Chapter 2

Differentiation in higher dimensions

2.1 The Total Derivative

Recall that if $f : \mathbb{R} \to \mathbb{R}$ is a 1-variable function, and $a \in \mathbb{R}$, we say that f is differentiable at x = a if and only if the ratio $\frac{f(a+h)-f(a)}{h}$ tends to a finite limit, denoted f'(a), as h tends to 0.

There are two possible ways to generalize this for vector fields

$$f: \mathcal{D} \to \mathbb{R}^m, \ \mathcal{D} \subseteq \mathbb{R}^n,$$

for points a in the *interior* \mathcal{D}^0 of \mathcal{D} . (The interior of a set X is defined to be the subset X^0 obtained by removing all the boundary points. Since every point of X^0 is an interior point, it is open.) The reader seeing this material for the first time will be well advised to stick to vector fields f with domain all of \mathbb{R}^n in the beginning. Even in the one dimensional case, if a function is defined on a closed interval [a, b], say, then one can properly speak of differentiability only at points in the open interval (a, b).

The first thing one might do is to fix a vector v in \mathbb{R}^n and say that f is **differentiable** along v iff the following limit makes sense:

$$\lim_{h \to 0} \frac{1}{h} \left(f(a+hv) - f(a) \right).$$

When it does, we write f'(a; v) for the limit. Note that this definition makes sense because a is an interior point. Indeed, under this hypothesis, \mathcal{D} contains a basic open set U containing a, and so a + hv will, for small enough h, fall into U, allowing us to speak of f(a + hv). This

derivative behaves exactly like the one variable derivative and has analogous properties. For example, we have the following

Theorem 1 (Mean Value Theorem for scalar fields) Suppose f is a scalar field. Assume f'(a + tv; v) exists for all $0 \le t \le 1$. Then there is a t_o with $0 \le t_o \le 1$ for which $f(a + v) - f(a) = f'(a + t_0v; v)$.

Proof. Put $\phi(t) = f(a + tv)$. By hypothesis, ϕ is differentiable at every t in [0, 1], and $\phi'(t) = f'(a + tv; v)$. By the one variable mean value theorem, there exists a t_0 such that $\phi'(t_0)$ is $\phi(1) - \phi(0)$, which equals f(a + v) - f(a). Done.

When v is a **unit vector**, f'(a; v) is called the **directional derivative** of f at a in the direction of v.

The disadvantage of this construction is that it forces us to study the change of f in one direction at a time. So we revisit the one-dimensional definition and note that the condition for differentiability there is equivalent to requiring that there exists a constant c (= f'(a)), such that $\lim_{h\to 0} \left(\frac{f(a+h) - f(a) - ch}{h}\right) = 0$. If we put L(h) = f'(a)h, then $L : \mathbb{R} \to \mathbb{R}$ is clearly a linear map. We generalize this idea in higher dimensions as follows:

Definition. Let $f : \mathcal{D} \to \mathbb{R}^m$ ($\mathcal{D} \subseteq \mathbb{R}^n$) be a vector field and a an interior point of \mathcal{D} . Then f is differentiable at x = a if and only if there exists a linear map $L : \mathbb{R}^n \to \mathbb{R}^m$ such that

(*)
$$\lim_{u \to 0} \frac{||f(a+u) - f(a) - L(u)||}{||u||} = 0$$

Note that the norm $|| \cdot ||$ denotes the length of vectors in \mathbb{R}^m in the numerator and in \mathbb{R}^n in the denominator. This should not lead to any confusion, however.

Lemma 1 Such an L, if it exists, is unique.

Proof. Suppose we have $L, M : \mathbb{R}^n \to \mathbb{R}^m$ satisfying (*) at x = a. Then

$$\lim_{u \to 0} \frac{||L(u) - M(u)||}{||u||} = \lim_{u \to 0} \frac{||L(u) + f(a) - f(a + u) + (f(a + u) - f(a) - M(u))||}{||u||} \\ \leq \lim_{u \to 0} \frac{||L(u) + f(a) - f(a + u)||}{||u||} \\ + \lim_{u \to 0} \frac{||f(a + u) - f(a) - M(u)||}{||u||} = 0.$$

Pick any non-zero $v \in \mathbb{R}^n$, and set u = tv, with $t \in \mathbb{R}$. Then, the linearity of L, M implies that L(tv) = tL(v) and M(tv) = tM(v). Consequently, we have

$$\lim_{t \to 0} \frac{||L(tv) - M(tv)||}{||tv||} = 0$$

=
$$\lim_{t \to 0} \frac{|t| ||L(v) - M(v)||}{|t| ||v||}$$

=
$$\frac{1}{||v||} ||L(v) - M(v)||.$$

Then L(v) - M(v) must be zero.

