Chapter 13

Differential Calculus and Variational Methods

In many of the preceding chapters, we studied linear spaces of functions and linear operators acting on them. This theory provides a natural framework for the majority of linear equations that arise in applied mathematics. Many problems lead to nonlinear equations that may be formulated in terms of nonlinear maps acting on Banach spaces. There is no general theory of nonlinear maps that is as powerful as, for example, the spectral theory of linear operators. If, however, we can approximate a nonlinear map locally by a linear map, then we can reduce various questions about nonlinear problems to ones about associated linear problems. The linearization of nonlinear maps is one of the most useful and widely applicable methods for the study of nonlinear problems, and accounts for the importance of linear analysis in nonlinear settings.

13.1 Linearization

Linearization is closely connected with differentiation: the central idea of differentiation is the local approximation of a nonlinear map by a linear map. A map $f : X \to Y$ between Banach spaces X, Y is *differentiable* at $x \in X$ if there is a bounded linear map $f'(x) : X \to Y$ such that

$$f(x + \epsilon h) = f(x) + \epsilon f'(x)h + o(\epsilon) \tag{13.1}$$

as $\epsilon \to 0$ for every $h \in X$. Here, $o(\epsilon)$ stands for a term that approaches zero faster than ϵ as $\epsilon \to 0$. We call the linear map $f'(x)$ the *derivative* of f at x.

In this section, we describe some problems where the linearization of a nonlinear map is useful. First, suppose that we want to find solutions $x \in X$ of a nonlinear equation of the form

$$f(x) = y, \tag{13.2}$$

where $f : X \to Y$ is a map between Banach spaces X, Y, and $y \in Y$ is given. If we know a solution $x_0 \in X$ for a particular $y_0 \in Y$, meaning that

$$f(x_0) = y_0, \tag{13.3}$$

then we can try to solve (13.2) when y is close to y_0 by looking for a solution x that is close to x_0. We write y as

$$y = y_0 + \epsilon y_1, \tag{13.4}$$

where ϵ is a small real or complex parameter. If f is differentiable at x_0, we may look for a solution $x(\epsilon)$ of the form

$$x(\epsilon) = x_0 + \epsilon x_1 + o(\epsilon). \tag{13.5}$$

Then, using (13.1), (13.4), and (13.5) in (13.2), we get

$$f(x_0) + \epsilon f'(x_0)x_1 = y_0 + \epsilon y_1 + o(\epsilon).$$

From (13.3), the leading order terms in ϵ are equal. Cancelling the leading order terms, dividing the equation by ϵ, and letting $\epsilon \to 0$, we find that x_1 and y_1 satisfy

$$f'(x_0)x_1 = y_1. \tag{13.6}$$

If $f'(x_0)$ is nonsingular, then we can solve (13.6) for x_1. It is then reasonable to expect that we can also solve the nonlinear equation (13.2) when y is sufficiently close to y_0. The *inverse function theorem* states that this expectation is correct, provided that f is continuously differentiable at x_0.

A second application of linearization concerns the stability of solutions of a nonlinear evolution equation of the form

$$x_t = f(x), \qquad x(0) = x_0, \tag{13.7}$$

where the solution $x : [0, \infty) \to X$ takes values in a Banach space X, and $f : X \to X$ is a vector field on X. For some equations, such as partial differential equations, the vector field f may only be defined on a dense subspace of X. A point $\overline{x} \in X$ is an *equilibrium solution*, or *stationary solution*, or *fixed point* of (13.7) if

$$f(\overline{x}) = 0.$$

In that case, the constant function $x(t) = \overline{x}$ is a solution of (13.7). Even though an equilibrium solution is an exact solution of (13.7), it may not be observed in practice if it is *unstable*, meaning that a small perturbation of the equilibrium grows in time.

To study the effect of a small perturbation on the equilibrium state, we look for solutions of (13.7) of the form $x(t) = \overline{x} + \epsilon y(t)$, where ϵ is small, and linearize the right hand side of (13.7) about $x = \overline{x}$. Neglecting higher order terms, we find that y satisfies the linear evolution equation

$$y_t = f'(\overline{x})\, y. \tag{13.8}$$

It is reasonable to expect that, under suitable conditions on f, the study of solutions of (13.8) will provide information about the stability of the equilibrium solution $\overline{x}$ of (13.7). Similar ideas may be used to study the stability of time-dependent solutions — for example, time-periodic solutions — of (13.7), but we will not describe them here.

As a third example of linearization, we consider the minimization of a functional $I : X \to \mathbb{R}$. We suppose that I is bounded from below and look for a minimizer $\overline{x} \in X$ such that

$$I(\overline{x}) = \inf_{x \in X} I(x). \tag{13.9}$$

We have already discussed the *direct method* for solving variational problems, in which we choose a minimizing sequence and attempt to show that it has a subsequence that converges to a minimizer. An alternative approach, called the *indirect method*, is to look for *critical points* of I, which are solutions of the equation

$$I'(x) = 0. \tag{13.10}$$

If I is differentiable, then any minimizer that is an interior point of the domain of I is a critical point of I. A point x at which $I'(x) \neq 0$ is called a *regular point*. Conversely, if an equation $f(x) = 0$ can be written in the form (13.10) for some functional I, then we may be able to use the associated variational principle (13.9) to construct solutions. When applicable, variational methods are one of the most powerful methods for analyzing equations.

The above examples illustrate the need for a notion of the derivative of a map between Banach spaces. There are many different definitions of the derivative. The most important is the Fréchet derivative, which generalizes the notion of the derivative or differential of a vector-valued function of several variables. We will also introduce the Gâteaux derivative, which generalizes the notion of the directional derivative.

13.2 Vector-valued integrals

In this section, we define the derivative and the Riemann integral of a vector-valued function of a real variable, and prove some of their basic properties. The definitions are essentially identical to the ones in elementary calculus for a real-valued function. We will need these tools, especially the estimate in Theorem 13.4, to prove results about differentiable functions, such as the inverse function theorem.

A vector-valued function of a real variable is a mapping from a subset of the real numbers into a Banach space, which could be finite or infinite-dimensional. Geometrically, such a function defines a parametrized curve in the Banach space. The derivative of the function is the tangent, or velocity, vector of the curve.

Definition 13.1 A function $f : (a, b) \to X$ from an open interval (a, b) into a Banach space X is *differentiable* at $a < t < b$, with derivative $f'(t) \in X$, if the following limit exists in X:

$$f'(t) = \lim_{h \to 0} \frac{f(t+h) - f(t)}{h}.$$

The function f is differentiable in (a, b) if it is differentiable at each point in (a, b), and continuously differentiable in (a, b) if $f' : (a, b) \to X$ is continuous.

Next, we define the *Riemann integral* of a vector-valued function $f : [a, b] \to X$ defined on a closed, bounded interval $[a, b]$. We say that $\varphi : [a, b] \to X$ is a *step function* if there is a partition $a = t_0 < t_1 < \ldots < t_n = b$ of the interval $[a, b]$, and constant vectors $c_i \in X$, with $i = 1, \ldots, n$, such that

$$\varphi(t) = c_i \qquad \text{for } t_{i-1} < t < t_i. \tag{13.11}$$

We denote the space of step functions from $[a, b]$ into X by $S([a, b])$, and regard it as a subspace of the Banach space $B([a, b])$ of bounded functions $f : [a, b] \to X$ equipped with the sup-norm

$$\|f\|_\infty = \sup_{a \le t \le b} \|f(t)\|.$$

We define a linear map

$$\Lambda : S([a, b]) \to X$$

that takes a step function φ, defined in (13.11), to its Riemann integral by

$$\Lambda\varphi = \sum_{i=1}^{n} (t_i - t_{i-1})\, c_i.$$

Thus, the integral of a step function is a finite linear combination of the values c_i of the step function. The vectors c_i need not be parallel, and the integral need not be parallel to any of the c_i's, but it does lie in the linear subspace spanned by $\{c_1, \ldots, c_n\}$. The map Λ is well defined, since its value does not depend on how the step-function is represented. From the triangle inequality, we have

$$\|\Lambda\varphi\| \le \left(\max_{1 \le i \le n} \|c_i\| \right) \sum_{i=1}^{n} (t_i - t_{i-1}) = \|\varphi\|_\infty (b - a),$$

so Λ is bounded. We denote the closure of $S([a, b])$ in $B([a, b])$ by $R([a, b])$. Elements in the space $R([a, b])$ of uniform limits of step functions are sometimes called *regulated functions*. Theorem 5.19 implies that there is a unique bounded linear extension of Λ to $R([a, b])$, which we also denote by $\Lambda : R([a, b]) \to X$. For

$f \in R([a,b])$, we call Λf the *Riemann integral* of f, and write it as

$$\Lambda f = \int_a^b f(t)\,dt.$$

The uniform continuity of a continuous function on the compact interval $[a,b]$ implies that $R([a,b])$ contains the space $C([a,b])$ of continuous functions from $[a,b]$ to X, so every continuous function is Riemann integrable (see Exercise 13.11). The space $R([a,b])$ also contains the piecewise continuous functions, which have a finite number of jump discontinuities in $[a,b]$, meaning that the left and right limits of the function exist at its points of discontinuity. In fact, it is possible to show [9] that a function f is in $R([a,b])$ if and only if the left and right hand limits,

$$\lim_{h\to 0^-} f(t+h), \qquad \lim_{h\to 0^+} f(t+h),$$

exist at every point of $[a,b]$ (except, of course, for the left limit at a and the right limit at b). The Riemann integral can be defined on a larger class of functions than the regulated functions, but once one has to deal with functions that are less regular than continuous or piecewise continuous functions, it is preferable to use the Lebesgue integral. One can also define integrals of functions taking values in an infinite-dimensional Banach space for which the Riemann sums, or the integrals of approximating simple functions, converge weakly instead of strongly. We will not consider such integrals in this book.

The estimate

$$\left\| \int_a^b f(t)\,dt \right\| \le \int_a^b \|f(t)\|\,dt \le M(b-a), \tag{13.12}$$

where

$$M = \sup_{a\le t\le b} \|f(t)\|,$$

follows from the continuity of Λ and the corresponding estimate for step functions. The usual algebraic properties of the Riemann integral also follow by continuity from the corresponding properties for step functions.

Next, we prove that if the derivative of a function is zero, then the function is constant. To do this, we use linear functionals on X to reduce to the real-valued case.

Proposition 13.2 If $f : (a,b) \to X$ is differentiable in (a,b) and $f' = 0$, then f is a constant function.

Proof. Let $\varphi : X \to \mathbb{R}$ be a bounded linear functional on X. We define $f_\varphi : (a,b) \to \mathbb{R}$ by

$$f_\varphi(t) = \varphi\left(f(t)\right).$$

The chain rule (see Theorem 13.8 below) implies that f_φ is differentiable and has zero derivative. The mean value theorem of elementary calculus (see Exercise 1.14) implies that f_φ is constant. Hence, for every $\varphi \in X^*$ and $s, t \in (a, b)$ we have

$$\varphi\left(f(s) - f(t)\right) = f_\varphi(s) - f_\varphi(t) = 0.$$

It follows from the Hahn-Banach theorem and Exercise 5.6 that $f(s) = f(t)$ for all $s, t \in (a, b)$, so f is constant. □

The fundamental theorem of calculus holds for vector-valued maps.

Theorem 13.3 (Fundamental theorem of calculus) Suppose that X is a Banach space.

(a) If $f : [a, b] \to X$ is continuous, then

$$F(t) = \int_a^t f(s)\, ds$$

is continuously differentiable in (a, b) and $F' = f$.

(b) If f is continuously differentiable in an open interval containing $[a, b]$, then

$$f(b) - f(a) = \int_a^b f'(t) dt. \tag{13.13}$$

Proof. To prove the first part, suppose that $a < t < b$ and h is sufficiently small. Then

$$F(t + h) - F(t) = \int_t^{t+h} f(s)\, ds.$$

It follows that

$$\frac{F(t + h) - F(t)}{h} - f(t) = \frac{1}{h} \int_t^{t+h} [f(s) - f(t)]\, ds.$$

Taking the norm of this equation, and using (13.12), we obtain that

$$\left\| \frac{F(t + h) - F(t)}{h} - f(t) \right\| \le \sup \{\|f(s) - f(t)\| \mid t \le s \le t + h\} \to 0$$

as $h \to 0$, by the continuity of f. Thus F is differentiable in (a, b), with continuous derivative f.

To prove the second part, suppose that f is continuously differentiable, and define

$$g(t) = \int_a^t f'(s)\, ds.$$

Then, from the first part, we have that g is continuously differentiable and $g' = f'$, so that the derivative of $(f - g)$ is zero. Since $g(a) = 0$, Proposition 13.2 implies that $f(t) - g(t) = f(a)$. Evaluation of this equation at $t = b$ gives (13.13). □

The mean value theorem for real-valued functions does not hold for vector-valued functions, but the following estimate substitutes for the mean value theorem in many contexts.

Theorem 13.4 (Mean value) If f is continuously differentiable in an open interval that contains the closed, bounded interval $[a, b]$, with values in a Banach space, then

$$\|f(b) - f(a)\| \leq M\,(b - a) \quad \text{where} \quad M = \sup_{a \leq t \leq b} \|f'(t)\|\,.$$

Proof. Using (13.12) and (13.13), we have

$$\|f(b) - f(a)\| = \left\| \int_a^b f'(t)\,dt \right\| \leq \int_a^b \|f'(t)\|\;dt \leq M(b - a).$$

□

As an application of vector-valued integrals, we briefly consider the solution of a linear evolution equation

$$x_t = Ax, \qquad x(0) = x_0, \tag{13.14}$$

where $A : X \to X$ is a bounded linear operator on a Banach space X. For example, if $X = \mathbb{R}^n$, then (13.14) is an $n \times n$ system of ODEs. Similar ideas apply to PDEs, where $A : \mathcal{D}(A) \subset X \to X$ is an unbounded linear operator that generates a C_0-semigroup. Let

$$y(\lambda) = \int_0^\infty e^{-\lambda t} x(t)\,ds$$

denote the *Laplace transform* of $x : [0, \infty) \to X$. Then, taking the Laplace transform of (13.14), and integrating by parts, we find that

$$(\lambda I - A)\,y = x_0.$$

Thus, for $\lambda \in \rho(A)$, we have

$$y(\lambda) = R(\lambda)x_0,$$

where $R(\lambda) = (\lambda I - A)^{-1}$ is the resolvent operator of the generator A. The resolvent operator is related to the solution operator $T(t) = e^{At}$ by

$$R(\lambda) = \int_0^\infty e^{-\lambda s} T(s)\,ds,$$

meaning that the solution operator is the inverse Laplace transform of the resolvent. A nonhomogeneous linear evolution equation may be solved in terms of the solution operator of the homogeneous equation (see Exercise 13.12).

13.3 Derivatives of maps on Banach spaces

In this section, we define the derivative of a map between Banach spaces. The dimensions of the Banach spaces play little role in what follows, and a geometric understanding of the derivative is essential for a clear understanding of multivariable calculus on $\mathbb{R}^n$.

