.

Of these generic behaviours, all except the centre are said to be **structurally stable**, in the sense that small changes in the parameters or elements of the key matrix M will not change the character of the fixed point. It seems reasonable that the centre is more fragile (indeed it is **structurally unstable**) since a small change is highly likely to introduce a real part into the eigenvalues, thus changing the centre into a spiral. Interestingly, the eigenvalues do not in themselves determine the direction of flow for the solutions around spirals and centres. As we shall see (by example of course!) it is straightforward to determine this direction by considering solution curves, typically at just one point.

Chapter 23

Nonlinear dynamics

In this chapter, we consider the truly wonderful world of systems of nonlinear differential equations, showing that the **linear** techniques developed in the previous chapter are still useful.

23.1 Stability of equilibrium (fixed) points

Consider the second order autonomous system

$$\dot{x} = f(x, y); \;\; \dot{y} = g(x, y),$$

where $x(t)$ and $y(t)$, yet f and g do not depend on t explicitly. We can learn a lot about the phase-space trajectories of solutions by considering equilibria (fixed points) and their stability.

Fixed points correspond to $\dot{x} = \dot{y} = 0$. Determining a fixed point (x_0, y_0) therefore requires solving

$$f(x_0, y_0) = g(x_0, y_0) = 0.$$

It is then typically appropriate to consider the stability of such a fixed point.

Write $x = x_0 + \xi$, $y = y_0 + \eta$ where ξ and η are small in some appropriate sense. Then, expanding f in terms of a multivariate Taylor series:

$$\dot{\xi} \;\; = \;\; f(x_0 + \xi, y_0 + \eta) = f(x_0, y_0) + \xi \frac{\partial f}{\partial x}(x_0, y_0) + \eta \frac{\partial f}{\partial y}(x_0, y_0) + H.O.T.,$$

where the "Higher Order Terms" involve at least second order powers of small quantities, and $f(x_0, y_0) = 0$ by definition. A similar expansion for $\dot{y}$ leads to a **linear** system for ξ and η:

$$\begin{pmatrix} \dot{\xi} \\ \dot{\eta} \end{pmatrix} = \begin{pmatrix} f_x & f_y \\ g_x & g_y \end{pmatrix} \begin{pmatrix} \xi \\ \eta \end{pmatrix}. \tag{23.1}$$

The properties of this linear system, and hence the behaviour of the underlying nonlinear system near the fixed points can be determined from the eigenvalues and eigenvectors of this linear system.

23.2 Population dynamics

As an example, let us consider a classic **predator prey** system. The time evolution of the size x of the population of the "prey" in the presence of a population of size y of a "predator" is determined by the equation

$$\dot{x} = \alpha x - \beta x^2 - \gamma xy.$$

The first term on the right-hand side of this equation describes the net rate of growth associated with more births than deaths (i.e. $\alpha > 0$). The second term describes a death rate associated with mutual competition, while the third time describes death at the hands of the predators. On the other hand the evolution of the population y of the predators is given by the equation

$$\dot{y} = -\delta y + \epsilon xy.$$

Here, there are more deaths than births, and so the only way for the predators to survive is to eat some of the prey. So the game is on... and to understand the rules it is best to consider the properties of the fixed points ...

Example

Let us consider the specific example

$$\begin{aligned}\dot{x} &= 8x - 2x^2 - 2xy = f(x,y),\\ \dot{y} &= -y + xy = g(x,y).\end{aligned}$$

Therefore:

$$f_x = 8 - 4x - 2y,\ f_y = -2x;\ g_x = y,\ g_y = -1 + x.$$

Fixed points require

$$f(x,y) = 0 \to 2x(4 - x - y) = 0 \to x = 0 \ \text{ or } \ y = 4 - x,$$

and

$$g(x,y) = 0 \to y(x-1) = 0 \to y = 0 \text{ or } \ x = 1.$$

Therefore, there are three fixed points: $(0,0)$, $(4,0)$ and $(1,3)$.

Behaviour near $(0, 0)$

Substituting $x_0 = 0$, $y_0 = 0$ into (23.2), (23.1) becomes

$$\begin{pmatrix} \dot{\xi} \\ \dot{\eta} \end{pmatrix} = \begin{pmatrix} 8 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \xi \\ \eta \end{pmatrix}.$$

Hopefully it is "clear" that this fixed point is a saddle, with the $x-$direction being unstable, and the $y-$direction being stable.

