

Differential Properties of Functions Defined on \mathbb{R}^n

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Let S be an open subset of \mathbb{R}^n and let $f : S \rightarrow \mathbb{R}$ be a function. The partial derivatives of f are denoted by $\frac{\partial f}{\partial x_i}$ for $1 \leq i \leq n$. The second order partial derivatives are denoted by

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

Definition

The linear form

$$f'(\mathbf{x}, \mathbf{h}) = \sum_{i=1}^n \frac{\partial f}{\partial x_i} h_i$$

is the **first differential** of f at \mathbf{x} .

It is also the derivative at $t = 0$ of the function $g(t) = f(\mathbf{x} + t\mathbf{h})$.

$f'(\mathbf{x}, \mathbf{h})$ can be interpreted as the derivative of f at \mathbf{x} in the direction \mathbf{h} .

Definition

The **gradient** of f at \mathbf{x} is the vector

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

We have $f'(\mathbf{x}, \mathbf{h}) = \nabla f(\mathbf{x})' \mathbf{h}$.

The quadratic form

$$f''(\mathbf{x}, \mathbf{h}) = \sum_{i=1}^n \sum_{j=1}^n \frac{\partial^2 f}{\partial x_i \partial x_j} h_i h_j$$

is **the second order differential** of f at \mathbf{x} .

It is also the second order derivative of the function $g(t) = f(\mathbf{x} + t\mathbf{h})$; accordingly, it is the second order derivative of f at \mathbf{x} in the direction \mathbf{h} .

The matrix of second derivatives of f is

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

is called the *Hessian* of f at \mathbf{x} .

Taylor Theorem for One Argument Functions

Theorem

(Taylor's Theorem for One-Argument Functions) Let $f : [a, b] \rightarrow \mathbb{R}$ be a function such that f together with its first $n - 1$ derivatives $f^{(1)}, \dots, f^{(n-1)}$ are continuous on the interval $[a, b]$. If $f^{(n)}$ exists on (a, b) , then there exists $c \in (a, b)$ such that

$$\begin{aligned} f(b) = & f(a) + f^{(1)}(a)(b-a) + \frac{f^{(2)}(a)}{2!}(b-a)^2 + \dots \\ & + \frac{f^{(n-1)}(a)}{(n-1)!}(b-a)^{n-1} + \frac{f^{(n)}(c)}{n!}(b-a)^n. \end{aligned}$$

Proof

Let $\phi : [a, b] \longrightarrow \mathbb{R}$ be the function defined by

$$\begin{aligned}\phi(x) = & f(b) - f(x) - f^{(1)}(x)(b-x) - \frac{f^{(2)}(x)}{2!}(b-x)^2 - \dots \\ & - \frac{f^{(n-1)}(x)}{(n-1)!}(b-x)^{n-1}.\end{aligned}$$

The derivative of ϕ exists for any $x \in (a, b)$ and is easily seen to be

$$\phi'(x) = -\frac{f^{(n)}(x)}{(n-1)!}(b-x)^{n-1}.$$

Define the function $g : [a, b] \longrightarrow \mathbb{R}$ as

$$g(x) = \phi(x) - \left(\frac{b-x}{b-a}\right)^n \phi(a).$$

Proof (cont'd)

Since $g(a) = g(b) = 0$, by Rolle's Theorem from elementary analysis, there exists $c \in (a, b)$ such that $g'(c) = 0$. Note that

$$g'(x) = \phi'(x) + n \frac{(b-x)^{n-1}}{(b-a)^n} \phi(a),$$

so

$$\phi'(c) + n \frac{(b-c)^{n-1}}{(b-a)^n} \phi(a) = 0.$$

Proof (cont'd)

Since $\phi'(c) = -\frac{f^{(n)}(c)}{(n-1)!}(b-c)^{n-1}$, it follows that

$$\phi(a) = (b-a)^n n! f^{(n)}(c),$$

which implies the desired equality

$$\begin{aligned} f(b) - f(a) - f^{(1)}(a)(b-a) - \frac{f^{(2)}(a)}{2!}(b-a)^2 - \dots - \frac{f^{(n-1)}(a)}{(n-1)!}(b-a)^{n-1} \\ = \frac{(b-a)^n}{n!} f^{(n)}(c). \end{aligned}$$