In order to generalize the notion of the derivative of a function of a real variable to a function defined on a Banach space, it is important to view the derivative in a slightly different way than is usual in elementary calculus. There, the derivative of a differentiable function $f : (a,b) \to \mathbb{R}$ is typically thought of as another function $f' : (a,b) \to \mathbb{R}$. Instead, we think of the derivative $f'(x)$ of f at a point x as a linear map that approximates f near x. For real-valued functions, this linear map is just multiplication by the value of the derivative at x.

Definition 13.5 A map $f : U \subset X \to Y$ whose domain U is an open subset of a Banach space X and whose range is a Banach space Y is *differentiable* at $x \in U$ if there is a bounded linear map $A : X \to Y$ such that

$$\lim_{h\to 0} \frac{\|f(x+h) - f(x) - Ah\|}{\|h\|} = 0.$$

This definition of the derivative is sometimes called the *Fréchet derivative*, to distinguish it from the directional, or Gâteaux, derivative in Definition 13.9 below. When we refer to the derivative of a function, without other qualifications, we will mean the Fréchet derivative, but there is little consistency in the literature in the usage of the words "derivative," "differential," and "differentiable."

We can restate the definition using the following o-notation. Suppose that

$$r : U \subset X \to Y$$

is a function whose domain U is a neighborhood of the origin in a Banach space X, with values in a Banach space Y. We write

$$r(h) = o(h^n) \qquad \text{as } h \to 0,$$

pronounced r is "small oh" of h^n, if

$$\lim_{h\to 0} \frac{\|r(h)\|}{\|h\|^n} = 0,$$

meaning that $\|r(h)\|$ approaches zero as $h \to 0$ faster than $\|h\|^n$. We also write

$$r(h) = O(h^n) \qquad \text{as } h \to 0,$$

pronounced r is "big oh" of h^n, if there are constants $\delta > 0$ and $C > 0$ such that

$$\|r(h)\| \leq C\|h\|^n \qquad \text{when } \|h\| < \delta.$$

If $f, g : U \subset X \to Y$, we write

$$f(h) = g(h) + o(h^n) \quad \text{if} \quad f(h) - g(h) = o(h^n) \quad \text{as } h \to 0,$$
$$f(h) = g(h) + O(h^n) \quad \text{if} \quad f(h) - g(h) = O(h^n) \quad \text{as } h \to 0.$$

Thus, $o(h^n)$ denotes a term that approaches zero faster than $\|h\|^n$, and $O(h^n)$ denotes a term that is bounded by a constant factor of $\|h\|^n$ near 0.

The function f is differentiable at x if and only if there is a bounded linear map $A : X \to Y$ such that

$$f(x + h) = f(x) + Ah + o(h) \qquad \text{as } h \to 0.$$

If such a linear map exists, then it is unique (see Exercise 13.1), and we write it as $A = f'(x)$. If f is differentiable at each point of U, then

$$f' : U \to \mathcal{B}(X, Y)$$

is the map that assigns to each point $x \in U$ the bounded linear map $f'(x) : X \to Y$ that approximates f near x. We say that f is *continuously differentiable* at x if the map f' is continuous at x, where the domain U is equipped with the norm on X and the range $\mathcal{B}(X, Y)$ is equipped with the operator norm. We say that f is continuously differentiable in U if it is continuously differentiable at each point $x \in U$. Other common notations for the derivative are df, Df, and f_x.

Example 13.6 Suppose that $f : U \subset \mathbb{R}^n \to \mathbb{R}^m$. We use coordinates $(x_1, x_2, \ldots, x_n)$ on $\mathbb{R}^n$ and $(y_1, y_2, \ldots, y_m)$ on $\mathbb{R}^m$. Then the component expression for f is

$$\begin{aligned} y_1 &= f_1(x_1, x_2, \ldots, x_n), \\ y_2 &= f_2(x_1, x_2, \ldots, x_n), \\ &\vdots \\ y_m &= f_m(x_1, x_2, \ldots, x_n), \end{aligned}$$

where $f_i : \mathbb{R}^n \to \mathbb{R}$. We assume that the partial derivatives of the coordinate functions f_i exist and are continuous in U. Then it follows from the remark below Theorem 13.11 that f is differentiable, and the matrix of $f' : U \to \mathcal{B}(\mathbb{R}^n, \mathbb{R}^m)$ is the *Jacobian matrix* of f:

$$f' = \begin{pmatrix} \partial f_1/\partial x_1 & \partial f_1/\partial x_2 & \ldots & \partial f_1/\partial x_n \\ \partial f_2/\partial x_1 & \partial f_2/\partial x_2 & \ldots & \partial f_2/\partial x_n \\ \vdots & \vdots & \ddots & \vdots \\ \partial f_m/\partial x_1 & \partial f_m/\partial x_2 & \ldots & \partial f_m/\partial x_n \end{pmatrix}.$$

Example 13.7 Let Ω be a smooth domain in $\mathbb{R}^n$, $X = H^1(\Omega)$, and $Y = L^1(\Omega)$. We consider real-valued functions $u : \Omega \to \mathbb{R}$ for simplicity. We will show that the quadratic map $f : X \to Y$ defined by

$$f(u) = \frac{1}{2}|\nabla u|^2 + \frac{1}{2}u^2$$

is differentiable, and find its derivative. We have

$$f(u+h) = f(u) + A(u)h + f(h),$$

where $A(u) : H^1(\Omega) \to L^1(\Omega)$ is defined by

$$A(u)h = \nabla u \cdot \nabla h + uh.$$

From the Cauchy-Schwarz inequality, we have

$$\|A(u)h\|_{L^1} \leq \|u\|_{H^1}\|h\|_{H^1},$$

so $A(u)$ is a bounded linear map. The term $f(h) = o(h)$ as $h \to 0$, since

$$\|f(h)\|_{L^1} = \frac{1}{2}\int_\Omega \left(|\nabla h|^2 + h^2\right) \, dx = \frac{1}{2}\|h\|_{H^1}^2,$$

so

$$\frac{\|f(h)\|_{L^1}}{\|h\|_{H^1}} = \|h\|_{H^1} \to 0 \qquad \text{as } h \to 0.$$

Thus, f is differentiable in $H^1(\Omega)$, and $f'(u) = A(u)$.

One of the most important results concerning derivatives is the *chain rule*. Geometrically, the chain rule states that the linear approximation of the composition of two differentiable maps is the composition of their linear approximations.

Theorem 13.8 (Chain rule) Suppose that X, Y, Z are Banach spaces, and

$$f : U \subset X \to Y, \qquad g : V \subset Y \to Z,$$

where U and V are open subsets of X and Y, respectively. If f is differentiable at $x \in U$ and g is differentiable at $f(x) \in V$, then $g \circ f$ is differentiable at x and

$$(g \circ f)'(x) = g'(f(x))\, f'(x).$$

Proof. By the differentiability of f, we have

$$f(x+h) = f(x) + f'(x)h + r(h),$$

where $r(h)/\|h\| \to 0$ as $h \to 0$. Let $y = f(x)$ and $k = f'(x)h + r(h)$. Then

$$g(y+k) = g(y) + g'(y)k + s(k),$$

where $s(k)/\|k\| \to 0$ as $k \to 0$. Hence,

$$g(f(x+h)) = g(y) + g'(y)\, f'(x)h + t(h),$$

where

$$\begin{aligned} t(h) &= g'(y)\, r(h) + s(k) \\ &= g'(f(x))\, r(h) + s(f'(x)h + r(h)) . \end{aligned}$$

Since $f'(x)$ and $g'(y)$ are bounded linear maps, we have

$$\frac{\|t(h)\|}{\|h\|} \le \frac{\|g'(y)\|\, \|r(h)\|}{\|h\|} + \frac{\|s(k)\|}{\|k\|} \left(\frac{\|f'(x)\|\, \|h\| + \|r(h)\|}{\|h\|} \right).$$

It follows that $\|t(h)\|/\|h\| \to 0$ as $h \to 0$, which proves the result. □

A useful way to compute the derivative of a function is in terms of its *directional derivative*, or *Gâteaux derivative*. For example, the matrix of the derivative of a map on $\mathbb{R}^n$ is the Jacobian matrix of its partial derivatives.

Definition 13.9 Let X and Y be Banach spaces, and $f : U \subset X \to Y$, where U is an open subset of X. The *directional derivative* of f at $x \in U$ in the direction $h \in X$ is given by

$$\delta f(x; h) = \lim_{t \to 0} \frac{f(x + th) - f(x)}{t}. \tag{13.15}$$

If this limit exists for every $h \in X$, and $f'_G(x) : X \to Y$ defined by $f'_G(x)h = \delta f(x; h)$ is a linear map, then we say that f is *Gâteaux differentiable* at x, and we call f'_G the *Gâteaux derivative* of f at x.

The directional derivative may also be written as

$$\delta f(x; h) = \left. \frac{d}{dt} f(x + th) \right|_{t=0}.$$

If f is Fréchet differentiable at x, then it is Gâteaux differentiable at x (Exercise 13.4), and the Fréchet derivative $f'(x)$ is given by

$$f'(x)h = \delta f(x; h).$$

The converse is not true. Even for functions defined on $\mathbb{R}^2$, the existence and linearity of directional derivatives does not imply the differentiability, or even the continuity, of the function (see Exercise 13.5). To give a sufficient condition for the existence of directional derivatives to imply differentiability, we first prove the following immediate consequence of the mean value theorem in Theorem 13.4.

Theorem 13.10 Suppose that $f : U \subset X \to Y$ is a Gâteaux differentiable function from an open subset U of a Banach space X to a Banach space Y. If $x, y \in U$ and the line segment $\{tx + (1 - t)y \mid 0 \le t \le 1\}$ connecting x and y is contained in U, then

$$\|f(x) - f(y)\| \le M\|x - y\| \quad \text{where} \quad M = \sup_{0 \le t \le 1} \|f'_G(tx + (1 - t)y)\|.$$

Proof. The definition of the Gâteaux derivative implies that the function

$$h(t) = f\left(tx + (1-t)y\right)$$

is differentiable in an open interval that contains $[0,1]$ and

$$h'(t) = f'_G\left(tx + (1-t)y\right)(x-y).$$

The result then follows from an application of Theorem 13.4 to h. □

Theorem 13.11 Suppose that $f : U \subset X \to Y$ is a Gâteaux differentiable function from an open subset U of a Banach space X to a Banach space Y. If the Gâteaux derivative $f'_G : U \subset X \to \mathcal{B}(X,Y)$ is continuous at $x \in U$, then f is Fréchet differentiable at x and $f'(x) = f'_G(x)$.

Proof. For sufficiently small $\|h\|$, we define

$$r(h) = f(x+h) - f(x) - f'_G(x)h. \tag{13.16}$$

The Gâteaux differentiability of f implies that r is Gâteaux differentiable, and

$$r'_G(h) = f'_G(x+h) - f'_G(x).$$

From Theorem 13.10, we have that

$$\|r(h)\| \le M(h)\|h\|,$$

where

$$M(h) = \sup_{0 \le t \le 1} \left\| r'_G(th) \right\|.$$

The continuous Gâteaux differentiability of f implies that $M(h) \to 0$ as $h \to 0$, so $r(h) = o(h)$ as $h \to 0$. Equation (13.16) implies that f is Fréchet differentiable at x, and $f'(x) = f'_G(x)$. □

A more refined argument shows that f is Fréchet differentiable at a point if its directional derivatives $\delta f(x;h)$ exist in a neighborhood of the point and are uniformly continuous functions of x and continuous functions of h (see Lusternik and Sobolev [33], for example).

Next, we consider some examples of directional derivatives.

Example 13.12 Let $X = L^p(\Omega)$, where $1 \le p < \infty$. We will compute the Gâteaux derivative of the L^p-norm. We define $F : X \to \mathbb{R}$ by $F(u) = \|u\|_p^p$. Then

$$\delta F(u;h) = \frac{d}{dt}\int |u+th|^p \bigg|_{t=0}.$$

First, we show that we can interchange the derivative and the integral by the dominated convergence theorem (Theorem 12.35). For each $x \in X$ we have

$$\frac{d}{dt}|u(x) + th(x)|^p \bigg|_{t=0} = \lim_{t \to 0} \frac{1}{t} \left(|u(x) + th(x)|^p - |u(x)|^p\right).$$

Since the function $x \mapsto |x|^p$ is convex for $p \geq 1$, we have

$$|u(x) + th(x)|^p \leq t|u(x) + h(x)|^p + (1-t)|u(x)|^p \qquad \text{for } 0 < t < 1.$$

Hence

$$\frac{|u(x) + th(x)|^p - |u(x)|^p}{t} \leq |u(x) + h(x)|^p - |u(x)|^p,$$

and similarly

$$|u(x)|^p - |u(x) - h(x)|^p \leq \frac{|u(x) + th(x)|^p - |u(x)|^p}{t}.$$

These two inequalities imply that

$$\left|\frac{|u(x) + th(x)|^p - |u(x)|^p}{t}\right| \leq |u(x)|^p + |u(x) + h(x)|^p + |u(x) - h(x)|^p. \tag{13.17}$$

The left-hand side of (13.17) converges pointwise a.e. as $t \to 0$, since

$$\begin{aligned} \lim_{t \to 0^+} \frac{1}{t} \left||u(x) + th(x)|^p - |u(x)|^p\right| &= \frac{d}{dt} \left||u(x) + th(x)|^p - |u(x)|^p\right| \bigg|_{t=0} \\ &= \frac{p}{2}|u(x)|^{p-2} \left(\overline{u(x)}h(x) + u(x)\overline{h(x)}\right), \end{aligned}$$

where we write $|z|^p$ as $(z\overline{z})^{p/2}$ before differentiating. The right-hand side of (13.17) is in L^1. Therefore, the dominated convergence theorem implies that

$$\lim_{t \to 0} \frac{1}{t} \int \left||u(x) + th(x)|^p - |u(x)|^p\right| = \frac{p}{2} \int |u(x)|^{p-2} \left(\overline{u(x)}h(x) + u(x)\overline{h(x)}\right).$$

Hence, the directional derivative is given by

$$\delta F(u; h) = \frac{p}{2} \int |u|^{p-2} \left(\overline{u}h + u\overline{h}\right).$$

Since $|u|^{p-1} \in L^{p'}$ when $u \in L^p$ where p' is the Hölder conjugate of p, Hölder's inequality implies that $\delta F(u; \cdot)$ is a bounded linear functional on L^p. It follows that F is Gâteaux differentiable.