Behaviour near $(4, 0)$

Now substituting $x_0 = 4$, $y_0 = 0$ into (23.2), (23.1) becomes

$$\begin{pmatrix} \dot{\xi} \\ \dot{\eta} \end{pmatrix} = \begin{pmatrix} -8 & -8 \\ 0 & 3 \end{pmatrix} \begin{pmatrix} \xi \\ \eta \end{pmatrix}.$$

Once again this fixed point is a saddle, since $\lambda_1 = -8$ and $\lambda_2 = 3$. The associated eigenvectors are $\mathbf{v}_1 = (1, 0)$ and $\mathbf{v}_2 = (8, -11)$.

Behaviour near $(1, 3)$

Finally substituting $x_0 = 1$, $y_0 = 3$ into (23.2), (23.1) becomes

$$\begin{pmatrix} \dot{\xi} \\ \dot{\eta} \end{pmatrix} = \begin{pmatrix} -2 & -2 \\ 3 & 0 \end{pmatrix} \begin{pmatrix} \xi \\ \eta \end{pmatrix}. \tag{23.2}$$

(As an exercise, can you use perturbation methods as in chapter 10 to determine the form of the matrix?) Here, the eigenvalues must satisfy

$$(-2 - \lambda)(-\lambda) + 6 = 0 \to \lambda = -1 \pm i\sqrt{5}.$$

Since the eigenvalues are complex conjugate with negative real part, this fixed point is a spiral.

The sense of the flow towards the fixed point for spirals and centres can be determined by considering the property of the solution at a **single** nearby well-chosen point, though it is often easier to visualize if several (still well-chosen) points are considered. From (23.2), it is apparent that

$$\dot{\xi}\Big|_{\xi=0} = -2\eta, \;\; \dot{\eta}|_{\eta=0} = 3\xi.$$

Therefore, nearby but directly above the fixed point, ($\xi = 0$, $\eta > 0$) the solution goes to the left, while directly below the fixed point, ($\xi = 0$, $\eta < 0$) the solution goes to the right. Similarly, directly to the right of the fixed

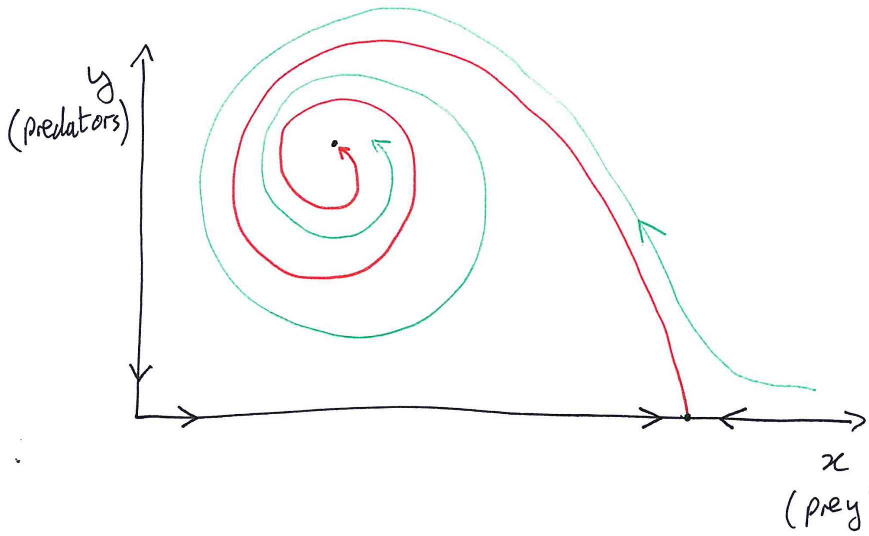

Figure 23.1: Schematic representation of the time evolution of the populations of prey $x(t)$ and predators $y(t)$. The anti-clockwise spiralling of the two populations into the fixed point $(1, 3)$ is clearly apparent.

point, ($\eta = 0$, $\xi > 0$) the solution goes upwards, while directly to the left of the fixed point, ($\eta = 0$, $\xi < 0$) the solution goes downwards. Taken all together, it is now possible to deduce that the solution spirals into this fixed point in a counter-clockwise sense.