Definition. If the limit condition (*) holds for a linear map L, we call L the **total deriva**tive of f at a, and denote it by $T_a f$.

It is mind boggling at first to think of the derivative as a linear map. A natural question which arises immediately is to know what the value of $T_a f$ is at any vector v in \mathbb{R}^n . We will show in section 2.3 that this value is precisely f'(a; v), thus linking the two generalizations of the one-dimensional derivative.

Sometimes one can guess what the answer should be, and if (*) holds for this choice, then it must be the derivative by uniqueness. Here are **two examples** which illustrate this.

(1) Let f be a **constant vector field**, i.e., there exists a vector $w \in \mathbb{R}^m$ such that f(x) = w, for all x in the domain \mathcal{D} . Then we claim that f is differentiable at any $a \in \mathcal{D}^0$ with **derivative zero**. Indeed, if we put L(u) = 0, for any $u \in \mathbb{R}^n$, then (*) is satisfied, because f(a+u) - f(a) = w - w = 0.

(2) Let f be a **linear map**. Then we claim that f is differentiable everywhere with $T_a f = f$. Indeed, if we put L(u) = f(u), then by the linearity of f, f(a+u) - f(a) = f(u), and so f(a+u) - f(a) - L(u) is zero for any $u \in \mathbb{R}^n$. Hence (*) holds trivially for this choice of L.

Before we leave this section, it will be useful to take note of the following:

Lemma 2 Let f_1, \ldots, f_m be the component (scalar) fields of f. Then f is differentiable at a iff each f_i is differentiable at a. Moreover, $Tf(v) = (Tf_1(v), Tf_2(v), \ldots, Tf_n(g))$.

An easy consequence of this lemma is that, when $\mathbf{n} = \mathbf{1}$, f is differentiable at a iff the following familiar looking limit exists in \mathbb{R}^m :

$$\lim_{h \to 0} \frac{f(a+h) - f(a)}{h},$$

allowing us to suggestively write f'(a) instead of $T_a f$. Clearly, f'(a) is given by the vector $(f'_1(a), \ldots, f'_m(a))$, so that $(T_a f)(h) = f'(a)h$, for any $h \in \mathbb{R}$.

Proof. Let f be differentiable at a. For each $v \in \mathbb{R}^n$, write $L_i(v)$ for the *i*-th component of $(T_a f)(v)$. Then L_i is clearly linear. Since $f_i(a + u) - f_i(u) - L_i(u)$ is the *i*-th component of f(a + u) - f(a) - L(u), the norm of the former is less than or equal to that of the latter. This shows that (*) holds with f replaced by f_i and L replaced by L_i . So f_i is differentiable for any *i*. Conversely, suppose each f_i differentiable. Put $L(v) = ((T_a f_1)(v), \ldots, (T_a f_m)(v))$. Then L is a linear map, and by the triangle inequality,

$$||f(a+u) - f(a) - L(u)|| \le \sum_{i=1}^{m} |f_i(a+u) - f_i(a) - (T_a f_i)(u)|.$$

It follows easily that (*) exists and so f is differentiable at a.

2.2 Partial Derivatives

Let $\{e_1, \ldots, e_n\}$ denote the standard basis of \mathbb{R}^n . The directional derivatives along the unit vectors e_j are of special importance.

Definition. Let $j \leq n$. The *j*th partial derivative of f at x = a is $f'(a; e_j)$, denoted by $\frac{\partial f}{\partial x_i}(a)$ or $D_j f(a)$.

Just as in the case of the total derivative, it can be shown that $\frac{\partial f}{\partial x_j}(a)$ exists iff $\frac{\partial f_i}{\partial x_j}(a)$ exists for each coordinate field f_i .