Example 13.13 Suppose that $\varphi : \mathbb{R} \to \mathbb{R}$ is a continuous function such that

$$|\varphi(t)| \leq a + b|t|^{p/q} \tag{13.18}$$

for suitable constants $a, b > 0$ and $p, q \geq 1$, and Ω is a bounded, measurable subset of $\mathbb{R}^n$. We define a nonlinear map $N_\varphi : L^p(\Omega) \to L^q(\Omega)$ by

$$(N_\varphi u)(x) = \varphi(u(x)).$$

Thus, N_φ is the operation of composition with the function φ, regarded as a map on L^p. Such an operator is called a *Nemitski operator*. It follows from (13.18) that N_φ is bounded, meaning that it maps bounded sets in L^p into bounded sets in L^q. It is also possible to show that if $u_n \to u$ in L^p, then $N_\varphi(u_n) \to N_\varphi(u)$ in L^q, so N_φ is continuous. This continuity does not follow from the boundedness of N_φ because N_φ is nonlinear.

Now suppose that $\varphi : \mathbb{R} \to \mathbb{R}$ is continuously differentiable. The pointwise calculation

$$\frac{d}{d\epsilon}\varphi(u(x) + \epsilon h(x))\bigg|_{\epsilon=0} = \varphi'(u(x))\, h(x)$$

suggests that, when it exists, the derivative of N_φ at u is multiplication by the function $\varphi'(u)$. To give conditions under which this is true, suppose that $p > 2$ and

$$|\varphi'(t)| \leq a + b|t|^{p-2}. \tag{13.19}$$

Then, if $u, h \in L^p(\Omega)$, we have $\varphi'(u)\, h \in L^q(\Omega)$, where q is the Hölder conjugate of p. Thus the map $h \mapsto \varphi'(u)\, h$ is a bounded linear map from L^p to L^q. It is possible to show that, in this case, the Nemitski operator $N_\varphi : L^p \to L^q$ is Fréchet differentiable, and

$$(N_\varphi)'(u)h = \varphi'(u)\, h.$$

In the limiting case, when $p = 2$ and $|\varphi'(t)| \leq a$, the Nemitski operator $N_\varphi : L^2 \to L^2$ is Gâteaux differentiable, but not Fréchet differentiable, unless $\varphi(t) = a + bt$ is a linear function of t. The proof of these facts requires some measure-theoretic arguments which we omit.

If $f : X \times Y \to Z$ is a differentiable map on the product of two Banach spaces, then we have

$$f(x + h, y + k) = f(x, y) + Ah + Bk + o(h, k)$$

for suitable linear maps $A : X \to Z$ and $B : Y \to Z$. We call A and B the *partial derivatives* of f with respect to x and y, repectively, and denote them by

$$A = D_x f(x, y), \qquad B = D_y f(x, y).$$

Other common notations for the partial derivatives $(D_x f, D_y f)$ are

$$(d_x f, d_y f), \quad (D_1 f, D_2 f), \quad (f_x, f_y).$$

We may define higher order derivatives as multilinear maps in a similar way to the definition of the first derivative as a linear map. For example, we say that $f : U \subset X \to Y$ is twice differentiable at $x \in U$ if there is a continuous, bilinear map $f''(x) : X \times X \to Y$ such that

$$f(x+h) = f(x) + f'(x)h + \frac{1}{2}f''(x)(h,h) + o(h^2) \qquad \text{as } h \to 0.$$

If $f : U \subset X \to Y$ is k-times continuously differentiable at each point of U, then we say that f belongs to $C^k(U)$.

Example 13.14 If $f = (f_1, f_2, \dots, f_m) : \mathbb{R}^n \to \mathbb{R}^m$, where $f_i : \mathbb{R}^n \to \mathbb{R}$ is twice continuously differentiable, and $h = (h_1, h_2, \dots, h_n) \in \mathbb{R}^n$, then

$$[f''(x)(h,h)]_i = \sum_{j,k=1}^{n} \frac{\partial f_i}{\partial x_j \partial x_k}(x) h_j h_k.$$

Just as we defined the equivalence of the topological properties of two spaces in terms of homeomorphisms, and the equivalence of metric space properties in terms of metric space isomorphisms, we may define the equivalence of the smoothness properties of two spaces in terms of diffeomorphisms.

Definition 13.15 If $f : U \subset X \to V \subset Y$ is a one-to-one, onto map from an open subset U of a Banach space X to an open subset V of a Banach space Y such that $f \in C^k(U)$ and $f^{-1} \in C^k(V)$, where $k \geq 1$, then f is called a C^k*-diffeomorphism*, or a *diffeomorphism*. Two open sets $U \subset X$, $V \subset Y$ are *diffeomorphic* if there is a diffeomorphism $f : U \to V$.

13.4 The inverse and implicit function theorems

In this section, we prove the inverse function theorem, which states that a continuously differentiable function is locally invertible if its derivative is invertible.

Theorem 13.16 (Inverse function) Suppose that $f : U \subset X \to Y$ is a differentiable map from an open subset U of a Banach space X to a Banach space Y. If f is continuously differentiable in U and $f'(x)$ has a bounded inverse at $x \in U$, then there are open neighborhoods $V \subset U$ of x and $W \subset Y$ of $f(x)$ such that $f : V \to W$ is a one-to-one, onto continuous map with continuous inverse $f^{-1} : W \to V$. Moreover, the local inverse is continuously differentiable at $f(x)$ and

$$\left(f^{-1}\right)'(f(x)) = \left[f'(x)\right]^{-1}. \tag{13.20}$$

Proof. We want to show that for a given sufficiently small $k \in Y$ there is a solution $h \in X$ of the equation

$$f(x+h) = f(x) + k. \tag{13.21}$$

The idea of the proof is to use the contraction mapping theorem to show that there is a solution of the nonlinear equation close to the solution of the linearized equation. We write

$$f(x+h) = f(x) + f'(x)h + r(h),$$

where $r(h) = o(h)$ as $h \to 0$. Since f is continuously differentiable at x, we see that r is continuously differentiable at 0, and $r'(0) = 0$. Since $f'(x)$ is invertible, we may rewrite (13.21) as a fixed point equation

$$h = T(h) \qquad \text{where} \quad T(h) = [f'(x)]^{-1}(k - r(h)). \tag{13.22}$$

The vector k occurs in this equation as a parameter.

First, we show that T contracts distances when $\|h\|$ is sufficiently small. From (13.22), we have

$$\|T(h_1) - T(h_2)\| \le \left\|[f'(x)]^{-1}\right\| \|r(h_1) - r(h_2)\|.$$

Theorem 13.10 implies that

$$\|r(h_1) - r(h_2)\| \le \sup_{0\le t\le 1} \|r'(th_1 + (1-t)h_2)\| \|h_1 - h_2\|.$$

Since $r'(0) = 0$ and r is continuously differentiable at 0, there is a $\delta > 0$ such that

$$\|r'(h)\| \le \frac{1}{2\left\|[f'(x)]^{-1}\right\|} \qquad \text{for } \|h\| \le \delta.$$

We denote the closed ball in X of radius δ and center zero by

$$B_\delta = \{h \in X \mid \|h\| \le \delta\}.$$

It follows that

$$\|r(h_1) - r(h_2)\| \le \frac{\|h_1 - h_2\|}{2\left\|[f'(x)]^{-1}\right\|} \qquad \text{for } h_1, h_2 \in B_\delta, \tag{13.23}$$

and therefore that

$$\|T(h_1) - T(h_2)\| \le \frac{1}{2}\|h_1 - h_2\| \qquad \text{for } h_1, h_2 \in B_\delta.$$

To apply the contraction mapping theorem, we need to show that T maps B_δ into itself when k is sufficiently small. Taking the norm of $T(h)$ in (13.22), we get

$$\|T(h)\| \le \|[f'(x)]^{-1}\| (\|k\| + \|r(h)\|). \tag{13.24}$$

Equation (13.23), with $h_1 = h$ and $h_2 = 0$, implies that

$$\|r(h)\| \le \frac{\|h\|}{2\left\|[f'(x)]^{-1}\right\|} \qquad \text{for } h \in B_\delta.$$

It therefore follows from (13.24) that if $\|h\| \le \delta$ and

$$\|k\| \le \eta \qquad \text{where} \quad \eta = \frac{\delta}{2\| [f'(x)]^{-1} \|}, \tag{13.25}$$

then $\|T(h)\| \le \delta$. Thus $T : B_\delta \to B_\delta$ is a contraction on the complete set B_δ when $k \in B_\eta$, where B_η is the closed ball in Y of radius η and center zero. The contraction mapping theorem implies that T has a unique fixed point in B_δ. We may therefore define $g : B_\eta \to B_\delta$ by the requirement that $h = g(k)$ is the unique solution of (13.22) belonging to B_δ. From (13.21), the function g provides a local inverse of f, with

$$f^{-1}(f(x) + k) = x + g(k). \tag{13.26}$$

To complete the proof, we need to show that f^{-1} is continuously differentiable.

From (13.22), if $h = g(k)$, then

$$h = [f'(x)]^{-1}(k - r(h)). \tag{13.27}$$

Subtracting the equations corresponding to (13.27) for $h_1 = g(k_1)$ and $h_2 = g(k_2)$, taking the norm of the result, and using (13.23), we find that

$$\begin{aligned} \|h_1 - h_2\| &\le \left\| [f'(x)]^{-1} \right\| (\|k_1 - k_2\| + \|r(h_1) - r(h_2)\|) \\ &\le \left\| [f'(x)]^{-1} \right\| \|k_1 - k_2\| + \frac{1}{2}\|h_1 - h_2\|. \end{aligned}$$

Rewriting this inequality, we obtain that

$$\|g(k_1) - g(k_2)\| \le 2\| [f'(x)]^{-1} \| \|k_1 - k_2\| \qquad \text{for } k_1, k_2 \in B_\eta. \tag{13.28}$$

Thus, g is Lipschitz continuous in B_η.

Setting $h = g(k)$ in (13.27), we find that

$$g(k) = [f'(x)]^{-1} k + s(k), \tag{13.29}$$

where the remainder $s : B_\eta \to Y$ is defined by

$$s(k) = -[f'(x)]^{-1} r(g(k)).$$

From (13.28), with $k_1 = k$ and $k_2 = 0$, we have

$$\|g(k)\| \le 2\|k\| \| [f'(x)]^{-1} \| \qquad \text{for } k \in B_\eta.$$

Hence, $s(k) = o(k)$ as $k \to 0$ because

$$\frac{\|s(k)\|}{\|k\|} = \frac{\|h\|}{\|k\|} \frac{\| [f'(x)]^{-1} r(h)\|}{\|h\|} \le 2\| [f'(x)]^{-1} \|^2 \frac{\|r(h)\|}{\|h\|} \to 0 \qquad \text{as } k \to 0.$$

Equation (13.29) therefore implies that g is differentiable at $k = 0$ with $g'(0) = [f'(x)]^{-1}$. It follows from (13.26) that f^{-1} is differentiable at $f(x)$, and its derivative is given by (13.20).

The continuous differentiability of f^{-1} follows from the continuous differentiability of f, and the continuity of inversion on the set of bounded, nonsingular linear operators. □

The fact that the derivative of the inverse is the inverse of the derivative may also be deduced from the chain rule. Exercise 13.7 shows that the continuity requirement on the derivative of f in the hypotheses of the inverse function theorem cannot be dropped.

Example 13.17 The map $s : \mathbb{R} \to \mathbb{R}$ given by $s(x) = x^2$ is locally invertible at every $x \neq 0$. If $x > 0$, a local inverse is $r : (0, \infty) \to (0, \infty)$ where $r(y) = \sqrt{y}$. If $x < 0$, a local inverse is $r : (0, \infty) \to (-\infty, 0)$ where $r(y) = -\sqrt{y}$. The map s is not locally invertible at 0 where its derivative vanishes. The map $c : \mathbb{R} \to \mathbb{R}$ given by $c(x) = x^3$ is globally invertible on $\mathbb{R}$, with continuous inverse $c^{-1} : \mathbb{R} \to \mathbb{R}$ where $c^{-1}(x) = x^{1/3}$. The inverse function is not differentiable at $x = 0$ where the derivative of c vanishes. Thus, $c : \mathbb{R} \to \mathbb{R}$ is a homeomorphism, but not a diffeomorphism.

Example 13.18 Consider the map $\exp : \mathbb{C} \to \mathbb{C}$ defined by $\exp z = e^z$. This map may also be regarded as a map $\exp : \mathbb{R}^2 \to \mathbb{R}^2$ defined by $\exp(x, y) = (u, v)$, where

$$u = e^x \cos y, \qquad v = e^x \sin y.$$

The derivative of exp is nonsingular at every point, so it is locally invertible. The map is not globally invertible, however, since $\exp(z + 2\pi i n) = \exp z$ for every $n \in \mathbb{Z}$.

Example 13.19 Suppose that $f : U \subset \mathbb{R}^n \to \mathbb{R}^n$ is a continuously differentiable map. From Example 13.6, the matrix of the derivative f' is the Jacobian matrix of f. The determinant of this matrix, $J : U \subset \mathbb{R}^n \to \mathbb{R}$,

$$J = \det\left(\frac{\partial f_i}{\partial x_j}\right)$$

is called the *Jacobian* of f. The inverse function theorem implies that the map f is locally invertible near x if its Jacobian is nonzero at x. Moreover, the local inverse f^{-1} is differentiable, and its Jacobian matrix is the inverse of the Jacobian matrix of f.

Example 13.20 The *hodograph method* is a method for linearizing certain nonlinear PDEs by exchanging the role of independent and dependent variables. As an example, we consider the *transonic small disturbance equation*, which provides a simplified model of the equations for steady fluid flows near the speed of sound (such as the flow around an aircraft flying at a speed close to the speed of sound):

$$\begin{aligned} uu_x + v_y &= 0, \\ u_y - v_x &= 0, \end{aligned} \tag{13.30}$$

where $u = u(x, y)$, $v = v(x, y)$. If the Jacobian

$$J = \begin{vmatrix} u_x & u_y \\ v_x & v_y \end{vmatrix} = u_x v_y - u_y v_x$$

is nonzero, then we may locally invert the map $(x, y) \mapsto (u, v)$ and write $x = x(u, v)$, $y = y(u, v)$. Moreover, we have

$$\begin{pmatrix} u_x & u_y \\ v_x & v_y \end{pmatrix} = \begin{pmatrix} x_u & x_v \\ y_u & y_v \end{pmatrix}^{-1} = \frac{1}{j} \begin{pmatrix} y_v & -x_v \\ -y_u & x_u \end{pmatrix},$$

where

$$j = x_u y_v - x_v y_u = \frac{1}{J}.$$

Hence,

$$u_x = \frac{y_v}{j}, \quad u_y = \frac{-x_v}{j}, \quad v_x = \frac{-y_u}{j}, \quad v_y = \frac{x_u}{j}.$$

The use of these equations in (13.30) implies that

$$\begin{aligned} u y_v + x_u &= 0, \\ x_v - y_u &= 0. \end{aligned}$$

The Jacobian j cancels, because all terms are linear in a first order derivative of u or v, and consequently the resulting system for $x = x(u, v)$, $y = y(u, v)$ is linear. From the second equation, we may write $x = \varphi_u$ and $y = \varphi_v$ for some function φ. The first equation then implies that $\varphi = \varphi(u, v)$ satisfies

$$\varphi_{uu} + u\varphi_{vv} = 0.$$

This PDE is called the *Tricomi equation*. It is one of the simplest equations of mixed type, being elliptic when $u > 0$ (corresponding to subsonic flow) and hyperbolic when $u < 0$ (corresponding to supersonic flow). Despite the greater simplicity of the linear equations for (x, y) than the nonlinear equations for (u, v), the hodograph method has a significant drawback: solutions may contain curves or regions where the Jacobians j or J vanish, and then the local invertibility between (x, y) and (u, v) is lost.

