Module MA2321: Analysis in Several Real Variables
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Part IV (Sections 10 and 11)

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Contents

10 Second Order Partial Derivatives and the Hessian Matrix

10.1 Second Order Partial Derivatives

Let X be an open subset of $\mathbb{R}^n$ and let $f\colon X \to \mathbb{R}$ be a real-valued function on X. We consider the second order partial derivatives of the function f defined by

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

We shall show that if the partial derivatives

$$\frac{\partial f}{\partial x_i}, \quad \frac{\partial f}{\partial x_j}, \quad \frac{\partial^2 f}{\partial x_i \partial x_j} \text{ and } \frac{\partial^2 f}{\partial x_j \partial x_i}$$

all exist and are continuous then

$$\frac{\partial^2 f}{\partial x_i \partial x_j} = \frac{\partial^2 f}{\partial x_j \partial x_i}.$$

First though we give a counterexample which demonstrates that there exist functions f for which

$$\frac{\partial^2 f}{\partial x_i \partial x_j} \neq \frac{\partial^2 f}{\partial x_j \partial x_i}.$$

Example Let $f\colon \mathbb{R}^2 \to \mathbb{R}$ be the function defined by

$$f(x,y) = \begin{cases} \dfrac{xy(x^2 - y^2)}{x^2 + y^2} & \text{if } (x,y) \neq (0,0); \\ 0 & \text{if } (x,y) = (0,0). \end{cases}$$

For convenience of notation, let us write

$$\begin{aligned} f_x(x,y) &= \frac{\partial f(x,y)}{\partial x}, \\ f_y(x,y) &= \frac{\partial f(x,y)}{\partial y}, \\ f_{xy}(x,y) &= \frac{\partial^2 f(x,y)}{\partial x \partial y}, \\ f_{yx}(x,y) &= \frac{\partial^2 f(x,y)}{\partial y \partial x}. \end{aligned}$$

If $(x, y) \neq (0, 0)$ then

$$\begin{aligned} f_x &= \frac{(3x^2y - y^3)(x^2 + y^2) - 2x^2y(x^2 - y^2)}{(x^2 + y^2)^2} \\ &= \frac{3x^4y + 3x^2y^3 - x^2y^3 - y^5 - 2x^4y + 2x^2y^3}{(x^2 + y^2)^2} \\ &= \frac{x^4y + 4x^2y^3 - y^5}{(x^2 + y^2)^2}. \end{aligned}$$

Similarly

$$f_y = \frac{-xy^4 - 4x^3y^2 + x^5}{(x^2 + y^2)^2}.$$

(This can be deduced from the formula for f_x on noticing that $f(x, y)$ changes sign on interchanging the variables x and y.)

Differentiating again, when $(x, y) \neq (0, 0)$, we find that

$$\begin{aligned} f_{xy}(x, y) &= \frac{\partial f_y}{\partial x} \\ &= \frac{(-y^4 - 12x^2y^2 + 5x^4)(x^2 + y^2)}{(x^2 + y^2)^3} \\ &\qquad + \frac{-4x(-xy^4 - 4x^3y^2 + x^5)}{(x^2 + y^2)^3} \\ &= \frac{-x^2y^4 - 12x^4y^2 + 5x^6 - y^6 - 12x^2y^4 + 5x^4y^2}{(x^2 + y^2)^3} \\ &\qquad + \frac{4x^2y^4 + 16x^4y^2 - 4x^6}{(x^2 + y^2)^3} \\ &= \frac{x^6 + 9x^4y^2 - 9x^2y^4 - y^6}{(x^2 + y^2)^3}. \end{aligned}$$

Now the expression just obtained for f_{xy} when $(x, y) \neq (0, 0)$ changes sign when the variables x and y are interchanged. The same is true of the expression defining $f(x, y)$. It follows that f_{yx}. We conclude therefore that if $(x, y) \neq (0, 0)$ then

$$f_{xy} = f_{yx} = \frac{x^6 + 9x^4y^2 - 9x^2y^4 - y^6}{(x^2 + y^2)^3}.$$

Now if $(x, y) \neq (0, 0)$ and if $r = \sqrt{x^2 + y^2}$ then

$$|f_x(x, y)| = \frac{|x^4y + 4x^2y^3 - y^5|}{r^4} \leq \frac{6r^5}{r^4} = 6r.$$

It follows that

$$\lim_{(x,y)\to(0,0)} f_x(x,y) = 0.$$

Similarly

$$\lim_{(x,y)\to(0,0)} f_y(x,y) = 0.$$

However

$$\lim_{(x,y)\to(0,0)} f_{xy}(x,y)$$

does not exist. Indeed

$$\begin{aligned}
\lim_{x\to 0} f_{xy}(x,0) = \lim_{x\to 0} f_{yx}(x,0) &= \lim_{x\to 0} \frac{x^6}{x^6} = 1, \\
\lim_{y\to 0} f_{xy}(0,y) = \lim_{y\to 0} f_{yx}(0,y) &= \lim_{y\to 0} \frac{-y^6}{y^6} = -1.
\end{aligned}$$

Next we show that f_x, f_y, f_{xy} and f_{yx} all exist at $(0,0)$, and thus exist everywhere on $\mathbb{R}^2$. Now $f(x,0) = 0$ for all x, hence $f_x(0,0) = 0$. Also $f(0,y) = 0$ for all y, hence $f_y(0,0) = 0$. Thus

$$f_y(x,0) = x, \qquad f_x(0,y) = -y$$

for all $x, y \in \mathbb{R}$. We conclude that

$$\begin{aligned}
f_{xy}(0,0) &= \left.\frac{d(f_y(x,0))}{dx}\right|_{x=0} = 1, \\
f_{yx}(0,0) &= \left.\frac{d(f_x(0,y))}{dy}\right|_{y=0} = -1,
\end{aligned}$$

Thus

$$\frac{\partial^2 f}{\partial x \partial y} \neq \frac{\partial^2 f}{\partial y \partial x}$$

at $(0,0)$.

Observe that in this example the functions f_{xy} and f_{yx} are continuous throughout $\mathbb{R}^2 \setminus \{(0,0\}$ and are equal to one another there. Although the functions f_{xy} and f_{yx} are well-defined at $(0,0)$, they are not continuous at $(0,0)$ and $f_{xy}(0,0) \neq f_{yx}(0,0)$.

Theorem 10.1 *Let X be an open set in $\mathbb{R}^2$ and let $f\colon X \to \mathbb{R}$ be a real-valued function on X. Suppose that the partial derivatives*

$$\frac{\partial f}{\partial x}, \quad \frac{\partial f}{\partial y} \quad \textit{and} \quad \frac{\partial^2 f}{\partial x \partial y}$$

exist and are continuous throughout X. Then the partial derivative

$$\frac{\partial^2 f}{\partial y \partial x}$$

exists and is continuous on X, and

$$\frac{\partial^2 f}{\partial x \partial y} = \frac{\partial^2 f}{\partial y \partial x}.$$

Proof Let

$$f_x(x,y) = \frac{\partial f}{\partial x}, \quad f_y(x,y) = \frac{\partial f}{\partial y}, \quad f_{xy} = \frac{\partial^2 f}{\partial x \partial y} \text{ and } f_{yx} = \frac{\partial^2 f}{\partial y \partial x}$$

and let (a,b) be a point of X. The set X is open in $\mathbb{R}^n$ and therefore there exists some positive real number L such that $(a+h, b+k) \in X$ for all $(h,k) \in \mathbb{R}^2$ satisfying $|h| < L$ and $|k| < L$. Let

$$S(h,k) = f(a+h, b+k) - f(a+h, b) - f(a, b+k) + f(a,b)$$

for all real numbers h and k satisfying $|h| < L$ and $|k| < L$. We use the Mean Value Theorem (Theorem 2.2) to prove the existence of real numbers u and v, where u lies between a and $a+h$ and v lies between b and $b+k$, for which

$$S(h,k) = hk \left. \frac{\partial^2 f}{\partial x \partial y} \right|_{(x,y)=(u,v)} = hk f_{xy}(u,v).$$

Let h be fixed, where $|h| < L$, and let $q\colon (b-L, b+L) \to \mathbb{R}$ be defined so that $q(t) = f(a+h, t) - f(a,t)$ for all real numbers t satisfying $b - L < t < b + L$. Then $S(h,k) = q(b+k) - q(b)$. But it follows from the Mean Value Theorem (Theorem 2.2) that there exists some real number v lying between b and $b+k$ for which $q(b+k) - q(b) = kq'(v)$. But $q'(v) = f_y(a+h, v) - f_y(a,v)$. It follows that

$$S(h,k) = k(f_y(a+h, v) - f_y(a,v)).$$

The Mean Value Theorem can now be applied to the function sending real numbers s in the interval $(a-L, a+L)$ to $f_y(s,v)$ to deduce the existence of a real number u lying between a and $a+h$ for which

$$S(h,k) = hk f_{xy}(u,v).$$

Now let some positive real number ε be given. The function f_{xy} is continuous. Therefore there exists some real number δ satisfying $0 < \delta < L$ such that $|f_{xy}(a+h,b+k)-f_{xy}(a,b)| \leq \varepsilon$ whenever $|h| < \delta$ and $|k| < \delta$. It follows that

$$\left| \frac{S(h,k)}{hk} - f_{xy}(a,b) \right| \leq \varepsilon$$

for all real numbers h and k satisfying $0 < |h| < \delta$ and $0 < |k| < \delta$. Now

$$\begin{aligned} \lim_{h \to 0} \frac{S(h,k)}{hk} &= \frac{1}{k} \lim_{h \to 0} \frac{f(a+h,b+k) - f(a,b+k)}{h} \\ &\qquad - \frac{1}{k} \lim_{h \to 0} \frac{f(a+h,b) - f(a,b)}{h} \\ &= \frac{f_x(a,b+k) - f_x(a,b)}{k}. \end{aligned}$$