Example: Define $f : \mathbb{R}^3 \to \mathbb{R}^2$ by

$$f(x, y, z) = (e^{x\sin(y)}, z\cos(y)).$$

All the partial derivatives exist at any $a = (x_0, y_0, z_0)$. We will show this for $\frac{\partial f}{\partial y}$ and leave it to the reader to check the remaining cases. Note that

$$\frac{1}{h}(f(a+he_2)-f(a)) = \left(\frac{e^{x_0\sin(y_0+h)}-e^{x_0\sin(y_0)}}{h}, z_0\frac{\cos(y_0+h)-\cos(y_0)}{h}\right).$$

We have to understand the limit as h goes to 0. Then the methods of one variable calculus show that the right hand side tends to the finite limit $(x_0\cos(y_0)e^{x_0\sin(y_0)}, -z_0\sin(y_0))$, which is $\frac{\partial f}{\partial y}(a)$. In effect, the partial derivative with respect to y is calculated like a one variable derivative, keeping x and z fixed. Let us note without proof that $\frac{\partial f}{\partial x}(a)$ is $(\sin(y_0)e^{x_0\sin(y_0)}, 0)$ and $\frac{\partial f}{\partial z}(a)$ is $(0, \cos(y_0))$.

It is easy to see from the definition that f'(a;tv) equals tf'(a;v), for any $t \in \mathbb{R}$. This follows as $\frac{1}{h}(f(a+h(tv))-f(a)) = t\frac{1}{th}(f(a+(ht)v)-f(a))$. In particular the Mean Value Theorem for scalar fields gives $f_i(a+hv) - f(a) = hf'_i(a+t_0hv) = hf_i(a+\tau v)$ for some $0 \le \tau \le h$.

We also have the following

Lemma 3 Suppose the derivatives of f along any $v \in \mathbb{R}^n$ exist near a and are continuous at a. Then

$$f'(a; v + v') = f'(a; v) + f'(a; v'),$$

for all v, v' in \mathbb{R}^n . In particular, the directional derivatives of f are all determined by the n partial derivatives.

We will do this for the scalar fields f_i . Notice

$$f_i(a + hv + hv') - f_i(a) = f_i(a + hv + hv') - f_i(a + hv) + f_i(a + hv) - f(a)$$

= $hf_i(a + hv + \tau v') + hf_i(a + \tau'v)$

where here $0 \le \tau \le h$ and $0 \le \tau' \le h$. Now dividing by h and taking the limit and $h \to 0$ gives $f'_i(a; v + v')$ for the first expression. The last expression gives a sum of two limits

$$\lim_{h\to 0} f'_i(a+hv+\tau v') + \lim_{h\to 0} f'_i(a+\tau'v;v').$$

But this is $f'_i(a; v) + f'_i(a; v')$. Recall both τ and τ' are between 0 and h and so as h goes to 0 so do τ and τ' . Here we have used the continuity of the derivatives of f along any line in a neighborhood of a.

Now pick e_1, e_2, \ldots, e_n the usual orthogonal basis and recall $v = \sum \alpha_i e_i$. Then $f'(a; v) = f'(a; \sum \alpha_i e_i) = \sum \alpha_i f'(a; e_i)$. Also the $f'(a; e_i)$ are the partial derivatives. The Lemma now follows easily.

In the next section (Theorem 1a) we will show that the conclusion of this lemma remains valid without the continuity hypothesis **if** we assume instead that f has a total derivative at a.

The **gradient** of a scalar field g at an interior point a of its domain in \mathbb{R}^n is defined to be the following vector in \mathbb{R}^n :

$$\nabla g(a) = \operatorname{grad} g(a) = \left(\frac{\partial g}{\partial x_1}(a), \dots, \frac{\partial g}{\partial x_n}(a)\right),$$

assuming that the partial derivatives exist at a.

Given a vector field f as above, we can then put together the gradients of its component fields f_i , $1 \le i \le m$, and form the following important matrix, called the **Jacobian matrix** at a:

$$Df(a) = \left(\frac{\partial f_i}{\partial x_j}(a)\right)_{1 \le i \le m, 1 \le j \le n} \in M_{mn}(\mathbb{R}).$$

The *i*-th row is given by $\nabla f_i(a)$, while the *j*-th column is given by $\frac{\partial f}{\partial x_j}(a)$. Here we are using the notation $M_{mn}(\mathbb{R})$ for the collection of all $m \times n$ -matrices with real coefficients. When m = n, we will simply write $M_n(\mathbb{R})$.