Example 13.21 Neglecting friction, the angle of $u(t)$ of a forced pendulum satisfies

$$\ddot{u} + \sin u = h, \tag{13.31}$$

where $h(t)$ is a given forcing function. We suppose that h is a T-periodic function, where $T > 0$, and ask if (13.31) has T-periodic solutions. When $h = 0$, (13.31) has the trivial T-periodic solution $u = 0$, and we can use the implicit function theorem to prove the existence of T-periodic solutions for small, nonzero h. Let

$$X = \left\{u \in C^2(\mathbb{R}) \mid u(t + T) = u(t)\right\}, \quad Y = \left\{u \in C(\mathbb{R}) \mid u(t + T) = u(t)\right\}.$$

Then we may write (13.31) as $f(u) = h$ where $f : X \to Y$ is defined by

$$f(u) = \ddot{u} + \sin u.$$

The map f is continuously differentiable, and its derivative $f'(0) : X \to Y$ is given by

$$f'(0)v = \ddot{v} + v.$$

The linear map $f'(0) : X \to Y$ is nonsingular if and only if $T \neq 2n\pi$ for some $n \in \mathbb{N}$. In that case, there is a unique T-periodic solution of (13.31) when $\|h\|_\infty$ is sufficiently small. The case $T = 2n\pi$ corresponds to a *resonance* of the external forcing with the linearized oscillator.

The implicit function theorem is a generalization of the inverse function theorem.

Theorem 13.22 (Implicit function theorem) Suppose that X, Y, Z are Banach spaces, and $F : U \subset X \times Y \to Z$ is a continuously differentiable map defined on an open subset U of $X \times Y$. If $(x_0, y_0) \in U$ is a point such that $F(x_0, y_0) = 0$, and $D_y F(x_0, y_0) : Y \to Z$ is a one-to-one, onto, bounded linear map, then there is an open neighborhood $V \subset X$ of x_0, an open neighborhood $W \subset Y$ of y_0, and a unique function $f : V \to W$ such that

$$F\left(x, f(x)\right) = 0 \qquad \text{for all } x \in V.$$

The function f is continuously differentiable, and

$$f'(x) = -\left[D_y F\left(x, f(x)\right)\right]^{-1} D_x F\left(x, f(x)\right).$$

The proof of this theorem is similar to the proof of the inverse function theorem, so we will omit it. The implicit function theorem reduces to the inverse function theorem when $F(x, y) = x - f(y)$.

Example 13.23 If $F = (F_1, F_2, \ldots, F_m) : \mathbb{R}^n \times \mathbb{R}^m \to \mathbb{R}^m$ is a continuously differentiable function, then the matrix of the partial derivative $D_y F$ is

$$\begin{pmatrix} \partial F_1/\partial y_1 & \partial F_1/\partial y_2 & \ldots & \partial F_1/\partial y_m \\ \partial F_2/\partial y_1 & \partial F_2/\partial y_2 & \ldots & \partial F_2/\partial y_m \\ \vdots & \vdots & \ddots & \vdots \\ \partial F_m/\partial y_1 & \partial F_m/\partial y_2 & \ldots & \partial F_m/\partial y_m \end{pmatrix}. \tag{13.32}$$

The $m \times m$ system of nonlinear equations

$$F(x, y) = 0$$

has a unique local solution for y in terms of x near any point where $F(x, y) = 0$ and the determinant of the Jacobian matrix in (13.32) is nonzero.

Many problems lead to an equation that depends on a parameter $\mu \in \mathbb{R}$. For example, μ may be a dimensionless parameter characteristic of the system being modeled by the equation. For a time-independent problem, we may write such an equation in the abstract form

$$F(x, \mu) = 0, \tag{13.33}$$

where $F : X \times \mathbb{R} \to Y$ and X, Y are Banach spaces. The study of how the solution set of (13.33) varies as μ varies is part of *bifurcation theory*. We assume that F is a smooth function. A *solution branch* of (13.33) is a smooth map $\overline{x} : I \subset \mathbb{R} \to X$ from an open interval I in $\mathbb{R}$ into X such that

$$F\left(\overline{x}(\mu), \mu\right) = 0 \qquad \text{for all } \mu \in I.$$

We say that μ_* is a *bifurcation point* of (13.33) from the solution branch $\overline{x}$, if there is a sequence of solutions (x_n, μ_n) in $X \times I$ such that

$$\begin{aligned} &F(x_n, \mu_n) = 0, \qquad x_n \neq \overline{x}(\mu_n), \\ &x_n \to \overline{x}(\mu_*), \quad \mu_n \to \mu_* \qquad \text{as } n \to \infty. \end{aligned}$$

The implicit function theorem implies that if the derivative

$$D_x F\left(\overline{x}(\mu), \mu\right) \tag{13.34}$$

is a nonsingular, bounded linear map from X to Y, then there is a unique local solution branch. Thus, a necessary condition for μ_* to be a bifurcation point is that the derivative in (13.34) is singular at $\mu = \mu_*$.

Example 13.24 Consider the equation

$$x^3 - \mu x = 0,$$

where $x, \mu \in \mathbb{R}$, corresponding to $F(x, \mu) = x^3 - \mu x$. The zero solution $x = 0$ is a solution branch. We have $F_x(0, \mu) = -\mu$, so the only possible bifurcation point from the zero solution is at $\mu = 0$. The solutions in this case are $x = 0$, and $x = \pm\sqrt{\mu}$ when $\mu > 0$. Thus, a new branch of solutions appears at $\mu = 0$. This bifurcation is called a *pitchfork bifurcation*.

The next example shows that the singularity of the derivative in (13.34) is a necessary but not sufficient condition for a bifurcation to occur.

Example 13.25 Consider the following system of equations for $(x, y) \in \mathbb{R}^2$:

$$\begin{aligned} y^3 - \mu x &= 0, \\ x^3 + \mu y &= 0. \end{aligned}$$

The zero solution $(x,y) = (0,0)$ satisfies this system for all $\mu \in \mathbb{R}$. The derivative of the left-hand side with respect to (x,y) has the matrix

$$\begin{pmatrix} -\mu & 3y^2 \\ 3x^2 & \mu \end{pmatrix}.$$

This matrix is singular at $x = y = 0$ if and only if $\mu = 0$, in which case it has a two-dimensional null space. Elimination of μ from the original system of equations implies that $x^4 + y^4 = 0$. Therefore, the zero solution is the only solution, and $\mu = 0$ is not a bifurcation point.

The same ideas apply to bifurcation problems for equations on infinite-dimensional spaces.

Example 13.26 Consider the following nonlinear Dirichlet problem on a smooth, bounded domain $\Omega \subset \mathbb{R}^n$:

$$\begin{aligned} -\Delta u &= \mu \sin u \qquad && \text{in } \Omega, \\ u &= 0 && \text{on } \partial\Omega. \end{aligned}$$

We write this equation in the form (13.33), where $F : X \times \mathbb{R} \to Y$ with

$$\begin{aligned} &F(u,\mu) = -\Delta u + \mu \sin u, \\ &X = \left\{ u \in C^{2,r}\left(\overline{\Omega}\right) \mid u = 0 \text{ on } \partial\Omega \right\}, \qquad Y = C^{0,r}\left(\overline{\Omega}\right). \end{aligned}$$

Here $0 < r \leq 1$, and $C^{k,r}\left(\overline{\Omega}\right)$ denotes a space of Hölder continuous functions. One can show that F is differentiable at $u = 0$, and

$$D_u F(0,\mu) h = -\Delta h - \mu h.$$

The theory of elliptic PDEs implies that $D_u F(0,\mu) : X \to Y$ is a bounded, nonsingular map unless μ is an eigenvalue of $-\Delta$. Thus, the possible bifurcation points from the trivial solution $u = 0$ are the eigenvalues of the Laplacian operator on Ω. It is possible to show that a bifurcation must occur at a simple eigenvalue, but need not occur at a multiple eigenvalue.

13.5 Newton's method

Newton's method is an iterative method for the solution of a finite or infinite-dimensional system of nonlinear equations,

$$f(x) = 0, \tag{13.35}$$

where f is a smooth mapping between Banach spaces. Suppose that x_n is an approximate solution. As $x \to x_n$, we have

$$f(x) = f(x_n) + f'(x_n)(x - x_n) + o(x - x_n).$$

If $f'(x_n)$ is nonsingular and x_n is sufficiently close to a solution of (13.35), then it is reasonable to expect that the solution $x = x_{n+1}$ of the linearized equation,

$$f(x_n) + f'(x_n)(x - x_n) = 0,$$

is a better approximation to the solution of the nonlinear equation than x_n. The resulting iteration scheme, called *Newton's method*, is given by

$$x_{n+1} = x_n - [f'(x_n)]^{-1} f(x_n) \qquad \text{for } n \geq 0. \tag{13.36}$$

After the choice of a starting point, x_0, Newton's method generates a sequence (x_n) of iterates, provided that $f'(x_n)$ is nonsingular for every n. The Newton iterates may be obtained from an iteration of the fixed point problem

$$x = x - [f'(x)]^{-1} f(x),$$

which is clearly equivalent to (13.35) when $f'(x)$ is nonsingular. A basic question concerning Newton's method is: When does the sequence of Newton iterates converge to a solution of (13.35)?

There are many variants of Newton's method. One of the simplest is the *modified Newton's method*:

$$x_{n+1} = x_n - [f'(x_0)]^{-1} f(x_n) \qquad \text{for } n \geq 0. \tag{13.37}$$

This method has the numerical advantage that the derivative $f'(x_0)$ only has to be computed and inverted once, at the starting point x_0; the sequence of approximations, however, does not converge as rapidly as the sequence obtained from Newton's method. The modified Newton's method is simpler to analyze than Newton's method, and, following Lusternik and Sobolev [33], we will prove a convergence result for it here. A proof of the convergence of Newton's method, under suitable assumptions on f and x_0, may be found in Kantorovich and Akilov [27].

In order to prove convergence, we will assume that f' satisfies a Lipschitz condition. If $f : U \subset X \to Y$ is a differentiable function, then we say that the derivative $f' : U \subset X \to \mathcal{B}(X, Y)$ is *Lipschitz continuous* in U if there is a constant C, called a *Lipschitz constant*, such that

$$\|f'(x) - f'(y)\| \leq C\|x - y\| \qquad \text{for all } x, y \in U. \tag{13.38}$$

Theorem 13.27 Let $f : U \subset X \to Y$ be a differentiable map from an open subset U of a Banach space X into a Banach space Y such that f' is Lipschitz continuous in U with Lipschitz constant C. Suppose that $x_0 \in U$, $f'(x_0)$ is nonsingular, and

$$h = C \left\| [f'(x_0)]^{-1} \right\| \left\| [f'(x_0)]^{-1} f(x_0) \right\| \leq \frac{1}{4}. \tag{13.39}$$

Define $\delta \geq 0$ by

$$\delta = \left\| [f'(x_0)]^{-1} f(x_0) \right\| \left(\frac{1 - \sqrt{1 - 4h}}{2h} \right), \tag{13.40}$$

and suppose further that the closed ball B_δ of radius δ centered at x_0,

$$B_\delta = \{x \in X \mid \|x - x_0\| \leq \delta\}, \tag{13.41}$$

is contained in U. Then there is a unique solution of the equation $f(x) = 0$ in B_δ, and the sequence (x_n) of modified Newton iterates, defined in (13.37), converges to the solution of $f(x) = 0$ in B_δ as $n \to \infty$.

Proof. The modified Newton iterates are obtained from the fixed point iteration $x_{n+1} = T(x_n)$, where

$$T(x) = x - [f'(x_0)]^{-1} f(x).$$

First, we show that $T : B_\delta \to B_\delta$. We may write

$$T(x) - x_0 = -[f'(x_0)]^{-1} [r(x) + f(x_0)], \tag{13.42}$$

where

$$r(x) = f(x) - f(x_0) - f'(x_0)(x - x_0). \tag{13.43}$$

Taking the norm of (13.42), we find that

$$\|T(x) - x_0\| \leq M \|r(x)\| + \eta, \tag{13.44}$$

where

$$M = \left\| [f'(x_0)]^{-1} \right\|, \qquad \eta = \left\| [f'(x_0)]^{-1} f(x_0) \right\|. \tag{13.45}$$

Computing the derivative of r, and using the Lipschitz condition (13.38) for f', we obtain that

$$\|r'(x)\| = \|f'(x) - f'(x_0)\| \leq C \|x - x_0\|.$$

Since $r(x_0) = 0$, the mean value theorem implies that

$$\|r(x)\| = \|r(x) - r(x_0)\| \leq \sup_{0 \leq t \leq 1} \|r'(tx + (1-t)x_0)\| \, \|x - x_0\| \leq C \|x - x_0\|^2.$$

Using this result in (13.44), we find that

$$\|T(x) - x_0\| \leq CM \|x - x_0\|^2 + \eta.$$

Hence, T maps the ball $\{x \mid \|x - x_0\| \leq \epsilon\}$ into itself provided that

$$CM\epsilon^2 + \eta \leq \epsilon. \tag{13.46}$$

This inequality can be satisfied for some $\epsilon > 0$ if

$$h = CM\eta \leq \frac{1}{4}. \tag{13.47}$$

Using (13.45), we see that this is the condition in (13.39). In that case, the smallest value δ of ϵ for which (13.46) holds is

$$\delta = \eta\tau, \tag{13.48}$$

where τ is the smallest root of the equation $h\tau^2 - \tau + 1 = 0$, or

$$\tau = \frac{1 - \sqrt{1-4h}}{2h}. \tag{13.49}$$

Using (13.45) and (13.49) in (13.48), we find that δ is given by (13.40). This proves that $T : B_\delta \to B_\delta$.

Next, we prove that T is a contraction on B_δ. Differentiating (13.42) and (13.43), we find that

$$T'(x) = -\left[f'(x_0)\right]^{-1}\left[f'(x) - f'(x_0)\right].$$

Hence, using (13.45) and the Lipschitz condition on f' in (13.38), we have

$$\|T'(x)\| \le M\,\|f'(x) - f'(x_0)\| \le CM\|x - x_0\| \le CM\delta \qquad \text{for all } x \in B_\delta.$$

It follows from (13.47), (13.48), and (13.49) that

$$CM\delta = \frac{1-\sqrt{1-4h}}{2} \le \frac{1}{2}.$$

We therefore have $\|T'(x)\| \le 1/2$ in B_δ, so from the mean value theorem

$$\|T(x) - T(y)\| \le \frac{1}{2}\|x - y\| \qquad \text{for all } x, y \in B_\delta.$$

The theorem now follows from the contraction mapping theorem. □

Note that the conditions (13.39) and $B_\delta \subset U$ in the hypotheses of the theorem are satisfied when x_0 is sufficiently close to a solution of $f(x) = 0$ at which the derivative of f is nonsingular.

