Taylor expansion

Main theorems

Theorem 1. *Let $U \subseteq \mathbb{R}^N$ be open and $\boldsymbol{x}_0 \in U$. Let $f: U \mapsto \mathbb{R}$ be $n+1$ times continuously partially differentiable, and let $\boldsymbol{x} \in U$ be such that $\{t\,\boldsymbol{x} + (1-t)\,\boldsymbol{x_0} |\, t \in [0,1]\} \subseteq U$. Then there is $\boldsymbol{\xi} = \theta\,\boldsymbol{x} + (1-\theta)\,\boldsymbol{x}_0$ for some $\theta \in [0,1]$ such that*

$$f(\boldsymbol{x}) = \sum_{|\alpha| \leqslant n} \frac{1}{\alpha!} \frac{\partial^\alpha f}{\partial \boldsymbol{x}^\alpha}(\boldsymbol{x}_0)\,(\boldsymbol{x} - \boldsymbol{x}_0)^\alpha + R_n(\boldsymbol{x}, \boldsymbol{x}_0) \tag{1}$$

where $\alpha = (\alpha_1, \ldots, \alpha_N)$ is a multi-index (explained below), and the remainder

$$R_n(\boldsymbol{x}, \boldsymbol{x}_0) := \sum_{|\alpha| = n+1} \frac{1}{\alpha!} \frac{\partial^\alpha f}{\partial \boldsymbol{x}^\alpha}(\boldsymbol{\xi})\,(\boldsymbol{x} - \boldsymbol{x}_0)^{n+1} \tag{2}$$

Notation. (Multi-index) *A multi-index $(\alpha_1, \ldots, \alpha_N)$ is a vector in $(\mathbb{N} \cup \{0\})^N$ that is each $\alpha_i \in \{0, 1, 2, 3, \ldots\}$. Then*

- $|\alpha| := \alpha_1 + \cdots + \alpha_N$;
- $\alpha! := (\alpha_1!) \cdots (\alpha_N!)$
- *For any $\boldsymbol{x} \in \mathbb{R}^N$,*

$$\boldsymbol{x}^\alpha := x_1^{\alpha_1} \cdots x_N^{\alpha_N}. \tag{3}$$

- *For any $f: \mathbb{R}^N \mapsto \mathbb{R}$ with all $|\alpha|$-th order partial derivatives continuous,*

$$\frac{\partial^{|\alpha|} f}{\partial \boldsymbol{x}^\alpha} := \frac{\partial^{|\alpha|} f}{\partial x_1^{\alpha_1} \cdots \partial x_N^{\alpha_N}}. \tag{4}$$

Exercise 1. Let α, β be multi-indices. Let $f: \mathbb{R}^N \mapsto \mathbb{R}$ be such that all its $(|\alpha| + |\beta|)$-th order partial derivatives are continuous. Prove that

$$\frac{\partial^{|\beta|}}{\partial \boldsymbol{x}^\beta}\left(\frac{\partial^{|\alpha|} f}{\partial \boldsymbol{x}^\alpha}\right) = \frac{\partial^{|\alpha|}}{\partial \boldsymbol{x}^\alpha}\left(\frac{\partial^{|\beta|} f}{\partial \boldsymbol{x}^\beta}\right) \tag{5}$$

and thus can simply be denoted $\frac{\partial^{|\alpha+\beta|} f}{\partial \boldsymbol{x}^{\alpha+\beta}}$.

Proof. Set $g(t) := f(t\,\boldsymbol{x} + (1-t)\,\boldsymbol{x}_0) = f(\boldsymbol{x}_0 + t\,(\boldsymbol{x} - \boldsymbol{x}_0))$. Denote $\boldsymbol{\xi} := (\boldsymbol{x} - \boldsymbol{x}_0)$. Then applying the change rule we have

$$g'(t) = \sum_{i=1}^N \xi_i \frac{\partial f}{\partial x_i}, \quad g''(t) = \sum_{i,j=1}^N \xi_i\,\xi_j \frac{\partial^2 f}{\partial x_i \partial x_j} \ldots \tag{6}$$

Note that formally we can write

$$g''(t) = \left(\xi_1 \frac{\partial}{\partial x_1} + \cdots + \xi_N \frac{\partial}{\partial x_N}\right)^2 f. \tag{7}$$

In general,

$$g^{(n)}(t) = \left(\xi_1 \frac{\partial}{\partial x_1} + \cdots + \xi_N \frac{\partial}{\partial x_N} \right)^n f. \tag{8}$$

Now consider a particular multi-index α with $|\alpha| = n$. We need to figure out the factor before $\frac{\partial^n f}{\partial \boldsymbol{x}^\alpha}$ in $g^{(n)}(t)$.

