Derivatives for multivariate functions

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Multivariate functions

 A function depending on more than one variable is called multivariate function.

Example:

 $f(x,y) := x^2 + 2xy + 1$



Let
$$f(x) = f(x_1, x_2, ..., x_n)$$
 be a multivariate function

The partial derivative in the x_i direction in $x^{(0)} = (x_1^{(0)}, x_2^{(0)}, \dots, x_n^{(0)})$ is

$$\frac{\partial}{\partial x_i} f(x^{(0)}) := \lim_{x \to x_i^{(0)}} \frac{f(x_1^{(0)}, \dots, x_{i-1}^{(0)}, x, x_{i+1}^{(0)}, \dots, x_n^{(0)}) - f(x^{(0)})}{x - x_i^{(0)}}$$

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The partial derivative is just the derivative wrt. x_i where the other values are treated as constants.

Function f



 $f(x,y) = x^2 + 2xy + 1$

Function *f*



 $f(x,y) = x^2 + 2xy + 1$

Function *f* with fixed $y_0 = -1$



 $f_{y=-1}(x) = x^2 - 2x + 1$

Function *f*



 $f(x,y) = x^2 + 2xy + 1$

Function *f* with fixed $y_0 = -1$



Function *f*



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

Function *f* with fixed $y_0 = -1$



■ The partial derivative ∂∂x_i f(x) again depends on the whole vector x = (x₁,..., x_n).

The vector of all partial derivatives

$$\nabla f(\mathbf{x}) := \begin{pmatrix} \frac{\partial}{\partial x_1} f(\mathbf{x}) \\ \vdots \\ \frac{\partial}{\partial x_n} f(\mathbf{x}) \end{pmatrix}$$

is called the **gradient** of f.

The gradient is a vector that points in the direction of steepest increase

Extrema of multivariate functions

A point $x^{(0)} \in \mathbb{R}^n$ is a **local maximum** of $f : \mathbb{R}^n \to \mathbb{R}$ if there is a $\epsilon > 0$ with

$$f(x_0) \ge f(x)$$
 for all x with $||x - x_0|| < \epsilon$

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 for all x with $||x - x_0|| < \epsilon$



Theorem

If $x^{(0)}$ is a extreme point, then

$$\nabla f(\mathbf{x}^{(0)}) := \begin{pmatrix} \frac{\partial}{\partial \mathbf{x}_1} f(\mathbf{x}^{(0)}) \\ \vdots \\ \frac{\partial}{\partial \mathbf{x}_n} f(\mathbf{x}^{(0)}) \end{pmatrix} = \mathbf{0}.$$

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 $\nabla f(x) = 0$ is only a **necessary condition** for an extreme point.

Definition

The symmetric matrix

$$H^{f}(\mathbf{x}^{(0)}) := \begin{pmatrix} \frac{\partial^{2}}{\partial x_{1}} f(\mathbf{x}^{(0)}) & \frac{\partial^{2}}{\partial x_{1} \partial x_{2}} f(\mathbf{x}^{(0)}) & \cdots & \frac{\partial^{2}}{\partial x_{1} \partial x_{n}} f(\mathbf{x}^{(0)}) \\ \frac{\partial^{2}}{\partial x_{2} \partial x_{1}} f(\mathbf{x}^{(0)}) & \frac{\partial^{2}}{\partial^{2} x_{2}} f(\mathbf{x}^{(0)}) & \cdots & \frac{\partial^{2}}{\partial x_{2} \partial x_{n}} f(\mathbf{x}^{(0)}) \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^{2}}{\partial x_{n} \partial x_{1}} f(\mathbf{x}^{(0)}) & \frac{\partial^{2}}{\partial x_{n} \partial x_{2}} f(\mathbf{x}^{(0)}) & \cdots & \frac{\partial^{2}}{\partial^{2} x_{n}} f(\mathbf{x}^{(0)}) \end{pmatrix}$$

is called **Hessian matrix** of f at x_0 .

Theorem

A function f has a local maximum/minimum at x_0 if

•
$$\nabla f(\mathbf{x}^{(0)}) = 0$$
 and

•
$$H^{f}(x^{(0)})$$
 is positive/negative definite

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Theorem

A function f has a local maximum/minimum at x_0 if

- $\nabla f(x^{(0)}) = 0$ and
- $H^{f}(\mathbf{x}^{(0)})$ is positive/negative definite $\Leftrightarrow All$ eigenvalues of $H^{f}(\mathbf{x}^{(0)})$ are positive/negative

Criteria for local extrema for n = 2

$$f: \mathbb{R}^2 \to \mathbb{R}^2 \text{ has a local maximum/minimum at } (x^{(0)}, y^{(0)}) \text{ if}$$

$$= \frac{\partial}{\partial x} f(x^{(0)}, y^{(0)}) = \frac{\partial}{\partial y} f(x^{(0)}, y^{(0)}) = 0 \quad \text{(Necessary condition)}$$

$$= \det \left(H^f(x^{(0)}, y^{(0)}) \right) > 0 \text{ and}$$

$$= \frac{\partial^2}{\partial^2 x} f(x^{(0)}, y^{(0)}) < 0 \text{ or } \quad \text{(Sufficient condition for maximum)}$$

$$= \frac{\partial^2}{\partial^2 x} f(x^{(0)}, y^{(0)}) > 0 \quad \text{(Sufficient condition for minimum)}$$

■ The determinant of *H^f* can be computed as

$$\det\left(H^{f}(x^{(0)}, y^{(0)})\right) = \frac{\partial^{2}}{\partial^{2}x} f(x^{(0)}, y^{(0)}) \cdot \frac{\partial^{2}}{\partial^{2}y} f(x^{(0)}, y^{(0)}) - \left(\frac{\partial^{2}}{\partial x \partial y} f(x^{(0)}, y^{(0)})\right)^{2}$$