It follows that

$$\left| \frac{f_x(a,b+k) - f_x(a,b)}{k} - f_{xy}(a,b) \right| \leq \varepsilon$$

whenever $0 < |k| < \delta$. Thus the difference quotient $\dfrac{f_x(a,b+k) - f_x(a,b)}{k}$ tends to $f_{xy}(a,b)$ as k tends to zero, and therefore the second order partial derivative f_{yx} exists at the point (a,b) and

$$f_{yx}(a,b) = \lim_{k \to 0} \frac{f_x(a,b+k) - f_x(a,b)}{k} = f_{xy}(a,b),$$

as required. ∎

Corollary 10.2 *Let X be an open set in $\mathbb{R}^n$ and let $f\colon X \to \mathbb{R}$ be a real-valued function on X. Suppose that the partial derivatives*

$$\frac{\partial f}{\partial x_i} \text{ and } \frac{\partial^2 f}{\partial x_i \partial x_j}$$

exist and are continuous on X for all integers i and j between 1 and n. Then

$$\frac{\partial^2 f}{\partial x_i \partial x_j} = \frac{\partial^2 f}{\partial x_j \partial x_i}$$

for all integers i and j between 1 and n.

10.2 Maxima and Minima for Functions of Several Real Variables

Let $f\colon X \to \mathbb{R}$ be a real-valued function defined over some open subset X of $\mathbb{R}^n$ whose first and second order partial derivatives exist and are continuous throughout X. Suppose that f has a local minimum at some point $\mathbf{p}$ of X, where $\mathbf{p} = (p_1, p_2, \ldots, p_n)$. Now for each integer i between 1 and n the map

$$t \mapsto f(p_1, \ldots, p_{i-1}, t, p_{i+1}, \ldots, p_n)$$

has a local minimum at $t = p_i$, hence the derivative of this map vanishes there. Thus if f has a local minimum at $\mathbf{p}$ then

$$\left.\frac{\partial f}{\partial x_i}\right|_{\mathbf{x}=\mathbf{p}} = 0.$$

In many situations the values of the second order partial derivatives of a twice-differentiable function of several real variables at a stationary point determines the qualitative behaviour of the function around that stationary point, in particular ensuring, in some situations, that the stationary point is a local minimum or a local maximum.

Lemma 10.3 *Let f be a continuous real-valued function defined throughout an open ball in $\mathbb{R}^n$ of radius R about some point $\mathbf{p}$. Suppose that the partial derivatives of f of orders one and two exist and are continuous throughout this open ball. Then there exists some real number θ satisfying $0 < \theta < 1$ for which*

$$f(\mathbf{p} + \mathbf{h}) = f(\mathbf{p}) + \sum_{k=1}^{n} h_k \left.\frac{\partial f}{\partial x_k}\right|_{\mathbf{p}} + \tfrac{1}{2} \sum_{j,k=1}^{n} h_j h_k \left.\frac{\partial^2 f}{\partial x_j\, \partial x_k}\right|_{\mathbf{p}+\theta\mathbf{h}}$$

for all $\mathbf{h} \in \mathbb{R}^n$ satisfying $|\mathbf{h}| < \delta$.

Proof Let $\mathbf{h}$ satisfy $|\mathbf{h}| < R$, and let

$$q(t) = f(\mathbf{p} + t\mathbf{h})$$

for all $t \in [0, 1]$. It follows from the Chain Rule for functions of several variables (Theorem 8.12) that

$$q'(t) = \sum_{j=1}^{n} h_k (\partial_k f)(\mathbf{p} + t\mathbf{h})$$

and

$$q''(t) = \sum_{j,k=1}^{n} h_j h_k (\partial_j \partial_k f)(\mathbf{p} + t\mathbf{h}),$$

where

$$(\partial_j f)(x_1, x_2, \ldots, x_n) = \frac{\partial f(x_1, x_2, \ldots, x_n)}{\partial x_j}$$

and

$$(\partial_j \partial_k f)(x_1, x_2, \ldots, x_n) = \frac{\partial^2 f(x_1, x_2, \ldots, x_n)}{\partial x_j \, \partial x_k}.$$

Now

$$q(1) = q(0) + q'(0) + \tfrac{1}{2} q''(\theta)$$

for some real number θ satisfying $0 < \theta < 1$. (see Proposition 2.3). It follows that

$$\begin{aligned} f(\mathbf{p} + \mathbf{h}) &= f(\mathbf{p}) + \sum_{k=1}^{n} h_k (\partial_k f)(\mathbf{p}) + \tfrac{1}{2} \sum_{j,k=1}^{n} h_j h_k (\partial_j \partial_k f)(\mathbf{p} + \theta \mathbf{h}) \\ &= f(\mathbf{p}) + \sum_{k=1}^{n} h_k \left. \frac{\partial f}{\partial x_k} \right|_{\mathbf{p}} + \tfrac{1}{2} \sum_{j,k=1}^{n} h_j h_k \left. \frac{\partial^2 f}{\partial x_j \, \partial x_k} \right|_{\mathbf{p} + \theta \mathbf{h}}, \end{aligned}$$

as required. ∎

Let f be a real-valued function of several variables whose first second order partial derivatives exist and are continuous throughout some open neighbourhood of a given point $\mathbf{p}$, and let $R > 0$ be chosen such that the function f is defined throughout the open ball of radius R about the point $\mathbf{p}$. It follows from Lemma 10.3 that if

$$\left. \frac{\partial f}{\partial x_j} \right|_{\mathbf{p}} = 0$$

for $j = 1, 2, \ldots, n$, and if $|\mathbf{h}| < R$ then

$$f(\mathbf{p} + \mathbf{h}) = f(\mathbf{p}) + \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} h_i h_j \left. \frac{\partial^2 f}{\partial x_i \partial x_j} \right|_{\mathbf{x} = \mathbf{p} + \theta \mathbf{h}}$$

for some θ satisfying $0 < \theta < 1$.

Let us denote by $(H_{i,j}(\mathbf{p}))$ the *Hessian matrix* at the point $\mathbf{p}$, defined by

$$H_{i,j}(\mathbf{p}) = \left. \frac{\partial^2 f}{\partial x_i \partial x_j} \right|_{\mathbf{x} = \mathbf{p}}.$$

If the partial derivatives of f of second order exist and are continuous then $H_{i,j}(\mathbf{p}) = H_{j,i}(\mathbf{p})$ for all i and j, by Corollary 10.2. Thus the Hessian matrix is symmetric.

We now recall some facts concerning symmetric matrices.

Let $(c_{i,j})$ be a symmetric $n \times n$ matrix.

The matrix $(c_{i,j})$ is said to be *positive semi-definite* if $\displaystyle\sum_{i=1}^{n}\sum_{j=1}^{n} c_{i,j}h_ih_j \geq 0$ for all $(h_1, h_2, \ldots, h_n) \in \mathbb{R}^n$.

The matrix $(c_{i,j})$ is said to be *positive definite* if $\displaystyle\sum_{i=1}^{n}\sum_{j=1}^{n} c_{i,j}h_ih_j > 0$ for all non-zero $(h_1, h_2, \ldots, h_n) \in \mathbb{R}^n$.

The matrix $(c_{i,j})$ is said to be *negative semi-definite* if $\displaystyle\sum_{i=1}^{n}\sum_{j=1}^{n} c_{i,j}h_ih_j \leq 0$ for all $(h_1, h_2, \ldots, h_n) \in \mathbb{R}^n$.

The matrix $(c_{i,j})$ is said to be *negative definite* if $\displaystyle\sum_{i=1}^{n}\sum_{j=1}^{n} c_{i,j}h_ih_j < 0$ for all non-zero $(h_1, h_2, \ldots, h_n) \in \mathbb{R}^n$.

The matrix $(c_{i,j})$ is said to be *indefinite* if it is neither positive semi-definite nor negative semi-definite.

Lemma 10.4 *Let $(c_{i,j})$ be a positive definite symmetric $n \times n$ matrix. Then there exists some $\varepsilon > 0$ with the following property: if all of the components of a symmetric $n \times n$ matrix $(b_{i,j})$ satisfy the inequality $|b_{i,j} - c_{i,j}| < \varepsilon$ then the matrix $(b_{i,j})$ is positive definite.*

Proof Let S^{n-1} be the unit $n-1$-sphere in $\mathbb{R}^n$ defined by

$$S^{n-1} = \{(h_1, h_2, \ldots, h_n) \in \mathbb{R}^n : h_1^2 + h_2^2 + \cdots + h_n^2 = 1\}.$$

Observe that a symmetric $n \times n$ matrix $(b_{i,j})$ is positive definite if and only if

$$\sum_{i=1}^{n}\sum_{j=1}^{n} b_{i,j}h_ih_j > 0$$

for all $(h_1, h_2, \ldots, h_n) \in S^{n-1}$. Now the matrix $(c_{i,j})$ is positive definite, by assumption. Therefore

$$\sum_{i=1}^{n}\sum_{j=1}^{n} c_{i,j}h_ih_j > 0$$

for all $(h_1, h_2, \ldots, h_n) \in S^{n-1}$.

