Module MAU23203: Analysis in Several Real Variables
Michaelmas Term 2022
Section 9: Second Order Partial Derivatives and the Hessian Matrix

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9 Second Order Partial Derivatives and the Hessian Matrix

9.1 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

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

Now it would be incorrect to assert that if the second order partial derivatives of a real-valued function f of real variables $x_1, x_2, \ldots, x_n$ all exist at some point of the domain of the function then

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

are equal for all values of i and j. 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

$$f_x(x, y) = \frac{\partial f(x, y)}{\partial x},$$

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

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

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

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

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

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 9.1 *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*

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

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

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

and let (a,b) be a point of X. The set X is open in $\mathbb{R}^2$ 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

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

for all real numbers h and k satisfying $|h| < L$ and $|k| < L$. First consider h to 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 $S(h,k) = q(b+k) - q(b)$. It then follows from the Mean Value Theorem (Theorem 7.5) 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

$$\begin{aligned} S(h,k) &= k(f_y(a+h,v) - f_y(a,v)) \\ &= hk f_{xy}(u,v) \\ &= hk \left. \frac{\partial^2 f}{\partial x \partial y} \right|_{(x,y)=(u,v)}. \end{aligned}$$

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 9.2 *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.

9.2 Local Maxima and Minima

Definition A function $\varphi\colon X \to \mathbb{R}^p$, defined over an open set X in $\mathbb{R}^n$ and mapping that open set into $\mathbb{R}^p$ for some positive integers n and p, is said to be *k times continuously differentiable* if the partial derivatives of the components of the functions φ of all orders less than or equal to k exist and are continuous throughout the domain X of the function φ.

Let $f\colon X \to \mathbb{R}$ be a twice continuously differentiable real-valued function defined over some open subset X of $\mathbb{R}^n$. (In other words, let f be a real-valued function defined on an open set X in $\mathbb{R}^n$ whose first and second order partial derivatives exist and are continuous throughout the domain X of the function f.) 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 $t = p_i$. It follows that 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 continuously 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.

Proposition 9.3 *Let f be a twice continuously differentiable real-valued function defined over an open ball in $\mathbb{R}^n$ of radius δ centred on some point $\mathbf{p}$ of $\mathbb{R}^n$. Then, given any vector $\mathbf{h}$ in $\mathbb{R}^n$ satisfying $|\mathbf{h}| < \delta$, there exists some real number θ satisfying $0 < \theta < 1$ for which*

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

Proof Let $\mathbf{h}$ satisfy $|\mathbf{h}| < \delta$, and let $q(t) = f(\mathbf{p} + t\mathbf{h})$ for all real numbers t in some appropriately chosen open interval in the real line that contains the real numbers 0 and 1. The function q is the composition function in which the function f follows the function that sends real numbers t in the domain of q to the point $\mathbf{p} + t\mathbf{h}$ of $\mathbb{R}^n$. It follows, on applying the Chain Rule for differentiable functions of several real variables (Theorem 8.20) that

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

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 7.10). Consequently

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

as required. ∎

Let f be a twice continuously differentiable real-valued function defined over an open ball of radius δ about some given point $\mathbf{p}$ of $\mathbb{R}^n$. It follows from Proposition 9.3 that if

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

for $j = 1, 2, \ldots, n$, and if $|\mathbf{h}| < \delta$ then there exists some real number θ satisfying $0 < \theta < 1$ for which

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

Let f be a real-valued function defined over an open set in $\mathbb{R}^n$ whose second order partial derivative are defined at a point $\mathbf{p}$ of its domain. Let us denote by $(H_{i,j}(\mathbf{p}))$ the *Hessian matrix* at the point $\mathbf{p}$, defined by

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

Suppose now that the function f is twice continuously differentiable on its domain. Then $H_{i,j}(\mathbf{p}) = H_{j,i}(\mathbf{p})$ for all integers i and j between 1 and n, by Corollary 9.2, and 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 $\displaystyle\sum_{i=1}^{n}\sum_{j=1}^{n} c_{i,j} h_i h_j \geq 0$ 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 $\displaystyle\sum_{i=1}^{n}\sum_{j=1}^{n} c_{i,j} h_i h_j > 0$ 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 $\displaystyle\sum_{i=1}^{n}\sum_{j=1}^{n} c_{i,j} h_i h_j \leq 0$ 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 $\displaystyle\sum_{i=1}^{n}\sum_{j=1}^{n} c_{i,j} h_i h_j < 0$ 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 9.4 *Let $(c_{i,j})$ be a positive definite symmetric $n \times n$ matrix. Then there exists some positive real number ε that is small enough to ensure that any symmetric $n \times n$ matrix $(b_{i,j})$ whose components all satisfy the inequality $|b_{i,j} - c_{i,j}| < \varepsilon$ 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

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

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

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

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 5.10 that there exists some $(k_1, k_2, \ldots, k_n) \in S^{n-1}$ with the property that

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

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 coefficients satisfy the inequality $|b_{i,j} - c_{i,j}| < \varepsilon$ 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 $f\colon X \to \mathbb{R}$ be a twice continuously differentiable real-valued function defined over some open set X in $\mathbb{R}^n$, and let $\mathbf{p}$ be a point of the open set 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 9.5 *Let $f\colon X \to \mathbb{R}$ be a twice continuously differentiable real-valued function defined over an open set X in $\mathbb{R}^n$, and let $\mathbf{p}$ be a point of the open set 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 the point $\mathbf{p}$ 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 Proposition 9.3).

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 $f: X \to \mathbb{R}$ be a twice continuously differentiable real-valued function defined over some open set in $\mathbb{R}^n$, and let $\mathbf{p}$ be a point of the domain of f at which the first order partial derivatives of f are zero. The above lemma shows that if the function f has a local minimum at $\mathbf{p}$ 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 $f: \mathbb{R}^2 \to \mathbb{R}$ defined by $f(x, y) = x^2 - y^3$. The first order partial derivatives of f are zero at $(0, 0)$. The Hessian matrix of f at $(0, 0)$ is the matrix

$$\left(\begin{array}{cc} 2 & 0 \\ 0 & 0 \end{array}\right).$$

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

The following theorem shows that if the Hessian matrix 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 9.6 *Let $f: X \to \mathbb{R}$ be a twice continuously differentiable real-valued function defined over 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 $(H_{i,j}(\mathbf{p}))$ of the function f at the point $\mathbf{p}$ is positive definite. Then f has a local minimum at $\mathbf{p}$.

Proof The first order partial derivatives of f take the value 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 Proposition 9.3). Suppose that the Hessian matrix $(H_{i,j}(\mathbf{p}))$ is positive definite. Then there exists some positive real number ε small enough to ensure 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 (see Lemma 9.4).

But it follows from the continuity of the second order partial derivatives of f that there exists some positive real number δ small enough to ensure that $\mathbf{x} \in X$ and $|H_{i,j}(\mathbf{x}) - H_{i,j}(\mathbf{p})| < \varepsilon$ for all integers i and j between 1 and n whenever $|\mathbf{x} - \mathbf{p}| < \delta$. Thus if $0 < |\mathbf{h}| < \delta$ 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 the function 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

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

Now

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

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 9.6 that the function f has a local minimum at $(0, 0)$.