Notations

Let $f : S \rightarrow \mathbb{R}$ be a function, where $S \subseteq \mathbb{R}^n$. If all partial derivatives $\frac{\partial^k f}{\partial x_{i_1} \cdots \partial x_{i_k}}$ exist for $1 \leq k \leq n$ and $\mathbf{h} \in \mathbb{R}^n$, define the expression

$$f^{[k]}(\mathbf{x}; \mathbf{h}) = \sum_{i_1=1}^n \cdots \sum_{i_k=1}^n \frac{\partial^k f}{\partial x_{i_1} \cdots \partial x_{i_k}}(\mathbf{x}) h_{i_1} \cdots h_{i_k}.$$

This notation is needed for formulating Taylor's Theorem for functions of n variables. Note that

$$f^{[k]}(\mathbf{x}; \lambda \mathbf{h}) = \lambda^k f^{[k]}(\mathbf{x}; \mathbf{h}).$$

The function $f^{[1]}(\mathbf{x}; \mathbf{h})$ is $f'(\mathbf{x}, \mathbf{h})$, the *differential* of the function f .

Notations

For $k = 2$, we have

$$\begin{aligned} f^{[2]}(\mathbf{x}; \mathbf{h}) &= \sum_{i_1=1}^n \sum_{i_2=1}^n \frac{\partial^2 f}{\partial x_{i_1} \partial x_{i_2}}(\mathbf{x}) h_{i_1} h_{i_2} \\ &= \mathbf{h}' H_f(\mathbf{x}) \mathbf{h}, \end{aligned}$$

where $H_f(\mathbf{x}) \in \mathbb{R}^{n \times n}$, the matrix defined by

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

is the as the *Hessian matrix* of the function f at \mathbf{x} .

$f^{[2]}(\mathbf{x}; \mathbf{h})$ is $f''(\mathbf{x}, \mathbf{h})$ the second order differential of f at \mathbf{x} .

Taylor's Theorem for Functions of Several Arguments

Theorem

Let $f : S \longrightarrow \mathbb{R}$ be a function, where $S \subseteq \mathbb{R}^n$ is an open set. If f and all its partial derivatives of order less or equal to m are differentiable on S , $\mathbf{a}, \mathbf{b} \in S$ such that $[\mathbf{a}, \mathbf{b}] \subseteq S$, then there exists a point $\mathbf{c} \in [\mathbf{a}, \mathbf{b}]$ such that

$$f(\mathbf{b}) = f(\mathbf{a}) + \sum_{k=1}^{m-1} \frac{1}{k!} f^{[k]}(\mathbf{a}, \mathbf{b} - \mathbf{a}) + \frac{1}{m!} f^{[m]}(\mathbf{c}, \mathbf{b} - \mathbf{a}).$$

Proof

Let $g : \mathbb{R} \longrightarrow \mathbb{R}$ be the function defined by $g(t) = f(\mathbf{p}(t))$, where $\mathbf{p}(t) = \mathbf{a} + t(\mathbf{b} - \mathbf{a})$ for $t \in [0, 1]$. We have $g(0) = f(\mathbf{a})$ and $g(1) = f(\mathbf{b})$. The Taylor's formula applied to g yields the existence of $c \in (0, 1)$ such that

$$g(1) = g(0) + \sum_{k=1}^{m-1} \frac{1}{k!} g^{(k)}(0) + g^{(m)}(c).$$

We claim that

$$g^{(m)}(t) = f^{[m]}(\mathbf{p}(t), \mathbf{b} - \mathbf{a}).$$

Indeed, for $m = 1$, by applying the chain rule we have

$$g'(t) = \sum_{j=1}^m \frac{\partial f}{\partial x_j}(\mathbf{p}(t))(b_j - a_j) = f^{[1]}(\mathbf{x}; \mathbf{b} - \mathbf{a}).$$