But S^{n-1} is a closed bounded set in $\mathbb{R}^n$, it therefore follows from Theorem 5.5 that there exists some $(k_1, k_2, \ldots, k_n) \in S^{n-1}$ with the property that

$$\sum_{i=1}^{n}\sum_{j=1}^{n} c_{i,j}h_ih_j \geq \sum_{i=1}^{n}\sum_{j=1}^{n} c_{i,j}k_ik_j$$

for all $(h_1, h_2, \ldots, h_n) \in S^{n-1}$. Let

$$A = \sum_{i=1}^{n} \sum_{j=1}^{n} c_{i,j} k_i k_j.$$

Then $A > 0$ and

$$\sum_{i=1}^{n} \sum_{j=1}^{n} c_{i,j} h_i h_j \geq A$$

for all $(h_1, h_2, \ldots, h_n) \in S^{n-1}$. Set $\varepsilon = A/n^2$.

If $(b_{i,j})$ is a symmetric $n \times n$ matrix all of whose components satisfy $|b_{i,j} - c_{i,j}| < \varepsilon$ then

$$\left| \sum_{i=1}^{n} \sum_{j=1}^{n} (b_{i,j} - c_{i,j}) h_i h_j \right| < \varepsilon n^2 = A,$$

for all $(h_1, h_2, \ldots, h_n) \in S^{n-1}$, hence

$$\sum_{i=1}^{n} \sum_{j=1}^{n} b_{i,j} h_i h_j > \sum_{i=1}^{n} \sum_{j=1}^{n} c_{i,j} h_i h_j - A \geq 0$$

for all $(h_1, h_2, \ldots, h_n) \in S^{n-1}$. Thus the matrix $(b_{i,j})$ is positive-definite, as required. ∎

Using the fact that a symmetric $n \times n$ matrix $(c_{i,j})$ is negative definite if and only if the matrix $(-c_{i,j})$ is positive-definite, we see that if $(c_{i,j})$ is a negative-definite matrix then there exists some $\varepsilon > 0$ with the following property: if all of the components of a symmetric $n \times n$ matrix $(b_{i,j})$ satisfy the inequality $|b_{i,j} - c_{i,j}| < \varepsilon$ then the matrix $(b_{i,j})$ is negative definite.

Let $f: X \to \mathbb{R}$ be a real-valued function whose partial derivatives of first and second order exist and are continuous throughout some open set X in $\mathbb{R}^n$. Let $\mathbf{p}$ be a point of X. We have already observed that if the function f has a local maximum or a local minimum at $\mathbf{p}$ then

$$\left. \frac{\partial f}{\partial x_i} \right|_{\mathbf{x}=\mathbf{p}} = 0 \qquad (i = 1, 2, \ldots, n).$$

We now study the behaviour of the function f around a point $\mathbf{p}$ at which the first order partial derivatives vanish. We consider the Hessian matrix $(H_{i,j}(\mathbf{p}))$ defined by

$$H_{i,j}(\mathbf{p}) = \left. \frac{\partial^2 f}{\partial x_i \partial x_j} \right|_{\mathbf{x}=\mathbf{p}}.$$

Lemma 10.5 *Let $f\colon X \to \mathbb{R}$ be a real-valued function whose partial derivatives of first and second order exist and are continuous throughout some open set X in $\mathbb{R}^n$, and let $\mathbf{p}$ be a point of X at which*

$$\left.\frac{\partial f}{\partial x_i}\right|_{\mathbf{x}=\mathbf{p}} = 0 \qquad (i = 1, 2, \ldots, n).$$

If f has a local minimum at a point $\mathbf{p}$ of X then the Hessian matrix $(H_{i,j}(\mathbf{p}))$ at $\mathbf{p}$ is positive semi-definite.

Proof The first order partial derivatives of f are zero at $\mathbf{p}$. It follows that, given any vector $\mathbf{h} \in \mathbb{R}^n$ which is sufficiently close to $\mathbf{0}$, there exists some θ satisfying $0 < \theta < 1$ (where θ depends on $\mathbf{h}$) such that

$$f(\mathbf{p}+\mathbf{h}) = f(\mathbf{p}) + \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} h_i h_j H_{i,j}(\mathbf{p}+\theta\mathbf{h}),$$

where

$$H_{i,j}(\mathbf{p}+\theta\mathbf{h}) = \left.\frac{\partial^2 f}{\partial x_i \partial x_j}\right|_{\mathbf{x}=\mathbf{p}+\theta\mathbf{h}}$$

(see Lemma 10.3).

It follows from this result that

$$\sum_{i=1}^{n}\sum_{j=1}^{n} h_i h_j H_{i,j}(\mathbf{p}) = \lim_{t\to 0} \frac{2(f(\mathbf{p}+t\mathbf{h}) - f(\mathbf{p}))}{t^2} \geq 0.$$

The result follows. ∎

Let $f\colon X \to \mathbb{R}$ be a real-valued function whose partial derivatives of first and second order exist and are continuous throughout some open set X in $\mathbb{R}^n$, and let $\mathbf{p}$ be a point at which the first order partial derivatives of f vanish. The above lemma shows that if the function f has a local minimum at $\mathbf{h}$ then the Hessian matrix of f is positive semi-definite at $\mathbf{p}$. However the fact that the Hessian matrix of f is positive semi-definite at $\mathbf{p}$ is not sufficient to ensure that f is has a local minimum at $\mathbf{p}$, as the following example shows.

Example Consider the function $f\colon \mathbb{R}^2 \to \mathbb{R}$ defined by $f(x,y) = x^2 - y^3$. Then the first order partial derivatives of f vanish at $(0,0)$. The Hessian matrix of f at $(0,0)$ is the matrix

$$\begin{pmatrix} 2 & 0 \\ 0 & 0 \end{pmatrix}$$

and this matrix is positive semi-definite. However $(0,0)$ is not a local minimum of f since $f(0,y) < f(0,0)$ for all $y > 0$.

The following theorem shows that if the Hessian of the function f is positive definite at a point at which the first order partial derivatives of f vanish then f has a local minimum at that point.

Theorem 10.6 *Let $f: X \to \mathbb{R}$ be a real-valued function whose partial derivatives of first and second order exist and are continuous throughout some open set X in $\mathbb{R}^n$, and let $\mathbf{p}$ be a point of X at which*

$$\left.\frac{\partial f}{\partial x_i}\right|_{\mathbf{x}=\mathbf{p}} = 0 \qquad (i = 1, 2, \ldots, n).$$

Suppose that the Hessian matrix $(H_{i,j}(\mathbf{p}))$ at $\mathbf{p}$ is positive definite. Then f has a local minimum at $\mathbf{p}$.

Proof The first order partial derivatives of f vanish at $\mathbf{p}$. It therefore follows from Taylor's Theorem that, for any $\mathbf{h} \in \mathbb{R}^n$ which is sufficiently close to $\mathbf{0}$, there exists some θ satisfying $0 < \theta < 1$ (where θ depends on $\mathbf{h}$) such that

$$f(\mathbf{p} + \mathbf{h}) = f(\mathbf{p}) + \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} h_i h_j H_{i,j}(\mathbf{p} + \theta \mathbf{h}),$$

where

$$H_{i,j}(\mathbf{p} + \theta \mathbf{h}) = \left.\frac{\partial^2 f}{\partial x_i \partial x_j}\right|_{\mathbf{x}=\mathbf{p}+\theta\mathbf{h}}$$

(see Lemma 10.3). Suppose that the Hessian matrix $(H_{i,j}(\mathbf{p}))$ is positive definite. It follows from Lemma 10.4 that there exists some $\varepsilon > 0$ such that if $|H_{i,j}(\mathbf{x}) - H_{i,j}(\mathbf{p})| < \varepsilon$ for all i and j then $(H_{i,j}(\mathbf{x}))$ is positive definite.

But it follows from the continuity of the second order partial derivatives of f that there exists some $\delta > 0$ such that $|H_{i,j}(\mathbf{x}) - H_{i,j}(\mathbf{p})| < \varepsilon$ whenever $|\mathbf{x} - \mathbf{p}| < \delta$. Thus if $|\mathbf{h}| < \delta$ then $(H_{i,j}(\mathbf{p} + \theta \mathbf{h}))$ is positive definite for all $\theta \in (0, 1)$ so that $f(\mathbf{p} + \mathbf{h}) > f(\mathbf{p})$. Thus $\mathbf{p}$ is a local minimum of f. ∎

A symmetric $n \times n$ matrix C is positive definite if and only if all its eigenvalues are strictly positive. In particular if $n = 2$ and if λ_1 and λ_2 are the eigenvalues of a symmetric 2×2 matrix C, then

$$\lambda_1 + \lambda_2 = \operatorname{trace} C, \qquad \lambda_1 \lambda_2 = \det C.$$

Thus a symmetric 2×2 matrix C is positive definite if and only if its trace and determinant are both positive.