Combining all the behaviours of the fixed points, the evolution of the system is shown schematically in figure 23.1. In the absence of prey (i.e. along the $y-$axis) the population of the predators decays monotonically. Analogously, in the absence of predators, (i.e. along the $x-$axis) the population of the prey approaches the fixed point at $(4, 0)$. However, both these situations are not stable. As soon as there is both prey and predators, the system spirals into the fixed point at $(1, 3)$, and there is a stable equilibrium with just enough rabbit to go round! Such an approach, involving a geometric interpretation of the nonlinear evolution is an extremely powerful way to gain insight into the behaviour of nonlinear systems when the differential equations may well not be solvable explicitly. As discussed in gory detail in other courses such as Dynamical Systems, one particular point of interest is the solution curve marked in red (formally referred to as the **unstable manifold**) of the saddle on the $x-$axis which is shown connecting to the stable spiral fixed point. Seems like a fun trip.

Chapter 24

Partial differential equations

In this last chapter, we will consider the briefest of introductions to **partial differential equations** (PDEs) i.e. differential equations where there are more than one **independent variables**. A particularly common example is of course where dependent variables depend on both space and time, and such equations occur all over the place in scientific (and indeed economic) systems. We will introduce two different kinds: **wave** equations and **diffusion** equations. You will hear much more about these equations in future years.

24.1 First order wave equation

As a first simplest example consider the equation for $y(x,t)$

$$\frac{\partial y}{\partial t} = c\frac{\partial y}{\partial x} \to \frac{\partial y}{\partial t} - c\frac{\partial y}{\partial x} = 0, \tag{24.1}$$

for c a constant. Note that c has the dimensions of a velocity, and is indeed the **phase speed** of the waves which satisfy this equation. We also typically need to know the **initial condition** that $y(x,0) = f(x)$.

Remember (4.9) in chapter 4, which describes the evolution of y along a given path $x(t)$:

$$\frac{dy}{dt} = \frac{\partial y}{\partial t} + \frac{\partial y}{\partial x}\frac{dx}{dt}.$$

Comparing this to (24.1), we see that

$$\frac{dy}{dt} = 0 \to y = \text{constant},$$

along paths

$$\frac{dx}{dt} = -c \to x = x_0 - ct;\ x + ct = x_0,$$

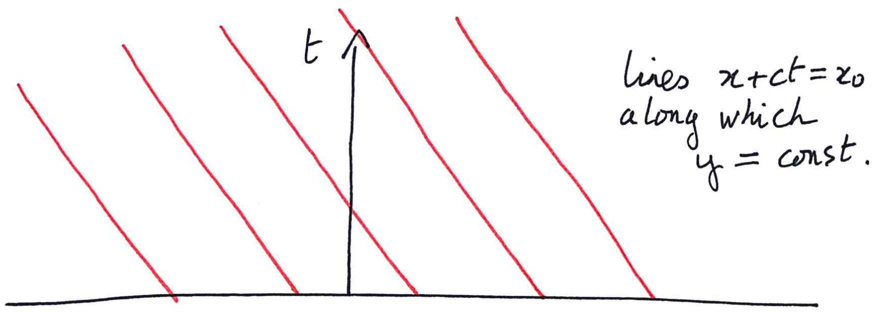

Figure 24.1: Schematic representation of the characteristics of the first order wave equation.

where x_0 is also a constant.

Therefore $y = f(x_0) = f(x + ct)$. The lines $x + ct = x_0$ along which y are constant are called **characteristics** of the PDE. They are shown schematically in figure 24.1. Effectively, x_0 is the label of each of the characteristics on the initial condition line $t = 0$. Usually **initial conditions** are indeed given, and the problem is typically well-posed provided the initial conditions are given on a curve which is not coincident with a characteristic. In fact, as you shall see in other courses, characteristics do not have to be straight lines, it is just that the mathematics is more straightforward if they are.

Example 1: Unforced waves

As a specific example, if $y(x, 0) = x^2 - 3$, and y satisfies (24.1) for $t \geq 0$, then $y = (x + ct)^2 - 3$.