Proof (cont'd)

Suppose that the equality holds for m . Then

$$\begin{aligned}
 g^{(m+1)}(t) &= (f^{[m]}(\mathbf{p}(t), \mathbf{b} - \mathbf{a}))' \\
 &= \left(\sum_{i_1=1}^n \cdots \sum_{i_m=1}^n \frac{\partial^m f}{\partial x_{i_1} \cdots \partial x_{i_m}}(\mathbf{p}(t))(b_{i_1} - a_{i_1}) \cdots (b_{i_m} - a_{i_m}) \right)' \\
 &= \sum_{i_1=1}^n \cdots \sum_{i_m=1}^n \sum_{i_{m+1}=1}^n \frac{\partial^{m+1} f}{\partial x_{i_1} \cdots \partial x_{i_{m+1}}}(\mathbf{p}(t))(b_{i_1} - a_{i_1}) \cdots (b_{i_m} - a_{i_m})(b_{i_{m+1}} - a_{i_{m+1}}) \\
 &= f^{[m+1]}(\mathbf{p}(t), \mathbf{b} - \mathbf{a}).
 \end{aligned}$$

When the values of the derivatives of g are substituted we obtain the equality of the theorem.

Proof

Example

For $m = 2$, Taylor's Theorem yields the existence of $\mathbf{c} \in [\mathbf{a}, \mathbf{b}]$ such that

$$\begin{aligned} f(\mathbf{b}) &= f(\mathbf{a}) + f^{[1]}(\mathbf{a}, \mathbf{b} - \mathbf{a}) + \frac{1}{2}(\mathbf{b} - \mathbf{a})' H_f(\mathbf{c})(\mathbf{b} - \mathbf{a}) \\ &= f(\mathbf{a}) + (\nabla f)'_{\mathbf{a}}(\mathbf{b} - \mathbf{a}) + \frac{1}{2}(\mathbf{b} - \mathbf{a})' H_f(\mathbf{c})(\mathbf{b} - \mathbf{a}). \end{aligned}$$

Example

Let $f : \mathbb{R}^3 \rightarrow \mathbb{R}$ be the function given by $f(\mathbf{x}) = \|\mathbf{x}\|$ for $\mathbf{x} \in \mathbb{R}^3$. We have

$$\frac{\partial f}{\partial x_1} = \frac{x_1}{\sqrt{x_1^2 + x_2^2 + x_3^2}} = \frac{x_1}{\|\mathbf{x}\|},$$

and similar expressions for $\frac{\partial f}{\partial x_2}$ and $\frac{\partial f}{\partial x_3}$ and we have

$$(\nabla f)_{\mathbf{x}_0} = \frac{1}{\|\mathbf{x}_0\|} \mathbf{x}_0$$

if $\mathbf{x}_0 \neq \mathbf{0}_3$. The gradient $\nabla(f)_{\mathbf{x}_0}$ is a unit vector for every $\mathbf{x}_0 \in \mathbb{R}^3 - \{\mathbf{0}_3\}$.

Example (cont'd)

The function $R(\mathbf{x}_0, \mathbf{x})$ is given by

$$\begin{aligned} R(\mathbf{x}_0, \mathbf{x}) &= \frac{f(\mathbf{x}) - f(\mathbf{x}_0) - (\nabla f)'_{\mathbf{x}_0}(\mathbf{x} - \mathbf{x}_0)}{\|\mathbf{x} - \mathbf{x}_0\|} \\ &= \frac{\|\mathbf{x}\| - \|\mathbf{x}_0\| - \frac{1}{\|\mathbf{x}_0\|} \mathbf{x}'_0(\mathbf{x} - \mathbf{x}_0)}{\|\mathbf{x} - \mathbf{x}_0\|} \end{aligned}$$

Therefore, the function f is differentiable in \mathbf{x}_0 if $\mathbf{x}_0 \neq \mathbf{0}_3$.