Example Consider the function $f\colon \mathbb{R}^2 \to \mathbb{R}$ defined by

$$f(x,y) = 4x^2 + 3y^2 - 2xy - x^3 - x^2y - y^3.$$

Now

$$\left.\frac{\partial f(x,y)}{\partial x}\right|_{(x,y)=(0,0)} = (0,0), \qquad \left.\frac{\partial f(x,y)}{\partial y}\right|_{(x,y)=(0,0)} = (0,0).$$

The Hessian matrix of f at $(0,0)$ is

$$\begin{pmatrix} 8 & -2 \\ -2 & 6 \end{pmatrix}.$$

The trace and determinant of this matrix are 14 and 44 respectively. Hence this matrix is positive definite. We conclude from Theorem 10.6 that the function f has a local minimum at $(0,0)$.

11 Repeated Differentiation and Smoothness

11.1 Repeated Differentiation of Functions of Several Variables

Let $\varphi: X \to \mathbb{R}^n$ be a function mapping some open subset X of a Euclidean space $\mathbb{R}^m$ into a Euclidean space $\mathbb{R}^n$. The function φ is "C^1" if and only if it is continuously differentiable, and this requires that the function be differentiable throughout X and also that the function each point $\mathbf{p}$ of X to the derivative $(D\varphi)_\mathbf{p}$ of φ at the point $\mathbf{p}$ is a continuous function from X to the space $L(\mathbb{R}^m, \mathbb{R}^n)$ of linear maps from $\mathbb{R}^m$ to $\mathbb{R}^n$. Moreover this is the case if and only if the partial derivatives of the Cartesian components of φ exist and are continuous throughout the open set X (see Corollary 8.17).

The process of differentiation can be repeated. Let $\varphi: V \to \mathbb{R}^n$ be a differentiable function defined over an open set V in $\mathbb{R}^n$. Suppose that the function φ is differentiable at each point $\mathbf{p}$. Then the derivative of φ can itself be regarded as a function on V taking values in the real vector space $L(\mathbb{R}^m, \mathbb{R}^n)$ of linear transformations between the real vector spaces $\mathbb{R}^m$ and $\mathbb{R}^n$. Moreover $L(\mathbb{R}^m, \mathbb{R}^n)$ can itself be regarded as a Euclidean space whose Euclidean norm is the Hilbert-Schmidt norm on $L(\mathbb{R}^m, \mathbb{R}^n)$. It follows that the definition of differentiability can be applied to derivative of a differentiable function of several real variables to obtain the second derivative of a twice-differentiable function. Continuing the process, one can obtain the kth derivative of a k-times differentiable function for any positive integer k.

A more detailed analysis of this process shows that if φ is a k-times differentiable function, and if the Cartesian components of φ are $f_1, f_2, \ldots, f_n$, so that

$$\varphi(\mathbf{x}) = (f_1(\mathbf{x}), f_2(\mathbf{x}), \ldots, f_n(\mathbf{x}))$$

for all $\mathbf{x} \in V$, then the kth derivative of φ at each point of V is represented by the multilinear transformation that maps each k-tuple $(\mathbf{v}^{(1)}, \mathbf{v}^{(2)}, \ldots, \mathbf{v}^{(k)})$ of vectors in $\mathbb{R}^m$ to the vector in $\mathbb{R}^n$ whose ith component is

$$\sum_{j_1=1}^{m} \sum_{j_2=1}^{m} \cdots \sum_{j_k=1}^{m} \frac{\partial^k f_i}{\partial x_{j_1}\, \partial x_{j_2} \cdots \partial x_{j_k}}\, v_{j_1}^{(1)} v_{j_2}^{(2)} \cdots v_{j_k}^{(k)},$$

where $v_j^{(s)}$ denotes the jth component of the vector $\mathbf{v}^{(s)}$ for $j = 1, 2, \ldots, m$ and $s = 1, 2, \ldots, k$. The kth derivative of the function φ is thus represented by a function from the open set V to some real vector space of multilinear transformations. Such a function is said to be a (Cartesian) *tensor field* on V. Such tensor fields are ubiquitous in differential geometry and theoretical physics.

We can formally define the concept of functions of several variables being *differentiable* of order k by recursion on k.

Definition Let V be an open set in $\mathbb{R}^m$. A function $\varphi: V \to \mathbb{R}^n$ is *k-times differentiable*, where $k > 1$, if it is differentiable and the $D\varphi: V \to L(\mathbb{R}^m, \mathbb{R}^n)$ that maps each point $\mathbf{x}$ of V to the derivative of φ at that point is a $(k-1)$-times differentiable function on V.

Definition Let V be an open set in $\mathbb{R}^m$. A function $\varphi: V \to \mathbb{R}^n$ is *k-times continuously differentiable*, where $k > 1$, if the function $D\varphi: V \to L(\mathbb{R}^m, \mathbb{R}^n)$ that maps each point $\mathbf{x}$ of V to the derivative of φ at that point is a $(k-1)$-times continuously differentiable function on V.

A function of several real variables is said to be "C^k" for some positive integer k if and only if it is k-times continuously differentiable.

Definition A function $\varphi: V \to \mathbb{R}^n$ is said to be *smooth* (or C^∞) if it is k-times differentiable for all positive integers k.

If a function of several real variables is $(k+1)$-times differentiable, then the components of its kth order derivative must be continuous functions, because differentiability implies continuity (see Lemma 8.8). It follows that a function of several real variables is smooth if and only if it is C^k for all positive integers k.

Lemma 11.1 *Let V be an open set in $\mathbb{R}^m$. A function $\varphi: V \to \mathbb{R}^n$ is k-times continuously differentiable (or C^k) if and only if the partial derivatives of the components of φ of all orders up to and including k exist and are continuous throughout V.*

Proof The result can be proved by induction on k. The result is true for $k = 1$ by Lemma 8.13. Suppose as our induction hypothesis that $k > 1$ and that continuously differentiable vector-valued functions on V are C^{k-1} if and only if their partial derivatives of orders up to and including $k-1$ exist and are continuous throughout V.

Now a vector-valued function is continuously differentiable if and only if its components are continuously differentiable. Moreover a vector-valued function is C^{k-1} if and only if its components are all C^{k-1}. It follows that the function φ is C^k if and only if the components of its derivative are C^{k-1}. These components are the first-order partial derivatives of φ. The induction hypothesis ensures that these first order partial derivatives of φ are C^{k-1} if and only if their partial derivatives of orders less than or equal to $k-1$ exist and are continuous throughout V. It follows that the function φ itself is C^k if and only if its partial derivatives of orders less than or equal to k exist and are continuous throughout V, as required. ∎

Lemma 11.2 *Let V be an open set in $\mathbb{R}^m$, and let $f: V \to \mathbb{R}$ and $g: V \to \mathbb{R}$ be real-functions on V, and let $f+g$, $f-g$ and $f \,.\, g$ denote the sum, difference and product of these functions, where*

$$(f+g)(\mathbf{x}) = f(\mathbf{x}) + g(\mathbf{x}), \quad (f-g)(\mathbf{x}) = f(\mathbf{x}) - g(\mathbf{x}),$$

$$(f \,.\, g)(\mathbf{x}) = f(\mathbf{x})g(\mathbf{x})$$

for all $\mathbf{x} \in V$. Suppose that the functions f and g are C^k for some positive integer k. Then so are the functions $f+g$, $f-g$ and $f \,.\, g$.

Proof The result can be proved by induction on k. It follows from Proposition 8.10 and Proposition 8.11 that the result is true when $k = 1$.

A real-valued function on V is C^k for some positive integer k if and only if all the partial derivatives of its components of degree less than or equal to k exist and are continuous throughout the open set V. It follows from this that a real-valued function f on V is C^k if and only if its first order partial derivatives $\partial_i f$ are C^{k-1}, where $\partial_i f = \dfrac{\partial f}{\partial x_i}$ for $i = 1, 2, \ldots, m$.

Thus suppose as our induction hypothesis that $k > 1$ and that all sums, differences and products of C^{k-1} functions are known to be C^{k-1}. Let f and g be C^k functions. Then

$$\partial_i(f+g) = \partial_i f + \partial_i g, \quad \partial_i(f-g) = \partial_i f - \partial_i g,$$

$$\partial_i(f \,.\, g) = f \,.\, (\partial_i g) + (\partial_i f) \,.\, g$$

for $i = 1, 2, \ldots, m$. Now the functions f, g, $\partial_i f$ and $\partial_i g$ are all C^{k-1}. The induction hypothesis then ensures that $\partial_i(f+g)$, $\partial_i(f-g)$ and $\partial_i(f \,.\, g)$ are all C^{k-1} for $i = 1, 2, \ldots, m$, and therefore the functions $f+g$, $f-g$ and $f \,.\, g$ are C^k.

The required result therefore follows by induction on the degree k of the derivatives required to be continuous. ∎

Lemma 11.3 *Let V and W be open sets in $\mathbb{R}^m$ and $\mathbb{R}^n$ respectively, and let $\varphi: V \to \mathbb{R}^n$ and $\psi: W \to \mathbb{R}^l$ be functions mapping V and W into $\mathbb{R}^n$ and $\mathbb{R}^l$ respectively, where $\varphi(V) \subset W$. Suppose that the functions $\varphi: V \to \mathbb{R}^n$ and $\psi: W \to \mathbb{R}^l$ are C^k. Then the composition function $\psi \circ \varphi: V \to \mathbb{R}^l$ is also C^k.*

Proof We prove the result by induction on k. The Chain Rule for functions of several real variables (Proposition 8.12) ensures that the result is true for $k = 1$.

