1. Taylor Expansion

Please read §3.5 of Dr. Runde's Notes.

1.1. Higher order derivatives.

- When $N=1$, defining higher order derivatives is relatively intuitive, as $f'(x)$ is a similarly defined function as f.
- When $N>1$, if we denote by $\mathcal{L}(X,Y)$ the space of all linear functions with domain X and target Y, we have the following. For simplicity of notation we assume f is smooth over the whole $\mathbb{R}^N$.

	f	Df	$D^2 f$	$D^3 f$	$\cdots$
Domain	$\mathbb{R}^N$	$\mathbb{R}^N$	$\mathbb{R}^N$	$\mathbb{R}^N$	
Target	$\mathbb{R}^M$	$\mathcal{L}(\mathbb{R}^N,\mathbb{R}^M)$	$\mathcal{L}(\mathbb{R}^N,\mathcal{L}(\mathbb{R}^N,\mathbb{R}^M))$	$\mathcal{L}(\mathbb{R}^N,\mathcal{L}(\mathbb{R}^N,\mathcal{L}(\mathbb{R}^N,\mathbb{R}^M)))$	
Representation of target	N/A	$\mathbb{R}^{N\times M}$	$\mathbb{R}^{N\times N\times M}$	$\mathbb{R}^{N\times N\times N\times M}$	

Table 1. Higher order derivatives

- The key result that makes the above representation possible is the following:

$$\mathcal{L}(X,\mathcal{L}(Y,Z)) \approx \mathcal{L}(X\times Y, Z). \tag{1}$$

For now we just understand "$\approx$" as "somehow equivalent".

- Thus for $f\colon\mathbb{R}^N\mapsto\mathbb{R}^M$, at every point x_0, we need MN numbers to represent $Df(x_0)$, MN^2 numbers to represent $D^2 f(x_0)$, and so on. It turns out that these numbers are exactly the partial derivatives of the corresponding order.

  Exercise 1. Can you prove this?

- By (1), we see that $Df(x_0)\colon \mathbb{R}^N\mapsto\mathbb{R}^M$, $D^2 f(x_0)\colon\mathbb{R}^N\times\mathbb{R}^N\mapsto\mathbb{R}^M$, $D^3 f\colon\mathbb{R}^N\times\mathbb{R}^N\times\mathbb{R}^N\mapsto\mathbb{R}^M$, and so on.

  Exercise 2. Prove that $D^2 f(x_0)$ is symmetric. What about $D^3 f(x_0)$?

  Exercise 3. Prove or disprove:

$$\frac{\partial}{\partial v_1}\left[\frac{\partial f}{\partial v_2}\right](x_0) = D^2 f(x_0)(v_1,v_2), \tag{2}$$

  where $v_1, v_2\in\mathbb{R}^N$.

- Multiindex. $\alpha=(\alpha_1,\ldots,\alpha_N)$. Define $|\alpha| := |\alpha_1| + \cdots + |\alpha_N|$.
- Due to symmetry of $D^k f(x_0)$, we can write a generic k-th order partial derivative as

$$\frac{\partial^k f(x_0)}{\partial x_1^{\alpha_1}\cdots\partial x_N^{\alpha_N}}, \qquad |\alpha|=k. \tag{3}$$

There are

$$\binom{k}{\alpha_1,\ldots,\alpha_N} := \frac{k!}{\alpha_1!\cdots\alpha_N!} \tag{4}$$

different k-th order partial derivatives.

- For simplicity, we use the notation

$$\alpha! := \alpha_1!\cdots\alpha_N!. \tag{5}$$

Thus (4) can be written as

$$\frac{k!}{\alpha!} = \frac{|\alpha|!}{\alpha!}. \tag{6}$$

- Furthermore, for $x\in\mathbb{R}^N$, we write

$$x^\alpha := x_1^{\alpha_1}\cdots x_N^{\alpha_N}. \tag{7}$$

- By the chain rule, we see that, if

$$g(t) := f(x_0 + t\,\xi), \qquad t \in \mathbb{R},\ x_0, \xi \in \mathbb{R}^N, \tag{8}$$

then

$$\frac{\mathrm{d}^k g}{\mathrm{d}t^k} = \sum_{|\alpha|=k} \frac{k!}{\alpha!} \frac{\partial^k f(x_0)}{\partial x_1^{\alpha_1} \cdots \partial x_N^{\alpha_N}} \xi_1^{\alpha_1} \xi_2^{\alpha_2} \cdots \xi_N^{\alpha_N} = \sum_{|\alpha|=k} \frac{k!}{\alpha!} D^k f(x_0)\,(\xi, \xi, \ldots, \xi) \tag{9}$$

where there are k ξ's in the last expression.