2.3 The main theorem

In this section we collect the main properties of the total and partial derivatives.

Theorem 2 Let $f : \mathcal{D} \to \mathbb{R}^m$ be a vector field, and a an interior point of its domain $\mathcal{D} \subseteq \mathbb{R}^n$.

(a) If f is differentiable at a, then for any vector v in \mathbb{R}^n ,

$$(T_a f)(v) = f'(a, v).$$

In particular, since $T_a f$ is linear, we have

$$f'(a;\alpha v + \beta v') = \alpha f'(a;v) + \beta f'(a;v'),$$

for all v, v' in \mathbb{R}^n and α, β in \mathbb{R} .

- (b) Again assume that f is differentiable. Then the matrix of the linear map $T_a f$ relative to the standard bases of \mathbb{R}^n , \mathbb{R}^m is simply the Jacobian matrix of f at a.
- (c) f differentiable at $a \Rightarrow f$ continuous at a.
- (d) Suppose all the partial derivatives of f exist near a and are continuous at a. Then $T_a f$ exists.

(e) (chain rule) Consider

Suppose f is differentiable at a and g is differentiable at b = f(a). Then the composite function $h = g \circ f$ is differentiable at a, and moreover,

$$T_a h = T_b g \circ T_a f.$$

In terms of the Jacobian matrices, this reads as

$$Dh(a) = Dg(b)Df(a) \in M_{kn}.$$

(f) (m = 1) Let f, g be scalar fields, differentiable at a. Then

(i)
$$T_a(f+g) = T_a f + T_a g$$
 (additivity)
(ii) $T_a(fg) = f(a)T_a g + g(a)T_a f$ (product rule)
(iii) $T_a(\frac{f}{g}) = \frac{g(a)T_a f - f(a)T_a g}{g(a)^2}$ if $g(a) \neq 0$ (quotient rule)

The following corollary is an immediate consequence of the theorem, which we will make use of, in the next chapter on normal vectors and extrema.

Corollary 1 Let g be a scalar field, differentiable at an interior point b of its domain \mathcal{D} in \mathbb{R}^n , and let v be any vector in \mathbb{R}^n . Then we have

$$\nabla g(b) \cdot v = g'(b; v).$$

Furthermore, let ϕ be a function from a subset of \mathbb{R} into $\mathcal{D} \subseteq \mathbb{R}^n$, differentiable at an interior point a mapping to b. Put $h = g \circ \phi$. Then h is differentiable at a with

$$h'(a) = \nabla g(b) \cdot \phi'(a).$$

Proof of main theorem. (a) It suffices to show that $(T_a f_i)(v) = f_i(a; v)$ for each $i \le n$. By definition,

$$\lim_{u \to 0} \frac{||f_i(a+u) - f_i(a) - (T_a f_i)(u)||}{||u||} = 0$$

This means that we can write for $u = hv, h \in \mathbb{R}$,

$$\lim_{h \to 0} \frac{f_i(a+hv) - f_i(a) - h(T_a f_i)(v)}{|h| ||v||} = 0$$

In other words, the limit $\lim_{h\to 0} \frac{f_i(a+hv)-f_i(a)}{h}$ exists and equals $(T_a f_i)(v)$. Done.

(b) By part (a), each partial derivative exists at a (since f is assumed to be differentiable at a). The matrix of the linear map $T_a f$ is determined by the effect on the standard basis vectors. Let $\{e'_i | 1 \le i \le m\}$ denote the standard basis in \mathbb{R}^m . Then we have, by definition,

$$(T_a f)(e_j) = \sum_{i=1}^m (T_a f_i)(e_j) e'_i = \sum_{i=1}^m \frac{\partial f_i}{\partial x_j}(a) e'_i.$$

The matrix obtained is easily seen to be Df(a).

(c) First we need the following simple

Lemma 4 Let $T : \mathbb{R}^n \to \mathbb{R}^m$ be a linear map. Then, $\exists c > 0$ such that $||Tv|| \leq c||v||$ for any $v \in \mathbb{R}^n$.