First notice that when α is fixed, the $\boldsymbol{\xi}$-part of the factor must be $\boldsymbol{\xi}^\alpha$. All we need to do now is to count how many times $\boldsymbol{\xi}^\alpha \frac{\partial^n}{\partial \boldsymbol{x}^\alpha}$ appears. This number is $\frac{n!}{\alpha!}$. Consequently

$$g^{(n)}(t) = \sum_{|\alpha| = n} \frac{n!}{\alpha!} \boldsymbol{\xi}^\alpha \frac{\partial^n f}{\partial \boldsymbol{x}^\alpha}. \tag{9}$$

Now recall the single variable Taylor expansion:

$$g(1) - g(0) = \sum_{k \leqslant n} \frac{g^{(k)}(0)}{k!} + g^{(n+1)}(\theta). \tag{10}$$

This translates exactly to

$$f(\boldsymbol{x}) = \sum_{|\alpha| \leqslant n} \frac{1}{\alpha!} \frac{\partial^\alpha f}{\partial \boldsymbol{x}^\alpha}(\boldsymbol{x}_0) (\boldsymbol{x} - \boldsymbol{x}_0)^\alpha + \sum_{|\alpha| = n+1} \frac{1}{\alpha!} \frac{\partial^\alpha f}{\partial \boldsymbol{x}^\alpha}(\boldsymbol{\xi}) (\boldsymbol{x} - \boldsymbol{x}_0)^{n+1} \tag{11}$$

as desired. □

If we require less differentiability, the explicit formula (2) is not available anymore. But we can still conclude that $R_n(\boldsymbol{x}, \boldsymbol{x}_0)$ is small compared to other terms.

Theorem 2. *Let $U \subseteq \mathbb{R}^N$ be open and $\boldsymbol{x}_0 \in U$. Let $f: U \mapsto \mathbb{R}$ be n times continuously partially differentiable, and let $\boldsymbol{x} \in U$ be such that $\{t\, \boldsymbol{x} + (1-t)\, \boldsymbol{x}_0 |\, t \in [0,1]\} \subseteq U$. Then there is $\boldsymbol{\xi} = \theta\, \boldsymbol{x} + (1-\theta)\, \boldsymbol{x}_0$ for some $\theta \in [0,1]$ such that*

$$f(\boldsymbol{x}) = \sum_{|\alpha| \leqslant n} \frac{1}{\alpha!} \frac{\partial^\alpha f}{\partial \boldsymbol{x}^\alpha}(\boldsymbol{x}_0) (\boldsymbol{x} - \boldsymbol{x}_0)^\alpha + R_n(\boldsymbol{x}, \boldsymbol{x}_0) \tag{12}$$

with $\lim_{\boldsymbol{x} \longrightarrow \boldsymbol{x}_0} \frac{R_n(\boldsymbol{x}, \boldsymbol{x}_0)}{(\boldsymbol{x} - \boldsymbol{x}_0)^n} = 0$.

Proof. From the previous theorem we have

$$f(\boldsymbol{x}) = \sum_{|\alpha| \leqslant n-1} \frac{1}{\alpha!} \frac{\partial^\alpha f}{\partial \boldsymbol{x}^\alpha}(\boldsymbol{x}_0) (\boldsymbol{x} - \boldsymbol{x}_0)^\alpha + \sum_{|\alpha| = n} \frac{1}{\alpha!} \frac{\partial^\alpha f}{\partial \boldsymbol{x}^\alpha}(\boldsymbol{\xi}) (\boldsymbol{x} - \boldsymbol{x}_0)^n \tag{13}$$