We have shown that sums, differences and products of C^k functions are C^k (see Lemma 11.2). We suppose as our induction hypothesis that all compositions of C^{k-1} functions of several real variables are C^{k-1} for some positive integer k, and show that this implies that all compositions of C^k functions of several real variables are C^k.

Let $\varphi: V \to \mathbb{R}^n$ and $\psi: W \to \mathbb{R}^l$ be C^k functions, where V is an open set in $\mathbb{R}^m$, W is an open set in $\mathbb{R}^n$ and $\varphi(V) \subset W$. Let the components of φ be $f_1, f_2, \ldots, f_m$ and let the components of ψ be $g_1, g_2, \ldots, g_n$, where $f_1, f_2, \ldots, f_m$ are real-valued functions on V, $g_1, g_2, \ldots, g_n$ are real-valued functions on W,

$$\varphi(\mathbf{x}) = (f_1(\mathbf{x}), f_2(\mathbf{x}), \ldots, f_m(\mathbf{x}))$$

for all $\mathbf{x} \in V$ and

$$\psi(\mathbf{y}) = (g_1(\mathbf{y}), g_2(\mathbf{y}), \ldots, f_n(\mathbf{y}))$$

for all $\mathbf{y} \in W$.

It then follows from the Chain Rule (Proposition 8.12) that

$$\frac{\partial}{\partial x_i}\Big(g_j(\varphi(x_1, x_2, \ldots, x_m))\Big) = \sum_{s=1}^{n} \left(\frac{\partial g_j}{\partial u_s} \circ \varphi\right) \frac{\partial f_s}{\partial x_i}.$$

Now the functions $\dfrac{\partial g_j}{\partial u_s} \circ \varphi$ are compositions of C^{k-1} functions. The induction hypothesis therefore ensures that these functions are C^{k-1}. This then ensures that the functions $\dfrac{\partial}{\partial x_i}\Big(g_j(\varphi(x_1, x_2, \ldots, x_m))\Big)$ are expressible as sums of products of C^{k-1} functions, and must therefore themselves be C^{k-1} functions (see Lemma 11.2). We have thus shown that the first order partial derivatives of the components of the composition function $\psi \circ \varphi$ are C^{k-1} functions. It follows that $\psi \circ \varphi$ must itself be a C^k function.

The required result therefore follows by induction on the degree k of the derivatives required to be continuous. ∎

It follows from Lemma 11.2 and Lemma 11.3 that functions that are constructed from smooth vector-valued functions defined over open sets in Euclidean spaces by means of the operations of additions, subtraction, multiplication and composition of functions must themselves be smooth functions over the open sets over which they are defined.

We now prove a lemma that guarantees the smoothness of matrix-valued functions obtained from smooth matrix-valued functions through the operation of matrix inversion. The lemma applies to functions $F: V \to \mathrm{GL}(n, \mathbb{R})$ defined over an open subset V of a Euclidean space $\mathbb{R}^m$ and taking values in the set $\mathrm{GL}(n, \mathbb{R})$ of invertible $n \times n$ matrices. The value $F(\mathbf{x})$ of such a function at a point $\mathbf{x}$ of V is thus an invertible $n \times n$ matrix, and thus the function $F: V \to \mathrm{GL}(n, \mathbb{R})$ determines a corresponding function $G: V \to \mathrm{GL}(n, \mathbb{R})$, where $G(\mathbf{x}) = F(\mathbf{x})^{-1}$ for all $\mathbf{x} \in V$. The coefficients of the matrices $F(\mathbf{x})$ and $G(\mathbf{x})$ are then functions of $\mathbf{x}$ as $\mathbf{x}$ varies over the open set V. Now the function F is C^k if and only if, for all i and j between 1 and n, the coefficient of the matrix $F(\mathbf{x})$ in the ith row and jth column is a C^k function of $\mathbf{x}$ throughout the open set V. We prove that if the function F is C^k for some positive integer k then the function G is also C^k. It follows that if the function F is smooth, then the function G is smooth.

Lemma 11.4 *Let n be a positive integer, let $M_n(\mathbb{R})$ denote the real vector space consisting of all $n \times n$ matrices with real coefficients, and let $\mathrm{GL}(n, \mathbb{R})$ be the open set in $M_n(\mathbb{R})$ whose elements are the invertible $n \times n$ matrices with real coefficients. Let V be an open set in $\mathbb{R}^m$ let $F: V \to \mathrm{GL}(n, \mathbb{R})$ be a function mapping V into $\mathrm{GL}(n, \mathbb{R})$, and let $G: V \to \mathrm{GL}(n, \mathbb{R})$ be defined such that $G(\mathbf{x}) = F(\mathbf{x})^{-1}$ for all $\mathbf{x} \in V$. Suppose that the function F is C^k. Then the function G is C^k.*

Proof For each $\mathbf{x} \in V$, the matrices $F(\mathbf{x})$ and $G(\mathbf{x})$ satisfy $F(\mathbf{x})G(\mathbf{x}) = I$, where I is the identity matrix. On differentiating this identity with respect to the ith coordinate function x_i on V, where $\mathbf{x} = (x_1, x_2, \ldots, x_m)$, we find that

$$\frac{\partial F(\mathbf{x})}{\partial x_i}\, G(\mathbf{x}) + F(\mathbf{x})\, \frac{\partial G(\mathbf{x})}{\partial x_i} = 0,$$

and therefore

$$\frac{\partial G(\mathbf{x})}{\partial x_i} = -F(\mathbf{x})^{-1} \frac{\partial F(\mathbf{x})}{\partial x_i}\, G(\mathbf{x}) = -G(\mathbf{x}) \frac{\partial F(\mathbf{x})}{\partial x_i}\, G(\mathbf{x}).$$

(In the above equation $F(\mathbf{x})$, $G(\mathbf{x})$ and their inverses and partial derivatives are $n \times n$ matrices that are multiplied using the standard operation of matrix multiplication.) Now sums and products of C^k real-valued functions are themselves C^k (see Lemma 11.2). It follows that if matrices are multiplied together, where the coefficients of those matrices are C^k real-valued functions defined over the open set V, the coefficients of the resultant matrix will also be C^k real-valued functions defined over V.

The equation above ensures that if the matrix-valued function F is C^k (so that the functions determining the coefficients of the matrix are real-valued C^k functions on V), then the first order partial derivatives of the function G are continuous, and therefore the function G itself is C^1, where $G(\mathbf{x}) = F(\mathbf{x})^{-1}$ for all $\mathbf{x} \in V$. Moreover if G is C^j, where $1 \leq j < k$ then the coefficients of the first order partial derivatives of G are expressible as a sums of products of C^j real-valued functions and thus are themselves C^j functions. Thus the matrix-valued function G itself is C^{j+1}. Repeated applications of this result ensure that G is a C^k function as required. ∎

11.2 Smoothness of Local Inverses

Lemma 11.5 *Let $\varphi: X \to \mathbb{R}^n$ be a continuously differentiable function defined over an open set X in $\mathbb{R}^n$ that is locally invertible around some point of X and let $\mu: W \to \mathbb{R}^n$ be a local inverse for φ. Suppose that $\varphi: X \to \mathbb{R}^n$ is C^k and that the local inverse $\mu: W \to \mathbb{R}^n$ is differentiable throughout W. Then $\mu: W \to \mathbb{R}^n$ is C^k throughout W.*

Proof The functions φ and μ are differentiable, and $\mu(\varphi(\mathbf{x})) = \mathbf{x}$ for all $\mathbf{x} \in \mu(W)$. The Chain Rule (Proposition 8.12) then ensures that $(D\mu)_{\varphi(\mathbf{x})} \circ (D\varphi)_{\mathbf{x}}$ is the identity operator. Let $F(\mathbf{x})$ denote the Jacobian matrix representing the derivative $(D\varphi)_{\mathbf{x}}$ of φ at each point $\mathbf{x}$ of $\mu(W)$, and let $G(\mathbf{x})$ denote the Jacobian matrix representing the derivative $(D\mu)_{\varphi(\mathbf{x})}$ of μ at $\varphi(\mathbf{x})$. Then the Chain Rule ensures that $G(\mathbf{x})F(\mathbf{x})$ is the identity matrix. It follows that $F(\mathbf{x})$ and $G(\mathbf{x})$ are invertible matrices and $G(\mathbf{x}) = F(\mathbf{x})^{-1}$ for all $\mathbf{x} \in \mu(W)$. Now the function φ is C^k on X and therefore the matrix-valued function $F: \mu(W) \to \mathrm{GL}(n, \mathbb{R})$ is is C^k on $\mu(W)$. It follows from Lemma 11.4 that the matrix-valued function $G: \mu(W) \to \mathrm{GL}(n, \mathbb{R})$ is also C^k on $\mu(W)$.