Proof of Lemma. Let A be the matrix of T relative to the standard bases. Put $C = \max_{j}\{||T(e_j)||\}$. If $v = \sum_{j=1}^{n} \alpha_j e_j$, then

$$\begin{aligned} ||T(v)|| &= ||\sum_{j} \alpha_{j} T(e_{j})|| &\leq C \sum_{j=1}^{n} |\alpha_{j}| \cdot 1 \\ &\leq C (\sum_{j=1}^{n} |\alpha_{j}|^{2})^{1/2} (\sum_{j=1}^{n} 1)^{1/2} \leq C \sqrt{n} ||v||, \end{aligned}$$

by the Cauchy–Schwarz inequality. We are done by setting $c = C\sqrt{n}$.

This shows that a linear map is continuous as if $||v - w|| < \delta$ then $||T(v) - T(w)|| = ||T(v - w)|| < c||v - w|| < c\delta$.

(c) Suppose f is differentiable at a. This certainly implies that the limit of the function $f(a + u) - f(a) - (T_a f)(u)$, as u tends to $0 \in \mathbb{R}^n$, is $0 \in \mathbb{R}^m$ (from the very definition of $T_a f$, $||f(a + u) - f(a) - (T_a f)(u)||$ tends to zero "faster" than ||u||, in particular it tends to zero). Since $T_a f$ is linear, $T_a f$ is continuous (everywhere), so that $\lim_{u\to 0} (T_a f)(u) = 0$. Hence $\lim_{u\to 0} f(a + u) = f(a)$ which means that f is continuous at a.

(d) By hypothesis, all the partial derivatives exist near $a = (a_1, \ldots, a_n)$ and are continuous there. It suffices to show that each f_i is differentiable at a by lemma 2. So we have only to show that (*) holds with f replaced by f_i and $L(u) = f'_i(a; u)$. Write $u = (h_1, \ldots, h_n)$. By Lemma 3, we know that $f'_i(a; -)$ is linear. So

$$L(u) = \sum_{j=1}^{n} h_j \frac{\partial f_i}{\partial x_j}(a),$$

and we can write

$$f_i(a+u) - f_i(a) = \sum_{j=1}^n (\phi_j(a_j + h_j) - \phi_j(a_j)),$$

where each ϕ_j is a one variable function defined by

$$\phi_j(t) = f_i(a_1 + h_1, \dots, a_{j-1} + h_{j-1}, t, a_{j+1}, \dots, a_n).$$

By the mean value theorem,

$$\phi_j(a_j + h_j) - \phi_j(a_j) = h_j \phi'_j(t_j) = h_j \frac{\partial f_i}{\partial x_j}(y(j)),$$

for some $t_j \in [a_j, a_j + h_j]$, with

$$y(j) = (a_1 + h_1, \dots, a_{j-1} + h_{j-1}, t_j, a_{j+1}, \dots, a_n).$$

Putting these together, we see that it suffices to show that the following limit is zero:

$$\lim_{u \to 0} \frac{1}{||u||} \sum_{j=1}^n h_j \left(\frac{\partial f_i}{\partial x_j}(a) - \frac{\partial f_i}{\partial x_j}(y(j)) \right) |.$$

Clearly, $|h_j| \leq ||u||$, for each j. So it follows, by the triangle inequality, that this limit is bounded above by the sum over j of $\lim_{h_j\to 0} |\frac{\partial f_i}{\partial x_j}(a) - \frac{\partial f_i}{\partial x_j}(y(j))|$, which is zero by the continuity of the partial derivatives at a. Here we are using the fact that each y(j) approaches a as h_j goes to 0. Done.