Example

Let $f : \mathbb{R}^3 \rightarrow \mathbb{R}$ be the function given by $f(\mathbf{x}) = \|\mathbf{x}\|^2$ for $\mathbf{x} \in \mathbb{R}^3$. We have

$$\frac{\partial f}{\partial x_1} = 2x_1, \frac{\partial f}{\partial x_2} = 2x_2, \frac{\partial f}{\partial x_3} = 2x_3,$$

so $(\nabla f)_{\mathbf{x}} = 2\mathbf{x}$ and this function is differentiable for all $\mathbf{x} \in \mathbb{R}^3$.

Definition

Let $f : \mathbb{R}^n \rightarrow \mathbb{R}$ be a function.

A point $\mathbf{x}_0 \in \mathbb{R}^n$ is a **local minimum** for f if there exists a closed sphere $B(\mathbf{x}_0, \epsilon)$ such that $f(\mathbf{x}_0) \leq f(\mathbf{x})$ for every $\mathbf{x} \in B(\mathbf{x}_0, \epsilon)$. If we have $f(\mathbf{x}_0) < f(\mathbf{x})$ for every $\mathbf{x} \in B(\mathbf{x}_0, \epsilon) - \{\mathbf{x}_0\}$, then \mathbf{x}_0 is a **strict local minimum**.

A **global minimum** for f is a point \mathbf{x}_0 such that $f(\mathbf{x}_0) \leq f(\mathbf{x})$ for $\mathbf{x} \in \mathbb{R}^n$; \mathbf{x}_0 is a **strict global minimum** if $f(\mathbf{x}_0) < f(\mathbf{x})$ for $\mathbf{x} \in \mathbb{R}^n - \{\mathbf{x}_0\}$.

Similar definitions can be formulated for local maxima, strict local maxima, global maxima, and strict global maxima:

$\mathbf{x}_0 \in \mathbb{R}^n$ is a **local maximum** if there exists a closed sphere $B(\mathbf{x}_0, \epsilon)$ such that $f(\mathbf{x}_0) \geq f(\mathbf{x})$ for every $\mathbf{x} \in B(\mathbf{x}_0, \epsilon)$. If $f(\mathbf{x}_0) > f(\mathbf{x})$ for every $\mathbf{x} \in B(\mathbf{x}_0, \epsilon) - \{\mathbf{x}_0\}$, then \mathbf{x}_0 is a **strict local maximum**.

A **global maximum** for f is a point \mathbf{x}_0 such that $f(\mathbf{x}_0) \geq f(\mathbf{x})$ for $\mathbf{x} \in \mathbb{R}^n$; \mathbf{x}_0 is a **strict global maximum** if $f(\mathbf{x}_0) > f(\mathbf{x})$ for $\mathbf{x} \in \mathbb{R}^n - \{\mathbf{x}_0\}$.

A local minimum or maximum of f is said to be a *local extremum*.

An **unconstraint optimization problem consists** in finding a local minimum or a local maximum of a function $f : \mathbb{R}^n \rightarrow \mathbb{R}$, when such a minimum exists. The function f is referred to as the **objective function**. Finding a local minimum of a function f is equivalent to finding a local maximum for the function $-f$.

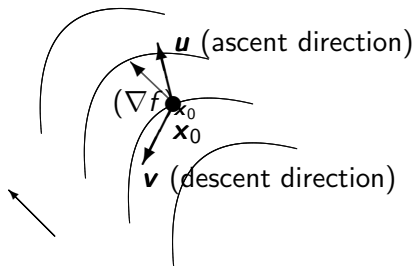
Definition

Let $f : \mathbb{R}^n \rightarrow \mathbb{R}$ be a function.

An **ascent direction** for f in \mathbf{x}_0 is a vector $\mathbf{h} \in \mathbb{R}^n$ such that there exists a positive number ϵ for which $0 < t < \epsilon$ implies $f(\mathbf{x}_0 + t\mathbf{h}) \geq f(\mathbf{x}_0)$.