Now $(D\mu)_{\mathbf{y}}$ is represented by the matrix $G(\mu(\mathbf{y}))$ for all $\mathbf{y} \in W$. It follows from the continuity of μ and G that the derivative $D\mu$ of μ is continuous on W. It follows that μ is C^1. Moreover if $\mu: W \to X$ is C^j for any integer j satisfying $1 \leq j < k$ then $G \circ \mu$ is a composition of C^j functions and is therefore C^j (Lemma 11.3). But the coefficients of the matrix $G(\mu(\mathbf{y}))$ are the first order partial derivatives of the components of μ at $\mathbf{y}$ at each point $\mathbf{y}$ of W. It follows therefore that the first order partial derivatives of μ are C^j and therefore the function μ itself is C^{j+1}. It follows by repeated application of this process that the function μ is C^k on W, as required. ∎

11.3 The Inverse and Implicit Function Theorems for Smooth Maps

Theorem 11.6 (Inverse Function Theorem for Smooth Maps) *Let $\varphi: V \to \mathbb{R}^n$ be a smooth function defined over an open set V in n-dimensional Euclidean space $\mathbb{R}^n$ and mapping V into $\mathbb{R}^n$, and let $\mathbf{p}$ be a point of V. Suppose that the derivative $(D\varphi)_{\mathbf{p}}: \mathbb{R}^n \to \mathbb{R}^n$ of the map φ at the point $\mathbf{p}$ is an invertible linear transformation. Then there exists an open set W in $\mathbb{R}^n$ and a smooth function $\mu: W \to V$ that satisfies the following conditions:—*

(i) $\mu(W)$ is an open set in $\mathbb{R}^n$ contained in V, and $\mathbf{p} \in \mu(W)$;

(ii) $\varphi(\mu(\mathbf{y})) = \mathbf{y}$ for all $\mathbf{y} \in W$.

Proof The existence of continuously differentiable local inverse $\mu: W \to V$ follows from the Inverse Function Theorem (Theorem 9.5). The result that this local inverse is smooth when φ is smooth then follows from Lemma 11.5. ∎

Definition Let V and W be open sets in n-dimensional Euclidean space $\mathbb{R}^n$, and let $\varphi: V \to W$ be a function from V to W. The function φ is said to be a *diffeomorphism* if it has a well-defined inverse $\varphi^{-1}: W \to V$ and both the function $\varphi: V \to W$ and its inverse $\varphi^{-1}: W \to V$ are smooth functions.

Definition Let V be an open set in n-dimensional Euclidean space $\mathbb{R}^n$, and let $\varphi: V \to \mathbb{R}^n$ be a smooth function from V to $\mathbb{R}^n$. Let U be an open subset of V. We say that φ maps U *diffeomorphically* onto an open set of $\mathbb{R}^n$ if $\varphi(U)$ is an open set in $\mathbb{R}^n$ and the restriction of the function φ to U is a diffeomorphism from U to $\varphi(U)$.

The following corollary is simply a restatement of the Inverse Function Theorem (Theorem 11.6) for smooth maps, using the language of diffeomorphisms.

Corollary 11.7 *Let V be an open set in n-dimensional Euclidean space $\mathbb{R}^n$, and let $\varphi: V \to \mathbb{R}^n$ be a smooth function from V to $\mathbb{R}^n$, and let $\mathbf{p} \in V$. Suppose that the derivative $(D\varphi)_{\mathbf{p}}$ of φ is invertible at the point $\mathbf{p}$. Then there exists an open subset U of V, where $\mathbf{p} \in U$, that is mapped diffeomorphically by φ onto an open set in $\mathbb{R}^n$.*

The following theorem is a version of the Implicit Function Theorem (Theorem 9.6 applicable when the functions $u_1, u_2, \ldots, u_m$ satisfying the conditions of Theorem 9.6 are all smooth.

Theorem 11.8 *Let* $\mathbf{p}$ *be a point of* $\mathbb{R}^n$*, where* $\mathbf{p} = (p_1, p_2, \ldots, p_n)$ *and let* $u_1, u_2, \ldots, u_m$ *be a smooth real-valued functions defined over an open neighbourhood* V *of the point* $\mathbf{p}$ *in* $\mathbb{R}^n$*, where* $m < n$*, and let*

$$M = \{\mathbf{x} \in V : u_j(\mathbf{x}) = 0 \text{ for } j = 1, 2, \ldots, m\}.$$

Suppose that $u_1, u_2, \ldots, u_n$ *are zero at* $\mathbf{p}$ *and that the matrix*

$$\begin{pmatrix} \dfrac{\partial u_1}{\partial x_1} & \dfrac{\partial u_1}{\partial x_2} & \cdots & \dfrac{\partial u_1}{\partial x_m} \\ \dfrac{\partial u_2}{\partial x_1} & \dfrac{\partial u_2}{\partial x_2} & \cdots & \dfrac{\partial u_2}{\partial x_m} \\ \vdots & \vdots & & \vdots \\ \dfrac{\partial u_m}{\partial x_1} & \dfrac{\partial u_m}{\partial x_2} & \cdots & \dfrac{\partial u_m}{\partial x_m} \end{pmatrix}$$

is invertible at the point $\mathbf{p}$*. Then there exists an open neighbourhood* U *of* $\mathbf{p}$ *and smooth functions* $f_1, f_2, \ldots, f_m$ *of* $n - m$ *real variables, defined around* $(p_{m+1}, \ldots, p_n)$ *in* $\mathbb{R}^{n-m}$*, such that*

$$\begin{aligned} M \cap U = \{ & (x_1, x_2, \ldots, x_n) \in U : \\ & x_j = f_j(x_{m+1}, \ldots, x_n) \text{ for } j = 1, 2, \ldots, m\}. \end{aligned}$$

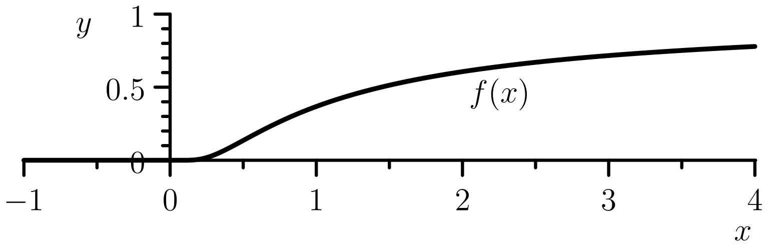
Proof The Implicit Function Theorem for continuously differentiable maps (Theorem 9.6) establishes the existence of continuously differentiable functions $f_1, f_2, \ldots, f_m$. Examination of the proof of that theorem shows that these functions are determined by a continuously differentiable local inverse of a smooth map. Lemma 11.5 ensures that this local inverse is itself smooth. It follows that that functions $f_1, f_2, \ldots, f_m$ defined as described in the proof of Theorem 9.6 are also smooth, and therefore satisfy the requirements of this theorem. ∎

11.4 Smooth Partitions of Unity

Proposition 11.9 *Let* $f: \mathbb{R} \to \mathbb{R}$ *be the function mapping the set* $\mathbb{R}$ *of real numbers to itself defined such that*

$$f(x) = \begin{cases} \exp\left(-\dfrac{1}{x}\right) & \text{if } x > 0; \\ 0 & \text{if } x \leq 0. \end{cases}$$

Then the function $f: \mathbb{R} \to \mathbb{R}$ *is smooth on* $\mathbb{R}$*. In particular* $f^{(k)}(0) = 0$ *for all positive integers* k*.*



Proof We show by induction on k that the function f is k times differentiable on $\mathbb{R}$ and $f^{(k)}(0) = 0$ for all positive integers k. Now it follows from standard rules for differentiating functions that

$$f^{(k)}(x) = \frac{p_k(x)}{x^{2k}} \exp\left(-\frac{1}{x}\right)$$

for all strictly positive real numbers x, where $p_1(x) = 1$ and

$$p_{k+1}(x) = x^2 p_k'(x) + (1 - 2kx)p_k(x)$$

for all k. A straightforward proof by induction shows that $p_k(x)$ is a polynomial in x of degree $k - 1$ for all positive integers k with leading term $(-1)^{k-1}k!x^{k-1}$.

Now

$$\frac{d}{dt}\left(t^n e^{-t}\right) = t^{n-1}(n - t)e^{-t}$$

for all positive real numbers t. It follows that function sending each positive real number t to $t^n e^{-t}$ is increasing when $0 \leq t < n$ and decreasing when $t > n$, and therefore $t^n e^{-t} \leq M_n$ for all positive real numbers t, where $M_n = n^n e^{-n}$. It follows that

$$0 \leq \frac{1}{x^{2k+1}} \exp\left(-\frac{1}{x}\right) \leq M_{2k+2}x$$

for all positive real numbers x, and therefore

$$\lim_{h\to 0^+} \frac{1}{h^{2k+1}} \exp\left(-\frac{1}{h}\right) = 0.$$

It then follows that

$$\begin{aligned}
\lim_{h\to 0^+} \frac{f^{(k)}(h)}{h} &= \lim_{h\to 0^+} \left(\frac{p_k(h)}{h^{2k+1}} \exp\left(-\frac{1}{h}\right)\right) \\
&= \lim_{h\to 0^+} p_k(h) \times \lim_{h\to 0^+} \left(\frac{1}{h^{2k+1}} \exp\left(-\frac{1}{h}\right)\right) \\
&= p_k(0) \times 0 = 0
\end{aligned}$$

for all positive integers k. Now

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

It follows that the function f is differentiable at zero, and $f'(0) = 0$.

Suppose that the function $f(x)$ is k-times differentiable at zero for some positive integer k, and that $f^{(k)}(0) = 0$. Then

$$\lim_{h \to 0^+} \frac{f^{(k)}(h) - f^{(k)}(0)}{h} = \lim_{h \to 0^+} \frac{f^{(k)}(h)}{h} = 0 = \lim_{h \to 0^-} \frac{f^{(k)}(h) - f^{(k)}(0)}{h}.$$

It then follows that the function $f^{(k)}$ is differentiable at zero, and moreover the derivative $f^{(k+1)}(0)$ of this function at zero is equal to zero. The function f is thus $(k+1)$-times differentiable at zero.