Example 2: Forced wave equation

Furthermore, the solution can evolve along the characteristic if the wave equation is forced/inhomogeneous, in that it involves a term which does not depend on y. As an example, consider the problem:

$$\frac{\partial y}{\partial t} + 5\frac{\partial y}{\partial x} = e^{-t};\ y(x, 0) = e^{-x^2}.$$

Here

$$\frac{dy}{dt} = e^{-t},$$

on paths (characteristics) defined by

$$\frac{dx}{dt} = 5.$$

Therefore,

$$y = A - e^{-t}, \text{ on } \; x = x_0 + 5t,$$

where A is a constant **on** a particular characteristic. We can determine A by applying the initial conditions. At $t = 0$,

$$x = x_0; \; y = A - 1 = e^{-x_0^2} \to A = 1 + e^{-x_0^2}.$$

Therefore, the general solution is

$$y = 1 + \exp[-(x - 5t)^2] - e^{-t},$$

re-expressing the label x_0 in terms of x and t along the characteristic for later times.

24.2 Second-order wave equation

In the previous section we considered waves which only went to the left. In general, as all guitarists know when they pluck strings, waves can go in more than one direction. So let us consider the second order wave equation

$$\frac{\partial^2 y}{\partial t^2} = c^2 \frac{\partial^2 y}{\partial x^2}; \; y(x, 0) = \phi(x); \; \frac{\partial y}{\partial t}(x, 0) = \psi(x), \tag{24.2}$$

where the initial disturbance and velocity are both specified.

Since c is a constant, the differential operator can be straightforwardly factorised:

$$\frac{\partial^2 y}{\partial t^2} - c^2 \frac{\partial^2 y}{\partial x^2} = 0 \to \left(\frac{\partial}{\partial t} + c\frac{\partial}{\partial x} \right) \left(\frac{\partial}{\partial t} - c\frac{\partial}{\partial x} \right) y = 0.$$

These operators commute, and so both $y = f(x + ct)$ and $y = g(x - ct)$ are solutions, and since the equation is linear $y = f(x + ct) + g(x - ct)$ is also a solution.

This can be derived directly from the properties of the characteristics. Since the equation is second order, there are now two sets of characteristics, $\xi = x + ct$ leaning to the left as before, and $\eta = x - ct$ leaning to the right. Now, from the chain rule, just for a change:

$$\begin{aligned} \frac{\partial}{\partial x} &= \frac{\partial \xi}{\partial x}\frac{\partial}{\partial \xi} + \frac{\partial \eta}{\partial x}\frac{\partial}{\partial \eta} = \frac{\partial}{\partial \xi} + \frac{\partial}{\partial \eta}, \\ \frac{\partial}{\partial t} &= c\frac{\partial}{\partial \xi} - c\frac{\partial}{\partial \eta}. \end{aligned}$$

Therefore, applying these relationships twice to each side of (24.2),

$$c^2\left(\frac{\partial^2}{\partial\xi^2}y+\frac{\partial^2}{\partial\eta^2}y+2\frac{\partial^2}{\partial\xi\partial\eta}y\right) = c^2\left(\frac{\partial^2}{\partial\xi^2}y+\frac{\partial^2}{\partial\eta^2}y-2\frac{\partial^2}{\partial\xi\partial\eta}y\right),$$

and so

$$\begin{aligned}\frac{\partial^2}{\partial\xi\partial\eta}y &= 0\to\frac{\partial}{\partial\eta}y=G(\eta),\\ \to y &= \int^\eta G(y)dy+g(\xi)=f(\eta)+g(\xi),\\ &= f(x+ct)+g(x-ct),\end{aligned}\tag{24.3}$$

for arbitrary functions f and g.

Therefore, solutions propagate along the characteristics (lines $x+ct=$ constant, and $x-ct=$ constant) without change. For $c>0$, the characteristics $\xi=A_1$ correspond to motion to the left, while characteristics $\eta=A_2$ correspond to motion to the right. Importantly, discontinuities can also propagate along the characteristics too, as can be seen by applying the initial conditions to the general solution (24.3). Any discontinuity in the initial conditions propagate along a characteristic.

