Notes on the Calculus of Variations

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1 Introduction

The main practical construction here is the calcuation of the first variation of a functional. This is given, informally, by

$$\delta \mathcal{F} = \frac{d}{dt} \mathcal{F}[u + t\phi]_{\Big|_{t=0}}.$$

And one can make sense of this without (really) knowing what one is doing. For example, if

$$\mathcal{F}[u] = \int_a^b \sqrt{1 + u'^2} \, dt$$

gives the length of the graph of a function $u \in c^1[a, b]$, then

$$\delta \mathcal{F} = \frac{d}{dt} \mathcal{F}[u + t\phi]_{|_{t=0}}$$

$$= \frac{d}{dt} \int_{a}^{b} \sqrt{1 + [(u + t\phi)']^{2}} dt_{|_{t=0}}$$

$$= \int_{a}^{b} \frac{\partial}{\partial t} \sqrt{1 + [(u + t\phi)']^{2}} dt_{|_{t=0}}$$

$$= \int_{a}^{b} \frac{\partial}{\partial t} \sqrt{1 + (u' + t\phi')^{2}} dt_{|_{t=0}}$$

$$= \int_{a}^{b} \frac{(u' + t\phi')\phi'}{\sqrt{1 + (u' + t\phi')^{2}}} dt_{|_{t=0}}$$

$$= \int_{a}^{b} \frac{u'\phi'}{\sqrt{1 + u'^{2}}} dt.$$

The immediate point is that if u is a minimizer of \mathcal{F} , then this kind of "derivative" should vanish for every admissible function ϕ . This leads, in turn, to an immediate question: What can you say about a function u for which

$$\int_{a}^{b} \frac{u'\phi'}{\sqrt{1+u'^2}} dt = 0 \quad \text{for every } \phi?$$
 (1)

This is where the fundamental lemma comes in.

Exercise 1 Assume $\phi(a) = 0 = \phi(b)$ and integrate by parts in (1) to obtain a condition

$$\int_{a}^{b} M[u] \, \phi \, dt = 0 \qquad \text{for every } \phi.$$

Conclude that u must satisfy the ordinary differential equation M[u] = 0. What kind of ODE have you obtained?

For our purposes, we need to understand what is going on with the first variation in a somewhat more detailed fashion. We need to consider the following questions:

- 1. What is the domain of \mathcal{F} ?
- 2. What is the set of admissible (or allowed) functions ϕ ?
- 3. What kind of function is the first variation?

These questions and several others are addressed below.

2 Calculus of Variations

The calculus of variations is, roughly speaking, a theory of minimization.

In the broadest sense, if A is any set and f is a real valued function with domain A, i.e.,

$$f: A \to \mathbb{R}$$
,

then we can define what it means to minimize the function f in the following terms:

An element $a \in A$ is a minimizer if

$$f(a) \le f(x)$$
 for all $x \in A$.

Given a minimizer $a \in A$, the real number f(a) is called the **minimum value** of f.

It is pretty obvious that a minimum value is unique while there may be many minimizers. Also, it is not difficult to see that it is quite possible for no minimizer to exist.

In order to proceed further with any kind of theory of minimization, we need more structure on the domain set A. It is also usual to introduce some kind of structure on the function f. If the set A is an interval in the real line, and the function f is differentiable, then the minimization of f is considered in a first course in calculus, or what is often called 1-D (one dimensional) calculus. This simple case is rather important for us, so let's review it.

Theorem 1 If $x_0 \in (a,b)$ is a minimizer of $f:(a,b) \to \mathbb{R}$ where f is a differentiable function, then

$$f'(x_0) = 0. (2)$$

The condition (2) is called a **necessary condition** for a minimizer because any minimizer x_0 (of this sort) must satisfy this condition.

Exercise 2 Give an example of a minimizer $x_0 \in [a,b]$ of a differentiable function $f:[a,b] \to \mathbb{R}$ for which (2) fails to hold. Note: When we say a function $f:[a,b] \to \mathbb{R}$, defined on a closed interval [a,b], is differentiable we usually mean there is an extension $\bar{f}:(\bar{a},\bar{b}) \to \mathbb{R}$ for some $\bar{a} < \bar{b}$ with $\bar{a} < a \le b < \bar{b}$, and

$$\bar{f}_{\mid_{[a,b]}} = f. \tag{3}$$

The function $\bar{f}_{|_{[a,b]}}:[a,b]\to\mathbb{R}$ is called the **restriction** of \bar{f} to the interval [a,b], and its values are given (of course) by

$$\bar{f}_{|a,b|}(x) = \bar{f}(x)$$
 for every $x \in [a,b]$.

Exercise 3 Give an example of a differentiable function $f:(a,b)\to\mathbb{R}$ and a point $x_0\in(a,b)$ with $f'(x_0)=0$ which illustrates that (2) is not sufficient to imply x_0 is a minimizer.

Exercise 4 What is the definition of the derivative f'(x) at $x \in (a,b)$ for a differentiable function $f:(a,b) \to \mathbb{R}$?

Exercise 5 Prove the necessary condition (2) for an interior minimizer x_0 of $f:(a,b)\to\mathbb{R}$.

There is also a second order necessary condition for interior minimizers, but it requires more **regularity** for the function f.

Theorem 2 If $x_0 \in (a,b)$ is a minimizer of $f:(a,b) \to \mathbb{R}$ where f is a twice differentiable function, then

$$f''(x_0) \ge 0. \tag{4}$$

Exercise 6 The following conditions on a function $f:(a,b)\to\mathbb{R}$ are called **regularity conditions**:

- 1. (continuity) For each $x \in (a,b)$, the function f is continuous at x.
- 2. (differentiability) For each $x \in (a, b)$, the derivative f'(x) exists (as a well-defined real number).
- 3. (continuous differentiability) For each $x \in (a,b)$, the derivative f'(x) exists and the function $f':(a,b) \to \mathbb{R}$ is continuous.
- 4. (twice differentiability) For each $x \in (a,b)$, the derivative f'(x) exists and the function $f'(a,b) \to \mathbb{R}$ is differentiable.

The set of continuous real valued functions on the interval (a,b) is denoted by $C^0(a,b)$. Let us denote the set of differentiable real valued functions on (a,b) by Diff(a,b). The set of continuously differentiable real valued functions on (a,b) is denoted by $C^1(a,b)$. Let us denote the set of twice differentiable real valued functions on (a,b) by $Diff^2(a,b)$. Show

$$\operatorname{Diff}^2(a,b) \subsetneq C^1(a,b) \subsetneq \operatorname{Diff}(a,b) \subsetneq C^0(a,b).$$

Exercise 7 Prove Theorem 2.

Exercise 8 Give an example showing the conclusions/necessary conditions (2) and (4) of Theorem 1 and Theorem 2 respectively, taken together, are not sufficient to imply x_0 is a minimizer.

Exercise 9 Give an example showing the conditions

$$f'(x_0) = 0$$
 and $f''(x_0) > 0$

are also not sufficient to imply $x_0 \in (a, b)$ is a minimizer of the function $f \in \text{Diff}^2(a, b)$.

If $f: A \to \mathbb{R}$ and the set A is taken to be an open subset of \mathbb{R}^2 or \mathbb{R}^3 , then the minimization problem for f is discussed in a course on multivariable calculus. Some understanding of what happens in these cases, and when A is an open subset of \mathbb{R}^n for any natural number n, is important for us too, and we will review that situation below. These cases fall under the heading of finite dimensional calculus.

A minimization problem in the calculus of variations is distinguished, roughly speaking, by the condition that the set A is infinite dimensional. This terminology is a tiny bit misleading because the notion of dimensionality relies on a vector space structure. On the other hand, an open set $\Omega \subset \mathbb{R}^n$ is usually not a vector space, but there is an obvious (finite dimensional) vector space of which Ω is a subset. Perhaps the best way to proceed is with a relatively simple example in which the domain does happen to be an infinite dimensional vector space:

2.1 2-D Capillary Surfaces

Consider $\mathcal{E}: C^1[-r,r] \to \mathbb{R}$ by

$$\mathcal{E}[u] = \int_{-r}^{r} \left[\sqrt{1 + u'(x)^2} + \kappa \frac{u(x)^2}{2} \right] dx - \beta [u(-r) + u(r)].$$
 (5)

Notice that \mathcal{E} assigns to each continuously differentiable function $u \in C^1[-r,r]$ a real number. Such a function is called a **functional**, and minimizing such functionals is the main objective in the calculus of variations. Put another way, the calculus of variations is the theory of minimizing functionals, more or less, like the functional \mathcal{E} above. Generally speaking, this is a very difficult problem.

It is always a good idea, with a problem like this, to have some understanding of what your functional is computing—or what is the meaning of its value. With this in mind, let us take a somewhat careful look at \mathcal{E} before we proceed to look for minimizers directly.¹

As in the previous chapter, the graph of the function u represents a possible interface separating the liquid in a capillary tube from the vapor exterior to that liquid. The idea is that the observed interface should, for some reason, be the one minimizing the functional \mathcal{E} . In particular, \mathcal{E} should, roughly speaking, measure the energy associated with any proposed interface, and the one that is observed is (the one) minimizing that energy.

We can recognize three terms that make up \mathcal{E} . The first one might be

$$\int_{-r}^{r} \sqrt{1 + u'(x)^2} \, dx.$$

Hopefully, you recognize this as the length of the graph of u. The idea is that a certain amount of energy is required to maintain an interface between a liquid and the vapor exterior to that liquid. There are a few different ways to look at this. First of all, it is almost surely true that on some microscopic level the separation between the liquid and vapor is much more messy and complicated than the simple C^1 curve we are using to model it. There are molecules of liquid moving around near the separation region. Some are evaporating into the vapor where there is probably a region of higher density near the bulk liquid; some are condensing back into the bulk liquid. In the liquid itself molecules near the separation experience an attraction to more molecules located deeper in the liquid than those closer to the separation. It is assumed this results in a net force pulling those molecules deeper into the liquid. On the other hand, the overall volume of the liquid does not appear to change position appreciably. Thus, it must be assumed other molecules of liquid are either condensing to replace those near the surface which are sinking deeper or deeper molecules are moving (being pushed) outward.

¹This is a little bit of an obscure math joke because we are actually only going to consider what are called the indirect methods in the calculus of variations. Thus, we will actually look for minimizers "indirectly." There are also what are called the "direct methods in the calculus of variations," but we won't really consider those methods in this course.

The bottom line of this point of view is that there is kinetic energy associated with the separation region called **free surface** (or interface) **energy**, and two assumptions are made about this energy (in this 2-D case):

- 1. The free surface energy is proportional to the length of the interface.
- 2. The observed interface "prefers" to minimize this energy.

The first assumption is probably a relatively reasonable one if the identification of the energy is with the kinetic energy of moving molecules near the separation region—modeled by the interface curve. The units we have are not quite correct since energy is force times length, and in fact, a more physically accurate expression for the free surface energy is

$$\sigma \int_{-r}^{r} \sqrt{1 + u'(x)^2} \, dx$$

where σ is a constant with units of force called the **surface tension**. One can simply think of this as a tension inherent to the particular liquid and vapor (subject to ambient—temperature and pressure—conditions) along the interface. We have simply divided the entire energy by this surface tension constant to obtain a simpler form for \mathcal{E} .

The second assumption is quite a bit more mysterious. The word "prefers" is not intended to suggest that the liquid (and/or vapor, molecules, etc.) are sentient. Probably the best interpretation is the following:

If a competitor interface were somehow constructed or achieved near the observed equilibrium interface, then the motion of molecules would result in a redistribution of the liquid so as to minimize the length of the interface—subject to other constraints in the problem, including those imposed by the other terms in the energy.

We are really not saying anything more than that we assume the energy is minimized. However, in practice, this kind of interpretation can be important. Let's consider the next term in the energy, and I will try to explain how and why.

The second term in the energy \mathcal{E} is proportional to

$$\int_{-r}^{r} u(x) \, dx.$$

This term is much easier to understand. The idea is that there is a potential field associated with gravity having the form -g(0,1). If a point mass m is located at the height z in this field, say at the point (0,z), then we imagine it has been moved there from some reference level, say z=0, and the potential energy associated with the point mass is given by the force times the distance

$$\int_{0}^{z} mg(0,1) \cdot (0,1) = mgz.$$

Similarly, each liquid element ΔV in the area

$$\mathcal{V} = \{(x, z) : |x| < r \text{ and } 0 < z < u(x)\}$$

has associated with it a potential energy

$$\rho \Delta V qz^*$$

where ρ is an areal density and z^* is some representative height for the area element ΔV . Of course, the gravitational potential field -g(0,1) we have taken is not really representative of the inverse square gravitational field of the earth, but it is a reasonable (and usual) approximation near the surface of the

earth, where we expect most interesting every day capillary surfaces will be observed. We are also assuming in the definition of \mathcal{V} that u is positive. With these assumptions the total energy associated with a particular interface is approximated by a sum

$$\sum_{j} \rho g \Delta V_{j} z_{j}^{*}.$$

This is a Riemann sum for an area integral over V, and (under appropriate regularity assumptions) we can say the gravitational potential energy associated with an interface determined by u should be

$$\lim \sum_{j} \rho g \Delta V_{j} z_{j}^{*} = \int_{\mathcal{V}} \rho g z = \rho g \int_{\mathcal{V}} z.$$

For the integral we can also write

$$\int_{\mathcal{Y}} z = \int_{-r}^{r} \int_{0}^{u(x)} z \, dz \, dx = \int_{-r}^{r} \frac{u(x)^{2}}{2} \, dx.$$

The factor in front of this integral for a physical energy is ρg . It will be recalled that we have divided by the surface tension σ to obtain (5), and

$$\kappa = \frac{\rho g}{\sigma}$$

is called the capillary constant. The previous principle we attempted to delineate for free surface energy can be, in a sense, easily illustrated for gravitational energy:

If a competitor interface were somehow constructed or achieved near the observed equilibrium interface, then the motion of molecules would result in a redistribution of the liquid so as to minimize the gravitational potential energy of the interface—subject to other constraints in the problem, including those imposed by the other terms in the energy.

Imagine the observed interface modeled in the upper left of Figure 1 where the liquid is assumed to be below the interface curve. The suggestion is that were the modification of the observed interface indicated in the upper right constructed and "let go," then the liquid in the bulge would fall in order to lower the value of \mathcal{E} .

Exercise 10 Consider a modification of the unit square

$$\{(x,z): 0 \le x, z \le 1\} = [0,1] \times [0,1]$$

obtained by replacing the top edge

$$\{(x, u(x)) : 0 \le x \le 1, \ u(x) \equiv 0\}$$

with the graph of $v(x) = 1 + \epsilon x(x-1)$. How does the energy

$$\mathcal{E}[u] = \int_0^1 \left[\sqrt{1 + u'(x)^2} + \kappa \frac{u(x)^2}{2} \right] dx$$

change under this modification. There are several possible approaches you can take here. You can plot the value $f(\epsilon) = \mathcal{E}[u]$ numerically. You can also compute the derivative f'(0). In the end, you should try to obtain an understanding of the order to which the length term changes compared to the order to which the gravitational energy term changes.