Taking difference we have

$$R_n(\boldsymbol{x}, \boldsymbol{x}_0) = \sum_{|\alpha| = n} \frac{1}{\alpha!} \left[\frac{\partial^\alpha f}{\partial \boldsymbol{x}^\alpha}(\boldsymbol{\xi}) - \frac{\partial^\alpha f}{\partial \boldsymbol{x}^\alpha}(\boldsymbol{x}_0) \right] (\boldsymbol{x} - \boldsymbol{x}_0)^n. \tag{14}$$

The conclusion now follows from the continuity of the n-th partial derivatives of f. □

Exercise 2. Calculate the Taylor expansion of the following functions at $(0,0)$ and $(1,-1)$:

a) $f(x,y) = 2x^2 - x\,y - y^2 - 6x - 3y + 5$;

b) $g(x,y,z)=x^2+y^2+z^2-3\,x\,y\,z$.

Exercise 3. Calculate the second-order Taylor expansion of $f(x,y,z)=y^2\,z+x\,e^z$ at $(1,0,-2)$.

Exercise 4. Prove that

$$\lim_{(x,y)\longrightarrow(0,0)}\frac{(\cos x/\cos y)}{1-(x^2+y^2)/2}=1. \tag{15}$$

Exercise 5. State and prove theorems about Taylor expansion of functions $\boldsymbol{f}\colon\mathbb{R}^N\mapsto\mathbb{R}^M$.

Taylor expansion to degrees 1 and 2

The most useful Taylor exanpsions in practice are the following two cases:

1. $n=1$:

$$\begin{aligned} f(\boldsymbol{x}) &= \sum_{|\alpha|\leqslant 1}\frac{1}{\alpha!}\frac{\partial^\alpha f}{\partial\boldsymbol{x}^\alpha}(\boldsymbol{x}_0)\,(\boldsymbol{x}-\boldsymbol{x}_0)^\alpha+\sum_{|\alpha|=2}\frac{1}{\alpha!}\frac{\partial^\alpha f}{\partial\boldsymbol{x}^\alpha}(\boldsymbol{\xi})\,(\boldsymbol{x}-\boldsymbol{x}_0)^n \\ &= f(\boldsymbol{x}_0)+\sum_{i=1}^N\frac{\partial f}{\partial x_i}(\boldsymbol{x}_0)\,(x_i-x_{i0})+\sum_{i=1}^N\frac{1}{2}\frac{\partial^2 f}{\partial x_i^2}(\boldsymbol{\xi})\,(x_i-x_{i0})^2 \\ &\quad+\sum_{i<j}\frac{\partial^2 f}{\partial x_i\partial x_j}(\boldsymbol{\xi})\,(x_i-x_{i0})\,(x_j-x_{j0}) \\ &= f(\boldsymbol{x}_0)+(\mathrm{grad}\,f)(\boldsymbol{x}_0)\cdot(\boldsymbol{x}-\boldsymbol{x}_0)+(\boldsymbol{x}-\boldsymbol{x}_0)^T H_f(\boldsymbol{\xi})\,(\boldsymbol{x}-\boldsymbol{x}_0). \end{aligned}$$

   Here H_f is the "Hessian matrix" of f:

$$H_f=\left(\frac{\partial^2 f}{\partial x_i\partial x_j}\right). \tag{16}$$

   Exercise 6. Write down the Hessian matrix for $f(x,y,z)$.

2. $n=2$. Similarly we have

$$f(\boldsymbol{x})=f(\boldsymbol{x}_0)+(\mathrm{grad}\,f)(\boldsymbol{x}_0)\cdot(\boldsymbol{x}-\boldsymbol{x}_0)+(\boldsymbol{x}-\boldsymbol{x}_0)^T H_f(\boldsymbol{x_0})\,(\boldsymbol{x}-\boldsymbol{x}_0)+R_n(\boldsymbol{x},\boldsymbol{x}_0) \tag{17}$$

   where

$$\lim_{\boldsymbol{x}\to\boldsymbol{x}_0}\frac{R_n(\boldsymbol{x},\boldsymbol{x}_0)}{\|\boldsymbol{x}-\boldsymbol{x}_0\|^2}=0. \tag{18}$$