A **descent direction** for f in \mathbf{x}_0 is a vector $\mathbf{h} \in \mathbb{R}^n$ such that exists a positive number ϵ for which $0 < t < \epsilon$ implies $f(\mathbf{x}_0 + t\mathbf{h}) \leq f(\mathbf{x}_0)$.

If $f : \mathbb{R}^n \rightarrow \mathbb{R}$ is a differentiable function, the existence of the gradient provides new instruments for computing extrema. The vector $(\nabla f)_x$ points in the direction of increased values of the function f .



direction of increase of $f(x)$

An ascent direction u in x_0 makes an acute angle with the vector $(\nabla f)_{x_0}$, while a descent direction v makes an obtuse angle with the same vector, as we see in the next statement.

Theorem

Let $f : \mathbb{R}^n \rightarrow \mathbb{R}$ be a differentiable function at \mathbf{x}_0 .

If $(\nabla f)'_{\mathbf{x}_0} \mathbf{w} < 0$, then \mathbf{w} is a descent direction for f in \mathbf{x}_0 .

If $(\nabla f)'_{\mathbf{x}_0} \mathbf{w} > 0$, then \mathbf{w} is an ascent direction for f in \mathbf{x}_0 .

Proof

Since f is differentiable in \mathbf{x}_0 we can write

$$f(\mathbf{x}_0 + t\mathbf{w}) = f(\mathbf{x}_0) + t(\nabla f)'_{\mathbf{x}_0} \mathbf{w} + t \|\mathbf{w}\| R(\mathbf{x}_0, \mathbf{x}_0 + t\mathbf{w}),$$

for $t > 0$, where $\lim_{t \rightarrow 0} R(\mathbf{x}_0, \mathbf{x}_0 + t\mathbf{w}) = 0$. This implies

$$\frac{f(\mathbf{x}_0 + t\mathbf{w}) - f(\mathbf{x}_0)}{t} = (\nabla f)'_{\mathbf{x}_0} \mathbf{w} + \|\mathbf{w}\| R(\mathbf{x}_0, \mathbf{x}_0 + t\mathbf{w}).$$

Since $(\nabla f)'_{\mathbf{x}_0} \mathbf{w} < 0$ and $\lim_{t \rightarrow 0} R(\mathbf{x}_0, \mathbf{x}_0 + t\mathbf{w}) = 0$, there exists $\epsilon > 0$ such that $0 < t < \epsilon$ implies $f(\mathbf{x}_0 + t\mathbf{w}) - f(\mathbf{x}_0) \leq 0$, so \mathbf{w} is a descent direction. The argument for the second part of the theorem is similar.

Theorem

Let $f : \mathbb{R}^n \rightarrow \mathbb{R}$ be a function differentiable at \mathbf{x}_0 . If \mathbf{x}_0 is a local minimum or a local maximum, then $(\nabla f)_{\mathbf{x}_0} = \mathbf{0}_n$.

Proof

Let \mathbf{x}_0 be a local minimum of f . Suppose that $(\nabla f)_{\mathbf{x}_0} \neq \mathbf{0}_n$ and let $\mathbf{w} = -(\nabla f)_{\mathbf{x}_0}$. We have $(\nabla f)'_{\mathbf{x}_0} \mathbf{w} < 0$, so, by Theorem ??, \mathbf{w} is a descent direction, that is, there exists a positive number ϵ such that $0 < t < \epsilon$ implies $f(\mathbf{x}_0 + t\mathbf{w}) \leq f(\mathbf{x}_0)$, which contradicts the initial assumption concerning \mathbf{x}_0 . Therefore, $(\nabla f)_{\mathbf{x}_0} = \mathbf{0}_n$.

The case when \mathbf{x}_0 is a local maximum can be treated similarly.

Definition

A *stationary point* of a differentiable function $f : S \longrightarrow \mathbb{R}$ (where $S \subseteq \mathbb{R}^n$) is a point $\mathbf{x} \in S$ such that $(\nabla f)_{\mathbf{x}} = \mathbf{0}_n$.

