Higher order partial derivatives and the Hessian matrix

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The partial derivative of f w.r.t. x_i is the function denoted by $f_{x_i}\left(\underset{\sim}{x}\right)$ or $\frac{\partial f}{\partial x_i}\left(\underset{\sim}{x}\right)$ and defined as

$$\frac{\partial f}{\partial x_i}\left(\underset{\sim}{x}\right) = \lim_{h \to 0} \frac{f\left(\underset{\sim}{x} + he_i\right) - f\left(\underset{\sim}{x}\right)}{h} \quad .$$

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The partial derivative of f w.r.t. x_i at a point $\underset{\sim}{a}$ measures the rate of change of f at $\underset{\sim}{a}$ in the direction of the standard basis vector e_i (i.e. w.r.t. the variable x_i).

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Notation :

- $f_{xx} = (f_x)_x$ or $\dfrac{\partial^2 f}{\partial x^2} = \dfrac{\partial}{\partial x}\left(\dfrac{\partial f}{\partial x}\right)$
- $f_{yy} = (f_y)_y$ or $\dfrac{\partial^2 f}{\partial y^2} = \dfrac{\partial}{\partial y}\left(\dfrac{\partial f}{\partial y}\right)$
- $f_{xy} = (f_x)_y$ or $\dfrac{\partial^2 f}{\partial y \partial x} = \dfrac{\partial}{\partial y}\left(\dfrac{\partial f}{\partial x}\right)$
- $f_{yx} = (f_y)_x$ or $\dfrac{\partial^2 f}{\partial x \partial y} = \dfrac{\partial}{\partial x}\left(\dfrac{\partial f}{\partial y}\right)$

Mixed partial derivatives

Examples

$f(x, y) = x + y$

$$\frac{\partial f}{\partial x} = 1 \qquad \frac{\partial f}{\partial y} = 1.$$

$$\frac{\partial^2 f}{\partial x^2} = 0 \quad , \quad \frac{\partial^2 f}{\partial y^2} = 0, \quad \frac{\partial^2 f}{\partial x \partial y} = 0 \quad , \quad \frac{\partial^2 f}{\partial y \partial x} = 0.$$

$f(x, y) = sin(xy)$

$$\frac{\partial f}{\partial x} = y \cos(xy) \quad , \quad \frac{\partial f}{\partial y} = x \cos(xy).$$

$$\frac{\partial^2 f}{\partial x^2} = y \times \{-\sin(xy)\, y\} \quad , \quad \frac{\partial^2 f}{\partial y^2} = -x^2 \sin(xy).$$

$$= -y^2 \sin(xy)$$

$$\frac{\partial^2 f}{\partial x \partial y} = 1 \times \cos(xy) + x \times \{y \sin(xy)\}$$

$$= \cos(xy) - xy \sin(xy).$$

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$=$

Clairaut's Theorem about mixed partials

Theorem (Clairaut's theorem)

Let $f(x, y)$ be a function defined on a domain D in $\mathbb{R}^2$ containing a point $\underset{\sim}{a}$ and an open ball around it.

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Let $f(x, y)$ be a function defined on a domain D in $\mathbb{R}^2$ containing a point $\underset{\sim}{a}$ and an open ball around it.

If the second order mixed partial derivatives f_{xy} and f_{yx} are continuous in an open ball around $\underset{\sim}{a}$, then $f_{xy}\left(\underset{\sim}{a}\right) = f_{yx}\left(\underset{\sim}{a}\right)$.

Example advising caution

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

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

$$\frac{\partial f}{\partial y}(0,0) = 0.$$

$$\frac{\partial f}{\partial x}(x,y) = \frac{(x^2+y^2)\{y(x^2-y^2) + xy(2x)\} - xy(x^2-y^2)2x}{(x^2+y^2)^2} = \frac{-y^5 + x^4y + 4x^2y^3}{(x^2+y^2)^2}$$

if $(x,y) \neq (0,0)$.

$$\frac{\partial f}{\partial y}(x,y) = \frac{x^5 - xy^4 - 4x^3y^2}{(x^2+y^2)^2}$$

$$\frac{\partial^2 f}{\partial x \partial y}(0,0) = \lim_{h\to 0} \frac{\frac{\partial f}{\partial y}(h,0) - \frac{\partial f}{\partial y}(0,0)}{h} = \lim_{h\to 0} \frac{h^5/(h^2+0^2)^2 - 0}{h} = \lim_{h\to 0} \frac{h-0}{h} = 1.$$

$$\neq$$

$$\frac{\partial^2 f}{\partial y \partial x}(0,0) = \lim_{h\to 0} \frac{\partial f/\partial x\,(0,h) - \frac{\partial f}{\partial x}(0,0)}{h} = \lim_{h\to 0} \frac{-h^5/(0^2+h^2)^2 - 0}{h} = -1.$$

Second order partial derivatives

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Let $f(x_1, x_2, \ldots, x_n)$ be a function defined on a domain D in $\mathbb{R}^n$. Then the second order partial derivatives of f are defined analogously as the partial derivatives of the partial derivatives.