24.2.1 d'Alembert's solution

At $t=0$, the initial conditions in (24.1) imply that

$$\begin{aligned}y(x) &= f(x)+g(x)=\phi(x),\\ \left.\frac{\partial y}{\partial t}\right|_{t=0} &= cf'(x)-cg'(x)=\psi(x).\end{aligned}$$

Differentiating the initial condition on y, a little manipulation yields

$$\begin{aligned}\phi'(x) &= f'(x)+g'(x),\\ \frac{1}{c}\psi(x) &= f'(x)-g'(x),\\ f'(x) &= \frac{1}{2}\left[\phi'(x)+\frac{1}{c}\psi(x)\right],\\ f(x) &= \frac{1}{2}\phi(x)+\frac{1}{2c}\int_0^x\psi(y)dy,\\ g(x) &= \frac{1}{2}\phi(x)-\frac{1}{2c}\int_0^x\psi(y)dy.\end{aligned}$$

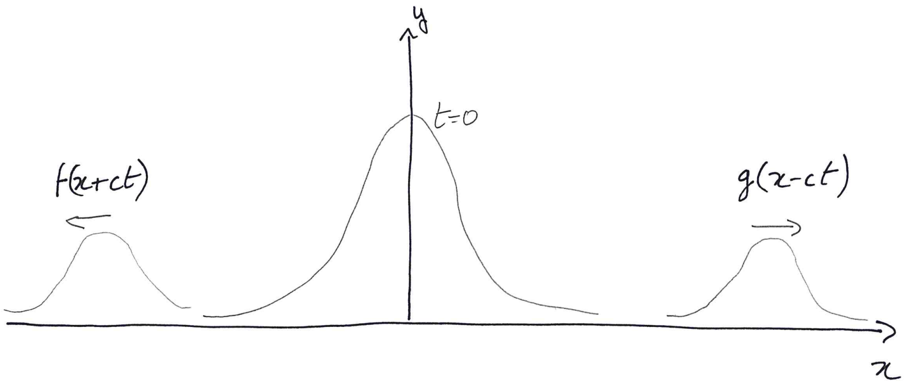

Figure 24.2: Schematic representation of the evolution of an initial displacement which satisfies the two-dimensional wave equation. Note that the initial displacement splits into two which travel to the left and right at speed c.

Therefore, at a general time, we obtain **d'Alembert's solution**

$$\begin{aligned} u(x,t) &= f(x+ct) + g(x-ct), \\ &= \frac{1}{2}\left[\phi(x+ct) + \phi(x-ct)\right] + \frac{1}{2c}\int_{x-ct}^{x+ct} \psi(y)dy. \end{aligned} \tag{24.4}$$

in quite a neat way.

Example

Consider the initial conditions that

$$y(x,0) = \phi(x) = \frac{1}{1+x^2}; \ \frac{\partial y}{\partial t}(x,0) = \psi(x) = 0.$$

Therefore, following the manipulation leading to (24.4), we find that

$$f(x) = g(x) = \frac{1}{2[1+x^2]} \to y(x,t) = \frac{1}{2}\left[\frac{1}{1+(x+ct)^2} + \frac{1}{1+(x-ct)^2}\right].$$

The solution is shown schematically in figure 24.2. Note that the initial mound splits into two, each of half the maximum amplitude, which travel to the left and right at speed c.

24.3 The diffusion equation

The (linear) wave equation is only one of many, many important partial differential equations. Another enormously important equation is the **diffusion** equation, which describes how substances, you know, diffuse. There is actually a beautifully simple probabilistic derivation of the diffusion equation, due to an obscure Austrian patent clerk called Albert something or other.

24.3.1 Random walk

Consider a lattice $x = 0, \pm\Delta x, \ldots$, and define the concentration $c(x,t)$ as the expected number of particles of something at x at time t. Now assume that at each time interval, each particle takes a random walk: i.e. at time $t+\Delta t$, there is a probability p that the particle moves left one lattice point, a probability p that the particle moves right one lattice point, and a probability $1-2p$ that it stays put. One way to visualise this is the decision making process of a student in a bar on Kings Street ...

Therefore

$$c(x, t+\Delta t) - c(x,t) \quad = \quad p[c(x+\Delta x, t) - 2c(x,t) + c(x-\Delta x, t)].$$

Expanding the left-hand side in terms of a Taylor series:

$$c(x, t+\Delta t) - c(x,t) = c(x,t) + \Delta t \frac{\partial c}{\partial t}(x,t) - c(x,t) + O(\Delta t^2),$$

we obtain for the left hand side

$$\Delta t \left[\frac{\partial c}{\partial t}(x,t) + O(\Delta t) \right].$$

We make explicit that the partial derivative is evaluated at x, t.