A significant practical difficulty in the implementation of Newton's method, and its modifications, is that the iterates may diverge unless the starting point is very close to the solution. For this reason, Newton's method is often used in conjunction with continuation methods, in which one slowly varies a parameter in the equation, and uses the solution for a previous parameter value as an initial guess for the Newton iterations for the next parameter value.

13.6 Linearized stability

We consider an equilibrium of the evolution equation

$$u_t = f(u), \tag{13.50}$$

where $f : \mathcal{D}(f) \subset X \to X$ is a vector field on a Banach space X. We assume that the initial value problem for (13.50) is well posed, meaning that there is a unique solution $u : [0, \infty) \to X$ for every initial condition $u(0) = u_0 \in X$, and $u(t)$ depends continuously on u_0 with respect to the normed topology on X. A state $\overline{u} \in X$ is an *equilibrium* of (13.50) if $f(\overline{u}) = 0$. There are many inequivalent ways to define the stability of an equilibrium. We only consider the two most common ways here.

Definition 13.28 An equilibrium $\overline{u}$ of (13.50) is *stable* if for every neighborhood U of $\overline{u}$ there is a neighborhood V of $\overline{u}$ such that if $u(0) \in V$, then $u(t) \in U$ for all $t \geq 0$. If $\overline{u}$ is not stable, then it is *unstable*. An equilibrium $\overline{u}$ is *asymptotically stable* if it is stable and there is a neighborhood W of $\overline{u}$ such that $u(t) \to \overline{u}$ as $t \to \infty$ whenever $u(0) \in W$.

Thus, if a stable equilibrium is perturbed, the perturbation remains small, and if an asymptotically stable equilibrium is perturbed, then the perturbation remains small and eventually dies out.

The linearization of (13.50) about $\overline{u}$ is

$$v_t = Av, \qquad \text{where } A = f'(\overline{u}). \tag{13.51}$$

We define the linear stability of an equilibrium $\overline{u}$ of (13.50) in terms of the stability of the equilibrium $v = 0$ of (13.51).

Definition 13.29 The equilibrium $u = \overline{u}$ of (13.50) is *linearly stable*, or *linearly asymptotically stable*, if $v = 0$ is a stable, or asymptotically stable, equilibrium of (13.51), respectively.

In the case of ODEs, we have the following result.

Theorem 13.30 Suppose that $f : \mathbb{R}^n \to \mathbb{R}^n$ is continuously differentiable and $f(\overline{u}) = 0$. If all the eigenvalues of $f'(\overline{u})$ have a strictly negative real part, then $\overline{u}$ is an asymptotically stable equilibrium of the system of ODEs $\dot{u} = f(u)$. If one of the eigenvalues of $f'(\overline{u})$ has a strictly positive real part, then $\overline{u}$ is unstable.

The stability part of this theorem is proved by the construction of a suitable quadratic *Liapunov function* $V : X \to \mathbb{R}$ for (13.50) that has a minimum at $\overline{u}$ and the property that $V_t \leq 0$ on solutions of (13.50) in a neighborhood of $\overline{u}$ (see [21]).

Example 13.31 Consider a 2×2 system of ODEs for $(u, v) \in \mathbb{R}^2$:

$$\dot{u} = f(u, v), \qquad \dot{v} = g(u, v). \tag{13.52}$$

The eigenvalues of the derivative

$$A = \begin{pmatrix} f_u(\overline{u}, \overline{v}) & f_v(\overline{u}, \overline{v}) \\ g_u(\overline{u}, \overline{v}) & g_v(\overline{u}, \overline{v}) \end{pmatrix} \tag{13.53}$$

have strictly negative real parts if and only if

$$\begin{aligned}\operatorname{tr} A &= f_u(\overline{u},\overline{v}) + g_v(\overline{u},\overline{v}) < 0,\\ \det A &= f_u(\overline{u},\overline{v})\, g_v(\overline{u},\overline{v}) - f_v(\overline{u},\overline{v})\, g_u(\overline{u},\overline{v}) > 0.\end{aligned} \tag{13.54}$$

Thus, an equilibrium $(\overline{u},\overline{v})$ of (13.52) is asymptotically stable when the condition in (13.54) holds.

If the spectrum of $f'(\overline{u})$ touches the imaginary axis, meaning that all points in the spectrum have nonpositive real parts and the real part of at least one point is equal to zero, then the equilibrium $\overline{u}$ may be linearly stable, but we cannot draw conclusions about the nonlinear stability of $\overline{u}$ from its linearized stability alone.

Example 13.32 Consider the following 2×2 system of ODEs for $(u,v) \in \mathbb{R}^2$:

$$\begin{aligned}\dot{u} &= \mu u - v - \alpha\left(u^2+v^2\right)u,\\ \dot{v} &= u + \mu v - \alpha\left(u^2+v^2\right)v,\end{aligned}$$

where α, μ are real parameters. It is convenient to write this equation in complex form for $w = u + iv \in \mathbb{C}$ as

$$\dot{w} = (\mu + i)\, w - \alpha |w|^2 w. \tag{13.55}$$

This equation may be solved by writing it in the polar form

$$\dot{r} = \mu r - \alpha r^3, \qquad \dot{\theta} = 1,$$

where

$$w = re^{i\theta}, \quad r = \sqrt{u^2+v^2}, \quad \tan\theta = \frac{v}{u}.$$

If $\mu < 0$, then the equilibrium $w = 0$ is asymptotically stable, and if $\mu > 0$ it is unstable. If $\mu = 0$, then the eigenvalues of the linearization are purely imaginary, and the equilibrium $w = 0$ is linearly stable. It is asymptotically stable if $\alpha > 0$, stable if $\alpha = 0$, and unstable if $\alpha < 0$.

When α and μ have the same sign, (13.55) has a periodic *limit cycle* solution

$$w(t) = \sqrt{\frac{\mu}{\alpha}}\, e^{it}.$$

As μ increases through zero, the equilibrium $w = 0$ becomes unstable. If $\alpha > 0$, then a stable limit cycle appears for $\mu > 0$, while if $\alpha < 0$, then an unstable limit cycle shrinks down to the equilibrium $w = 0$ and disappears for $\mu > 0$. This type of bifurcation is called a *Hopf bifurcation*. The Hopf bifurcation is said to be *supercritical* if $\alpha > 0$ and *subcritical* if $\alpha < 0$.

For PDEs, the relationship between different types of stability, and between linear and nonlinear stability, can be rather subtle. It is usually true that if the spectrum of $f'(\overline{u})$ is contained in a left-half plane $\{\lambda \in \mathbb{C} \mid \operatorname{Re}\lambda \leq \omega\}$ for some $\omega < 0$, then $\overline{u}$ is linearly asymptotically stable (see the discussion of (9.24)), and that linear asymptotic stability implies nonlinear asymptotic stability, but there are exceptions. Moreover, the linearized equation may have continuous or residual spectrum in addition to, or instead of, the pure point spectrum that occurs for ODEs.

We will illustrate the linearization of nonlinear PDEs by considering an important class of examples called *reaction-diffusion equations*. These nonlinear PDEs describe the dynamics of spatially dependent chemical concentrations and temperature in the presence of chemical reactions and the diffusion of reactants and heat. They also model the population of spatially distributed species in ecology. The general form of a reaction-diffusion equation for $u(x,t) \in \mathbb{R}^m$, where $x \in \mathbb{R}^n$ and $t \geq 0$, is

$$u_t = D\Delta u + f(u). \tag{13.56}$$

The effect of diffusion is described by the linear term $D\Delta u$, where D is a positive definite, symmetric $m \times m$ matrix, called the diffusion matrix. In most applications, D is diagonal, and, for simplicity, we assume that D is constant. The effect of reactions is described by the term $f(u)$, where $f : \mathbb{R}^m \to \mathbb{R}^m$ is a given nonlinear function. For models of chemical reactions, f is often a polynomial in the chemical concentrations, as follows from the *law of mass action*, with coefficients that depend exponentially on the temperature. To be specific, we consider a reaction-diffusion equation for a function u defined on a regular, bounded domain $\Omega \subset \mathbb{R}^n$ subject to Dirichlet boundary conditions. In that case, we supplement (13.56) with the initial and boundary conditions

$$\begin{aligned} u(x,t) &= 0 \qquad && \text{for } x \in \partial\Omega \text{ and } t > 0, \\ u(x,0) &= u_0(x) \qquad && \text{for } x \in \Omega. \end{aligned}$$

An equilibrium solution $\overline{u} : \Omega \subset \mathbb{R}^n \to \mathbb{R}^m$ of (13.56) satisfies the elliptic system of PDEs

$$\begin{aligned} &D\Delta\overline{u} + f(\overline{u}) = 0, \\ &\overline{u}(x) = 0 \qquad \text{for } x \in \partial\Omega. \end{aligned}$$

To study the linear stability of $\overline{u}$, we have to compute the Fréchet derivative of the map F given by

$$F(u) = D\Delta u + f(u). \tag{13.57}$$

The derivative of the linear term is trivial to compute, so we only need to compute the derivative of the nonlinear term, defined on a suitable space of functions.

Lemma 13.33 Suppose that $\Omega \subset \mathbb{R}^n$ is a regular, bounded open domain, and $f : \mathbb{R}^m \to \mathbb{R}^m$ is a twice continuously differentiable function with derivative $f' : \mathbb{R}^m \to \mathbb{R}^{m\times m}$. Then the map $N_f : H^k(\Omega) \to L^2(\Omega)$ defined by $N_f(u) = f(u)$ is differentiable for every $k > n/2$, and its derivative $N_f'(u) : H^k(\Omega) \to L^2(\Omega)$ at $u \in H^k(\Omega)$, is given by

$$N_f'(u)(v) = f'(u)v.$$

Proof. Let $|u|$ denote the Euclidean norm of $u \in \mathbb{R}^m$. Since f is twice continuously differentiable, for each $R > 0$ there is constant $C(R)$ such that

$$|f(u+h) - f(u) - f'(u)v| \le C(R)|v|^2$$

for all $u, v \in \mathbb{R}^n$ such that $|u| \le R$ and $|u+v| \le R$. By the Sobolev embedding theorem (Theorem 12.70) and the assumption that $k > n/2$, there is a constant M such that

$$\|u\|_\infty \le M\|u\|_{H^k}.$$

By combining these inequalities and integrating the result over Ω, we obtain for $\|v\|_{H^k} \le 1$ that

$$\begin{aligned} \|f(u+v) - f(u) - f'(u)v\|_{L^2} &\le C\left\|v^2\right\|_{L^2} \\ &\le C'\|v\|_\infty\|v\|_{L^2} \\ &\le C''\|v\|_{H^k}^2 \end{aligned}$$

where $C = C(R)$ with $R = \|u\|_\infty + M$, C', and C'' are constants depending on the bounded domain Ω and u, but not on v. The result follows by dividing this equation by $\|v\|_{H^k}$ and taking the limit of the result as $\|v\|_{H^k} \to 0$. □

The Laplacian maps H^k into L^2 if $k \ge 2$. Thus, it follows that if $k \ge 2$ and $k > n/2$, then the map F defined in (13.57), where

$$F : \mathcal{D}(F) \subset H^k(\Omega) \to L^2(\Omega), \qquad \mathcal{D}(F) = \left\{u \in H^k(\Omega) \mid u = 0 \text{ on } \partial\Omega\right\},$$

is differentiable, and the derivative of F at $\overline{u} \in \mathcal{D}(F)$ is given by

$$F'(\overline{u})\, v = D\Delta v + Av,$$

where $A = f'(\overline{u})$. The linearization of (13.56) is therefore

$$v_t = D\Delta v + Av. \tag{13.58}$$

As for the Laplacian on a regular bounded domain, the spectrum of $F'(\overline{u})$ consists entirely of eigenvalues. The matrix A need not be symmetric, and if it is not, then $F'(\overline{u})$ is not self-adjoint, so its eigenvalues need not be real. The equilibrium $\overline{u}$ is linearly asymptotically stable if every eigenvalue of $F'(\overline{u})$ has strictly negative real part.

In general, the equilibrium $\overline{u}$ is a function of x, so that $F'(\overline{u})$ is a variable coefficient elliptic differential operator. It is usually not possible to compute its eigenvalues explicitly, although the eigenvalues with the largest real parts can be computed numerically. If, however, $\overline{u}$ is a constant state and the reaction-diffusion equation is posed on $\mathbb{R}^n$, or $\mathbb{T}^n$, then we can use Fourier analysis to study the spectrum of the linearization. We illustrate this procedure with a discussion of the *Turing instability*, which was proposed by Turing in 1952 as a mechanism for the development of spatial patterns from a spatially uniform state, and in particular as a possible mechanism for morphogenesis.

The state $\overline{u} \in \mathbb{R}^m$ is a spatially uniform equilibrium of (13.56) if and only if $f(\overline{u}) = 0$. We look for solutions of the linearization (13.58) of (13.56) at $\overline{u}$ of the form

$$v(x,t) = e^{ik\cdot x+\lambda t}\widehat{v}, \tag{13.59}$$

where $k \in \mathbb{R}^n$, $\lambda \in \mathbb{C}$, and $\widehat{v} \in \mathbb{C}^m \setminus 0$. General solutions of the IVP for (13.58) may be obtained from these solutions by use of the Fourier transform. The solution (13.59) grows exponentially in time if $\operatorname{Re}\lambda > 0$. Thus, $\overline{u}$ is linearly unstable if $\operatorname{Re}\lambda > 0$ for some $k \in \mathbb{R}^n$. The use of (13.59) in (13.58) implies that

$$\left(-|k|^2 D + A\right)\widehat{v} = \lambda\widehat{v}. \tag{13.60}$$

It follows that λ is an eigenvalue of $-|k|^2D + A$. Turing observed that $-|k|^2D + A$ may have an eigenvalue with positive real part for some $|k| > 0$ even though all the eigenvalues of A have negative real part. In that case, $\overline{u}$ is an asymptotically stable equilibrium of the reaction equations $\dot{u} = f(u)$, and is therefore stable to spatially uniform perturbations, but is unstable to spatially nonuniform perturbations. The growth of spatially unstable perturbations, and the possible saturation of the growth by nonlinear effects, leads to the formation of spatial patterns from a spatially uniform state. This instability is called a *Turing instability* or a *diffusion-driven instability*.