1.2. Taylor expansion for $N = 1$.

1.2.1. Basic idea.

- Recall that $f'(x_0)$ can be defined through the idea of optimal approximation of f by affine functions:

$$\lim_{x \longrightarrow x_0, x \neq x_0} \frac{|f(x) - f(x_0) - f'(x_0)\,(x - x_0)|}{|f(x) - a - b\,(x - x_0)|} = 0 \tag{10}$$

unless $a = f(x_0), b = f'(x_0)$.

- This idea can be readily generalized to higher order derivatives. The n-th order Taylor polynomial $T_n(x)$ for a function f at x_0 is defined as follows:

$$\lim_{x \longrightarrow x_0, x \neq x_0} \frac{|f(x) - T_n(x)|}{|f(x) - P(x)|} = 0 \tag{11}$$

for all other n-th order polynomials.

Remark 1. The existence and uniqueness of such $T_n(x)$ now becomes a non-trivial claim.

- One can prove that, if such $T_n(x)$ exists, then it is given by

$$T_n(x) = f(x_0) + f'(x_0)\,(x - x_0) + \frac{f''(x_0)}{2!}\,(x - x_0)^2 + \cdots + \frac{f^{(n)}(x_0)}{n!}\,(x - x_0)^n. \tag{12}$$

- Often it is a better idea to remind us the dependence of T_n on x_0. In the following we do this by writing $T_{n,x_0}(x)$ or $T_n(x_0; x)$.

1.2.2. Remainders.

- It is now natural to try to understand how good $T_{n,x_0}(x)$ approximates $f(x)$ near x_0. Thus we define the "remainder term"

$$R_{n,x_0}(x) = R_n(x_0; x) := f(x) - T_{n,x_0}(x). \tag{13}$$

- It should be emphasized that $R_{n,x_0}(x)$ is a fixed function, depending on n, x_0, x. In particular, the various "remainder"s introduced below are just different representations of the same functions. Thus it is more accurate to say "Peano form of the remainder", "Lagrange form of the remainder", etc.

- Different forms of remainders.

  - Peano.

  $$R_{n,x_0}(x) = o((x - x_0)^n), \qquad i.e., \quad \lim_{x \to x_0, x \neq x_0} \frac{|R_{n,x_0}(x)|}{|x - x_0|^n} = 0. \tag{14}$$

  - Lagrange.

  $$R_{n,x_0}(x) = \frac{f^{(n+1)}(c)}{(n+1)!}\,(x - x_0)^{n+1}. \tag{15}$$

  - Cauchy.

  $$R_{n,x_0}(x) = \frac{f^{(n+1)}(c)}{n!}\,(x - c)^n\,(x - x_0) = \frac{f^{(n+1)}(c)}{n!}\,(1 - \theta)^n\,(x - x_0)^{n+1} \tag{16}$$

  where $\theta = \frac{c - x_0}{x - x_0}$.

- Schlomilich-Roche.

$$R_{n,x_0}(x) = \frac{f^{(n+1)}(c)}{n!\,p}\,(x-c)^{n-p+1}\,(x-x_0)^p = \frac{f^{(n+1)}(c)}{n!\,p}\,(1-\theta)^{n-p+1}\,(x-x_0)^{n+1} \tag{17}$$

  where $\theta = \frac{c-x_0}{x-x_0}$.

- Integral.

$$R_{n,x_0}(x) = \frac{1}{n!}\int_{x_0}^{x} f^{(n+1)}(t)\,(x-t)^n\,\mathrm{d}t. \tag{18}$$

Note. It should be kept in mind that different forms of remainder requires different regularity conditions on f.

Remark 2. See my Fall 2013 Math 217 lecture notes for hints on how to prove the above.

1.3. Taylor expansion for $N > 1$.

- The basic idea is to use the auxiliary function

$$g(t) := f(x_0 + t\,(x-x_0)) \tag{19}$$

  and apply Taylor expansion results for $N = 1$ together with the identity (9).

- The n-th order Taylor polynomial for f at x_0 is then given by

$$T_{n,x_0}(x) := \sum_{k=0}^{n}\left[\sum_{|\alpha|=k}\frac{1}{\alpha!}\,\frac{\partial^k f(x_0)}{\partial x_1^{\alpha_1}\cdots\partial x_N^{\alpha_N}}\,(x-x_0)^\alpha\right]. \tag{20}$$

- Remainders

  We still denote

$$R_{n,x_0}(x) := f(x) - T_{n,x_0}(x). \tag{21}$$

  - Peano.

$$R_{n,x_0}(x) = o(|x-x_0|^n). \tag{22}$$

  - Lagrange.

$$R_{n,x_0}(x) = \sum_{|\alpha|=n+1}\frac{1}{\alpha!}\,\frac{\partial^k f(\xi)}{\partial x_1^{\alpha_1}\cdots\partial x_N^{\alpha_N}}\,(x-x_0)^\alpha \tag{23}$$

    where ξ is located on the line segment connecting x_0 and x.

Exercise 4. Obtain Cauchy, Schlomilich-Roche, and Integral forms of the remainder for $N > 1$.