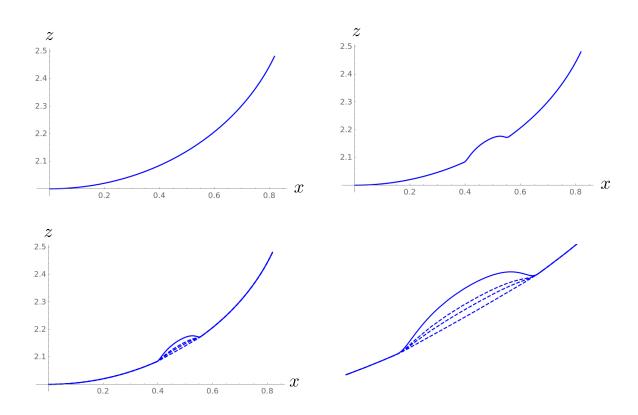


Figure 1: A modification of an observed interface (upper row). Clearly elimination of the bulge reduces the gravitational potential energy associated with the modified interface. Notice replacing the bulged portion with a straight line would both reduce the gravitational potential energy and the free surface length. In fact, this would reduce the free surface length to a minimum with respect to possible modification on the bulge region. It is at least plausible, however, that the energy can be reduced further by lowering the interface a little more (making it convex). This reduces the gravitational energy a relatively large amount while increasing the free surface length only slightly. See Exercise 10. The suggestion is that the observed interface is precisely the one obtaining the optimal balance to minimize the total energy. The lower row indicates (very roughly) how the liquid might "move" or migrate in a way that lowers energy. You should ask yourself the question: Is that what the liquid would actually do?

Finally, we consider the third term $-\beta[u(-r) + u(r)]$. This term is called the **wetting energy**. Technically, in order to have physically correct units the wetting energy is $\sigma\beta[u(-r) + u(r)]$. Nevertheless, β is a physical constant measuring the differential attraction between the molecules of the liquid and those of the container, or 2-D "tube" consisting of two vertical walls that are straight lines. The constant β is called the **adhesion coefficient**. If $\beta > 0$, then the molecules of the liquid are attracted to those of the walls so that the energy is lower when the wetted portions of the wall

$$\{(-r,z): 0 < z < u(-r)\}$$
 and $\{(r,z): 0 < z < u(r)\}$

are as long as possible. Notice again, the balance: If $\beta > 0$, then making these segments long tends to increase both the free surface energy and the gravitational potential energy. If $\beta = 0$, then the molecules of the liquid are indifferent toward those of the wall, and if $\beta < 0$, then the molecules of the liquid and those of the wall experience a mutual repelling force.

The discussion of the energy functional above is vague and inadequate. If you can think more deeply about why and how liquid interfaces minimize such a functional, many people will be interested to hear your thoughts. We have merely attempted to make the minimization of \mathcal{E} by observed interfaces seem plausible. What we can do is say more precise things about the model interfaces that do minimize \mathcal{E} . At the current time, the ultimate motivation for this description is that it leads to the equations of Young and Laplace and the resulting minimizing interfaces match experimental observations.

Returning to our illustration of the general subject of calculus of variations, we have a specific functional $\mathcal{E}: C^1[-r,r] \to \mathbb{R}$.

Exercise 11 Recall that a vector space E over a field F is a set with a binary operation of addition $+: E \times E \to E$ and a scaling operation $\cdot: F \times E \to E$ and having the following properties:

- 1. Addition is commutative: v + w = w + v for all $w, v \in E$.
- 2. Addition is associative: (v+w)+z=v+(w+z) for all $w,v,z\in E$.
- 3. There exists a zero vector 0 with

$$v + \mathbf{0} = \mathbf{0} + v = v$$
 for all $v \in E$.

4. For each vector $v \in E$, there exists an additive inverse, which is another vector $w \in E$ for which

$$v + w = w + v = 0$$
.

The additive inverse vector w of a vector v is denoted by -v. See Exercise 12 below.

- 5. Scaling is associative: (ab)v = a(bv) for all $a, b \in F$ and $v \in E$.
- 6. 0v = 0 and 1v = v for any $v \in E$ where 0 is the additive identity in the field F and 1 is the multiplicative identity in the field F.
- 7. There are two distributive laws for scaling.
 - (a) Scalars distribute across a sum of vectors:

$$a(v+w) = av + aw$$
 for all $a \in F$ and $v, w \in E$.

(b) A vector distributes across a sum of scalars:

$$(a+b)v = av + bv$$
 for all $a, b \in F$ and $v \in E$.

Definition 1 Given two vector spaces X and E over the same field F, a function $L: X \to E$ is linear if

$$L(av + bw) = aL(v) + bL(w)$$
 for all $a, b \in F$ and $v, w \in X$.

Show $C^1[-r,r]$ and \mathbb{R} are both vector spaces over \mathbb{R} , but $\mathcal{E}:C^1[-r,r]\to\mathbb{R}$ is not linear.

Exercise 12 The following are some basic exercises concerning the notion of a vector space.

- (a) Show that the zero vector in a vector space is unique.
- (b) Show that the additive inverse of any vector v in a vector space is unique.
- (c) Show that the compatibility properties for scaling involving the additive and multiplicative identities in the field given in condition 6 of the definition of a vector space follow independently from the other properties defining a vector space. Thus condition 6 may be omitted from the definition.
- (d) Look up and write down carefully the definition of a field.
- (e) Explain how the integers mod 3

$$\mathbb{Z}_3 = \{0, 1, 2\}$$

is a field.

Exercise 13 Let V be a vector space over a field F.

Definition 2 A set $B \subset V$ is a basis for V if the following conditions hold:

1. Given any vector $v \in V$ there exist (finitely many) vectors $v_1, v_2, \ldots, v_k \in V$ and there exist scalars $c_1, c_2, \ldots, c_k \in F$ for which

$$v = \sum_{j=1}^{k} c_j v_j.$$

2. Given elements $w_1, w_2, \ldots, w_\ell \in B$ and $a_1, a_2, \ldots, a_\ell \in F$ with the elements of B distinct, if

$$\mathbf{0} = \sum_{j=1}^{\ell} a_j w_j, \quad then \ a_1 = a_2 = \dots a_{\ell} = 0.$$

The following are basic exercises concerning the notion of a basis:

(a) Given any subset $A \subset V$, the span of A is defined to be the set of all linear combinations of elements from A, that is,

$$span(A) = \left\{ \sum_{j=1}^{k} c_j v_j : v_1, v_2, \dots, v_k \in A \text{ and } c_1, c_2, \dots, c_k \in F \right\}.$$

Show span(A) is a vector field over the same field F. Thus, the first condition defining a basis B may be written simply as span(B) = V, i.e., B is a spanning set.

(b) Any subset $A \subset V$ satisfying the second condition defining a basis for V, that is, given elements $w_1, w_2, \ldots, w_\ell \in A$ and $a_1, a_2, \ldots, a_\ell \in F$ with the elements of A distinct, if

$$\mathbf{0} = \sum_{j=1}^{\ell} a_j w_j, \quad then \ a_1 = a_2 = \dots a_{\ell} = 0,$$

is said to be linearly independent. Show any vector v in the span of a linearly independent set A can be written uniquely as a linear combination of distinct elements of A, i.e, if

$$\sum_{j=1}^{\ell} a_j w_j = \sum_{j=1}^{k} c_j v_j$$

for some distinct $w_1, w_2, \ldots, w_\ell \in A$, some distinct $v_1, v_2, \ldots, v_k \in A$ and some $a_1, a_2, \ldots, a_\ell, c_1, c_2, \ldots, c_k \in F$, then

$$\{v_1, v_2, \dots, v_k\} = \{w_1, w_2, \dots, w_\ell\},\$$

and in particular $k = \ell$, and there exists a **permutation**, i.e., a bijection $\phi : \{1, 2, ..., k\} \rightarrow \{1, 2, ..., \ell = k\}$, such that

$$v_j = w_{\phi(j)}$$
 and $c_j = a_{\phi(j)}$ for $j = 1, 2, \dots, k$.

Thus, an alternative definition of a basis B for a vector space V is a subset $B \subset V$ for which each element $v \in V$ can be written as a unique linear combination of distinct elements in B.

Exercise 14 A vector space V is said to be finite dimensional if there exists a basis B for V with finitely many elements. A vector space V is said to be infinite dimensional if it is not finite dimensional, i.e., if no basis with finitely many elements exists.

- (a) Two vector spaces E and V over the same field are said to be **isomorphic** (as vector spaces) if there is a linear bijection $L: E \to V$. Show any finite dimensional vector space V is isomorphic to F^n for some n.
- **(b)** Show $C^1[-r,r]$ is infinite dimensional.

According to the preceding exercises, we have a real valued nonlinear functional $\mathcal{E}: C^1[-r,r] \to \mathbb{R}$ defined on an infinite dimensional vector space $C^1[-r,r]$, and we can attempt to minimize \mathcal{E} . It turns out that, in the grand scheme of things, the fact that $C^1[-r,r]$ is an infinite dimensional vector space is not directly representative of the infinite dimensionality inherent to the problems of the calculus of variations, but the review of vector spaces, and infinite dimensional vector spaces in particular, will be useful and necessary. The functional $\mathcal{E}: C^1[-r,r] \to \mathbb{R}$ is, in fact, a rather typical example of the kinds of functionals considered in the calculus of variations.

The object corresponding to a first derivative of a functional like \mathcal{E} is called a **first variation** or **Gateaux differential**. Here is the construction: Let $u, \phi \in C^1[-r, r]$ and consider $v = u + \epsilon \phi$. The quantity

$$\delta \mathcal{E}[\phi] = \delta_u \mathcal{E}[\phi] = \left[\frac{d}{d\epsilon} \mathcal{E}[u + \epsilon \phi] \right]_{\epsilon=0}$$

is called the first variation of \mathcal{E} at u in the direction ϕ . In this definition, we are thinking of u and ϕ fixed. After the value of $\delta \mathcal{E}$ is computed, we may think of u and/or ϕ as arguments of the first variation. If u is a minimizer of \mathcal{E} , then $\mathcal{E}[v] = \mathcal{E}[u + \epsilon \phi] \geq \mathcal{E}[u]$, and $f(\epsilon) = \mathcal{E}[u + \epsilon \phi]$ (with ϕ fixed) is a real valued function of one variable, ϵ , with a minimum at $\epsilon = 0$. Therefore, if u is a minimizer of \mathcal{E} , then

$$\delta_u \mathcal{E}[\phi] \equiv 0$$
 for every $\phi \in C^1[-r, r]$.

We might be worried about whether or not the derivative with respect to ϵ exists and, if so, if the limit as ϵ tends to zero exists as well. Let's see if we can make a computation to determine if concerns about

this are valid. Writing out $\mathcal{E}[v]$ from (5) we have

$$\mathcal{E}[v] = \int_{-r}^{r} \left[\sqrt{1 + v'(x)^2} + \kappa \frac{v(x)^2}{2} \right] dx - \beta [v(-r) + v(r)]$$

$$= \int_{-r}^{r} \left[\sqrt{1 + [u'(x) + \epsilon \phi'(x)]^2} + \kappa \frac{[u(x) + \epsilon \phi(x)]^2}{2} \right] dx$$

$$- \beta [u(-r) + \epsilon \phi(-r) + u(r) + \epsilon \phi(r)].$$

Thus, forming the difference quotient

$$\frac{\mathcal{E}[u+\epsilon\phi] - \mathcal{E}[u+(\epsilon+h)\phi]}{h}$$

we obtain

$$\frac{1}{h} \int_{-r}^{r} \left[\sqrt{1 + [u'(x) + (\epsilon + h)\phi'(x)]^{2}} - \sqrt{1 + [u'(x) + \epsilon\phi'(x)]^{2}} \right] dx
+ \kappa \int_{-r}^{r} \left[[u(x) + \epsilon\phi(x)]\phi(x) + \frac{h\phi(x)^{2}}{2} \right] dx - \beta[\phi(-r) + \phi(r)].$$

The First term can be written as

$$\int_{-r}^{r} \frac{2[u'(x) + \epsilon \phi'(x)]\phi'(x) + h\phi'(x)}{\sqrt{1 + [u'(x) + (\epsilon + h)\phi'(x)]^2} + \sqrt{1 + [u'(x) + \epsilon \phi'(x)]^2}} dx.$$

From these expressions, it is clear the limit as h tends to zero exists and

$$\frac{d}{d\epsilon}\mathcal{E}[v] = \int_{-r}^{r} \frac{[u'(x) + \epsilon\phi'(x)]\phi'(x)}{\sqrt{1 + [u'(x) + \epsilon\phi'(x)]^2}} dx + \kappa \int_{-r}^{r} [u(x) + \epsilon\phi(x)] \phi(x) dx - \beta[\phi(-r) + \phi(r)].$$

The derivative with respect to ϵ does exist, and evaluation at $\epsilon = 0$ is also immediate:

$$\delta \mathcal{E}[\phi] = \int_{-r}^{r} \left[\frac{u'(x)}{\sqrt{1 + u'(x)^2}} \phi'(x) + \kappa u(x) \phi(x) \right] dx - \beta [\phi(-r) + \phi(r)].$$

We pause to remark/recall that if $u \in C^1[-r, r]$ is a minimizer of \mathcal{E} , then $\delta_u \mathcal{E}[\phi] = 0$ for all $\phi \in C^1[-r, r]$. Our computation allows us to write this condition as

$$\int_{-r}^{r} \left[\frac{u'(x)}{\sqrt{1 + u'(x)^2}} \phi'(x) + \kappa u(x) \phi(x) \right] dx = \beta [\phi(-r) + \phi(r)]$$
for all $\phi \in C^1[-r, r]$. (6)

It is not entirely clear what this (integral) condition implies about the minimizer u. We can say, more generally, however that **any** function $u \in C^1[-r, r]$ for which (6) holds is called a **weak extremal** for the functional \mathcal{E} . A weak extremal is an analogue of a (1-D calculus) *critical point* in the calculus of variations; a weak extremal need not be a minimum; it might be a maximum or neither a minimum nor maximum.

Theorem 3 (first necessary condition in the calculus of variations) A minimizer $u \in C^1[-r,r]$ of \mathcal{E} : $C^1[-r,r] \to \mathbb{R}$ given by (5) is a weak extremal for \mathcal{E} .

In order to proceed further, we assume additional regularity on a minimizer (or extremal) u.

Theorem 4 (C^2 weak extremals) If $u \in C^2[-r,r]$ is a weak extremal for \mathcal{E} given by (5), then

$$\frac{d}{dx}\left(\frac{u'(x)}{\sqrt{1+u'(x)^2}}\right) = \kappa u(x) \qquad \text{for } x \in (-r,r),\tag{7}$$

and

$$\frac{u'(\pm r)}{\sqrt{1 + u'(\pm r)^2}} = \pm \beta. \tag{8}$$

Proof: If $u \in C^2[-r, r]$, then the curvature of the graph

$$\frac{d}{dx} \left(\frac{u'(x)}{\sqrt{1 + u'(x)^2}} \right)$$

makes sense, and we may integrate the first term in (6) by parts to obtain

$$\left(\frac{u'(x)}{\sqrt{1+u'(x)^2}}\phi(x)\right)\Big|_{x=-r}^r - \int_{-r}^r \left[\frac{d}{dx}\left(\frac{u'(x)}{\sqrt{1+u'(x)^2}}\right) - \kappa u(x)\right]\phi(x) dx$$

$$= \beta[\phi(-r) + \phi(r)].$$

That is,

$$\int_{-r}^{r} \left[\frac{d}{dx} \left(\frac{u'(x)}{\sqrt{1 + u'(x)^2}} \right) - \kappa u(x) \right] \phi(x) dx$$

$$= \left[\frac{u'(r)}{\sqrt{1 + u'(r)^2}} - \beta \right] \phi(r) - \left[\frac{u'(-r)}{\sqrt{1 + u'(-r)^2}} + \beta \right] \phi(-r)$$
(9)

for all
$$\phi \in C^1[-r, r]$$
.