The simplest system that exhibits Turing instability is a 2×2 system of reaction diffusion equations for $(u, v) \in \mathbb{R}^2$ with a diagonal diffusion matrix $D = \operatorname{diag}(\mu, \nu)$, where $\mu, \nu > 0$:

$$\begin{aligned} u_t &= \mu\Delta u + f(u,v), \\ v_t &= \nu\Delta v + g(u,v). \end{aligned} \tag{13.61}$$

Here, $f, g : \mathbb{R}^2 \to \mathbb{R}$ are given functions that describe the reaction equations. The eigenvalue problem (13.60) for (13.61) is

$$\begin{pmatrix} -|k|^2\mu + f_u & f_v \\ g_u & -|k|^2\nu + g_v \end{pmatrix}\begin{pmatrix} \widehat{u} \\ \widehat{v} \end{pmatrix} = \lambda\begin{pmatrix} \widehat{u} \\ \widehat{v} \end{pmatrix},$$

where we do not indicate explicitly that the derivatives of f, g are evaluated at $u = \overline{u}$, $v = \overline{v}$.

The eigenvalues λ are solutions of the quadratic equation

$$\lambda^2 - \left[f_u + g_v - |k|^2 (\mu + \nu)\right] \lambda + h\left(|k|^2\right) = 0, \tag{13.62}$$

where

$$h\left(|k|^2\right) = \mu\nu |k|^4 - (\mu g_v + \nu f_u) |k|^2 + f_u g_v - f_v g_u.$$

From (13.54), the equilibrium state is stable to spatially uniform perturbations with $k = 0$ if

$$f_u + g_v < 0, \qquad f_u g_v - f_v g_u > 0. \tag{13.63}$$

The quadratic equation (13.62) for λ then has a root with positive real part if and only if $h\left(|k|^2\right) < 0$, and this can occur for some $|k| > 0$ only if

$$\mu g_v + \nu f_u > 0. \tag{13.64}$$

In that case, $h\left(|k|^2\right)$ has a minimum at $|k| = \kappa$, where

$$\kappa^2 = \frac{\mu g_v + \nu f_u}{2\mu\nu},$$

and $h\left(\kappa^2\right) < 0$ if and only if

$$\mu g_v + \nu f_u > 2\sqrt{\mu\nu \left(f_u g_v - f_v g_u\right)}. \tag{13.65}$$

Thus, the conditions (13.63)–(13.65) imply that a Turing instability occurs in the system defined by (13.61).

At first sight, it may seem surprising that diffusion can cause instability in a state that is stable to spatially uniform perturbations, but there is a simple explanation. It follows from (13.63) and (13.64) that f_u and g_v have opposite signs and $\mu \neq \nu$. This difference between the diffusivities is essential for the Turing instability. Exchanging u and v, if necessary, we may assume that $f_u < 0$ and $g_v > 0$, when $\mu > \nu$. Furthermore, replacing v by $-v$, if necessary, we find that the sign structure of the entries in the matrix A of the derivative of the reaction terms in a 2×2 system that is subject to a Turing instability can always be put in the form

$$A = \begin{pmatrix} - & + \\ - & + \end{pmatrix}.$$

In this case, we call v an *activator* because, in the absence of diffusion, it grows exponentially in time when $u = 0$, and we call u an *inhibitor* because positive values of u reduce the growth of v. If $v = 0$, then the inhibitor u decays exponentially to its equilibrium state. The equilibrium is a stable state of the reaction equations because a positive perturbation in the activator from its equilibrium value causes a growth in the inhibitor, and this in turn stabilizes the activator. We have seen that $\mu > \nu$, which means that the diffusivity of the inhibitor is greater than the diffusivity of the activator. If a spatially nonuniform perturbation in the activator begins to grow at some point, then the inhibitor diffuses away faster than the activator, and as a result the generation of inhibitor may not be sufficient to prevent the continued growth of the activator.

Morphogenesis is too complex to be explained by a Turing instability. It has been suggested, however, that some biological patterns, such as coat pigmentations, are the result of a Turing instability. Turing instability has been observed in chemically reacting systems in gels, although the first successful experimental observations took place almost forty years after Turing's original theoretical work.

13.7 The calculus of variations

The calculus of variations is an enormous subject, with applications to physics, geometry, and optimization theory, among many other areas. The following discussion is therefore only a brief, and incomplete, introduction.

A basic problem in the calculus of variations is the minimization of a functional. Suppose that $I : X \to \mathbb{R}$ is a real-valued functional defined on a Hilbert or Banach space X. If I has a local minimum at $\overline{x}$, then for each $h \in X$, the function $I(\overline{x}+\epsilon h)$ of the scalar parameter ϵ has a local minimum at $\epsilon = 0$. Therefore, if I is differentiable at $\overline{x}$, then

$$\left.\frac{d}{d\epsilon} I(\overline{x} + \epsilon h)\right|_{\epsilon=0} = I'(\overline{x})h = 0,$$

so the derivative of I at $\overline{x}$ is zero. We call a point where the derivative of a functional I vanishes a *critical point* or *stationary point* of I. Thus, a necessary condition for a differentiable functional I to have a minimum at an interior point $\overline{x}$ of its domain is that $\overline{x}$ is a critical point of I. In searching for the minimizers of I, we may therefore restrict attention to the critical points of I, as well as any boundary points of the domain of I, and points where I fails to be differentiable. A critical point need not be a local minimum. For example, it could be a local maximum or a saddle point. We will not discuss here sufficient conditions for a critical point to be a minimum, but critical points of functionals are often of interest in their own right.

In this section, we introduce the fundamental ideas in the calculus of variations by a study of functionals of the form

$$I(u) = \int_0^1 L\left(x, u(x), Du(x)\right)\, dx, \tag{13.66}$$

where $u : [0, 1] \to \mathbb{R}^m$ is a continuously differentiable function of one variable, and

$$L : [0, 1] \times \mathbb{R}^m \times \mathbb{R}^m \to \mathbb{R}$$

is a given smooth function, called the *Lagrangian*. It is convenient to use the notation D for the derivative with respect to x, so $Du = u'$.

We will derive a differential equation, called the *Euler-Lagrange* equation, that is satisfied by any sufficiently smooth critical point of I. Abusing notation slightly, we write

$$\begin{aligned} L_x\left(x, u(x), Du(x)\right) &= \left.\frac{\partial}{\partial x} L(x, y, v)\right|_{y=u(x),\, v=Du(x)}, \\ L_u\left(x, u(x), Du(x)\right) &= \left.\frac{\partial}{\partial y} L(x, y, v)\right|_{y=u(x),\, v=Du(x)}, \\ L_{Du}(x, u(x), Du(x)) &= \left.\frac{\partial}{\partial v} L(x, y, v)\right|_{y=u(x),\, v=Du(x)}. \end{aligned}$$

If $u = (u_1, u_2, \ldots, u_m)$ takes values in $\mathbb{R}^m$, then these partial derivatives denote the gradient, and

$$L_u = \left(L_{u_1}, L_{u_2}, \ldots, L_{u_m}\right), \qquad L_{Du} = \left(L_{Du_1}, L_{Du_2}, \ldots, L_{Du_m}\right)$$

also take values in $\mathbb{R}^m$. If $\varphi = (\varphi_1, \varphi_2, \ldots, \varphi_m) : [0,1] \to \mathbb{R}^m$, then we write

$$L_u \cdot \varphi = \sum_{i=1}^m L_{u_i} \varphi_i, \qquad L_{Du} \cdot \varphi = \sum_{i=1}^m L_{Du_i} \varphi_i.$$

For example, the chain rule implies that

$$\begin{aligned} DL\left(x, u(x), Du(x)\right) &= L_x\left(x, u(x), Du(x)\right) + L_u\left(x, u(x), Du(x)\right) \cdot Du(x) \\ &\quad + L_{Du}(x, u(x), Du(x)) \cdot D^2 u(x). \end{aligned}$$

There are many possible choices for the space X of admissible functions on which I is defined, and the "correct" space in which to look for a minimizer, if one exists at all, depends in general on the functional. For definiteness, we first suppose that u is a continuously differentiable function that satisfies the boundary conditions $u(0) = u(1) = 0$. Then $I : X \to \mathbb{R}$, where

$$X = \left\{ u \in C^1([0,1]) \mid u(0) = u(1) = 0 \right\}.$$

The functional I is differentiable on X, and $I'(u) : X \to \mathbb{R}$ is given by

$$\begin{aligned} I'(u)\varphi &= \left.\frac{d}{d\epsilon} I(u + \epsilon\varphi)\right|_{\epsilon=0} \\ &= \left.\frac{d}{d\epsilon} \int_0^1 L(x, u + \epsilon\varphi, Du + \epsilon D\varphi)\, dx\right|_{\epsilon=0} \\ &= \int_0^1 \left\{ L_u(x, u, Du) \cdot \varphi + L_{Du}(x, u, Du) \cdot D\varphi \right\}\, dx. \end{aligned}$$

Thus, if u is a critical point of I, we have

$$\int_0^1 \left\{ L_u(x, u, Du) \cdot \varphi + L_{Du}(x, u, Du) \cdot D\varphi \right\}\, dx = 0 \qquad \text{for all } \varphi \in X.$$

Suppose that the critical point u belongs to $C^2([0,1])$. We may then integrate by parts in this equation to obtain

$$\int_0^1 \{L_u(x,u,Du) - D\left[L_{Du}(x,u,Du)\right]\} \cdot \varphi \, dx = 0 \qquad \text{for all } \varphi \in X. \tag{13.67}$$

The boundary terms vanish because φ is zero at the endpoints. To obtain the differential equation satisfied by u, we use the following *fundamental lemma of the calculus of variations*, or *du Bois-Reymond lemma*.

Lemma 13.34 (Fundamental) If $f : [a,b] \to \mathbb{R}$ is a continuous function such that

$$\int_a^b f(x)\varphi(x)\, dx = 0 \qquad \text{for every } \varphi \in C_c^\infty\left((a,b)\right),$$

then $f(x) = 0$ for every $a \le x \le b$.

Proof. Suppose that f is not identically zero. Then there is an $x_0 \in (a,b)$ such that $f(x_0) \neq 0$. Multiplying f by -1, if necessary, we may assume that $f(x_0) > 0$. Since f is continuous, there is an interval $I \subset (a,b)$ such that

$$|f(x) - f(x_0)| \le \frac{1}{2} f(x_0) \qquad \text{for every } x \in I,$$

which implies that $f(x) \ge f(x_0)/2$ for every $x \in I$. Let $\varphi \in C_c^\infty\left((a,b)\right)$ be a nonnegative function with integral equal to one and support contained in I. Then

$$\int_a^b f(x)\varphi(x)\, dx \ge \frac{1}{2} f(x_0) > 0.$$

This contradiction proves the lemma. □

Applying the fundamental lemma componentwise to (13.67), we see that every C^2-critical point u of the functional I defined in (13.66) satisfies the following *Euler-Lagrange* equation:

$$-DL_{Du} + L_u = 0. \tag{13.68}$$

If $u = (u_1, u_2, \ldots, u_m)$ is an m-vector-valued function, where $u_i : [0,1] \to \mathbb{R}$, then the component form of the Euler-Lagrange equation (13.68) is

$$-DL_{Du_i} + L_{u_i} = 0, \qquad i = 1, 2, \ldots, m.$$

Using the chain rule to expand the derivative, we may write this equation as

$$-\sum_{j=1}^m \left\{L_{Du_i Du_j} D^2 u_j + L_{Du_i u_j} Du_j\right\} - L_{Du_i x} + L_{u_i} = 0, \qquad i = 1, 2, \ldots, m.$$

If the second derivative L_{DuDu} of L with respect to Du, with matrix

$$\left(L_{Du_i Du_j}\right)_{i,j=1}^{m},$$

is nonsingular, then we may solve this equation for D^2u to obtain a second-order system of equations of the form $D^2u = f(x, u, Du)$.

Exactly the same argument applies if we minimize I over the affine space of functions u that satisfy the nonhomogeneous boundary conditions

$$u(0) = a, \qquad u(1) = b, \tag{13.69}$$

since $u + \epsilon\varphi$ satisfies the same boundary conditions as u if and only if $\varphi(0) = \varphi(1) = 0$. A C^2-critical point of I on the space of functions $u \in C^1([0,1])$ such that $u(0) = a$ and $u(1) = b$ therefore satisfies the ODE (13.68) and the boundary conditions (13.69).

Example 13.35 Suppose that a curve $y = u(x)$ connects the origin $(0,0)$ and a point (a,b) in the (x,y)-plane. The length $I(u)$ of the curve is given by the arclength integral

$$I(u) = \int_0^a \sqrt{1 + (Du)^2}\, dx.$$

The corresponding Euler-Lagrange equation is

$$-D\left(\frac{Du}{\sqrt{1 + (Du)^2}}\right) = 0,$$

which simplifies to

$$D^2u = 0.$$

The solution is a linear function of x, and the shortest curve connecting two points is a straight line.

Example 13.36 One of the original problems in the calculus of variations was the *brachistochrone problem*, first formulated by Galileo in 1638, who suggested incorrectly that the solution is a circular arc. The problem was formulated independently and solved correctly by Johann Bernoulli in 1697. Suppose that a frictionless particle, or bead, slides along a curve $y = u(x)$ under the influence of gravity. We choose the y coordinate downwards, so that gravity acts in the positive y-direction. If the particle starts at the origin $O = (0,0)$ with zero velocity, then conservation of energy implies that after it has dropped a vertical distance y, the velocity v of the particle satisfies

$$\frac{1}{2}v^2 = gy,$$

where g is the acceleration due to gravity. Therefore, $v = \sqrt{2gy}$. The time $I(u)$ taken by the particle to move from the origin O to a point $P = (a, b)$ on the curve is given by the integral of arclength divided by velocity, or

$$I(u) = \int_0^a \sqrt{\frac{1 + (Du)^2}{2gu}}\, dx.$$

The brachistochrone problem is to find the curve connecting given points O and P such that a particle starting at rest slides from O to P along the curve in the shortest possible time. The curve should be steep initially, so the particle accelerates rapidly, but it should not be too steep, because this increases its arclength. The required curve satisfies the Euler-Lagrange equation associated with I, which is

$$-D\left(\frac{Du}{\sqrt{2gu\,[1 + (Du)^2]}}\right) - \frac{1}{2}\sqrt{\frac{1 + (Du)^2}{2gu^3}} = 0. \tag{13.70}$$

In order to solve (13.70), we will show that the Euler-Lagrange equation has a first integral whenever the Lagrangian does not depend explicitly on the independent variable x. This result is one of the simplest instances of *Noether's theorem*, which connects symmetries of the Lagrangian with conservation laws of the Euler-Lagrange equation.