The right-hand side is a little more complicated:

$$\begin{aligned} c(x+\Delta x, t) - c(x,t) &= c(x,t) + \Delta x \frac{\partial c}{\partial x}(x,t) + \frac{[\Delta x]^2}{2} \frac{\partial^2 c}{\partial x^2}(x,t) \\ &\quad -c(x,t) + O([\Delta x]^3), \\ c(x-\Delta x, t) - c(x,t) &= c(x,t) - \Delta x \frac{\partial c}{\partial x}(x,t) + \frac{[\Delta x]^2}{2} \frac{\partial^2 c}{\partial x^2}(x,t) \\ &\quad -c(x,t) + O([\Delta x]^3), \end{aligned}$$

and so

$$p[c(x+\Delta x, t) - 2c(x,t) + c(x-\Delta x, t)] = p\Delta x^2 \left[\frac{\partial^2 c}{\partial x^2}(x,t) + O(\Delta x) \right].$$

Recombining the two sides of the equation and dividing across by Δt, we obtain

$$\frac{\partial c}{\partial t}(x,t) + O(\Delta t) = \frac{p\Delta x^2}{\Delta t} \frac{\partial^2 c}{\partial x^2}(x,t) + O\left(\frac{\Delta x^3}{\Delta t} \right).$$

We now take a distinguished limit. We require that $\Delta t \to 0$, $\Delta x \to 0$, yet $p\Delta x^2/\Delta t \to \kappa$ where κ is a positive finite constant. Therefore, we obtain the **diffusion** equation:

$$\frac{\partial c}{\partial t} = \kappa \frac{\partial^2 c}{\partial x^2}, \tag{24.5}$$

where κ is the **diffusion coefficient** and has dimensions $L^2 T^{-1}$.

This equation is entirely consistent with a heuristic interpretation of the diffusion of, for example, heat in a metal bar in terms of **Fick's second law**. This empirical "law" states that the local rate of change of a diffusing substance is proportional to the divergence of a flux, which in turn is proportional to the gradient, with the substance of interest (heat, concentration etc) always flowing **downgradient** from high to low values.

24.4 Similarity solutions

Consider a specific example of an infinitely long metal bar heating at one end. The temperature $\theta(x,t)$ in the bar satisfies the diffusion equation (24.5):

$$\frac{\partial \Theta}{\partial t} = \kappa \frac{\partial^2 \Theta}{\partial x^2},$$

subject to the boundary and initial conditions

$$\Theta(x,0) = 0; \;\; \Theta(0,t) = H(t), \tag{24.6}$$

where $H(t)$ is the Heaviside step-function as defined in (17.4).

We can actually find a solution to this problem by considering a a **similarity variable** η, defined as

$$\eta \;\; = \;\; \frac{x}{2\sqrt{\kappa t}}.$$

Notice how this grouping (i.e. a square of a length and a first power of a time) is very suggestive of the grouping we found when constructing the diffusion equation from a random walk. This is no coincidence. Therefore, applying the chain rule once more with feeling:

$$\begin{aligned}
\frac{\partial}{\partial t} &= \frac{\partial \eta}{\partial t}\frac{\partial}{\partial \eta} = \frac{-x}{4\sqrt{\kappa t^3}}\frac{\partial}{\partial \eta} = \frac{-\eta}{2t}\frac{\partial}{\partial \eta}, \\
\frac{\partial}{\partial x} &= \frac{\partial \eta}{\partial x}\frac{\partial}{\partial \eta} = \frac{1}{2\sqrt{\kappa t}}\frac{\partial}{\partial \eta}, \\
\frac{\partial^2}{\partial x^2} &= \frac{1}{4\kappa t}\frac{\partial^2}{\partial \eta^2}.
\end{aligned}$$

Therefore, the diffusion equation can be reposed as a differential equation only in η:

$$\frac{-\eta}{2t}\left(\frac{d\theta}{d\eta}\right) = \frac{\kappa}{4\kappa t}\frac{d}{d\eta}\left(\frac{d\theta}{d\eta}\right), \rightarrow \theta'' + 2\eta\theta' = 0.$$

where $\Theta(x,t) = \theta(\eta)$. With the substitution,

$$\begin{aligned}
X &= \frac{d\theta}{d\eta}, \\
\frac{dX}{d\eta} &= -2\eta X, \\
\log X &= -\eta^2 + C_1, \\
X &= C_2 e^{-\eta^2}, \\
\theta(\eta) &= \alpha\frac{2}{\sqrt{\pi}}\int_0^\eta e^{-u^2}du + \beta, \\
\Theta(x,t) &= \alpha\mathrm{erf}\left[\frac{x}{2\sqrt{\kappa t}}\right] + \beta, \qquad (24.7)
\end{aligned}$$

where α and β are constants determined by the initial conditions and $\mathrm{erf}(y)$ is the **error function**.