Let us assume, by way of contradiction that the factor

$$\frac{d}{dx}\left(\frac{u'(x)}{\sqrt{1+u'(x)^2}}\right) - \kappa u(x)$$

in the integral in (9) is nonzero at some point $x = x_0 \in (-r, r)$. By continuity, then, there is some $\epsilon > 0$ for which

$$\frac{d}{dx}\left(\frac{u'(x)}{\sqrt{1+u'(x)^2}}\right) - \kappa u(x) \neq 0 \quad \text{for } |x-x_0| < \epsilon.$$

Notice that this assertion assumes ϵ is small enough so that $x \in [-r, r]$ for every x with $|x - x_0| < \epsilon$. We know, furthermore, by the intermediate value theorem that this integrand assumes a single sign on the entire interval $x_0 - \epsilon < x < x_0 + \epsilon$.

Exercise 15 Explain why (i.e., give explicit estimates showing) we can assume $\{x : |x-x_0| < \epsilon\} \subset (-r,r)$. Also, explain the application of the intermediate value theorem in detail.

Exercise 16 There exists a function $\phi \in C^1[-r,r]$ satisfying the following:

(a)
$$\phi(x) \equiv 0$$
 for $|x - x_0| \ge \epsilon$.

(b)
$$\phi(x) > 0$$
 for $|x - x_0| < \epsilon$.

Substituting the function ϕ from Exercise 16, for which $\phi(-r) = \phi(r) = 0$, into (9) we conclude

$$\int_{-r}^{r} \left[\frac{d}{dx} \left(\frac{u'(x)}{\sqrt{1 + u'(x)^2}} \right) - \kappa u(x) \right] \phi(x) dx = 0.$$

That is,

$$\int_{x_0 - \epsilon}^{x_0 + \epsilon} \left[\frac{d}{dx} \left(\frac{u'(x)}{\sqrt{1 + u'(x)^2}} \right) - \kappa u(x) \right] \phi(x) \, dx = 0.$$

The factors in the integrand here are both nonzero and neither changes sign on the interior interval $(x_0 - \epsilon, x_0 + \epsilon)$. This is a contradiction implying (7) must hold identically.

In view of what we have just shown (9) simplifies to

$$\left[\frac{u'(r)}{\sqrt{1+u'(r)^2}} - \beta\right] \phi(r) = \left[\frac{u'(-r)}{\sqrt{1+u'(-r)^2}} + \beta\right] \phi(-r)$$

for all $\phi \in C^1[-r, r]$.

Taking any $\phi \in C^1[-r,r]$ for which $\phi(r)=0$ but $\phi(-r)\neq 0$, we get

$$\frac{u'(-r)}{\sqrt{1+u'(-r)^2}} = -\beta.$$

Similarly, when $\phi(-r) = 0$ but $\phi(r) = 0$, we conclude

$$\frac{u'(r)}{\sqrt{1+u'(r)^2}} = \beta. \qquad \Box$$

Notice that we have obtained in Theorem 4 the 2-D capillary surface equation (and ordinary differential equation) and the boundary condition subject to the assumption that the adhesion coefficient β satisfies

$$|\beta| < 1$$

so that the equation $\cos \gamma = \beta$ defines a unique contact angle γ strictly between 0 and π . It may be observed that there was no particular physical restriction suggesting $|\beta| < 1$, and it can be fairly asked: What if we consider the functional \mathcal{E} with $|\beta| \geq 1$? Let us postpone consideration of this question until the next chapter where we discuss solutions of Euler's equation for elastic curves.

2.2 Calculus of Variations

With at least one example of the process (typical to the calculus of variations) by which one begins with a functional and, in an effort to minimize its value or find a minimizer, arrives at a differential equation, let us consider the process in a somewhat more general framework.

Problems in the calculus of variations always involve two important sets, which are usually sets of functions. These two sets are the admissible class \mathcal{A} and the set of **perturbations** \mathcal{V} . The admissible class is the domain of the functional under consideration. Thus, we consider

$$\mathcal{F}: \mathcal{A} \to \mathbb{R}$$
.

and we (typically) seek to minimize \mathcal{F} . The set \mathcal{A} is very often *not* a vector space, though it was in our example above. The set of perturbations \mathcal{V} is almost always a vector space—and an infinite dimensional vector space in the case of the calculus of variations. The perturbations can be thought of roughly as differences of admissible functions. In particular, given an admissible function $u \in \mathcal{A}$ and a perturbation $\phi \in \mathcal{V}$, we require

$$v = u + \epsilon \phi \in \mathcal{A}$$
 for $\epsilon \in \mathbb{R}$ with $|\epsilon|$ small.

We need this in order to compute the first derivative

$$\frac{d}{d\epsilon}\mathcal{F}[u+\epsilon\phi]$$

and hence the first variation

$$\delta_u \mathcal{F}[\phi] = \left(\frac{d}{d\epsilon} \mathcal{F}[u + \epsilon \phi]\right)_{\mid_{\epsilon=0}}.$$

If you think of \mathcal{V} as differences admissible functions with

$$v = u + a \phi \in \mathcal{A}$$
 and $w = u - b \psi \in \mathcal{A}$

both admissible with $\phi, \psi \in \mathcal{V}$, then $v - w = a \phi + b \psi$ should also be in \mathcal{V} (at least for small a and b). This means \mathcal{V} is closed under "small" linear combinations making \mathcal{V} a vector space at least on a small scale.

Also by assuming the set of perturbations \mathcal{V} is a vector space, the first variation (Gateaux derivative or functional derivative) is a functional defined on a vector space:

$$\delta_u \mathcal{F}: \mathcal{V} \to \mathbb{R}.$$

This makes it possible to understand the first variation as a **linear** functional. In fact, under the most common structural assumption for $\mathcal{F}: \mathcal{A} \to \mathbb{R}$, the first variation will always be a linear functional. Namely, if $\mathcal{F}: \mathcal{A} \to \mathbb{R}$ is an **integral functional** of the form

$$\mathcal{F}[u] = \int_{a}^{b} F(x, u(x), u'(x)) dx$$

where \mathcal{A} is some subset (not necessarily a subspace) of $C^1[a, b]$ and $F : [a, b] \times \mathbb{R} \times \mathbb{R} \to \mathbb{R}$ with F = F(x, z, p) is continuously differentiable, then $\delta_u \mathcal{F} : \mathcal{V} \to \mathbb{R}$ by

$$\delta_{u}\mathcal{F}[\phi] = \int_{a}^{b} \left(\frac{\partial F}{\partial z}(x, u(x), u'(x)) \phi(x) + \frac{\partial F}{\partial p}(x, u(x), u'(x)) \phi'(x) \right) dx$$

where \mathcal{V} is a subspace of $C^1[a, b]$. The first variational formula is often written in a shorter form obtained by suppressing the arguments of the functions in the integrand:

$$\delta_u \mathcal{F}[\phi] = \int_a^b \left(\frac{\partial F}{\partial z} \phi + \frac{\partial F}{\partial p} \phi' \right) dx \tag{10}$$

Exercise 17 Compute the first variation formula (10) for an integral functional and verify $\delta_u \mathcal{F}$ is linear (assuming \mathcal{V} is a vector subspace of $C^1[a,b]$).

At this point consideration of several other examples is in order. In particular, we should like to see an example where the admissible class is (naturally) not a vector space. This is easy to illustrate.

Exercise 18 Consider the length of the graph of a function $u : [a, b] \to \mathbb{R}$ with $u \in C^1[a, b]$. Write down the formula for the length functional $\mathcal{L} : \mathcal{A} \to \mathbb{R}$ where

$$\mathcal{A} = \{ u \in C^1[a, b] : u(a) = y_a \text{ and } u(b) = y_b \}.$$

Explain why A is **not** a vector space, but the set of perturbations

$$\mathcal{V} = \{u - v : u, v \in \mathcal{A}\}$$
 is a vector space.

What can you say about minimizers for this problem?

The shortest graph problem above is a very simple and popular example of a problem in the calculus of variations. The next problem is very similar to it in several ways.

Exercise 19 Again let us take

$$A = \{u \in C^1[a, b] : u(a) = y_a \text{ and } u(b) = y_b\}$$

and

$$\mathcal{V} = C_0^1[a, b] = \{ \phi \in C^1[a, b] : \phi(a) = \phi(b) = 0 \}.$$

This time consider $\mathcal{D}: \mathcal{A} \to \mathbb{R}$ by

$$\mathcal{D}[u] = \int_a^b u'(x)^2 \, dx.$$

This is called the **Dirichlet energy** of a function $u \in C^1[a, b]$.

- (a) Find the unique minimizer in the case $y_a = y_b$. Prove your answer is the only possible minimizer in this case.
- (b) Explain why the minimizer when $y_a = y_b$ is inadmissible when $y_a \neq y_b$ and that the minimum value of \mathcal{D} (if it exists when $y_a \neq y_b$) is positive. Hint: Use the mean value theorem. Can you find an explicit lower bound for the minimum value of \mathcal{D} (in terms of a, b, y_a , and y_b)?
- (c) Compute the first variation of \mathcal{D} .
- (d) Assume a minimizer u_0 exists and is in $C^2[a,b]$. Integrate by parts to find an ordinary differential equation satisfied by the minimizer u_0 . State and solve the natural boundary value problem for this ordinary differential equation for the minimizer.
- (e) Again assuming $y_a \neq y_b$, compare the values of $\mathcal{D}[u_c]$ where c is fixed with a < c < b and

$$u_c(x) = \begin{cases} y_a, & 0 \le x \le c, \\ (y_b - y_a)(x - c)/(b - c) + y_a, & c \le x \le b. \end{cases}$$

There is something quite interesting about the functions u_c in the last part of Exercise 19. Do you see what it is?

Here are two (much harder) but still quite popular calculus of variations problems:

Exercise 20 (Brachistochrone) Consider the points A = (0, H) and B = (1, h) in the plane with 0 < h < H. If we consider the path

$$\{(x, -(H-h)x + H) : 0 \le x \le 1\}$$

connecting A to B, we can imagine a point mass (or frictionless bead) that starts from rest at A and slides down to B (under the influence of a downward gravitational field -g(0,1)). Assuming the mass

is constrained to the specified path, notice that the gravitational force can be decomposed in components parallel and orthogonal to the path as

$$-mg(0,1) = -mg\sin\psi(\cos\psi,\sin\psi) + mg\cos\psi(\sin\psi,-\cos\psi)$$

where $\psi = \tan^{-1}(h - H) < 0$. The component orthogonal to the path must be absorbed by a reaction force and, according to Newton's second law the other component gives acceleration to the mass according to

$$\left(\frac{d^2x}{dt^2}, \frac{d^2y}{dt^2}\right) = -g\sin\psi(\cos\psi, \sin\psi).$$

In this case we can find an explicit expression for the motion, and then essentially everything is known.

(a) How long does it take for this mass to move from A to B?

In other cases, computing the time of travel is not so easy. Let us say a path is given by the graph of a function in the set $u \in C^1[0,1]$ with u(0) = H and u(1) = h.

Let us also assume, as with the straight line path given above, a frictionless bead starting from rest at A will move to B along the graph of this function (under the influence of gravity) and arrive at B in finite time T. Denote the motion of this mass by

$$\mathbf{r}(t) = (x(t), y(t)) = (x(t), u(x(t)))$$
 for $0 \le t \le T$.

(b) Recall the arclength relation

$$s = \int_0^x \sqrt{1 + u'(\xi)^2} \, d\xi.$$

Differentiate this expression twice with respect to time to obtain

$$\frac{d^2s}{dt^2} = -g\sin\psi$$

where the inclination angle ψ is defined by

$$(\cos \psi, \sin \psi) = \left(\frac{1}{\sqrt{1 + u'(x)^2}}, \frac{u'(x)}{\sqrt{1 + u'(x)^2}}\right)$$

as usual. Hint(s): Take the component of force along the path as we did for the straight line path to conclude

$$\frac{d^2\mathbf{r}}{dt^2} = -g\sin\psi(\cos\psi,\sin\psi)$$

in general. Then compute $d^2\mathbf{r}/dt^2$ directly and compare what you get to your expression for d^2s/dt^2 .

(c) Show the quantity

$$C = \frac{1}{2}m\left(\frac{ds}{dt}\right)^2 + mgu(x(t))$$

is constant. Hint: Differentiate \mathcal{C} with respect to t and use the previous part.

(d) Assume

$$\frac{dx}{dt} > 0$$

so that $x:[0,T]\to [0,1]$ has in inverse $\tau:[0,1]\to [0,T]$ giving the time $\tau=\tau(\xi)$ at which the mass has x-coordinate ξ . Show

$$T[u] = \frac{1}{\sqrt{2g}} \int_0^1 \sqrt{\frac{1 + u'(x)^2}{H - u(x)}} \, dx.$$

Hint: Use the fundamental theorem of calculus to write T as an integral of $d\tau/d\xi$. Then use the chain rule to show

$$\frac{d\tau}{d\xi} = \frac{\frac{ds}{dx}}{\frac{ds}{dt}}.$$

Finally, use the conserved quantity to express ds/dt in terms of u.

A minimizer of the time of travel functional $T: A \to \mathbb{R}$ where

$$\mathcal{A} = \left\{ u \in C^1[0, 1] : u(0) = H, \ u(1) = h, \text{ and } \int_0^1 \sqrt{\frac{1 + u'(x)^2}{H - u(x)}} \, dx < \infty \right\}$$

is called a brachistochrone or "shortest time" function. This is an example where the perturbation space

$$\mathcal{V} = \{ \phi \in C^1[0,1] : \phi(0) = 0 = \phi(1) \}$$

cannot be interpreted as the set of differences of admissible functions. Nevertheless, one has for each $u \in A$ the crucial condition

$$u + \epsilon \phi \in \mathcal{A}$$
 when $\phi \in \mathcal{V}$ and $|\epsilon|$ is small enough.

This is enough to compute the first variation and determine minimizers.

Incidentally, this problem was posed publicly (and somewhat flamboyantly) by Johann Bernoulli in 1696:

I, Johann Bernoulli, address the most brilliant mathematicians in the world. Nothing is more attractive to intelligent people than an honest, challenging problem, whose possible solution will bestow fame and remain as a lasting monument. Following the example set by Pascal, Fermat, etc., I hope to gain the gratitude of the whole scientific community by placing before the finest mathematicians of our time a problem which will test their methods and the strength of their intellect. If someone communicates to me the solution of the proposed problem, I shall publicly declare him worthy of praise.

It can certainly be argued that while the shortest path and minimum Dirichlet energy problems have (at least) obvious candidates for minimizers, this problem illustrates the fact that the calculus of variations can be used to obtain very non-obvious information.