Proposition 13.37 If $L = L(u, Du)$ is independent of x, then any solution u of the Euler-Lagrange equation (13.68) satisfies the conservation law

$$L_{Du}(u, Du) \cdot Du - L(u, Du) = \text{constant}.$$

Proof. We define $H : \mathbb{R}^m \times \mathbb{R}^m \to \mathbb{R}$ by

$$H(u, Du) = L_{Du}(u, Du) \cdot Du - L(u, Du).$$

Then, using the chain rule, we find that

$$DH = (DL_{Du} - L_u) \cdot Du.$$

Hence, if u satisfies (13.68), then H is constant. □

Example 13.38 The Lagrangian for brachistochrone problem in Example 13.36,

$$L(u, Du) = \sqrt{\frac{1 + (Du)^2}{2gu}},$$

is independent of x. Proposition 13.37 therefore implies that (13.70) has the first integral

$$\frac{(Du)^2}{\sqrt{2gu\left[1 + (Du)^2\right]}} - \sqrt{\frac{1 + (Du)^2}{2gu}} = c,$$

where c is a constant of integration. This equation simplifies to

$$2gc^2u\left[1 + (Du)^2\right] = 1.$$

Writing the curve $y = u(x)$ in the parametric form $x = x(t)$, $y = y(t)$, where $y(t) = u(x(t))$ so $Du = \dot{y}/\dot{x}$, and setting $y(t) = k(1 - \cos t)$ where $k = 1/(4gc^2)$, we find that

$$\dot{x} = k(1 - \cos t).$$

The solution through the points $(0,0)$ and (a,b) is therefore the cycloid

$$x(t) = k(t - \sin t), \qquad y(t) = k(1 - \cos t)$$

for $0 \leq t \leq T$. The constants of integration k, T are chosen so that

$$k(T - \sin T) = a, \qquad k(1 - \cos T) = b.$$

In view of the importance of the expression on the left-hand side of the Euler-Lagrange equation (13.68), we make the following definition.

Definition 13.39 The *variational derivative*, or *functional derivative*, of the functional I in (13.66) at a smooth function u is the function

$$\frac{\delta I}{\delta u} = -DL_{Du} + L_u.$$

The *Euler operator* L_I of I is the operator

$$L_I(u) = \frac{\delta I}{\delta u}$$

that maps a function u to the variational derivative of I at u.

Using this notation, we may write the Euler-Lagrange equation for I as

$$\frac{\delta I}{\delta u} = 0.$$

If u and φ are sufficiently smooth, and φ is compactly supported in $(0,1)$, then

$$\frac{d}{d\epsilon} I(u + \epsilon\varphi)\bigg|_{\epsilon=0} = \int_0^1 \frac{\delta I}{\delta u}(x) \cdot \varphi(x)\, dx. \tag{13.71}$$

We may think of the L^2-inner product

$$\langle u, v\rangle = \int_0^1 u(x) \cdot v(x)\, dx$$

as a continuous analog of the Euclidean inner product on $\mathbb{R}^n$,

$$\langle u, v\rangle = \sum_{i=1}^n u_i v_i,$$

in which an integral over the continuous index x replaces a sum over the discrete index i. Equation (13.71) is the continuous analog of the formula for the directional derivative of a function $I : \mathbb{R}^n \to \mathbb{R}$:

$$\frac{d}{d\epsilon} I(u + \epsilon\varphi)\bigg|_{\epsilon=0} = \sum_{i=1}^{n} \frac{\partial I}{\partial u_i} \varphi_i.$$

Thus, the variational derivative of a functional defined on a suitable subspace of L^2 is a formal continuous analog of the gradient of a function defined on $\mathbb{R}^n$. From (13.71), we may write the value of the variational derivative at x formally as

$$\frac{\delta I}{\delta u}(x) = \frac{d}{d\epsilon} I(u + \epsilon\delta_x)\bigg|_{\epsilon=0},$$

where δ_x is the delta-function supported at x. Thus, heuristically, the value of $\delta I/\delta u$ at the point x measures the sensitivity of I to changes in u at x.

In the above analysis, we looked for critical points of the functional I in (13.66), defined on a restricted class of admissible functions that satisfy prescribed Dirichlet conditions at the endpoints. Suppose, instead, we look for critical points of $I(u)$ without imposing any boundary conditions on the admissible functions u, so that $I : X \to \mathbb{R}$ where $X = C^1([0,1])$. If a critical point u belongs to $C^2([0,1])$, then exactly the same argument as before implies that

$$\int_0^1 \{L_u(x,u,Du) - DL_{Du}(x,u,Du)\} \cdot \varphi \, dx = -\left[L_{Du}(x,u,Du) \cdot \varphi\right]_0^1, \qquad (13.72)$$

for all $\varphi \in C^1([0,1])$. The boundary terms arising from the integration by parts need not vanish, since φ is not required to vanish at the endpoints. If, however, we first consider (13.72) for functions φ that do vanish at the endpoints, then we see, as before, that u must satisfy the Euler-Lagrange equation (13.68). It then follows from (13.72) that

$$\left[L_{Du}(x,u,Du) \cdot \varphi\right]_0^1 = 0 \qquad \text{for all } \varphi \in C^1([0,1]).$$

Choosing a smooth function $\varphi : [0,1] \to \mathbb{R}^m$ such that $\varphi_i(0) = 1$, $\varphi_i(1) = 0$, or $\varphi_i(0) = 0$, $\varphi_i(1) = 1$, with all other components zero at both endpoints, we see that the critical point u must satisfy the boundary conditions

$$L_{Du}(x,u,Du) = 0 \qquad \text{when } x = 0, 1.$$

These boundary conditions are called *natural boundary conditions* or *free boundary conditions* for I, since they are the ones picked out automatically by the variational principle.

A function $N(x,y,v)$ is called a *null Lagrangian* if the functional

$$F(u) = \int N(x,u,Du) \, dx$$

has the property that $L_F(u) = 0$ for all smooth functions u. If L and $\widetilde{L}$ are two Lagrangians that differ by a null Lagrangian, then the associated variational principles have the same Euler-Lagrange equations, but they may have different natural boundary conditions. Null Lagrangians are also of interest in other contexts.

Example 13.40 If $u : \mathbb{R} \to \mathbb{R}$, the Lagrangian $N = Du$ is a null Lagrangian, since the Euler operator of the associated functional $F = \int N\, dx$ is

$$L_F(u) = -DN_{Du} = -D1 = 0.$$

The Euler-Lagrange equation of the functional

$$I_\alpha(u) = \int_0^1 \left(\frac{1}{2}(Du)^2 + \alpha Du - fu\right) dx$$

is independent of α:

$$-D^2u - f = 0;$$

but the natural boundary conditions do depend on α:

$$Du + \alpha = 0 \qquad \text{when } x = 0, 1.$$

13.8 Hamilton's equation and classical mechanics

If the Lagrangian $L(x, y, v)$ is a convex function of v, we may use a *Legendre transform* to rewrite the second-order Euler-Lagrange equation (13.68) as a first-order, Hamiltonian system of ODEs. We begin by describing the Legendre transform.

Let $f : \Omega \subset \mathbb{R}^n \to \mathbb{R}$ be a twice continuously differentiable function defined on a convex, open set Ω. We say that f is *uniformly convex* if the second derivative

$$f''(x) : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$$

is positive definite for every $x \in \Omega$, meaning that

$$f''(x)\,(h, h) > 0 \qquad \text{for all } h \in \mathbb{R}^n \setminus \{0\}.$$

This condition is equivalent to the positive definiteness of the *Hessian matrix* of f,

$$\left(\frac{\partial^2 f}{\partial x_i \partial x_j}\right).$$

A uniformly convex function is strictly convex (see Exercise 13.16). We define the *gradient mapping* $\varphi : \Omega \to \Omega^*$ associated with f by

$$\varphi(x) = f'(x), \quad \Omega^* = \{x^* \in \mathbb{R}^n \mid x^* = \varphi(x) \text{ for some } x \in \Omega\}. \tag{13.73}$$

Geometrically, $f'(x) : \mathbb{R}^n \to \mathbb{R}$, so x^* belongs to the dual space of $\mathbb{R}^n$. Here, we will use the Euclidean inner product $\cdot$ to identify $\mathbb{R}^n$ with its dual.

Lemma 13.41 If $f : \Omega \to \mathbb{R}$ is a uniformly convex function on a convex, open subset Ω of $\mathbb{R}^n$ that belongs to $C^2(\Omega)$, then the gradient map $\varphi : \Omega \to \Omega^*$ defined in (13.73) is a C^1-diffeomorphism of Ω onto Ω^*.

Proof. Since $\varphi' = f''$ is nonsingular, the inverse function theorem implies that φ is a locally invertible C^1-map. By the definition of Ω^*, the gradient map φ is onto, so we only have to show that φ is globally one-to-one. Suppose that $x, y \in \Omega$. Then, since Ω is convex, we have

$$\begin{aligned}
[\varphi(x) - \varphi(y)]\,(x-y) &= \left[\int_0^1 \frac{d}{dt}\varphi\left(tx + (1-t)y\right)\, dt\right](x-y) \\
&= \int_0^1 f''\left(tx + (1-t)y\right)(x-y, x-y)\, dt.
\end{aligned}$$

Using the positive definiteness and continuity of f'', we see that

$$[\varphi(x) - \varphi(y)]\,(x-y) > 0 \qquad \text{if } x \neq y.$$

Hence $\varphi(x) \neq \varphi(y)$ if $x \neq y$, so φ is globally invertible. □

It follows from this lemma that $\varphi^{-1} : \Omega^* \to \Omega$ is a C^1-diffeomorphism. The following Legendre transform is therefore well defined.

Definition 13.42 Let $f : \Omega \to \mathbb{R}$ be a uniformly convex function on a convex, open subset Ω of $\mathbb{R}^n$ that belongs to $C^2(\Omega)$. The *Legendre transform* of f is the map $f^* : \Omega^* \to \mathbb{R}$ defined by

$$f^*(x^*) = x \cdot x^* - f(x), \qquad \text{where } x = \varphi^{-1}(x^*).$$

Here, $x \cdot x^*$ denotes the Euclidean inner product of x and x^* in $\mathbb{R}^n$, and $\varphi : \Omega \to \Omega^*$ is the gradient map associated with f defined in (13.73).

We call x, x^* *dual variables* or *conjugate variables*, and f, f^* *dual functions* or *conjugate functions*.

Example 13.43 If $f : \mathbb{R} \to \mathbb{R}$ is uniformly convex, then $x^* = \varphi(x)$ is the slope of the graph of f at x, which is a strictly increasing function of x. The value of f^* at x^* is the difference between the values of the linear function whose graph is a line through the origin of slope x^* and f at the point where the slope of f is equal to x^*.

We now return to the variational principle for the functional I in (13.66). We assume that the Lagrangian $L(x, y, v)$ is a uniformly convex function of v, and we define the *Hamiltonian* $H(x, y, p)$ to be the Legendre transform of $L(x, y, v)$ with respect to v, meaning that

$$H(x, y, p) = p \cdot v - L(x, y, v), \qquad p = L_v(x, y, v). \tag{13.74}$$

It follows from (13.74) that $L_u = -H_u$. The Euler-Lagrange equation (13.68) may therefore be written as a first-order system of ODEs:

$$Du = H_p(x, u, p), \qquad Dp = -H_u(x, u, p).$$

We call such a system a *Hamiltonian system.*

Variational principles provide a general formulation of the laws of classical mechanics, which may be written in either the Lagrangian or Hamiltonian forms. This formulation is essential in understanding the connection between classical and quantum mechanics. As an example, we consider the equations for a particle of mass m moving in $\mathbb{R}^n$, acted on by a conservative force field $F = -\nabla V$, where $V : \mathbb{R}^n \to \mathbb{R}$ is a smooth potential energy function. We change notation, and write the independent variable as t, instead of x, and the dependent variable as q, instead of u. We use a dot to denote the derivative with respect to t. A particle path for times $0 \le t \le T$ is given by a function $q : [0, T] \to \mathbb{R}^n$. We define the *action* $S(q)$ of a path q to be the time-integral of the difference between the particle's kinetic and potential energies along the path:

$$S(q) = \int_0^T \left(\frac{1}{2} m\dot{q}^2 - V(q) \right) dt.$$

Here, $\dot{q}^2 = \dot{q} \cdot \dot{q}$. The corresponding Lagrangian is

$$L(q, \dot{q}) = \frac{1}{2} m\dot{q}^2 - V(q).$$

Thus, the action $S : C^1([0, T]) \to \mathbb{R}$ is a functional defined on the space of possible particle paths. Hamilton's *principle of stationary action* states that the actual path traveled by a particle with given positions at $t = 0$ and $t = T$ is a stationary point of the action. The path therefore satisfies the Euler-Lagrange equation associated with S, which is

$$m\ddot{q} = -\nabla V. \tag{13.75}$$

This equation is Newton's second law.

The Lagrangian L is independent of t, and Proposition 13.37 implies that

$$\frac{1}{2} m\dot{q}^2 + V(q) = \text{constant} \tag{13.76}$$

on a solution, which expresses the conservation of energy. The correspondence between the invariance of the Lagrangian under time translations and the conservation of energy is a very general one.

Conservation of energy may be verified directly from (13.75). Taking the scalar product of (13.75) with $\dot{q}$, we obtain that

$$m\dot{q} \cdot \ddot{q} + \nabla V(q) \cdot \dot{q} = 0.$$

Using the chain rule, we find that

$$\frac{d}{dt}\left[\frac{1}{2}m\dot{q}^2 + V(q)\right] = 0,$$

which implies (13.76).

The reason why classical mechanics is given by a principle of stationary action is not at all clear at the classical level, but the principle may be derived from quantum mechanics. For example, in Feynman's path-integral formulation of quantum mechanics, the action is the phase of the quantum-mechanical amplitude of a particle path, and the classical paths are paths of stationary phase.

The Legendre transform (13.74) implies that the momentum $p = mv$ is the dual variable to the velocity $v = \dot{q}$, and the Hamiltonian H is the total energy of the particle:

$$H(q,p) = \frac{1}{2m}p^2 + V(q).$$

The Hamiltonian form of the Euler-Lagrange equation is

$$\dot{q} = \frac{1}{m}p, \qquad \dot{p} = -\nabla_q V.$$

Hamilton's equation may itself be given a variational formulation, as the Euler-Lagrange equation of the functional

$$\widetilde{S}(q,p) = \int_0^T \{p \cdot \dot{q} - H(p,q)\}\ dt.$$

The Lagrangian function is not a uniformly convex function of the derivatives, since it is a linear function of $\dot{q}$ and is independent of $\dot{p}$. This explains why the associated Euler-Lagrange equation is first-order, rather than second-order.