Proof of (e) Write $L = T_a f$, $M = T_b g$, $N = M \circ L$. To show: $T_a h = N$. Define F(x) = f(x) - f(a) - L(x - a), G(y) = g(y) - g(b) - M(y - b) and H(x) = h(x) - h(a) - N(x - a). Then we have

$$\lim_{x \to a} \frac{||F(x)||}{||x - a||} = 0 = \lim_{y \to b} \frac{||G(y)||}{||y - b||}$$

So we need to show:

$$\lim_{x \to a} \frac{||H(x)||}{||x - a||} = 0.$$

But

$$H(x) = g(f(x)) - g(b) - M(L(x - a))$$

Since L(x - a) = f(x) - f(a) - F(x), we get

$$H(x) = [g(f(x)) - g(b) - M(f(x) - f(a))] + M(F(x)) = G(f(x)) + M(F(x)).$$

Therefore it suffices to prove:

(i)
$$\lim_{x \to a} \frac{||G(f(x))||}{||x - a||} = 0$$
 and
(ii) $\lim_{x \to a} \frac{||M(F(x))||}{||x - a||} = 0.$

By Lemma 4, we have $||M(F(x))|| \le c||F(x)||$, for some c > 0. Then $\frac{||M(F(x))||}{||x-a||} \le c \lim_{x \to a} \frac{||F(x)||}{||x-a||} = 0$, yielding (ii).

On the other hand, we know $\lim_{y\to b} \frac{||G(y)||}{||y-b||} = 0$. So we can find, for every $\epsilon > 0$, a $\delta > 0$ such that $||G(f(x))|| < \epsilon ||f(x) - b||$ if $||f(x) - b|| < \delta$. But since f is continuous, $||f(x) - b|| < \delta$ whenever $||x - a|| < \delta_1$, for a small enough $\delta_1 > 0$. Hence

$$\begin{aligned} ||G(f(x))|| &< \epsilon ||f(x) - b|| = \epsilon ||F(x) + L(x - a)|| \\ &\le \epsilon ||F(x)|| + \epsilon ||L(x - a)||, \end{aligned}$$

by the triangle inequality. Since $\lim_{x \to a} \frac{||F(x)||}{||x-a||}$ is zero, we get

$$\lim_{x \to a} \frac{||G(f(x))||}{||x-a||} \le \epsilon \lim_{x \to a} \frac{||L(x-a)||}{||x-a||}.$$

Applying Lemma 4 again, we get $||L(x-a)|| \le c'||x-a||$, for some c' > 0. Now (i) follows easily.

(f) (i) We can think of f + g as the composite h = s(f, g) where (f, g)(x) = (f(x), g(x))and s(u, v) = u + v ("sum"). Set b = (f(a), g(a)). Applying (e), we get

$$T_a(f+g) = T_b(s) \circ T_a(f,g) = T_a(f) + T_a(g)$$

Done. The proofs of (ii) and (iii) are similar and will be left to the reader.

QED.

Remark. It is important to take note of the fact that a vector field f may be differentiable at a without the partial derivatives being continuous. We have a counterexample already when n = m = 1 as seen by taking

$$f(x) = x^2 \sin\left(\frac{1}{x}\right) \quad \text{if} \quad x \neq 0,$$

and f(0) = 0. This is differentiable everywhere. The only question is at x = 0, where the relevant limit $\lim_{h\to 0} \frac{f(h)}{h}$ is clearly zero, so that f'(0) = 0. But for $x \neq 0$, we have by the product rule,

$$f'(x) = 2x\sin\left(\frac{1}{x}\right) - \cos\left(\frac{1}{x}\right),$$

which does not tend to f'(0) = 0 as x goes to 0. So f' is not continuous at 0.

2.4 Mixed partial derivatives

Let f be a scalar field, and a an interior point in its domain $\mathcal{D} \subseteq \mathbb{R}^n$. For $j, k \leq n$, we may consider the second partial derivative

$$\frac{\partial^2 f}{\partial x_j \partial x_k}(a) = \frac{\partial}{\partial x_j} \left(\frac{\partial f}{\partial x_k}\right)(a),$$

when it exists. It is called the *mixed partial derivative* when $j \neq k$, in which case it is of interest to know whether we have the equality

(3.4.1)
$$\frac{\partial^2 f}{\partial x_j \partial x_k}(a) = \frac{\partial^2 f}{\partial x_k \partial x_j}(a).$$

Proposition 1 Suppose $\frac{\partial^2 f}{\partial x_j \partial x_k}$ and $\frac{\partial^2 f}{\partial x_k \partial x_j}$ both exist near a and are continuous there. Then the equality (3.4.1) holds.

The proof is similar to the proof of part (d) of Theorem 1.