Exercise 21 Consider $A: A \to \mathbb{R}$ by

$$A[u] = 2\pi \int_0^1 u(x)\sqrt{1 + u'(x)^2} \, dx$$

where

$$\mathcal{A} = \{ u \in C^1[0,1] : u(0) = z_0, \ u(1) = z_1, \ u > 0 \}.$$

This functional gives the area of a surface of rotation generated by rotating the graph of u around the x-axis. Find the first variation and the differential equation satisfied by C^2 minimizers. What you will obtain is called the axially symmetric **minimal surface equation**; it is in fact the equation of meridian curves for axially symmetric surfaces with zero mean curvature. (We will discuss mean curvature in the next section.)

Finding the actual minimizers for the functionals in the last two problems is relatively difficult.

Note on regularity of function classes

For reasons that should become clear later—and would also become clear if the brachistochrone and axially symmetric minimal surface problems were studied further—it is natural to require less regularity than we have required above for admissible functions and more regularity for perturbations. In fact, we already considered functions whose regularity was less than the nominal regularity of the admissible class in part (e) of Exercise 19 concerning Dirichlet energy. Taking the set

$$\{u \in C^1[a,b] : u(a) = y_a \text{ and } u(b) = y_b\}$$

used in some of the examples above, we usually replace this with the larger admissible class

$$\{u \in \Box^1[a,b] : u(a) = y_a \text{ and } u(b) = y_b\}$$

where $\Box^1[a,b]$ denotes the subspace of $C^0[a,b]$ consisting of **piecewise** C^1 **functions**. For each function $u \in \Box^1[a,b]$ there exists a partition $a = x_0 < x_1 < x_2 < \cdots < x_m = b$ such that for $j = 1, 2, \ldots, m$

$$u_{|_{[x_{j-1},x_j]}} \in C^1[x_{j-1},x_j].$$

Here are three reasons to consider admissible classes with lower regularity:

- 1. It is easier to find minimizers and prove minimizers exist—because you are allowing more possibilities. (This is particularly important in the direct methods of the calculus of variations which we will not really cover, and certainly wont emphasize, in this course.)
- 2. It is easier to make modifications/variations of a given admissible function and remain in the admissible class.
- 3. Sometimes minimizers do not have the regularity you would expect. For example sometimes minimizers turn out to be piecewise C^1 instead of C^1 . See Exercise 22 below.

Alternatives to the space of piecewise C^1 functions may be found among the spaces of functions with **weak** derivatives. These spaces are considered, for example, in the text *One-dimensional Variational Problems* by Buttazzo, Giaquinta, and Hildebrandt. The piecewise C^1 functions, however, are a quite traditional choice found, for example, in the classic text *Introduction to the Calculus of Variations* by Hans Sagan.

Exercise 22 (Newton's profile of minimal drag) Isaac Newton modeled the drag on an axially symmetric object of maximum radius R as proportional to

$$N[u] = \int_0^R \frac{x}{1 + u'(x)^2} \, dx$$

where the graph of $u \in [0, R]$ gives the rigid profile meeting the opposing fluid medium. For example, if $u(x) \equiv 0$, then one is considering a flat cylinder $\{(x, y, z) : x^2 + y^2 \leq R^2 \text{ and } z \leq 0\}$ or

$$\{(x, y, z) : x^2 + y^2 \le R^2 \text{ and } -L \le z \le 0\}$$

moving vertically upward and

$$N[u] = \frac{R^2}{2}$$

can be viewed as giving a measure of the resistance encountered.

(a) If one caps the cylinder with a hemisphere, what does Newton's resistance measurement give? Newton mentioned the comparison (of the value for the hemisphere to that for the cylinder) specifically and apparently viewed it as an encouraging sign that his functional was measuring the quantity he had in mind.

(b) Compute the Newtonian resistance N[u] for the conical cap determined by

$$u(x) = \frac{H}{R}(R - x).$$

In practice, it may be impractical to construct a nose cone of arbitrarily large height H. Thus, we introduce the admissible class

$$A = \{u \in \Box^1[0, R] : u(0) = H, \ u(R) = 0, \text{ and } u' \le 0\}$$

for H > 0 fixed. The next part gives some indication about the origin of the monotonicity requirement $u'(x) \le 0$ for $0 \le x \le R$.

- (c) Plot the profile determined by $u(x) = H \sin^2(2\pi nx/R)$ and compute N[u].
- (d) We may assume every function $u \in A$ has $u(x) \equiv H$ on some interval $0 \le x \le R_0 < R$. Among the admissible functions

$$u(x) = \begin{cases} H, & 0 \le x \le R_0, \\ H(R-x)/(R-R_0), & R_0 \le x \le R, \end{cases}$$

which has the least Newtonian resistance N[u]?

There are two more exercises at the end of this section on Newton's resistance functional. The first suggests a kind of justification/derivation for the functional itself, and the second gives a start at finding some actual minimizers and proving that every minimizer satisfies $u(x) \equiv H$ for $0 \le x \le R_0$ and some $R_0 > 0$ and that

$$\lim_{x \searrow R_0} u'(x) < 0$$

so that a minimizer satisfies $u \in \Box^1[0,R] \setminus C^1[0,R]$.

Let us now turn our attention to the vector space of perturbations. A typical collection of perturbations is $C_c^{\infty}(a,b)$ which is a relatively much smaller vector space than

$$C_0^1[a,b] = \{ \phi \in C^1[a,b] : \phi(a) = \phi(b) = 0 \}.$$

The functions in $C_c^{\infty}(a, b)$ are infinitely differentiable and have support compactly contained in the interior interval (a, b). This requires a little explanation.

Open and Closed Sets; Support

We have mentioned the **open interval** $(a,b) \subset \mathbb{R}^1$ and the **open disk**

$$B_r(x_0, y_0) = \{(x, y) : (x - x_0)^2 + (y - y_0)^2 < r^2\} \subset \mathbb{R}^2.$$

These are both examples of **open balls**. Note in particular, that the open interval can be expressed as the set of all points in \mathbb{R}^1 whose distance from the center (a+b)/2 is less than the radius (b-a)/2. In fact open balls are prototypical open sets in any **metric space** which is a set with a notion of distance between pairs of points. More precisely, a set X is a metric space if there is a function $d: X \times X \to [0, \infty)$ satisfying

- 1. d(x,y) = d(y,x) for all $x, y \in X$. (symmetry)
- 2. d(x,y) = 0 if and only if x = y. (positive definite)
- 3. $d(x,z) \le d(x,y) + d(y,z)$ for all $x,y,z \in X$. (triangle inequality)

The function d is called a distance function or metric (distance). Every finite dimensional Euclidean space \mathbb{R}^n is a metric space with

$$d(\mathbf{x}, \mathbf{y}) = \sqrt{\sum_{j=1}^{n} (y_j - x_j)^2}$$

where $\mathbf{x} = (x_1, x_2, \dots, x_n)$ and $\mathbf{y} = (y_1, y_2, \dots, y_n)$. This is called the Euclidean metric and the value of the Euclidean metric is also denoted $|\mathbf{y} - \mathbf{x}|$ or sometimes $||\mathbf{y} - \mathbf{x}||$ if one is worried about confusion with the absolute value function on \mathbb{R} .

Using any metric (on a metric space X) one defines the open ball of radius r > 0 and center $p \in X$ by

$$B_r(p) = \{ x \in X : d(x, p) < r \}.$$

Also a subset $U \subset X$ of any metric space X is said to be **open** if for each $p \in U$, there is some r > 0 such that

$$B_r(p) \subset U$$
.

Exercise 23 Show that an open ball in any Euclidean space is open.

Technically, there can be other notions of open sets and we should be a little more careful and say a set is *open with respect to the metric topology* if the condition above holds. For our purposes at the moment, however, we can assume the only topologies of interest are metric topologies of the sort just described.

Exercise 24 Show a finite intersection of open sets is open and any possible union of open sets is open.

Definition 3 The interior of any set (in a metric space) is the union of all open balls inside that set. If $A \subset X$ and X is a metric space, we denote the interior of A by $\operatorname{int}(A)$ and

$$int(A) = \bigcup_{\substack{x \in X, r > 0 \\ B_r(x) \subset A}} B_r(x).$$

Exercise 25 Show the interior of a set is always open.

A set $A \subset X$ is defined to be **closed** if the complement

$$A^c = X \setminus A = \{x \in X : x \notin A\}$$
 is open.

Exercise 26 Show any intersection of closed sets is closed.

This brings us to a crucial construction: The **closure** of any subset A of a metric space X is defined to be the smallest closed set containing A. That is, the closure of A is

$$\operatorname{clos}(A) = \overline{A} = \bigcap_{\substack{C \supset A \\ C: \operatorname{closed}}} C.$$

Exercise 27 Show a set is closed if and only if the set is its own closure.

Definition 4 (support) Given a function $u: A \to \mathbb{R}$ defined on a subset A of the Euclidean space \mathbb{R}^n , the support of u, denoted by supp(u), is the closure of the set of points where u is nonzero. That is,

$$\operatorname{supp}(u) = \overline{\{\mathbf{x} \in A : u(\mathbf{x}) \neq 0\}}.$$

Definition 5 A set $A \subset X$ where X is a metric space is **bounded** if there is some $p \in X$ and some r > 0 such that

$$A \subset B_r(p)$$
.

In the case where $X = \mathbb{R}^n$ is Euclidean space, we may take the center of the bounding ball to be the origin **0**. Then a set is bounded if there is some r > 0 such that

$$|\mathbf{x}| < r$$
 for all $\mathbf{x} \in A$.

Definition 6 A set $K \subset \mathbb{R}^n$ is compact if K is closed and bounded.

Definition 7 A function $u: A \to \mathbb{R}$ defined on a set $A \subset \mathbb{R}^n$ is said to have **compact support** in A if supp(u) is compact and

$$supp(u) \subset int(A).$$

This condition is often written as $supp(u) \subset A$, which is read "the function u has support compactly contained in A" or "the function u is compactly supported in A" for short.

We are now (almost) in a position to discuss $C_c^{\infty}(a,b)$. We have mentioned that the set of continuous real valued functions on [a,b] is denoted by $C^0[a,b]$, and the set of continuously differentiable real valued functions on [a,b] is denoted by $C^1[a,b]$. These are vector spaces over \mathbb{R} and $C^0[a,b] \supset C^1[a,b]$. Naturally, we can also require continuity or differentiability only at interior points of (a,b), and the corresponding vector spaces are denoted by $C^0(a,b) \supset C^1(a,b)$. We can also require the existence of more continuous derivatives: The functions in $C^k(a,b)$ have derivatives of order k which are continuous at each point in (a,b), and we have an infinite collection of nested vector subspaces:

$$C^0(a,b) \supset C^1(a,b) \supset C^2(a,b) \supset \cdots$$

Showing strict inequality in each of these inclusions is one way to show each of these vector subspaces is infinite dimensional.

$$C^{\infty}(a,b) = \bigcap_{k=0}^{\infty} C^k(a,b).$$

In some sense, most familiar functions are in this (kind of) space. Most familiar functions have derivatives of all orders: polynomials, exponentials, sine and cosine. The tangent function is in $C^{\infty}(-\pi/2, \pi/2)$.

$$C_c^{\infty}(a,b) = \{ u \in C^{\infty}(a,b) : \operatorname{supp}(u) \subset\subset (a,b) \}.$$

If you haven't been shown a function in $C_c^{\infty}(a,b)$, or thought carefully about it for a long time, then you probably do not know any nonzero functions in this set.

Exercise 28 Show there exists a nonzero C^{∞} function with compact support.

2.3 Calculus of Variations—second pass

One advantage of using a very small perturbation space is that the theorems above hold under less restrictive hypotheses. Notice that to require

$$\mathcal{F}[u] \le \mathcal{F}[u + h\phi]$$
 for every $\phi \in C_0^1[a, b]$

is much more than requiring

$$\mathcal{F}[u] \le \mathcal{F}[u + h\phi]$$
 for every $\phi \in C_c^{\infty}(a, b)$

simply because $C_c^{\infty}(a,b)$ is effectively a subset of $C_0^1[a,b]$.

Here is a somewhat more standard treatment of some of the results above for an integral functional $\mathcal{F}: \mathcal{A} \to \mathbb{R}$ defined on an admissible class in $\Box^1[a,b]$. If \mathcal{F} is given by

$$\mathcal{F}[u] = \int_a^b F(x, u, u') \, dx,$$

then the function F = F(x, z, p) is called the **Lagrangian** for the variational problem. The first variation of \mathcal{F} at u in the direction $\phi \in C_c^{\infty}(a, b)$ is defined by

$$\delta_u \mathcal{F}[\phi] = \left[\frac{d}{d\epsilon} \int_a^b F(x, u + \epsilon \phi, u' + \epsilon \phi') \, dx \right]_{\epsilon=0}.$$

Theorem 5 A function $u \in A$ for which

$$\delta_u \mathcal{F}[\phi] \equiv 0$$
 for all $\phi \in C_c^{\infty}(a, b)$

is called a weak extremal of \mathcal{F} , and one has the first necessary condition

$$\int_{a}^{b} \left[\frac{\partial F}{\partial z} \phi + \frac{\partial F}{\partial p} \phi' \right] dx = 0 \quad \text{for all } \phi \in C_{c}^{\infty}(a, b).$$

The key tool for the proof of the next result is called the **fundamental lemma of the calculus of variations**:

Lemma 1 If $f:(a,b)\to\mathbb{R}$ is a continuous function and

$$\int_{a}^{b} f(x)\phi(x) dx = 0 \quad \text{for every } \phi \in C_{c}^{\infty}(a,b),$$

then f(x) = 0 for $x \in (a, b)$.

Theorem 6 A weak extremal for \mathcal{F} which is C^2 on any open subinterval $(x_0 - \delta, x_0 + \delta) \subset (a, b)$ satisfies the ordinary differential equation

$$\frac{d}{dx}\left(\frac{\partial F}{\partial p}\right) = \frac{\partial F}{\partial z} \tag{11}$$

on the interval $(x_0 - \delta, x_0 + \delta)$.

The second order ordinary differential equation (11) is called the **Euler-Lagrange** equation for the functional \mathcal{F} .

There are various generalizations of these results, but understanding the simple concept that minimization problems for integral functionals lead to differential equations is a good start.

Exercise 29 Prove the fundamental lemma.

Exercise 30 Use the fundamental lemma (and integration by parts) to prove the Euler-Lagrange equation holds for C^2 weak extremals.

Local Minimizers

Exercise 9 illustrates that critical points can be local minimizers in finite dimensional calculus without being global minimizers. The same thing can happen in the calculus of variations, but up until this point we have not introduced enough structure to make sense of the notion of local versus global minimizers. The key is the introduction of a distance between elements in the admissible class \mathcal{A} . In particular, we already have discussed the notion of a metric distance and we certainly want to have such a distance on \mathcal{A} . Most commonly, however, the metric distance we will use comes from an additional abstract structure which it is well worth discussing:

Definition 8 Given a vector space V over the field \mathbb{R} , i.e., a real vector space, a function $\|\cdot\|:V\to[0,\infty)$ is called a **norm**, and the vector space V is called a **normed vector space**, if the following conditions hold:

- 1. ||cv|| = |c|||v|| for every $c \in \mathbb{R}$ and every $v \in V$ (non-negative homogeneity)
- 2. ||v|| = 0 if and only if $v = \mathbf{0}$ (positive definite)
- 3. $||v+w|| \le ||v|| + ||w||$ (triangle inequality)

Exercise 31 Show that every normed vector space is a metric space with metric distance d(v, w) = ||v - w||.