13.9 Multiple integrals in the calculus of variations

The Euler-Lagrange equation for a functional of functions of several variables is a PDE, rather than an ODE. Suppose that

$$I(u) = \int_\Omega L(x, u, Du)\ dx, \tag{13.77}$$

where Ω is a smooth bounded domain in $\mathbb{R}^n$, $u : \Omega \subset \mathbb{R}^n \to \mathbb{R}^m$, and

$$Du = (D_1 u, D_2 u, \ldots, D_n u)$$

is the derivative of u, where D_i is the partial derivative with respect to x_i keeping x_j fixed for $j \neq i$. A similar calculation to the one in Section 13.7 shows that the

Euler-Lagrange equation for I is

$$-\sum_{i=1}^{n} D_i L_{D_i u} + L_u = 0.$$

Example 13.44 The Euler-Lagrange equation associated with the functional

$$I(u) = \int_\Omega \left\{ \frac{1}{2} u_t^2 - \frac{1}{2}|Du|^2 - (1 - \cos u) \right\} dxdt$$

is the *sine-Gordon equation*,

$$-u_{tt} + \Delta u - \sin u = 0.$$

We will consider the variational principle for Laplace's equation. Similar ideas apply to variational principles of the form (13.77) in which L is a convex function of Du. We define a quadratic functional $I : H_0^1(\Omega) \to \mathbb{R}$ by

$$I(u) = \frac{1}{2} \int_\Omega |Du|^2 \, dx - f(u),$$

where $f : H_0^1(\Omega) \to \mathbb{R}$ is a bounded linear functional on $H_0^1(\Omega)$, meaning that $f \in H^{-1}(\Omega)$. From the Poincaré inequality in Theorem 12.77, we may use

$$\langle u, v \rangle = \int_\Omega Du \cdot Dv \, dx$$

as the H_0^1-inner product. Then

$$I(u) = \frac{1}{2}\|u\|^2 - f(u).$$

It follows from Theorem 8.50 (see Exercise 8.20) that I has a unique minimizer on $H_0^1(\Omega)$. This minimizer is a critical point of I, so that $I'(u)(\varphi) = 0$ for all $\varphi \in H_0^1(\Omega)$, meaning that

$$\int_\Omega Du \cdot D\varphi \, dx + f(\varphi) = 0 \qquad \text{for all } \varphi \in H_0^1(\Omega).$$

From Definition 12.79, the minimizer u is a weak solution of Laplace's equation,

$$-\Delta u = f,$$

providing another proof of the existence of weak solutions.

In many problems, we are interested in minimizing a functional $I : X \to \mathbb{R}$ subject to a nonlinear constraint $J(x) = 0$, where $J : X \to \mathbb{R}$. A constrained minimization problem may often be replaced by an unconstrained problem by the introduction of a *Lagrange multiplier* λ. We define $F : X \times \mathbb{R} \to \mathbb{R}$ by

$$F(x, \lambda) = I(x) - \lambda J(x).$$

If $(\overline{x}, \overline{\lambda})$ is a critical point of F, then taking the partial derivatives of F with respect to x and λ, we see that

$$I'(\overline{x}) - \overline{\lambda} J'(\overline{x}) = 0, \qquad J(\overline{x}) = 0.$$

It follows that $\overline{x}$ is a critical point of I on the constraint manifold $J(x) = 0$ (see Giaquinta and Hildebrandt [14] for a detailed discussion).

Example 13.45 Consider the problem of minimizing $I : H_0^1(\Omega) \to \mathbb{R}$ given by

$$I(u) = \frac{1}{2} \int_\Omega |Du|^2 \, dx$$

subject to the constraint

$$\frac{1}{2} \int_\Omega u^2 \, dx = 1.$$

A constraint on the value of an integral of an admissible function is called an *isoperimetric constraint.* Introducing a Lagrange multiplier $\lambda \in \mathbb{R}$, we consider critical points of the functional

$$F(u, \lambda) = \frac{1}{2} \int_\Omega |Du|^2 \, dx - \lambda \left(\frac{1}{2} \int_\Omega u^2 \, dx - 1 \right).$$

Taking the derivative of F with respect to u, we find that a smooth critical point satisfies

$$-\Delta u = \lambda u.$$

Thus, u is an eigenfunction of the Laplacian, and the Lagrange multiplier λ is an eigenvalue.

Example 13.46 Consider a function

$$u = (u_1, u_2, \ldots, u_{m+1}) : \Omega \subset \mathbb{R}^n \to \mathbb{S}^m \subset \mathbb{R}^{m+1}$$

from a subset Ω of n-dimensional Euclidean space into an m-dimensional sphere. We use the notation

$$|u|^2 = \sum_{j=1}^{m+1} u_j^2, \quad |Du|^2 = \sum_{i=1}^{n} \sum_{j=1}^{m+1} \left(\frac{\partial u_j}{\partial x_i} \right)^2.$$

A function u that minimizes the functional

$$I(u) = \frac{1}{2} \int_\Omega |Du|^2 \, dx, \tag{13.78}$$

subject to the constraint that $u(x) \in \mathbb{S}^m$, meaning that

$$|u(x)|^2 = 1, \tag{13.79}$$

is called a *harmonic map* from $\mathbb{R}^n$ into $\mathbb{S}^m$. A constraint on the pointwise values of an admissible function and its derivative is called a *holonomic constraint.*

In this case, the Lagrange multiplier is a function $\lambda : \Omega \subset \mathbb{R}^n \to \mathbb{R}$. We consider critical points of the functional

$$F(u, \lambda) = \frac{1}{2} \int_\Omega |Du|^2 \, dx - \int_\Omega \lambda \, |u|^2 \, dx.$$

The Euler-Lagrange equation is

$$-\Delta u = \lambda u. \tag{13.80}$$

Differentiating the constraint $|u|^2 = 1$, we find that $u \cdot Du = 0$. Hence, taking the scalar product of (13.80) with u, and rearranging the result, we find that

$$\lambda = -u \cdot \Delta u = -D \cdot (u \cdot Du) + |Du|^2 = |Du|^2 .$$

Thus the Euler-Lagrange equation for harmonic maps from Euclidean space into a sphere is the following nonlinear elliptic system of PDEs:

$$-\Delta u = |Du|^2 \, u.$$

Such harmonic maps provide a simple model for the steady state configuration of systems with orientational order, such as liquid crystal director fields. An interesting feature of the solutions is the possible presence of topological defects in the field u of unit vectors.

13.10 References

Newton's method is discussed in Kantorovich and Akilov [27]. For a discussion of evolution equations and Liapunov functions, see Walker [55]. For more on symmetries and variational principles, see Olver [42]. For classical mechanics, see Arnold [2] and Gallavotti [13]. The Legendre transformation in convex analysis is described in Rockafellar [46]. The classical calculus of variations is discussed in much more depth in Giaquinta and Hildebrandt [14]. An indication of the extent of the subject is that, despite the fact that these two volumes have a total length of over 1,000 pages, the authors state that their account is an introduction to the subject, and is not encyclopaedic!

13.11 Exercises

Exercise 13.1 Prove that the derivative of a differentiable map is unique.

Exercise 13.2 Prove that if $A : X \to Y$ is a bounded linear map, then A is differentiable in X, with constant Fréchet derivative equal to A itself.

Exercise 13.3 Suppose that $f, g : X \to Y$ are two differentiable maps between Banach spaces X, Y. Show that $f + g$ is differentiable, and $(f+g)' = f' + g'$.

Exercise 13.4 Prove that a Fréchet differentiable map is Gâteaux differentiable.

Exercise 13.5 Define the function $f : \mathbb{R}^2 \to \mathbb{R}$ by

$$f(x,y) = \frac{xy^2}{x^2 + y^4} \qquad \text{for } (x,y) \neq (0,0),$$

and $f(0,0) = 0$. Show that the directional derivatives of f at the origin exist in every direction, but f is not continuous or Fréchet differentiable at the origin.

Exercise 13.6 Let $k : \mathbb{R} \times [0,1] \to \mathbb{R}$ be a continuous function such that for each $t \in [0,1]$, the function $k(\cdot, t)$ is in $C^1(\mathbb{R})$. Define a functional $f : C([0,1]) \to \mathbb{R}$ by

$$f(u) = \int_0^1 k(u(t), t)\, dt.$$

Determine the differentiability properties of f.

Exercise 13.7 Let $f : \mathbb{R} \to \mathbb{R}$ be an increasing function such that

$$f(x) = \begin{cases} 1/n & \text{if } 1/n - 1/(4n^2) \leq x \leq 1/n + 1/(4n^2), \\ x + O(x^2) & \text{as } x \to 0, \end{cases}$$

where $n \in \mathbb{N}$. Show that $f'(0) \neq 0$, but f is not locally invertible at 0. Why doesn't this example contradict the inverse function theorem?

Exercise 13.8 Consider the BVP

$$\begin{aligned} &u'' = \mu^2 \sin v, \quad v'' = \mu^2 u \cos v, \\ &u'(0) = u(1) = 0, \quad v(0) = v'(1) = 0. \end{aligned}$$

Show that there are no solutions that bifurcate off the trivial solution $u = v = 0$ unless $\mu \in \mathbb{R}$ is a solution of

$$1 + \cos\mu \cosh\mu = 0.$$

Exercise 13.9 Suppose that $\mathcal{H}$ is a Hilbert space and $F : \mathcal{H} \times \mathbb{R} \to \mathcal{H}$ is a continuously differentiable operator such that $F(0, \mu) = 0$ for all $\mu \in \mathbb{R}$, so $u = 0$ is a solution branch of the equation $F(u, \mu) = 0$. Suppose that $D_u F(0,0) : \mathcal{H} \to \mathcal{H}$ is a singular Fredholm operator (see Definition 8.22), assumed self-adjoint for simplicity. Then $\mathcal{H} = \mathcal{M} \oplus \mathcal{N}$ where $\mathcal{M} = \operatorname{ran} D_u F(0,0)$ and $\mathcal{N} = \ker D_u F(0,0)$. Let P denote the orthogonal projection of $\mathcal{H}$ onto $\mathcal{M}$ and Q the orthogonal projection onto $\mathcal{N}$. Prove that there are open neighborhoods $U \subset \mathcal{H}$, $V \subset \mathcal{N}$, and $I \subset \mathbb{R}$ of 0 and a continuously differentiable function $\varphi : V \times I \to \mathcal{M}$ such that $(u, \mu) \in U \times I$

is a solution of $F(u, \mu) = 0$ if and only if $u = \varphi(v, \mu) + v$ where $v \in V$ is a solution of $G(v, \mu) = 0$ with $G : V \times \mathbb{R} \to \mathcal{N}$ defined by

$$G(v, \mu) = QF\left(\varphi(v, \mu) + v, \mu\right).$$

The finite-dimensional system of equations $G(v, \mu) = 0$ for $v \in \ker D_u F(0, 0)$ is called the *bifurcation equation* associated with the original, possibly infinite-dimensional, system of equations $F(u, \mu) = 0$. This procedure is called *Liapunov-Schmidt reduction*. With appropriate modifications, a similar procedure applies to a continuously differentiable map $F : X \times \mathbb{R} \to Y$ between Banach spaces X, Y.

Exercise 13.10 Suppose that $f : \mathcal{H} \to \mathbb{R}$ is a differentiable functional on a Hilbert space $\mathcal{H}$. Show that there is a function $\nabla f : \mathcal{H} \to \mathcal{H}$, called the *gradient* of f, such that

$$f'(x)h = \langle \nabla f(x), h \rangle.$$

Compute the gradient of the function $f(x) = \|x\|^2$.

Exercise 13.11 Prove that the closure $R([a, b])$ of the space $S([a, b])$ of step functions in the space $B([a, b])$ of bounded functions $f : [a, b] \to X$ on a compact interval $[a, b]$ into a Banach space X, equipped with the sup-norm, includes all continuous functions. Show that the characteristic function of the rationals in $[a, b]$ does not belong to $R([a, b])$.

Exercise 13.12 Let $A : X \to X$ be a bounded linear operator on a Banach space X, and $f : \mathbb{R} \to X$ a continuous, vector-valued function. Show that the solution of the nonhomogeneous linear evolution equation

$$x_t = Ax + f, \qquad x(0) = x_0$$

is given by

$$x(t) = T(t)x_0 + \int_0^t T(t - s) f(s)\, ds,$$

where $T(t) = e^{tA}$ is the solution operator of the homogeneous equation. This result is called *Duhamel's formula*.

Exercise 13.13 Suppose that $T > 0$ and $T \neq 2n\pi$ for any $n \in \mathbb{N}$. Write out the iteration scheme of the modified Newton method for finding T-periodic solutions of the forced pendulum,

$$\ddot{u} + \sin u = h,$$

where h is a given T-periodic function. Assume that the initial point for the modified Newton's method is $u_0 = 0$. Find an estimate on $\|h\|_\infty$ that is sufficient to ensure convergence of the modified Newton iterates, and estimate the norm $\|u\|_{C^2}$ of the corresponding T-periodic solution.

Exercise 13.14 Derive the Euler-Lagrange equation satisfied by C^4-critical points of a functional $I : C^2([0,1]) \to \mathbb{R}$ defined by

$$I(u) = \int_0^1 L\left(x, u, Du, D^2u\right)\, dx,$$

where the Lagrangian $L : \mathbb{R} \times \mathbb{R}^m \times \mathbb{R}^m \times \mathbb{R}^m \to \mathbb{R}$ is a twice continuously differentiable function.

Exercise 13.15 The area of a surface obtained by revolving the graph $y = u(x)$ about the x-axis, where $0 \leq x \leq 1$, is given by

$$I(u) = 2\pi \int_0^1 u(x)\sqrt{1 + [Du(x)]^2}\, dx.$$

Write out the Euler-Lagrange equation, and the first integral that follows from the independence of the Lagrangian of x. Show that the curve with smallest surface area of revolution connecting given endpoint $u(0) = a$, $u(1) = b$ is a catenary.

Exercise 13.16 Prove that a uniformly convex function $f : \Omega \subset \mathbb{R}^n \to \mathbb{R}$ on an open, convex set Ω is strictly convex.

Exercise 13.17 Compute the Legendre transform of:

(a) $f(x) = e^x - 1$, where $f : \mathbb{R} \to \mathbb{R}$;
(b) $f(x) = x^T Ax/2$ where A is an $n \times n$ positive definite matrix, and $f : \mathbb{R}^n \to \mathbb{R}$.

Exercise 13.18 Compute the Euler-Lagrange equation of the quadratic functional

$$I(u) = \int_\Omega \left\{ \sum_{i,j=1}^n \frac{1}{2} a_{ij}(x) \frac{\partial u}{\partial x_i} \frac{\partial u}{\partial x_j} - f(x)u \right\} dx,$$

where $a_{ij} = a_{ji}$ without loss of generality. Show that the resulting linear PDE is formally self-adjoint.

Exercise 13.19 Let Ω be a regular, bounded open subset of $\mathbb{R}^n$. Show that

$$\lambda = \inf_{\substack{u \in H_0^1(\Omega) \\ u \neq 0}} \left\{ \frac{\int_\Omega |\nabla u|^2\, dx}{\int_\Omega |u|^2 dx} \right\}$$

is the smallest eigenvalue of the Dirichlet problem for the Laplacian on Ω, and that the infimum is attained at the corresponding eigenfunctions. Use the trial function $u(x,y) = xy(1 - x - y)$ to obtain an upper bound on the lowest eigenvalue of the Dirichlet Laplacian on the triangle $\Omega = \left\{(x,y) \in \mathbb{R}^2 \mid 0 < x < 1,\, 0 < y < 1 - x\right\}$.