Observe that a stationary point of a function is not necessarily a local extremum of the function, as the next example shows.

Example

Consider the function $f : \mathbb{R}^2 \longrightarrow \mathbb{R}$ defined by $f(x_1, x_2) = x_1 x_2$ for $(x_1, x_2) \in \mathbb{R}^2$. We have

$$(\nabla f)_{\mathbf{x}} = \begin{pmatrix} x_2 \\ x_1 \end{pmatrix},$$

which shows that $\mathbf{0}_2$ is a stationary point of f . Note that in any sphere $B(\mathbf{0}_2, \epsilon)$ there are both positive and negative numbers. Since $f(\mathbf{0}_2) = 0$, it is clear that although $\mathbf{0}_2$ is a stationary point of f , $\mathbf{0}_2$ is not a local extremum.

For functions that are twice differentiable it is possible to give characterizations of local extrema.

The next theorem gives sufficient conditions for the existence of a local minimum.

Theorem

Let $f : \mathbb{R}^n \rightarrow \mathbb{R}$ be a twice differentiable function at \mathbf{x}_0 .

If $(\nabla f)_{\mathbf{x}_0} = \mathbf{0}_n$, and the Hessian matrix $H_f(\mathbf{x}_0)$ is positive definite, then \mathbf{x}_0 is a local minimum of f .

By Taylor's Theorem, taking into account that $(\nabla f)_{\mathbf{x}_0} = \mathbf{0}_n$, we have

$$\begin{aligned} f(\mathbf{x}) &= f(\mathbf{x}_0) + (\mathbf{x} - \mathbf{x}_0)' H_f(\mathbf{x}_0) (\mathbf{x} - \mathbf{x}_0) \\ &\quad + \|\mathbf{x} - \mathbf{x}_0\|^2 R(\mathbf{x}_0, \mathbf{x} - \mathbf{x}_0), \end{aligned}$$

where $\lim_{\mathbf{x} \rightarrow \mathbf{x}_0} R(\mathbf{x}_0, \mathbf{x} - \mathbf{x}_0) = 0$.

Suppose that \mathbf{x}_0 is not a minimum. Then, there exists a sequence $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n, \dots$ such that $\lim_{n \rightarrow \infty} \mathbf{x}_n = \mathbf{x}_0$ such that $f(\mathbf{x}_n) < f(\mathbf{x}_0)$ for each $n \geq 1$. Let \mathbf{r}_n be the unit vector $\mathbf{r}_n = \frac{1}{\|\mathbf{x}_n - \mathbf{x}_0\|} (\mathbf{x}_n - \mathbf{x}_0)$.

Proof (cont'd)

We have

$$\begin{aligned} f(\mathbf{x}_n) &= f(\mathbf{x}_0) + \|\mathbf{x}_n - \mathbf{x}_0\|^2 \mathbf{r}_n' H_f(\mathbf{x}_0) \mathbf{r}_n \\ &\quad + \|\mathbf{x}_n - \mathbf{x}_0\|^2 R(\mathbf{x}_0, \mathbf{x}_n - \mathbf{x}_0) < f(\mathbf{x}_0), \end{aligned}$$

which implies

$$\mathbf{r}_n' H_f(\mathbf{x}_0) \mathbf{r}_n + R(\mathbf{x}_0, \mathbf{x}_n - \mathbf{x}_0) < 0.$$

The sequence $(\mathbf{r}_1, \dots, \mathbf{r}_n, \dots)$ is bounded since it consists of unit vectors and, therefore, it contains a subsequence convergent subsequence $(\mathbf{r}_{i_1}, \dots, \mathbf{r}_{i_m}, \dots)$ such that $\lim_{m \rightarrow \infty} \mathbf{r}_{i_m} = \mathbf{r}$ and $\|\mathbf{r}\| = 1$. This implies $\mathbf{r}' H_f(\mathbf{x}_0) \mathbf{r} \leq 0$, which contradicts the fact that $H_f(\mathbf{x}_0)$ is positive definite. Therefore, \mathbf{x}_0 is a local minimum.