It now follows by induction on k that $f^{(k)}(x)$ exists for all positive integers k and real numbers x, and moreover

$$f^{(k)}(x) = \begin{cases} \dfrac{p_k(x)}{x^{2k}} \exp\left(-\dfrac{1}{x}\right) & \text{if } x > 0; \\ 0 & \text{if } x \leq 0. \end{cases}$$

The function $f\colon \mathbb{R} \to \mathbb{R}$ is thus a smooth function, as required. ∎

Definition Let $f\colon \mathbb{R}^n \to \mathbb{R}$ be a real-valued function defined on n-dimensional Euclidean space $\mathbb{R}^n$. The *support* of f is defined to be the closure in $\mathbb{R}^n$ of the set

$$\{\mathbf{x} \in \mathbb{R}^n : f(\mathbf{x}) \neq 0\}.$$

Example Let r be a positive real number, and let $f\colon \mathbb{R}^n \to \mathbb{R}$ be the real-valued function on $\mathbb{R}^n$ defined such that

$$f(\mathbf{x}) = \begin{cases} \exp\left(-\dfrac{1}{r^2 - |\mathbf{x}|^2}\right) & \text{if } |\mathbf{x}| < r; \\ 0 & \text{if } |\mathbf{x}| \geq r. \end{cases}$$

Then the set of points $\mathbf{x}$ of $\mathbb{R}^n$ for which $f(\mathbf{x}) \neq 0$ is the open ball of radius r about the origin. It follows that the support of the function f is the closed ball $\{\mathbf{x} \in \mathbb{R}^n : |\mathbf{x}| \leq r\}$ of radius r about the origin.

Proposition 11.10 *Let X be a closed bounded set in n-dimensional Euclidean space $\mathbb{R}^n$, and let $\mathcal{V}$ be a collection of open sets in $\mathbb{R}^n$ which covers the set X. Then there exist smooth real-valued functions $f_1, f_2, f_3 \ldots, f_N$, each defined throughout $\mathbb{R}^n$ such that the following properties are satisfied:—*

(i) $0 \leq f_j(\mathbf{x}) \leq 1$ *for* $j = 1, 2, \ldots, N$ *and for all points* $\mathbf{x}$ *of* $\mathbb{R}^n$*;*

(ii) $\sum_{j=1}^{n} f_j(\mathbf{x}) = 1$ *for all points* $\mathbf{x}$ *of the set* X*;*

(iii) given any integer j *between* 1 *and* N*, there exists an open set* V *belonging to the collection* $\mathcal{V}$ *which contains the support of the function* f_j*.*

Proof Let Y be a closed ball of radius R centred on the origin, where R is chosen large enough to ensure that the set X is contained within a ball of radius $R - 3$ about the origin. If we adjoin the set $\mathbb{R}^n \setminus X$ to the collection $\mathcal{V}$ we obtain a collection $\mathcal{W}$ of open sets in $\mathbb{R}^n$ which covers Y. Now every open cover of a closed bounded subset of $\mathbb{R}^n$ has a Lebesgue number (see Proposition 5.7). It follows that there exists a real number δ satisfying $0 < \delta < 1$ with the property that, given any point $\mathbf{p}$ of Y, then the closed ball of radius δ centred on the point $\mathbf{p}$ is a subset of one of the open sets belonging to the collection $\mathcal{W}$ of open sets covering Y.

The set Y is compact (see Theorem 5.9). Therefore there is a finite list

$$\mathbf{p}_1, \mathbf{p}_2, \ldots, \mathbf{p}_M$$

of points of Y with the property that the collection of open balls of radius δ centred on these points covers Y. We order these points so that, for some integer N between 1 and M, the open balls of radius δ about points $\mathbf{p}_j$ for $1 \leq j \leq N$ have non-empty intersection with the set X, whilst the open balls of radius δ about the points $\mathbf{p}_j$ for $N < j \leq M$ do not intersect the set X. For each integer j between 1 and M we define a real-valued function $g_j\colon \mathbb{R}^n \to \mathbb{R}$ on $\mathbb{R}^n$ so that

$$g_j(\mathbf{x}) = \begin{cases} \exp\left(-\dfrac{1}{\delta^2 - |\mathbf{x} - \mathbf{p}_j|^2}\right) & \text{if } |\mathbf{x} - \mathbf{p}_j| < \delta; \\ 0 & \text{if } |\mathbf{x} - \mathbf{p}_j| \geq \delta. \end{cases}$$

Then $g_j(\mathbf{x}) = h(|\mathbf{x} - \mathbf{p}_j|^2)$, for $j = 1, 2, \ldots, M$ and for all points $\mathbf{x}$ of $\mathbb{R}^n$, where $h\colon \mathbb{R} \to \mathbb{R}$ is defined so that

$$h(t) = \begin{cases} \exp\left(-\dfrac{1}{t}\right) & \text{if } t > 0; \\ 0 & \text{if } t \leq 0. \end{cases}$$

Now the function h is smooth on $\mathbb{R}$ (see Proposition 11.9) Also $|\mathbf{x} - \mathbf{p}_j|^2$ is a smooth function of $\mathbf{x}$ throughout $\mathbb{R}^n$, as this function is the sum of the squares of the components of the vector $\mathbf{x} - \mathbf{p}_j$. It follows that the functions $g_1, g_2, \ldots, g_M$ are smooth functions throughout Y. Now $g(\mathbf{x}) \geq 0$ for all $\mathbf{x} \in \mathbb{R}^n$. Also, given any point $\mathbf{x}$ of Y, there exists some integer j between 1 and M for which $|\mathbf{x} - \mathbf{p}_j| < \delta$, because the points $\mathbf{p}_1, \mathbf{p}_2, \ldots, \mathbf{p}_M$ have been chosen so that the open balls of radius δ about these points cover Y. It follows that $G(\mathbf{x}) > 0$ for all $\mathbf{x} \in Y$, where

$$G(\mathbf{x}) = \sum_{j=1}^{M} g_j(\mathbf{x})$$

for all $\mathbf{x} \in \mathbb{R}^m$. Also if $j > N$ then the open ball of radius δ about the point $\mathbf{p}_j$ does not intersect the set X, and therefore $g_j(\mathbf{x}) = 0$ for all $\mathbf{x} \in X$. Define real-valued functions $f_1, f_2, \ldots, f_N$ throughout $\mathbb{R}^n$ such that

$$f_j(\mathbf{x}) = \begin{cases} \dfrac{g_j(\mathbf{x})}{G(\mathbf{x})} & \text{if } |\mathbf{x}| < R; \\ 0 & \text{if } |\mathbf{x}| \geq R. \end{cases}$$

Now if j is an integer between 1 and N then the open ball of radius δ about the point $\mathbf{p}_j$ intersects the set X and therefore every point of $\mathbb{R}^n$ for which $g_j(\mathbf{x}) > 0$ lies within a distance 2δ of a point of X, where $\delta < 1$, and therefore lies within the closed ball of radius $R - 1$ about the origin in $\mathbb{R}^n$. It follows that, for each integer j between 1 and n, the function f_j satisfies $f_j(\mathbf{x}) = 0$ at all points $\mathbf{x}$ of $\mathbb{R}^n$ whose distance from the boundary sphere of the closed ball Y is less than one. The function f_j is therefore smooth around all points of the boundary sphere of Y (being identically equal to zero throughout some open neighbourhood of that boundary sphere), and thus each function f_j is smooth throughout $\mathbb{R}^n$. Now $0 \leq f_j(\mathbf{x}) \leq 1$ for all $\mathbf{x} \in \mathbb{R}^n$. The support of each function f_j is contained within a closed ball of radius δ about the point $\mathbf{p}_j$ and is therefore contained within one of the open sets belonging to the collection $\mathcal{W}$ of open sets that covers Y. But none of the functions $f_1, f_2, \ldots, f_N$ has support contained in $\mathbb{R}^n \setminus X$. It follows that, for each integer j between 1 and N, the support of the function f_j is contained within one of the open sets belonging to the given collection $\mathcal{V}$ of open sets covering the set X.

Finally we note that if $\mathbf{x}$ is a point of the set X then $g_j(\mathbf{x}) = 0$ for all integers j satisfying $N < j \leq M$, and therefore

$$\sum_{j=1}^{N} f_j(\mathbf{x}) = \sum_{j=1}^{N} \frac{g_j(\mathbf{x})}{G(x)} = \sum_{j=1}^{M} \frac{g_j(\mathbf{x})}{G(x)} = \frac{G(x)}{G(x)} = 1.$$

This completes the proof. ∎

11.5 Taylor's Theorem

Lemma 11.11 *Let s and h be real numbers, let f be a k times differentiable real-valued function defined on some open interval containing s and $s+h$, let $c_0, c_1, \ldots, c_{k-1}$ be real numbers, and let*

$$p(t) = f(s+th) - \sum_{n=0}^{k-1} c_n t^n.$$

for all real numbers t belonging to some open interval D for which $0 \in D$ and $1 \in D$. Then $p^{(n)}(0) = 0$ for all integers n satisfying $0 \leq n < k$ if and only if

$$c_n = \frac{h^n f^{(n)}(s)}{n!}$$

for all integers n satisfying $0 \leq n < k$.