Exercise 32 Show that $||u|| = \max\{|u(x)| : a \le x \le b\}$ defines a norm on $C^0[a,b]$. (You'll need some theorems from 1-D calculus for this.) This is called the "C zero" norm, the L^{∞} norm, the "sup" norm, and the uniform norm; it goes by many names.

Exercise 33 Show $C_B^0(a,b) = \{u \in C^0(a,b) : \sup\{|u(x)| : a < x < b\}\}\$ is a vector subspace of $C^0(a,b)$ and

$$\|u\|_{C^0} = \sup\{|u(x)| : a < x < b\}$$

is a norm on $C_B^0(a,b)$ (the subspace of bounded continuous functions on (a,b)).

Exercise 34 There are many important continuous functions which are not in $C_B^0(a,b)$, and the sup norm is not a norm on $C^0(a,b)$. Consider $d: C^0(a,b) \times C^0(a,b) \to [0,\infty)$ by

$$d(f,g) = \min\{1, \sup\{|f(x) - g(x)| : a < x < b\}.$$

Is d a metric on $C^0(a,b)$?

There are a good many important vector spaces, like $C^0(a,b)$, which are not (at least in any natural way) normed spaces. Please note/recall that normed spaces are required to be vector spaces but metric spaces, in general, are not required to be vector spaces. If the notion of a metric, however, is coupled with the condition of being a vector space by the introduction of certain axioms one is led to (or may stumble upon) the theory of **topological vector spaces**. Doing analysis in the framework of topological vector spaces can become somewhat complicated, so we will try to avoid that, but it's perhaps worth knowing such a thing/structure is out there.

Exercise 35 Consider $[\cdot]: C^1[a,b] \to [0,\infty)$ by

$$[u] = \max\{|u'(x)| : a \le x \le b\}.$$

The function $[\ \cdot\]$ is called the C^1 seminorm.

(a) Determine which properties of a norm $[\cdot]$ satisfies. Those are the defining properties of a seminorm.

(b) Show that $\|\cdot\|_1: X \to [0,\infty)$ given by

$$||v||_1 = ||v|| + [v]$$

where $\|\cdot\|$ is any norm on a vector space X and $[\cdot]$ is any seminorm on X is a norm on X.

The sum of the C^0 "sup" norm and the C^1 seminorm is called the C^1 norm on $C^1[a,b]$.

(c) Define a C^1 seminorm and a C^1 norm on a suitable subspace $C^1_B(a,b)$ of $C^1(a,b)$.

Definition 9 Let $\mathcal{F}: \mathcal{A} \to \mathbb{R}$ be a functional defined on a admissible class of functions \mathcal{A} which is a subset of a normed vector space X containing the subspace of variations \mathcal{V} . An admissible function $u \in \mathcal{A}$ is said to be a **local minimizer** of \mathcal{F} relative to the norm on X if there exists some $\delta > 0$ such that the following holds:

If $v \in A$ and $||u - v||_X \le \delta$, then $u - v \in V$ and

$$\mathcal{F}[u] \le \mathcal{F}[v].$$

This definition gives rise to the notion of local C^0 minimizers (if one takes the C^0 norm on $C^0[a,b]$) and of local C^1 minimizers (if one happens to have $\mathcal{A} \subset C^1[a,b]$ and takes the C^1 norm).

Theorem 7 (first order necessary conditions in the calculus of variations) A local C^0 minimizer $u \in \mathcal{A} \subset C^1(a,b) \cap C^0(a,b)$ of the integral functional $\mathcal{F} : \mathcal{A} \to \mathbb{R}$ given by

$$\mathcal{F}[u] = \int_{a}^{b} F(x, u, u') \, dx$$

is a weak extremal:

$$\int_{a}^{b} \left[\frac{\partial F}{\partial z} \phi + \frac{\partial F}{\partial p} \phi' \right] dx = 0 \quad \text{for all } \phi \in C_{c}^{\infty}(a, b).$$

If the local C^0 minimizer satisfies $u \in C^2(a,b)$, then u is a solution of the Euler-Lagrange equation in the interior of the interval (a,b):

$$\frac{d}{dx}\left(\frac{\partial F}{\partial p}\right) = \frac{\partial F}{\partial z} \qquad a < x < b.$$

Additional Exercises

Exercise 36 (Newton's drag functional) One can heuristically motivate the interpretation of the quantity

$$N[u] = \int_0^R \frac{x}{\sqrt{1 + u'(x)^2}} dx$$

as a measure of the resistance against a moving profile along the following lines: To a moving point mass m having velocity \mathbf{v} one can associate a **momentum vector** $m\mathbf{v}$ and a potential energy $m|\mathbf{v}|^2/2$. Assume we are given a very small mass m at rest that encounters a large moving profile, associated presumably to a large mass. We can shift reference frame and consider the profile at rest and the small mass as moving and striking the profile with a particular orientation. In particular, if we assume the initial momentum vector of the mass is $-m|\mathbf{v}|(0,1)$ and the profile is given by $\{(x,u(x)): 0 \le x \le R\}$, then the component of the momentum vector orthogonal to the profile at impact is

$$[-m|\mathbf{v}|(0,1)\cdot(\sin\psi,-\cos\psi)](\sin\psi,-\cos\psi) = m|\mathbf{v}|\cos\psi(\sin\psi,-\cos\psi)$$

where the inclination angle ψ is defined by

$$(\cos \psi, \sin \psi) = \left(\frac{1}{\sqrt{1 + u'(x)^2}}, \frac{u'(x)}{\sqrt{1 + u'(x)^2}}\right)$$

as usual. Assume this component of the momentum is completely absorbed by the profile. Accordingly, we assume the profile absorbs the kinetic energy associated with this component of momentum.

- (a) What is the absorbed kinetic energy from the mass m?
- (b) Instead of a finite point mass m, approximate the absorbed energy with a mass of the form

$$m_{ij} = \rho x_j^* (\theta_i - \theta_{i-1}) (x_j - x_{j-1})$$

where ρ is a constant areal mass density and $x_j^*(\theta_i - \theta_{i-1})(x_j - x_{j-1})$ is a local area element given in polar coordinates. Summing over i and j write an approximation for the total absorbed energy as a Riemann sum converging to an integral over the disk $B_R(0)$.

(c) Show the integral expression from the last part is proportional to Newton's functional.

Hint:

$$\sum_{i,j} \frac{1}{2} \rho x_j^* |\mathbf{v}|^2 \cos^2 \psi (\theta_i - \theta_{i-1}) (x_j - x_{j-1})$$
$$\sim \frac{\rho}{2} |\mathbf{v}|^2 \sum_{i,j} \frac{x_j^*}{1 + u'(x_j^*)^2} (\theta_i - \theta_{i-1}) (x_j - x_{j-1}).$$

Exercise 37 (flat tipped minimizers) We consider Newton's profile of minimal drag problem with R = H = 1. Consider the function $f : [1, \infty) \to \mathbb{R}$ by

$$f(t) = \frac{t}{(1+t^2)^2} \left(\frac{3}{4}t^4 + t^2 - \frac{7}{4} - \log t\right).$$

Set $t_0 = f^{-1}(1)$ and $r_0 = 4T/(1+T^2)^2$.

- (a) Find t_0 and r_0 numerically.
- (b) Use mathematical software to plot the profile $\{(x, u_0(x)) : 0 \le x \le 1\}$ satisfying $u_0(x) = 1$ for $0 \le x \le r_0$ with the remainder of the graph given parametrically by

$$(x(t), z(t)) = (0, 1) + \frac{r_0(1 + t^2)^2}{4t} (1, -f(t)), \qquad 1 \le t \le t_0.$$

- (c) Show $\lim_{x \searrow r_0} u'(x) < 0$.
- (d) Let R_0 be fixed with $0 \le R_0 < 1$. Consider a function $u : [0,1] \to [0,1]$ with
 - (i) $u \in C^0[0,1]$,
 - (ii) $u(x) \equiv 1 \text{ for } 0 \le x \le R_0$,
 - (iii) $u'(x) < 0 \text{ for } R_0 < x \le 1, \text{ and }$
 - (iv) u(1) = 0.

Note that the restriction

$$u_{|_{[R_0,1]}}: [R_0,1] \to [0,1]$$

has an inverse $w:[0,1] \to [R_0,1]$. Assume $w \in C^1[0,1]$ and set v(t) = w(1-t). Show

$$N[u] = \frac{v(0)^2}{2} + \int_0^1 \frac{v(t)v'(t)^3}{1 + v'(t)^2} dt.$$

(e) Consider $M: \mathcal{M} \to \mathbb{R}$ by

$$M[v] = \frac{v(0)^2}{2} + \int_0^1 \frac{v(t)v'(t)^3}{1 + v'(t)^2} dt$$

on

$$\mathcal{M} = \{ v \in C^2[0,1] : v(0) \ge 0, \ v(1) = 1, \text{ and } v' \ge 0 \}.$$

Compute the Euler-Lagrange equation and show the solution v leads to the function u_0 defined in part (b). (This is somewhat tricky, but at least you should be able to show the function v_0 obtained from u_0 solves the Euler-Lagrange equation.)

3 Partial Differential Equations

One generalization we do want to consider is exemplified by deriving the equations of Laplace and Young for a capillary surface in a vertical tube. Let us, in this instance, assume the tube has general cross-section \mathcal{U} where \mathcal{U} is a bounded open subset of \mathbb{R}^2 having boundary (which is a topological term we need to define) a smooth simple closed curve. What we mean by this is the following: The **boundary** of any set (in a metric space, e.g., \mathbb{R}^n) is the intersection of the closure of the set with the closure of the complement of the set. That is,

$$\partial \mathcal{U} = \overline{\mathcal{U}} \bigcap \overline{\mathbb{R}^2 \backslash \mathcal{U}}.$$

Exercise 38 Show a x is in the boundary ∂A of any set A if and only if for every r > 0

$$B_r(x) \cap A \neq \phi$$
 and $B_r(x) \cap A^c \neq \phi$.

There are a couple equivalent ways we can say what it means for an open bounded set $\mathcal{U} \subset \mathbb{R}^2$ to have a smooth simple closed curve as boundary. It is no easy task to show they are equivalent, but we can state the conditions

There exists a surjective² twice continuously differentiable vector valued function $\alpha: \mathbb{R} \to \partial\Omega \subset \mathbb{R}^2$ with the following properties

1. For some L > 0, the restriction

$$\alpha_{\big|_{[0,L)}}:[0,L)\to\partial\Omega$$
 is one-to-one and onto,

- 2. $\alpha(L) = \alpha(0)$, and
- 3. $\alpha(t+L) = \alpha(t)$ for all $t \in \mathbb{R}$.

Being twice continuously differentiable here means $x, y \in C^2(\mathbb{R})$ where $\alpha(t) = (x(t), y(t))$.

Alternatively, we can define a **homotopy** of a loop as follows: Given a loop, which is just a continuous function $\alpha : [0, L] \to \mathcal{U}$ with $\alpha(L) = \alpha(0)$, a homotopy of α (relative to \mathcal{U}) is a continuous function $h : [0, 1] \times [0, 1] \to \mathcal{U}$ satisfying the following

²Surjective means "onto" in the sense that for each $\mathbf{p} \in \Omega$, there is some $t \in \mathbb{R}$ with $\alpha(t) = \mathbf{p}$.

- 1. $\alpha(t) = h(t, 0)$ for $0 \le t \le 1$ and
- 2. h(0,s) = h(1,s) for $0 \le s \le 1$.

A homotopy h of the loop α is a **fixed point homotopy** if $h(0,s) = \alpha(0)$ for $0 \le s \le 1$. A homotopy if a **contraction to a point** if there is a point $\mathbf{p} \in \mathcal{U}$ for which $h(t,1) \equiv \mathbf{p}$ for $0 \le t \le 1$.

The open set $\mathcal{U} \subset \mathbb{R}^2$ is **simply connected** if for every loop $\alpha : [0,1] \to \mathcal{U}$ there exists a fixed point homotopy (relative to \mathcal{U}) which is a contraction of α to $\alpha(0)$.

A bounded open set $\mathcal{U} \subset \mathbb{R}^2$ has boundary a simple closed curve if (and only if) the following hold:

- 1. \mathcal{U} is simply connected, and
- 2. for each $\mathbf{p} \in \partial \mathcal{U}$, there exists some a > 0, a unit vector $\mathbf{u} = (u_1, u_2)$, and a function $g \in C^2[-a, a]$ with g'(0) = 0 such that

$$\mathcal{U} \cap \{\mathbf{p} + s\mathbf{u} + t\mathbf{u}^{\perp} : s, t \in [-a, a]\}$$
$$= \{\mathbf{p} + s\mathbf{u} + t\mathbf{u}^{\perp} : t \ge g(s) \text{ and } -a \le s \le a\}.$$

In these sets $\mathbf{u}^{\perp} = (-u_2, u_1)$.

Exercise 39 A collection of open sets $\{U_{\alpha}\}_{{\alpha}\in\Gamma}$ where Γ is any indexing set is called an open cover of a set A if

$$A \subset \bigcup_{\alpha \in \Gamma} U_{\alpha}.$$

A subset $A \subset \mathbb{R}^n$ is compact if and only if it has the following property: Given any open cover $\{U_\alpha\}_{\alpha\in\Gamma}$ of A, there exist finitely many sets $U_{\alpha_1}, U_{\alpha_2}, \ldots, U_{\alpha_k}$ in the open cover such that

$$\{U_{\alpha_1}, U_{\alpha_2}, \dots, U_{\alpha_k}\}$$
 is still an open cover of A.

This is called the Hiene-Borel Theorem. The finite subcollection of open sets in this result is called a finite subcover.

Exercise 40 Show that the boundary of an open bounded subset of \mathbb{R}^n is compact.

Returning to the capillary tube problem: Let \mathcal{U} be a bounded open subset of \mathbb{R}^2 with boundary a simple closed curve. Let σ be a surface tension constant with units (force)/distance. Let $\beta \in (0,1)$ be a dimensionless constant adhesion coefficient, i.e., β has units 1. Let g be the usual gravitational constant. Given $u \in C^1(\overline{\mathcal{U}})$, which means there exists an open set $U \supset \overline{\mathcal{U}}$ and an extension $\overline{u}: U \to \mathbb{R}$ with continuous partial derivatives

$$\frac{\partial \overline{u}}{\partial x}$$
 and $\frac{\partial \overline{u}}{\partial y}$,

both in $C^0(U)$, such that

$$\overline{u}_{|_{\mathcal{U}}} = u,$$

we define the **capillary energy** of u to be

$$\mathcal{E}[u] = \sigma \int_{\mathcal{U}} \sqrt{1 + |Du|^2} - \sigma \beta \int_{\partial \mathcal{U}} u + \frac{\rho g}{2} \int_{\mathcal{U}} u^2.$$

As in the 2-D case, the first term is called the free surface energy, the second term is called the wetting energy, and the third term is called the gravitational potential energy.

Exercise 41 Explain why

$$A[u] = \int_{\mathcal{U}} \sqrt{1 + |Du|^2}$$

is the area functional.

Exercise 42 Obtain the gravitational energy as a limit of a Riemann sum approximating an integral over the volume

$$\{(x, y, z) : (x, y) \in \mathcal{U} \text{ and } 0 < z < u(x, y)\}$$

(assuming u > 0).