The error function $\mathrm{erf}(x/2\sqrt{\kappa t})$ is plotted in figure 24.3 (for $\kappa = 1$) for times $t = 10^{-3}$, $t = 10^{-2}$, $t = 10^{-1}$, and $t = 10^{0}$. It appears frequently in diffusive, random processes, and has the nicely scaled properties that $\mathrm{erf}(0) = 0$ and $\mathrm{erf}(x) \rightarrow 1$ as $x \rightarrow \infty$. Applying the conditions (24.6) to the solution (24.7), we find that

$$\begin{aligned}
\Theta(0,t) &= 1 \;\forall\; t > 0 \rightarrow \theta(0) = 1 \rightarrow \beta = 1; \\
\Theta(x,0) &= 0 \rightarrow \lim_{\eta\rightarrow\infty}\theta = 0 \rightarrow \alpha = -1,
\end{aligned}$$

and so

$$\Theta(x,t) = 1 - \mathrm{erf}\left(\frac{x}{2\sqrt{\kappa t}}\right) = \mathrm{erfc}\left(\frac{x}{2\sqrt{\kappa t}}\right),$$

defining the **complementary** error function erfc. You will hear a lot more about this equation in Methods, but for now, in the immortal words of Bugs Bunny...

That's all folks!

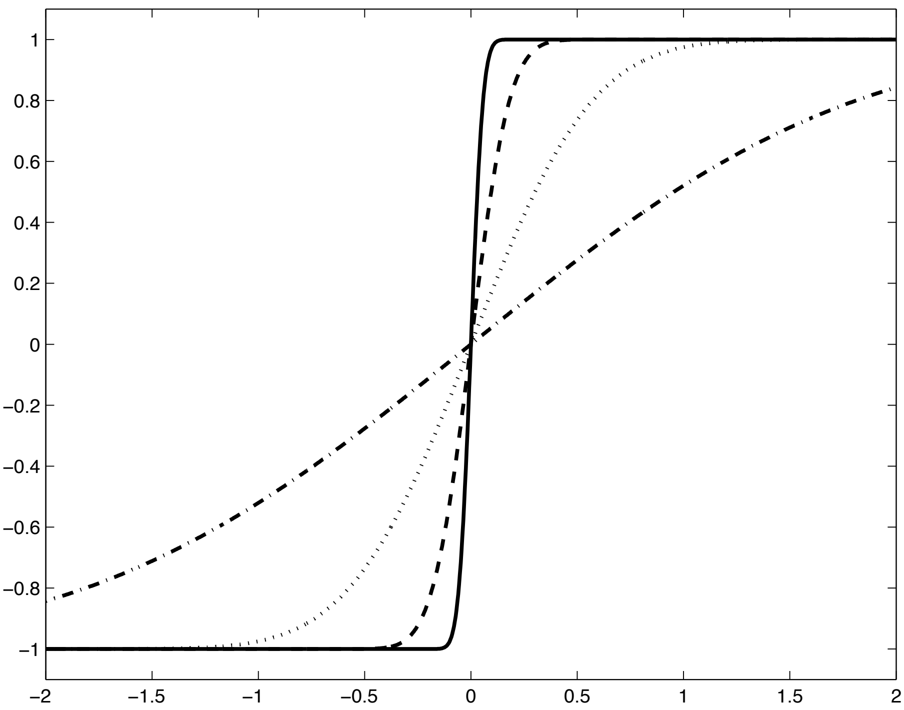

Figure 24.3: Plots (with $\kappa = 1$) of the error function $\operatorname{erf}(x/2\sqrt{\kappa t})$ for times $t = 10^{-3}$ (solid); $t = 10^{-2}$ (dashed); $t = 10^{-1}$ (dotted); and $t = 10^{0}$ (dot-dashed).