Proof On setting $t = 0$, we find that $p(0) = f(s) - c_0$, and thus $p(0) = 0$ if and only if $c_0 = f(s)$.

Let the integer n satisfy $0 < n < k$. On differentiating $p(t)$ n times with respect to t, we find that

$$p^{(n)}(t) = h^n f^{(n)}(s+th) - \sum_{j=n}^{k-1} \frac{j!}{(j-n)!} c_j t^{j-n}.$$

Then, on setting $t = 0$, we find that only the term with $j = n$ contributes to the value of the sum on the right hand side of the above identity, and therefore

$$p^{(n)}(0) = h^n f^{(n)}(s) - n! c_n.$$

The result follows. ∎

Theorem 11.12 *[Taylor's Theorem] Let s and h be real numbers, and let f be a k times differentiable real-valued function defined on some open interval containing s and $s+h$. Then*

$$f(s+h) = f(s) + \sum_{n=1}^{k-1} \frac{h^n}{n!} f^{(n)}(s) + \frac{h^k}{k!} f^{(k)}(s+\theta h)$$

for some real number θ satisfying $0 < \theta < 1$.

Proof Let D be an open interval, containing the real numbers 0 and 1, chosen to ensure that $f(s+th)$ is defined for all $t \in D$, and let $p: D \to \mathbb{R}$ be defined so that

$$p(t) = f(s+th) - f(s) - \sum_{n=1}^{k-1} \frac{t^n h^n}{n!} f^{(n)}(s)$$

for all $t \in D$. A straightforward calculation shows that $p^{(n)}(0) = 0$ for $n = 0, 1, \ldots, k-1$ (see Lemma 11.11). Thus if $q(t) = p(t) - p(1)t^k$ for all $s \in [0,1]$ then $q^{(n)}(0) = 0$ for $n = 0, 1, \ldots, k-1$, and $q(1) = 0$. We can therefore apply Rolle's Theorem (Theorem 2.1) to the function q on the interval $[0,1]$ to deduce the existence of some real number t_1 satisfying $0 < t_1 < 1$ for which $q'(t_1) = 0$. We can then apply Rolle's Theorem to the function q' on the interval $[0, t_1]$ to deduce the existence of some real number t_2 satisfying $0 < t_2 < t_1$ for which $q''(t_2) = 0$. By continuing in this fashion, applying Rolle's Theorem in turn to the functions $q'', q''', \ldots, q^{(k-1)}$, we deduce the existence of real numbers $t_1, t_2, \ldots, t_k$ satisfying $0 < t_k < t_{k-1} < \cdots < t_1 < 1$ with the property that $q^{(n)}(t_n) = 0$ for $n = 1, 2, \ldots, k$. Let $\theta = t_k$. Then $0 < \theta < 1$ and

$$0 = \frac{1}{k!} q^{(k)}(\theta) = \frac{1}{k!} p^{(k)}(\theta) - p(1) = \frac{h^k}{k!} f^{(k)}(s+\theta h) - p(1),$$

hence

$$\begin{aligned} f(s+h) &= f(s) + \sum_{n=1}^{k-1} \frac{h^n}{n!} f^{(n)}(s) + p(1) \\ &= f(s) + \sum_{n=1}^{k-1} \frac{h^n}{n!} f^{(n)}(s) + \frac{h^k}{k!} f^{(k)}(s+\theta h), \end{aligned}$$

as required. ∎

Corollary 11.13 *Let $f: D \to \mathbb{R}$ be a k-times continuously differentiable function defined over an open subset D of $\mathbb{R}$ and let $s \in \mathbb{R}$. Then given any strictly positive real number ε, there exists some strictly positive real number δ such that*

$$\left| f(s+h) - f(s) - \sum_{n=1}^{k} \frac{h^n}{n!} f^{(n)}(s) \right| < \varepsilon |h|^k$$

whenever $|h| < \delta$.

Proof The function f is k-times continuously differentiable, and therefore its kth derivative $f^{(k)}$ is continuous. Let some strictly positive real number ε be given. Then there exists some strictly positive real number δ that is small enough to ensure that $s + h \in D$ and $|f^{(k)}(s + h) - f^{(k)}(s)| < k!\varepsilon$ whenever $|h| < \delta$. If h is an real number satisfying $|h| < \delta$, and if θ is a real number satisfying $0 < \theta < 1$, then $s + \theta h \in D$ and $|f^{(k)}(s + \theta h) - f^{(k)}(s)| < k!\varepsilon$. Now it follows from Taylor's Theorem (Theorem 11.12) that, given any real number h satisfying $|h| < \delta$ there exists some real number θ satisfying $0 < \theta < 1$ for which

$$f(s+h) = f(s) + \sum_{n=1}^{k-1} \frac{h^n}{n!} f^{(n)}(s) + \frac{h^k}{k!} f^{(k)}(s + \theta h).$$

Then

$$\begin{aligned} \left| f(s+h) - f(s) - \sum_{n=1}^{k} \frac{h^n}{n!} f^{(n)}(s) \right| &= \frac{|h|^k}{k!} |f^{(k)}(s+\theta h) - f^{(k)}(s)| \\ &< \varepsilon |h|^k, \end{aligned}$$

as required. ∎

Theorem 11.14 (Taylor's Theorem in Higher Dimensions) *Let $f\colon X \to \mathbb{R}$ be a real-valued function defined on an open set X in $\mathbb{R}^n$ that is k-times continuously differentiable on X, let $\mathbf{p}$ be a point of X, and let δ be a positive number small enough to ensure that the open ball of radius δ about the point $\mathbf{p}$ is contained in X. Then, given any vector $\mathbf{h}$ satisfying $|\mathbf{h}| < \delta$, there exists some real number θ satisfying $0 < \theta < 1$ for which*

$$\begin{aligned} f(\mathbf{p}+\mathbf{h}) &= f(\mathbf{p}) \\ &\quad + \sum_{\substack{j_1 \geq 0, \ldots, j_n \geq 0 \\ 0 < j_1 + j_2 + \cdots + j_n < k}} \frac{h_1^{j_1} \cdots h_n^{j_n}}{j_1! j_2! \cdots j_n!} \left. \frac{\partial^{j_1+j_2+\cdots+j_n} f}{\partial^{j_1} x_1 \ldots \partial^{j_n} x_n} \right|_{\mathbf{p}} \\ &\quad + \sum_{\substack{j_1 \geq 0, \ldots, j_n \geq 0 \\ j_1 + j_2 + \cdots + j_n = k}} \frac{h_1^{j_1} \cdots h_n^{j_n}}{j_1! j_2! \cdots j_n!} \left. \frac{\partial^{j_1+j_2+\cdots+j_n} f}{\partial^{j_1} x_1 \ldots \partial^{j_n} x_n} \right|_{\mathbf{p}+\theta\mathbf{h}}. \end{aligned}$$

Proof Taylor's Theorem for functions of a single real variable (Theorem 11.12), applied to the function sending real numbers t in the interval $[0, 1]$ to $f(\mathbf{p} +$

$t\mathbf{h}$), ensures the existence of real constants $c_{j_1 \cdots j_n}$ independent of f for which

$$\begin{aligned} f(\mathbf{p}+\mathbf{h}) &= f(\mathbf{p}) \\ &\quad + \sum_{\substack{j_1 \geq 0, \ldots, j_n \geq 0 \\ 0 < j_1 + j_2 + \cdots + j_n < k}} c_{j_1, \ldots, j_n} h_1^{j_1} \cdots h_n^{j_n} \left. \frac{\partial^{j_1+j_2+\cdots+j_n} f}{\partial^{j_1} x_1 \ldots \partial^{j_n} x_n} \right|_{\mathbf{p}} \\ &\quad + \sum_{\substack{j_1 \geq 0, \ldots, j_n \geq 0 \\ j_1 + j_2 + \cdots + j_n = k}} c_{j_1, \ldots, j_n} h_1^{j_1} \cdots h_n^{j_n} \left. \frac{\partial^{j_1+j_2+\cdots+j_n} f}{\partial^{j_1} x_1 \ldots \partial^{j_n} x_n} \right|_{\mathbf{p}+\theta\mathbf{h}}. \end{aligned}$$

The values of these constants $c_{j_1 \cdots j_n}$ can then be determined by applying the identity with

$$f(x_1, x_2, \ldots, x_n) = x_1^{j_1} x_2^{j_2} \cdots x_n^{j_n}. \quad \blacksquare$$

11.6 Real-Analytic Functions

Definition A real-valued function $f \colon D \to \mathbb{R}$ defined over an open subset D of the set $\mathbb{R}$ of real numbers is said to be *real-analytic* if, given any real number s belonging to the domain D of the function, there exists some strictly positive real number δ such that

$$f(s+h) = f(s) + \sum_{n=1}^{+\infty} \frac{h^n}{n!} f^{(n)}(s)$$

for all real numbers h satisfying $|h| < \delta$.

It can be shown that sums, differences, products, quotients and compositions of real-analytic functions are themselves real-analytic over their domains of definition. In particular, polynomial functions and quotients of polynomial functions are real-analytic. The natural logarithm function is real-analytic over the set of positive real numbers because its derivative is real-analytic. The exponential, natural logarithm, sine and cosine functions are examples of real-analytic functions. Inverses of real-analytic functions are real-analytic.

All real-analytic functions are smooth. However not all smooth functions are real-analytic. The function considered in Proposition 11.9 is an example of such a function.