3.1 The first variation of area

We wish to compute a variation

$$\left[\frac{d}{d\epsilon} \int_{\mathcal{U}} \sqrt{1 + |D(u + \epsilon \phi)|^2}\right]_{\epsilon = 0}.$$

Let us first recall that the vector function $Du : \overline{\mathcal{U}} \to \mathbb{R}^2$ is the **gradient field** or total derivative of u given by the vector of first partials:

$$Du = \left(\frac{\partial \overline{u}}{\partial x}, \frac{\partial \overline{u}}{\partial y}\right),\,$$

and when we write $|Du|^2$ we are indicating the use of the Euclidean norm:

$$|Du|^2 = \left(\frac{\partial \overline{u}}{\partial x}\right)^2 + \left(\frac{\partial \overline{u}}{\partial y}\right)^2.$$

Thus, the value of the area functional

$$\int_{\mathcal{U}} \sqrt{1 + |Du|^2}$$

is an example of an integral of a real valued function of two variables x and y over an open subset $\mathcal{U} \subset \mathbb{R}^2$. Certainly such integrals are considered in a course on multivariable calculus. It is likely that we will need to understand such integrals, and what can be done with them, a bit better than they are understood by most students who have taken such a course. In view of this, I have typed up in the next section an exposition of certain aspects of integration. It might be worth looking at before reading further. I have also included a review of differentiation and verious kinds of derivatives which may be consulted if desired or necessary.

Let us write $A: C^1(\overline{\mathcal{U}}) \to \mathbb{R}$ to denote the area functional and calculate the first variation of area δA . The area of a perturbed graph given by $u + \epsilon \phi$ where $\phi \in C_c^{\infty}(\mathcal{U})$ is given by

$$\int_{\mathcal{U}} \sqrt{1 + |Du + \epsilon D\phi|^2}.$$

Thus, by the chain rule

$$\frac{d}{d\epsilon} \int_{\mathcal{U}} \sqrt{1 + |Du + \epsilon D\phi|^2} = \int_{\mathcal{U}} \frac{(Du + \epsilon D\phi) \cdot D\phi}{\sqrt{1 + |Du + \epsilon D\phi|^2}},$$

and

$$\delta A_u[\phi] = \int_{\mathcal{U}} \frac{Du \cdot D\phi}{\sqrt{1 + |Du + \epsilon D\phi|^2}} = \int_{\mathcal{U}} Tu \cdot D\phi$$

where $Tu = Du/\sqrt{1 + |Du|^2}$ is the projection projection of the downward unit normal field $(u_x, u_y, -1)/\sqrt{1 + |Du|}$ encountered in Chapter 1. To the real scaling ϕTu of this projection field and use the divergence theorem to write

$$\int_{\mathcal{U}} \operatorname{div}(\phi T u) = \int_{\partial \mathcal{U}} \phi T u = 0.$$

owing to the fact that ϕ has support compactly contained in \mathcal{U} . There is a general product formula for the divergence applying to a real scaling of a vector field, namely,

$$\operatorname{div}(w\mathbf{v}) = Dw \cdot \mathbf{v} + w \operatorname{div} \mathbf{v}.$$

Exercise 43 If \mathcal{U} is an open subset of \mathbb{R}^n with $w: \mathcal{U} \to \mathbb{R}$ satisfying $w \in C^1(\mathcal{U})$ and $\mathbf{v} \in C^1(\mathcal{U} \to \mathbb{R}^n)$, then

$$\operatorname{div}(w\mathbf{v}) = Dw \cdot \mathbf{v} + w \operatorname{div} \mathbf{v}.$$

Prove this identity two different ways

- (a) Use the definition of the divergence as a limit of flux density.
- (b) Verify the formula in terms of standard rectangular coordinates.

This is a good time to pause and note that when we restrict to perturbations $\phi \in C_c^{\infty}(\mathcal{U})$, we are considering what are called **interior variations**. As pointed out in the previous section, this is a commonly considered and convenient vector space of perturbations. In the capillary tube problem, however, it is also important to consider more general variations.

Theorem 8 If $u \in C^2(\mathcal{U})$, then the interior variation of area at u is given by

$$\delta A_u[\phi] = -\int_{\mathcal{U}} \operatorname{div}\left(\frac{Du}{\sqrt{1+|Du|^2}}\right) \phi \quad \text{for } \phi \in C_c^{\infty}(\mathcal{U}).$$

Thus, we encounter the mean curvature operator

$$\mathcal{M}u = \operatorname{div} Tu = \operatorname{div} \left(\frac{Du}{\sqrt{1 + |Du|^2}} \right)$$

of the previous chapter.

Exercise 44 Compute the interior variation of the full capillary energy \mathcal{E} to show that for $u \in C^2(\mathcal{U})$

$$\delta \mathcal{E}_u[\phi] = \int_{\mathcal{U}} \left[-\operatorname{div}\left(\frac{Du}{\sqrt{1+|Du|^2}}\right) + f(u) \right] \phi$$

for an appropriate function $f: \mathbb{R} \to \mathbb{R}$ and all $\phi \in C_c^{\infty}(\mathcal{U})$.

Mean Curvature

Now let us consider a little surface geometry in coordinates. Say $u \in C^2(\mathcal{U})$ has graph $\mathcal{G} = \{(x, y, u(x, y)) : (x, y) \in \mathcal{U}\}$. We have discussed the signed curvature of a plane curve with

$$k = \left(\frac{u'}{\sqrt{1 + u'^2}}\right)' = \frac{u''}{(1 + u'^2)^{3/2}}$$

when the curve is given as the graph of a function $\{(x, u(x)) : x \in (a, b)\}$. In this context, the signed curvature can also be realized as the derivative, with respect to arclength, of the inclination angle ψ with respect to the horizontal; see Exercise 20. In fact,

$$\sin \psi = \frac{u'}{\sqrt{1 + u'^2}}$$

so that

$$k = \frac{d}{dx}[\sin \psi] = \frac{d}{ds}[\sin \psi] \frac{ds}{dx} = \cos \psi \frac{d\psi}{ds} \frac{ds}{dx} = \frac{d\psi}{ds}.$$

Exercise 45 Reparameterize the graph $\{(x, u(x)) : x \in (a, b)\}$ by arclength to show

$$\frac{ds}{dx} = \sqrt{1 + u'^2}.$$

More generally, the **curvature vector** \vec{k} of a space curve $\alpha:(a,b)\to\mathbb{R}^n$ at a point $\alpha(t_0)$ with $t_0\in(a,b)$ is defined as follows: Reparameterize α by arclength obtaining, for some $\epsilon>0$, a parameterization of (perhaps a portion of) the same curve $\gamma:(-\epsilon,\epsilon)\to\mathbb{R}^n$ defined on $\{s:|s|<\epsilon\}$ and satisfying $\gamma(0)=\alpha(t_0)$. Then,

$$\vec{k} = \frac{d^2\gamma}{ds^2}(0).$$

This definition assumes reparameterization by arclength is possible and that the derivatives to be computed exist. Sufficient conditions for this to be the case are the following:

- 1. $\alpha \in C^2((a,b) \to \mathbb{R}^n)$ and
- 2. $\alpha'(t_0) \neq 0$.

Exercise 46 The arclength of a curve $\alpha \in C^1((a,b) \to \mathbb{R}^n)$ is

$$s = \int_{t_0}^t |\alpha'(\tau)| \, d\tau.$$

Assuming $\alpha'(t_0) \neq \mathbf{0}$, reparameterize α to obtain an arclength parameterization $\gamma: (-\epsilon, \epsilon) \to \mathbb{R}^n$ as in the definition above and compute

$$\frac{d\gamma}{ds}$$
.

Exercise 47 Given $u \in C^2(a,b)$ and $\alpha(x) = (x,u(x))$, find the curvature vector \vec{k} of the graph $\mathcal{G} = \{(x,u(x)) : x \in (a,b)\}$ at each point, and find an expression for the signed curvature of the graph with respect to the upward normal.

Exercise 48 Assuming $\alpha \in C^2((a,b) \to \mathbb{R}^n)$ with $\alpha'(t_0) \neq \mathbf{0}$, compute the curvature vector \vec{k} at $\alpha(t_0)$ in terms of γ .

In physics, it is often convenient to express derivatives with respect to time using a "dot" instead of a prime so that velocity v is given by the derivative of position \dot{x} with respect to time and acceleration a is given by the derivative of velocity \ddot{x} with respect to time. This seems to be a tradition started by Newton and it leaves open the prime notation for derivatives with respect to space. A similar tradition is convenient when one makes curvature calculations like those above: We denote derivatives with respect to the parameter t (or whatever parameter is used to define α) with a prime and derivatives with respect to arclength with a "dot." Thus, $\dot{\gamma} = \alpha'/|\alpha'|$ and $\vec{k} = \ddot{\gamma}$.

It will be noted that there is no immediately obvious notion of signed curvature for a space curve. There are certain situations, however, where such a notion does make sense. If that curve happens to lie in a two-dimensional plane and a particular unit normal N (to the curve within that plane) is specified at a point $\alpha(t_0)$, then we may define the signed curvature of α at $\alpha(t_0)$ with respect to N by

$$k = \vec{k} \cdot N$$

where \vec{k} is the curvature vector to the curve at $\alpha(t_0)$. The value of the signed curvature in this context is sometimes denoted by k_N .

Exercise 49 Show the new notion of signed curvature for a graph $\{(x, u(x)) : x \in (a, b)\}$ agrees with the previous definition if we take as the specified normal

$$N = \frac{(-u', 1)}{\sqrt{1 + u'^2}},$$

that is, the upward unit normal to the graph.

Perhaps this is a good start to understanding the curvature of curves.

Exercise 50 Find the curvature of the graph of the function $u(x) = \sqrt{r^2 - x^2}$ for |x| < r. Find the curvature of the graph of the function $u(x) = -\sqrt{r^2 - x^2}$ for |x| < r.

Let us return to our simple surface which is the graph of a function u:

$$G = \{(x, y, u(x, y)) : (x, y) \in U\}.$$

If we want to talk about the curvature of this surface, things are somewhat (more) complicated. We note that there are many curves passing through each point $(x_0, y_0, u(x_0, y_0))$ on the surface, and it is reasonable to imagine that the curvatures of these curves are somehow related to the curvature of the surface at this point. There are a several nominally different ways to think about (and compute) the kind of curvature (mean curvature) that is prescribed by the capillary equation. Probably we should think about at least a couple of them.

Take the upward unit normal to the surface \mathcal{G} is given by

$$N = \frac{(-u_x, -u_y, 1)}{\sqrt{1 + |Du|^2}}.$$

Exercise 51 Explain why the vectors $X_x = (1, 0, u_x)$ and $X_y = (0, 1, u_y)$ are linearly independent tangent vectors to \mathcal{G} and compute N using the cross product $X_x \times X_y$.

We denote the tangent plane to \mathcal{G} at X by $T_X\mathcal{G}$. Thus,

$$T_X \mathcal{G} = \{aX_x + bX_y : (a, b) \in \mathbb{R}^2\}.$$

Any nonzero tangent vector $\mathbf{v} = (v_1, v_2, v_3) \in T_X \mathcal{G}$ determines a unique plane $\Pi = \Pi(\mathbf{v})$ orthogonal to $\mathbf{v} \times N$. Such a **normal plane** intersects the surface \mathcal{G} in a curve, and we would like to compute the signed curvature of this curve in the plane Π with respect to N at the point X = (x, y, u(x, y)).

To illustrate how this computation works, we make a specific choice of unit tangent vector

$$\mathbf{v} = \frac{X_x}{|X_x|} = \frac{(1, 0, u_x)}{\sqrt{1 + u_x^2}}.$$

Let us denote the associated plane by Π_{α} where we imagine $\alpha:(-\epsilon,\epsilon)\to\mathbb{R}^3$ parameterizes the intersection curve on some interval $(-\epsilon,\epsilon)$ with $\alpha(0)=X$. A unit normal to Π is

$$\mathbf{w} = N \times \mathbf{v}$$
.

Computing and writing this vector as a column vector we have

$$\mathbf{w} = \frac{1}{\sqrt{1+|Du|^2}} \frac{1}{\sqrt{1+u_x^2}} \begin{pmatrix} -u_x u_y \\ 1+u_x^2 \\ u_y \end{pmatrix}.$$

We also write

$$\Pi_{\alpha} = \{ (\xi, \eta, \zeta) \in \mathbb{R}^3 : [(\xi, \eta, \zeta) - (x, y, u)] \cdot \mathbf{w} = 0 \}.$$

The intersection of Π_{α} with the graph of u

$$\mathcal{G} = \{ (\xi, \eta, u(\xi, \eta)) : (\xi, \eta) \in \mathcal{U} \}$$

in some small neighborhood of X=(x,y,u(x,y)) is a C^2 curve. This follows from the **implicit function** theorem. This is a touch tricky, so let's see if we can give the details of how it works: Consider the function $\Psi:\mathcal{U}\to\mathbb{R}^2$ by

$$\Psi\left(\begin{array}{c}\xi\\\eta\end{array}\right)=\left(\begin{array}{c}\xi\\[(\xi,\eta,u(\xi,\eta))-(x,y,u)]\cdot\mathbf{w}\end{array}\right).$$

I've written the arguments as columns here because they are (I think) a little easier to visualize and compute with in that form. Notice $\Psi(x,y)=(x,0)$. Also, the transformation Ψ has total derivative

$$D\Psi = \begin{pmatrix} 1 & 0 \\ (1, 0, u_x(\xi, \eta)) \cdot \mathbf{w} & (0, 1, u_y(\xi, \eta)) \cdot \mathbf{w} \end{pmatrix}.$$

In particular, at $(\xi, \eta) = (x, y)$, we have det $D\Psi \neq 0$. These are the hypotheses of the **inverse function theorem**, which then tells us there is an open ball $B_{\delta}(x, y) \subset \mathcal{U}$ such that Ψ restricted to $B_{\delta}(x, y)$ has a well-defined C^2 inverse with domain $\mathcal{V} = \Psi(B_{\delta}(x, y)) \subset \mathbb{R}^2$ and $(x, 0) \in \mathcal{V}$. We write the second component of Psi^{-1} as ϕ , so that

$$\Psi^{-1} \left(\begin{array}{c} \xi \\ p \end{array} \right) = \left(\begin{array}{c} \xi \\ \phi(\xi, p) \end{array} \right).$$

Setting $\eta(\xi) = \phi(\xi, 0)$ it is easy to check $\alpha : (x - \delta, x + \delta) \to \mathbb{R}^2$ by

$$\alpha(\xi) = (\xi, \eta(\xi), u(\xi, \eta(\xi)))$$

is a parameterization of the intersection curve near X with $\alpha' = (1, \eta', u_x + \eta' u_y) \neq \mathbf{0}$. What we have actually done here is give the proof of the implicit function theorem in this case applied directly would say that if

$$\frac{\partial}{\partial \eta} \left\{ \left[(\xi, \eta, u(\xi, \eta)) - (x, y, u) \right] \cdot \mathbf{w} \right\}_{|_{(x, y)}} \neq 0,$$

then there is some $\delta > 0$ for which the equation

$$[(\xi, \eta, u(\xi, \eta)) - (x, y, u)] \cdot \mathbf{w} = 0$$

determines η uniquely as a C^2 function of ξ for $x - \delta < \xi < x + \delta$. We get the same conclusion. Reparameterizing by arclength, we can assume the intersection curve is given locally by

$$\gamma(s) = (\xi(s), \eta(s), u(\xi(s), \eta(s)))$$

with $\gamma(0) = X = (x, y, u)$. Parameterization by arclength means that the tangent vector $\dot{\gamma} = (\dot{\xi}, \dot{\eta}, \dot{\xi}u_x + \dot{\eta}u_y)$ is a unit vector where $u_x = u_x(\xi, \eta)$ and $u_y = u_y(\xi, \eta)$. That is,

$$\dot{\xi}^2 + \dot{\eta}^2 + (\dot{\xi}u_x + \dot{\eta}u_y)^2 = 1. \tag{12}$$

In the particular case under consideration, we are also assuming

$$\dot{\gamma}(0) = \mathbf{v} = \frac{X_x}{|X_x|} = \frac{(1, 0, u_x)}{\sqrt{1 + u_x^2}}.$$

Exercise 52 Use the inverse/implicit function theorem to generalize the construction above with \mathbf{v} any unit vector in $T_X \mathcal{G}$.