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Let $f(x_1, x_2, \dots, x_n)$ be a function defined on a domain D in $\mathbb{R}^n$. Then the second order partial derivatives of f are defined analogously as the partial derivatives of the partial derivatives.

$$f_{x_i x_i} = (f_{x_i})_{x_i} \quad \text{or} \quad \frac{\partial^2 f}{\partial x_i^2} = \frac{\partial}{\partial x_i}\left(\frac{\partial f}{\partial x_i}\right)$$

$$f_{x_i x_j} = (f_{x_i})_{x_j} \quad \text{or} \quad \frac{\partial^2 f}{\partial x_j \partial x_i} = \frac{\partial}{\partial x_j}\left(\frac{\partial f}{\partial x_i}\right).$$

Example : $f(x, y) = xy + yz + zx$

$$\frac{\partial f}{\partial x} = y + z, \quad \frac{\partial f}{\partial y} = x + z, \quad \frac{\partial f}{\partial z} = x + y.$$

$$\frac{\partial^2 f}{\partial x^2} = 0, \quad \frac{\partial^2 f}{\partial y \partial x} = 1. \quad \frac{\partial^2 f}{\partial z \partial x} = 1.$$

$$\frac{\partial^2 f}{\partial x \partial y} = 1. \quad \frac{\partial^2 f}{\partial y^2} = 0 \quad \frac{\partial^2 f}{\partial z \partial y} = 1.$$

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Higher order partial derivatives

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Let $f(x_1, x_2, \ldots, x_n)$ be a function defined on a domain D in $\mathbb{R}^n$. Then the higher order partial derivatives of f are defined analogously by taking successive partial derivatives.

$$f_{x_{i_1} x_{i_2} \ldots x_{i_k}} = \left(\left(\left(f_{x_{i_1}}\right)_{x_{i_2}}\right)_{x_{i_3}} \cdots\right)_{x_{i_k}}$$

or

$$\frac{\partial^k f}{\partial x_{i_k} \ldots \partial x_{i_2} \partial x_{i_1}} = \frac{\partial}{\partial x_{i_k}}\left(\frac{\partial}{\partial x_{i_{k-1}}}\left(\frac{\partial}{\partial x_{i_{k-2}}}\left(\cdots\left(\frac{\partial f}{\partial x_{i_1}}\right)\right)\right)\right)$$

An appropriately modified statement of Clairaut's theorem holds.

Under suitable hypothesis

$$f_{x_{i_1} x_{i_2} \cdots x_{i_k}} = f_{x_{i_{j_1}} x_{i_{j_2}} \cdots x_{i_{j_k}}}.$$

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Then the Hessian matrix of f is defined as :

$$Hf = \begin{array}{cc}
\begin{array}{cccccc} & & & i^{th}\text{ column} & & \end{array} & \\
\begin{bmatrix}
\frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_j} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\
\frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_j} & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_n} \\
\cdots & \cdots & \ddots & \cdots & \cdots & \cdots \\
\frac{\partial^2 f}{\partial x_i \partial x_1} & \frac{\partial^2 f}{\partial x_i \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_i \partial x_j} & \cdots & \frac{\partial^2 f}{\partial x_i \partial x_n} \\
\cdots & \cdots & \ddots & \cdots & \cdots & \cdots \\
\frac{\partial^2 f}{\partial x_n \partial x_1} & \frac{\partial^2 f}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_n \partial x_j} & \cdots & \frac{\partial^2 f}{\partial x_n^2}
\end{bmatrix} & i^{th}\text{ row}
\end{array}$$

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Examples

$f(x, y) = x + y$

$$Hf = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}_{2\times 2}$$

$f(x, y) = sin(xy)$

$$Hf = \begin{bmatrix} -y^2 \sin(xy) & \cos(xy) - xy\sin(xy) \\ \cos(xy) - xy\sin(xy) & -x^2\sin(xy) \end{bmatrix}$$

$f(x, y, z) = xy + yz + zx$

$$Hf = \begin{bmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{bmatrix}_{3\times 3}$$

Thank you