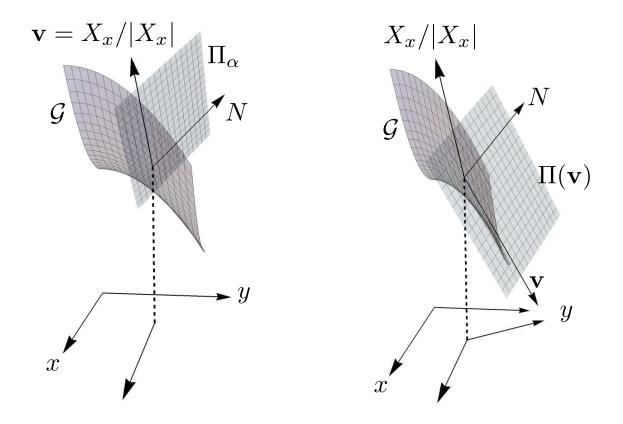


Figure 2: Planes normal to the graph of a function of two variables

If we differentiate the relation $[\gamma(s) - (x, y, u)] \cdot \mathbf{w} = 0$, noting that the vectors X = (x, y, u) and \mathbf{w} are independent of the arclength s, we conclude $\dot{\gamma} \cdot \mathbf{w} = 0$. Using the expression for \mathbf{w} computed above, we see this implies

$$-\dot{\xi}u_x u_y + \dot{\eta}(1 + u_x^2) + (\dot{\xi}u_x + \dot{\eta}u_y)u_y = 0.$$
(13)

We should be careful to recognize something about this dot product. Notice the three components of $\dot{\gamma}$ appearing here. Each involves dependence on the arclength s with $\dot{\xi} = \dot{\xi}(s)$ and $\dot{\eta} = \dot{\eta}(s)$. Note very carefully, the third component:

$$\dot{\xi}u_x + \dot{\eta}u_y = \dot{\eta}(s)u_x(\xi(s), \eta(s)) + \dot{\eta}(s)u_y(\xi(s), \eta(s)).$$

The remaining first partial derivatives in (13) are evaluated at (x, y). Thus, in the first and second terms

$$u_x u_y = u_x(x, y) u_y(x, y)$$
 and $1 + u_x^2 = 1 + [u_x(x, y)]^2$ independent of s.

Similarly, the second factor in the third term is $u_y = u_y(x, y)$, independent of s, and not $u_y(\xi(s), \eta(s))$. If we evaluate (13) at s = 0, however, there is a cancellation, and we obtain the useful relation $\dot{\eta}(0)(1+|Du|^2) = 0$ according to which $\dot{\eta}(0) = 0$. It follows from (12) that $\dot{\xi}(0) = \pm 1/\sqrt{1+u_x^2}$. With a choice according to which $\dot{\gamma}(0) = \dot{\xi}(0)X_u = \mathbf{v}$, we have

$$\dot{\xi}(0) = \frac{1}{\sqrt{1 + u_x^2}}.$$

As mentioned above, we would like to compute the curvature of the intersection curve—the signed curvature as a plane curve (graph) in Π_{α} with respect to N. This value is given by

$$k_{\alpha} = \ddot{\gamma} \cdot N = \ddot{\gamma}(0) \cdot N_X.$$

We find

$$\ddot{\gamma} = \ddot{\xi}(1,0,u_x) + \ddot{\eta}(0,1,u_y) + (0,0,\dot{\xi}^2 u_{xx} + 2\dot{\xi}\dot{\eta}u_{xy} + \dot{\eta}^2 u_{yy}).$$

Evaluating at s=0, this becomes

$$\ddot{\gamma}(0) = \ddot{\xi} X_x + \ddot{\eta} X_y + (0, 0, \dot{\xi}^2 u_{xx} + 2\dot{\xi}\dot{\eta} u_{xy} + \dot{\eta}^2 u_{yy}).$$

Since X_x and X_y are tangent vectors to \mathcal{G} , both orthogonal to N at the point $X \in \mathcal{G}$, the dot product is given by

$$k_{\alpha} = \frac{\dot{\xi}^2 u_{xx} + 2\dot{\xi}\dot{\eta}u_{xy} + \dot{\eta}^2 u_{yy}}{\sqrt{1 + |Du|^2}} = \frac{u_{xx}}{(1 + u_x^2)\sqrt{1 + |Du|^2}}.$$
 (14)

Let us now pause to think carefully (as carefully as we can) about this value. In particular, let us attempt to compare this value to what we know about the curvature of planar graphs. If N = (0, 0, 1), that is, if the tangent plane $T_X \mathcal{G}$ is horizontal with $u_x = u_y = 0$, then $k_\alpha = u_{xx}$ as we would expect. Now, if u_x is nonzero but $u_y = 0$, then $N = (-u_x, 0, 1)/\sqrt{1 + u_x^2}$, and

$$k_{\alpha} = \frac{u_{xx}}{(1 + u_{x}^{2})^{3/2}},\tag{15}$$

and this matches precisely what we would expect for a planar graph according to the familiar formula

$$k = \frac{u''}{(1 + u'^2)^{3/2}}$$

for the signed curvature. In this case, for the surface, the vector **w** is horizontal. In fact according to our formula for **w** in this case we will have $\mathbf{w} = (0, 1, 0)$. The normal plane is vertical and parallel to the x, z-plane, and the intersection curve is given by $\alpha(\xi) = (\xi, y, u(\xi, y))$. This is all as it should be: a second derivative reduced/scaled by the reciprocal of the cube of the length scaling factor.

The interesting, geometrically new, phenomenon here is how the curvature of the intersection curve changes with the tilt in the other (y) coordinate direction. First of all, when $u_y \neq 0$ the X_x normal plane is not vertical and parallel to the x, z-coordinate plane. The normal curvature, however, is still (just) a scaling of u_{xx} .

Exercise 53 Perhaps the simplest situation in which the phenomenon captured in (15) is operative and evident is when the graph \mathcal{G} is the graph of a circular cylinder. Start with the cylinder $x^2 + z^2 = r^2$, and then express half of this cylinder as a graph \mathcal{G} , and tilt \mathcal{G} using a rotation

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} \mapsto \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos \theta & -\sin \theta \\ 0 & \sin \theta & \cos \theta \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}.$$

Explain why it makes sense that the curvature of the tilted cylinder in the normal planes determined by X_x at each point are given by (15). Does it make any difference for, say the bottom half of the cylinder if one considers

$$u(x,y) = -\sqrt{r^2 - x^2} - \tan \theta \ y?$$

Notice the vectors \mathbf{w} and N also determine a unique plane

$$\Pi_{\beta} = \{ (\xi, \eta, \zeta) : [(\xi, \eta, \zeta) - (x, y, u)] \cdot (1, 0, u_x) = 0 \}$$

passing through $X = (x, y, u(x, y)) \in \mathcal{G}$ and orthogonal to \mathbf{v} , i.e. containing \mathbf{w} and N. The intersection $\Pi_{\beta} \cap \mathcal{G}$ is also a planar curve that can be parameterized by arclength with

$$\gamma(s) = (\xi, \eta, u(\xi, \eta))$$

as above. Several of the computations above apply, but differentiating the defining relation $(\gamma - X) \cdot X_x = 0$, we find

$$\dot{\gamma} \cdot X_x = (\dot{\xi}, \dot{\eta}, \dot{\xi}u_x + \dot{\eta}u_y) \cdot (1, 0, u_x) = 0$$

where, as above, $u_x = u_x(\xi, \eta)$ and $u_y = u_y(\xi, \eta)$ depend on s in the first vector, but $u_x = u_x(x, y)$ in the second tangent vector is independent of s. Evaluating at s = 0 this time, we obtain

$$(1 + u_x^2)\dot{\xi}(0) + u_x u_y \dot{\eta}(0) = 0.$$

It follows that for some nonzero constant c we must have

$$\dot{\xi}(0) = -cu_x u_y$$
 and $\dot{\eta}(0) = c(1 + u_x^2)$.

From the condition $|\dot{\gamma}| = 1$ and the choice $\dot{\eta}(0) > 0$, we find after some simplification that

$$c = \frac{1}{\sqrt{1 + |Du|^2} \sqrt{1 + u_x^2}}$$

so that

$$\dot{\xi}(0) = -\frac{u_x u_y}{\sqrt{1 + |Du|^2} \sqrt{1 + u_x^2}}$$
 and $\dot{\eta}(0) = \frac{\sqrt{1 + u_x^2}}{\sqrt{1 + |Du|^2}}$.

Substituting these values in the expression for $\ddot{\gamma}(0) \cdot N$ from above, we have the signed curvature of this intersection curve with respect to the normal N at the point X satisfies

$$k_{\beta} = \frac{\dot{\xi}^2 u_{xx} + 2\dot{\xi}\dot{\eta}u_{xy} + \dot{\eta}^2 u_{yy}}{\sqrt{1 + |Du|^2}}$$

$$= \frac{1}{(1+|Du|^2)^{3/2}} \left(\frac{u_x^2 u_y^2}{1+u_x^2} u_{xx} - 2u_x u_y u_{xy} + (1+u_x^2) u_{yy} \right).$$

It is quite easy to see from this expression that

$$k_{\alpha} + k_{\beta} = \mathcal{M}u$$

is the quantity we have called the mean curvature of the graph.

We have shown

The **mean curvature** given by the expression $\mathcal{M}u$ is the sum of the curvatures of two orthogonal planar curves lying on the graph \mathcal{G} of u, each taken as a signed curvature with respect to the surface normal N which also lies in the (normal) plane containing each curve.

The derivation above leaves open the possibility that one of the two normal planes determining one of the intersections curves must be the plane $\Pi(\mathbf{v})$ determined by the special tangent vector $\mathbf{v} = X_x/|X_x|$. Thus, we can ask: Is this quantity $\mathcal{M}u$ something of fundamental geometric meaning as curvature, or is it somehow dependent on the particular coordinates we have used, and consequently, the first normal plane we have chosen?

Perhaps the derivation suggests, however, a more general construction:

Let \mathbf{v} be any unit length vector in $T_X \mathcal{G}$, and let $\mathbf{w} = N \times \mathbf{v}$. Let k_{α} be the signed curvature of the intersection of the normal plane $\Pi(\mathbf{v})$ orthogonal to \mathbf{w} with respect to N, and let k_{β} be the signed curvature of the intersection of the normal plane $\Pi(\mathbf{w})$ orthogonal to \mathbf{v} with respect to N. Is the number

$$k_{\alpha} + k_{\beta}$$

always equal to $\mathcal{M}u$?

In fact, the suggested construction is correct:

If Π_{α} and Π_{β} are any pair of orthogonal planes intersecting along the normal line to a C^2 surface S at a point $X \in S$, then each of the two planes intersects S locally in a planar curve. The two resulting planar curves have some signed curvatures k_{α} and k_{β} with respect to a choice of normal N, and the average of these two numbers is called the **mean curvature** \mathcal{H} of the surface. The mean curvature is independent of the choice of orthogonal planes and depends only on the surface S and the (unit) normal N (chosen among two possibilities). According to this construction

$$\mathcal{H} = \frac{k_{\alpha} + k_{\beta}}{2}$$
 and $\mathcal{M} = 2\mathcal{H}$. (16)

The last expression relating the mean curvature operator \mathcal{M} and the value of the mean curvature assumes the surface \mathcal{S} is given by the graph of a function. In fact, every **surface** (a concept we have not actually defined carefully but which one can hope³ is a relatively intuitively clear concept) can be expressed as a union of graphs of functions, so in particular, coordinates ξ and η can be chosen so that all points in the surface \mathcal{S} near a given point $X \in \mathcal{S}$ are congruent to a graph

$$\mathcal{G} = \{ (\xi, \eta, u(\xi, \eta)) : (\xi, \eta) \in \mathcal{U} \}$$

for some open set $\mathcal{U} \subset \mathbb{R}^2$. According to the above assertion, it does not matter which graph is chosen to locally represent \mathcal{S} .

There are various ways to see the mean curvature \mathcal{H} is a geometric quantity as described above. The following is one way:

Say we take a different direction $\mathbf{v} \in T_X \mathcal{G}$ and an orthogonal direction $\mathbf{w} = N \times \mathbf{v} \in T_X \mathcal{G}$. Rather than try to generalize the computation above for $\mathbf{v} = X_x ||X_x||$ directly, note that this new tangent vector $\mathbf{v} = (v_1, v_2, v_3)$ must have some nonzero projection into the x, y-plane, namely $\mathbf{u}_1 = (v_1, v_2) / \sqrt{v_1^2 + v_2^2}$.

Exercise 54 Explain how we know $(v_1, v_2) \neq \mathbf{0} \in \mathbb{R}^2$.

We can represent \mathcal{G} as a graph in new coordinates as follows: We first write $\mathbf{u}_1 = (\cos \theta, \sin \theta)$ determining the angle θ uniquely in the interval $[0, 2\pi)$. We then consider the function $\tilde{u} : \tilde{\mathcal{U}} \to \mathbb{R}$ by

$$\tilde{u}(\xi, \eta) = u(x + \xi \cos \theta - \eta \sin \theta, y + \xi \sin \theta + \eta \cos \theta)$$

on an appropriate domain $\tilde{\mathcal{U}} \subset \mathbb{R}^2$.

Exercise 55 Find the "appropriate" domain $\tilde{\mathcal{U}}$ in terms of the domain $\mathcal{U} \subset \mathbb{R}^2$ for $u \in C^2(\mathcal{U})$, and show there exists a rigid motion $\rho : \mathbb{R}^3 \to \mathbb{R}^3$ (translation and rotation) such that

$$\tilde{\mathcal{G}} = \{(\xi, \eta, \tilde{u}(\xi, \eta)) : (\xi, \eta) \in \tilde{\mathcal{U}}\}$$

³If you do not know the technical definition of a surface and (for some reason) are not interested in looking it up and understanding it at the moment, then you might write down any example you can imagine being a surface and see if you can express every small enough piece of that surface as the graph of a function. For example, one might start with $\partial B_r(\mathbf{0}) = \{(x, y, z) : x^2 + y^2 + z^2 = r^2\}$. Perhaps we will also remedy this deficiency soon.

is the (congruent) image of \mathcal{G} under ρ , that is

$$\tilde{\mathcal{G}} = \{ \rho(X) : X \in \mathcal{G} \}$$

with $(1,0,\tilde{u}_{\xi}) = \rho(\mathbf{v})$. Thus, the sum of the normal curvatures associated with \mathbf{v} and \mathbf{w} is the same as calculating $\mathcal{M}\tilde{u}(0,0)$, which we know to be

$$\mathcal{M}\tilde{u} = \frac{(1 + \tilde{u}_{\eta}^2)\tilde{u}_{\xi\xi} - 2\tilde{u}_{\xi}\tilde{u}_{\eta}\tilde{u}_{\xi\eta} + (1 + \tilde{u}_{\xi}^2)\tilde{u}_{\eta\eta}}{(1 + |D\tilde{u}|^2)^{3/2}}.$$

In view of the above construction/exercise we compute $\mathcal{M}\tilde{u}$:

$$\tilde{u}_{\xi} = u_x \cos \theta + u_y \sin \theta$$
 and $\tilde{u}_{\eta} = -u_x \sin \theta + u_y \cos \theta$.

The denominator $(1 + |D\tilde{u}|^2)^{3/2}$ in $\mathcal{M}\tilde{u}$ is easily calculated at this point and found to be $(1 + |Du|^2)^{3/2}$, which is promising. The coefficients involving first order terms are more complicated, but straightforward to compute:

$$1 + \tilde{u}_{\xi}^2 = 1 + u_x^2 \cos^2 \theta + 2u_x u_y \cos \theta \sin \theta + u_y^2 \sin^2 \theta$$
$$\tilde{u}_{\xi} \tilde{u}_{\eta} = -u_x^2 \cos \theta \sin \theta + u_x u_y (\cos^2 \theta - \sin^2 \theta) + u_y^2 \cos \theta \sin \theta$$
$$1 + \tilde{u}_{\eta}^2 = 1 + u_x^2 \sin^2 \theta - 2u_x u_y \cos \theta \sin \theta + u_y^2 \cos^2 \theta.$$

Finally, for the second order derivatives we have

$$\tilde{u}_{\xi\xi} = u_{xx}\cos^2\theta + 2u_{xy}\cos\theta\sin\theta + u_{yy}\sin^2\theta$$

$$\tilde{u}_{\xi\eta} = -u_{xx}\cos\theta\sin\theta + u_{xy}(\cos^2\theta - \sin^2\theta) + u_{yy}\cos\theta\sin\theta$$

$$\tilde{u}_{\eta\eta} = u_{xx}\sin^2\theta - 2u_{xy}\cos\theta\sin\theta + u_{yy}\cos^2\theta.$$

Algebraically, the calculation of the expression

$$(1+\tilde{u}_{\eta}^2) \ \tilde{u}_{\xi\xi} - 2\tilde{u}_{\xi}\tilde{u}_{\eta} \ \tilde{u}_{\xi\eta} + (1+\tilde{u}_{\xi}^2) \ \tilde{u}_{\eta\eta}$$

becomes somewhat long and cumbersome. With this in mind, we compute the products giving the coefficients of the second order terms one by one. The coefficient of u_{xx} is the sum of three terms: The first is from the product $(1 + \tilde{u}_n^2)\tilde{u}_{\xi\xi}$ and is given by

$$\cos^2\theta(1+u_x^2\sin^2\theta-2u_xu_y\cos\theta\sin\theta+u_y^2\cos^2\theta). \tag{17}$$

The second is from $-2\tilde{u}_{\xi}\tilde{u}_{\eta}\tilde{u}_{\xi\eta}$ and is

$$2\cos\theta\sin\theta(-u_x^2\cos\theta\sin\theta + u_xu_y(\cos^2\theta - \sin^2\theta) + u_y^2\cos\theta\sin\theta). \tag{18}$$

The third comes from $(1 + \tilde{u}_{\varepsilon}^2)\tilde{u}_{\eta\eta}$:

$$\sin^2\theta(1+u_x^2\cos^2\theta+2u_xu_y\cos\theta\sin\theta+u_y^2\sin^2\theta). \tag{19}$$

It is not difficult to see that the sum of (17), (18), and (19) simplifies to

$$1 + u_y^2.$$

Thus, we have established

$$\mathcal{M}\tilde{u} = \frac{1}{(1+|Du|^2)^{3/2}} \left[(1+u_y^2) \ u_{xx} + \cdots \right].$$

The coefficient of u_{xy} is similarly the sum of three terms:

$$2\cos\theta\sin\theta(1+u_x^2\sin^2\theta-2u_xu_y\cos\theta\sin\theta+u_y^2\cos^2\theta)$$
$$-2(\cos^2\theta-\sin^2\theta)(-u_x^2\cos\theta\sin\theta+u_xu_y(\cos^2\theta-\sin^2\theta)+u_y^2\cos\theta\sin\theta)$$
$$-2\cos\theta\sin\theta(1+u_x^2\cos^2\theta+2u_xu_y\cos\theta\sin\theta+u_y^2\sin^2\theta).$$

This sum, as might be expected, simplifies to $2u_xu_y$. Finally, the coefficient of u_{yy} is

$$\sin^2 \theta (1 + u_x^2 \sin^2 \theta - 2u_x u_y \cos \theta \sin \theta + u_y^2 \cos^2 \theta)$$

$$- 2\cos \theta \sin \theta (-u_x^2 \cos \theta \sin \theta + u_x u_y (\cos^2 \theta - \sin^2 \theta) + u_y^2 \cos \theta \sin \theta)$$

$$+ \cos^2 \theta (1 + u_x^2 \cos^2 \theta + 2u_x u_y \cos \theta \sin \theta + u_y^2 \sin^2 \theta)$$

$$= 1 + u_x^2.$$

We have shown $\mathcal{M}\tilde{u}(0,0) = \mathcal{M}u(x,y)$ is independent of the choice of orthogonal vectors \mathbf{v} and \mathbf{w} in $T_X\mathcal{G}$.

Geometric meaning and curvature

Let us return to the discussion surrounding (14) and attempt to think about this expression a little more carefully and filling out a little more the connection with the curvature of curves and the broader idea of what it means for a quantity to be **geometric**.

If $u:(a,b)\to\mathbb{R}$ has $u\in C^2(a,b)$ and graph a curve $\{(x,u(x)):x\in(a,b)\}$, then the values of u are made geometric by the consideration of the graph.

When you think of the distance $\xi = \xi(t)$ traveled by someone walking, or someone in a car, or a baseball, or a rocket, then that distance alone (as a function of time) is analytic or physical but not necessarily geometric. It becomes geometric when we plot the curve $\{(t, \xi(t)) \in \mathbb{R}^2 : t \in (a, b)\}$ which is the graph of the distance as a function of time. Once we have this graph, then the value $\xi'(t)$ may be thought of as geometric: The **slope** of the tangent line to the graph. Without the graph, the **rate of change** $\xi'(t)$ of the distance with respect to time is merely analytic or physical.

We are quite accustomed to identify the physical/analytic meaning with the geometric meaning in this instance, and forget there is a difference. The point of this discussion is that the situation changes with the second derivative u''(x) of $u \in C^2(a,b)$. This quantity, **the second derivative** by itself, **has no geometric meaning**.

Though this startling declaration may be obvious, it also may be quite subtle for some people, so I will elaborate. Geometric meaning in relation to the function $u \in C^2(a, b)$ is associated, and only associated, with the graph of the function u, which is a curve. That curve, as a geometric object, may have a relation to a fixed direction, like a direction specified as horizontal, given by a quantity like slope or inclination. If we know which direction is horizontal, and we know u'(x) with respect to this horizontal direction (measured by the quantity x), then we know something about the geometry of the curve—the inclination of the curve at the point (x, u(x)) on the curve—just as u(x) tells us something about the orthogonal distance from (x, u(x)) to the horizontal. If we know u''(x), however, this tells us (almost) nothing about the geometry of the graph and, since that is the only geometry we have, nothing geometric (period).

As an illustration, consider the specific function $\xi(t) = t^2$. In Figure 3 I have plotted the graph of the function ξ along with three small disks focusing on three different portions of the graph and having centers on specific points $(t, \xi(t))$ on the graph. Now, if I were to tell you a particular point $(t, \xi(t))$ at the center of one of these disks is a point where $\xi'' = 2$, could you look at the three disks, and determine the point to which I was referring (from the geometry)? In fact, you cannot determine anything geometric from the information $\xi''(t) = 2$. If you know time is measured in seconds and ξ is measured in meters, you can tell something physical: The rate of change of ξ' with respect to time (or the **acceleration**) at this point (and every point) is 2 meters per second. More generally, you can tell something analytic, namely that

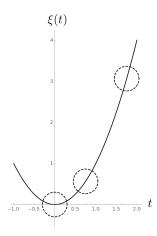


Figure 3: The graph of a "position" function $\xi = \xi(t) = t^2$.

the rate of change of ξ' with respect to the quantity t (whatever the appropriate units may happen to be) is 2. This kind of information can be useful both computationally (analytically) and physically, but it is not geometric.

Geometric information comes from the graph and the value of the second derivative is not simply related to the geometry of the graph. As we know, one quantity

$$k = \frac{u''}{(1 + u'^2)^{3/2}},$$

a combination of the first and second derivatives called curvature, does give precise quantitative geometric information. We may qualify our comments by pointing out that u''(x) does give some **qualitative geometric information**: If u''(x) is positive, we can infer the geometric convexity of the graph of u with respect to the horizontal. It is the quantitative measure of that convexity we cannot discern without the curvature. And, as we know, the formula says that if the inclination of the graph is zero (i.e., has slope zero) at a point, then u''(x) gives the curvature, but if the inclination is nonzero, then the number u''(x) is strictly larger in absolute value than the curvature and must be diminished by a factor

$$\frac{1}{(1+u'^2)^{3/2}} < 1.$$

This is how curvature works in relation to a second derivative. Why that particular scaling factor is the correct one is difficult to see geometrically, but that is what comes out from the computation using the chain rule. Maybe you can find a nice geometric interpretation for the scaling factor.

Exercise 56 Consider the vectors $u''(-u',1)/\sqrt{1+u'^2}$ and $u''(1,u')/\sqrt{1+u'^2}$ normal and tangent to the graph of $u \in C^2(a,b)$. Can you express the curvature vector $\vec{k} = u''(-u',1)/(1+u'^2)^2$ geometrically in terms of one (or both) of these vectors?

The expression

$$k_{\alpha} = \frac{u_{xx}}{(1 + u_x^2)\sqrt{1 + |Du|^2}}$$

given in (14) is telling us something new (and geometric) about the curvature of curves on a surface—and indirectly about the curvature of a surface. Let a surface \mathcal{S} be given locally as a graph

$$\mathcal{G} = \{(x, y, u(x, y)) : (x, y) \in \mathcal{U}\}$$

where \mathcal{U} is an open subset of \mathbb{R}^2 as usual.

If we intersect the surface S with a vertical plane, say a plane parallel to the x, z-plane, then the signed curvature of the intersection curve at a particular point is

$$\frac{u_{xx}}{(1+u_x^2)^{3/2}},\tag{20}$$

and this value is always larger in absolute value than (or possibly equal to) the normal curvature determined by the tangent vector $(1,0,u_x)$ at that point. If the slope in the orthogonal coordinate direction at the point, as measured by u_y , is zero, then the value (20) is the normal curvature. If, however, $u_y \neq 0$, then the value given in (20) must be diminished by a factor

$$\frac{\sqrt{1+u_x^2}}{\sqrt{1+|Du|^2}} < 1. \tag{21}$$

It will be noted that the factor in (21) is the ratio of the length scaling factor for the coordinate intersection

$$\{(\xi, y, u(\xi, y)) : (\xi, y) \in \mathcal{U}\}$$

to the area scaling factor for the surface. This is how the curvature of curves given by the intersection with normal planes works on a surface.

Exercise 57 Find the projection of the curvature vector

$$\vec{k}_x = \frac{u_{xx}}{(1 + u_x^2)^2} (-u_x, 0, 1)$$

of the intersection of the vertical plane

$$\Pi_x = \{ (\xi, y, \zeta) : (\xi, \zeta) \in \mathbb{R}^2 \}$$

with the graph

$$\mathcal{G} = \{(x, y, u(x, y)) : (x, y) \in \mathcal{U}\}$$

onto the normal $N = (-u_x, -u_y, 1)/\sqrt{1 + |Du|^2}$ of the surface.

In 1776 Jeen Baptiste Marie Charles Meusnier de la Place discovered⁴ a remarkable generalization of the construction we have given concerning k_{α} . The result is purely geometric and captures precisely what is happening.

Theorem 9 (Meusnier's theorem) Let S be a surface containing a point $X \in S$ and having a unit tangent vector $\mathbf{v} \in T_X S$ at X. If $\gamma : (-\epsilon, \epsilon) \to S$ is a parameterization by arclength of any curve on the surface S with $\gamma(0) = X \in S$, $\dot{\gamma}(0) = \mathbf{v}$, and well-defined curvature vector $\ddot{\gamma}(0)$, then the number

$$k_N = \ddot{\gamma}(0) \cdot N,$$

where N is a choice of unit normal to S at X, is independent of the curve γ . This is called the **normal** curvature of the surface S at the point X and depends only on

- 1. the surface S,
- 2. the tangent direction \mathbf{v} , and
- 3. the choice of unit normal to S (up to a sign).

⁴The French name Meusnier is pronounced like "moon yay."

Additional Exercises

Exercise 58 Compare the graphs of the functions $u: \mathbb{R} \to \mathbb{R}$ by $u(x) = x^2$ and $v: [x_0 - r, x_0 + r] \to \mathbb{R}$ by

$$v(x) = y_0 - \sqrt{r^2 - (x - x_0)^2}.$$

- (a) Discuss the regularity of each function.
- (b) Compute the curvature of the graph of each function.
- (c) Given a point (x, u(x)) on the graph of u, find a center (x_0, y_0) and radius r so that the graph of v "matches the graph of u to second order" at the point (x, u(x)). Show the center and radius you have found are unique.
- (d) Use numerical software to plot the graph of u and some osculating circles determined by the graph of u.

4 Integration

We wish to discuss the integration of real valued functions on (somewhat) general sets. The basic setup is this: You have a function

$$f: X \to \mathbb{R}$$

where X is a metric space with a **measure**. As we know, the metric on a metric space (or distance function) allows one to measure distances between points and diameters of sets with diam : $\mathcal{P}(X) \to [0, \infty]$ by

$$diam(A) = \sup\{d(x, y) : x, y \in A\}.$$

Here we have used $\mathcal{P}(X)$ to denote the collection of all subsets of X. This particular set is also called the **power set** of X and is sometimes denoted 2^X .

A measure μ is usually different from the diameter associated with a metric, though these functions can agree, for example on intervals in \mathbb{R} where the measure of an integral (and the diameter of an interval) is its length. Ideally, we can also measure all sets with $\mu : \mathcal{P}(X) \to [0, \infty]$, and little harm is done (usually) if we imagine that to be the case. Technically, it is sometimes only possible to define a measure on some proper subset \mathcal{M} of $\mathcal{P}(X)$ called the collection of measurable sets. Measurable sets should have the following properties:

- 1. $\phi, X \in \mathcal{M}$.
- 2. If $A \in \mathcal{M}$, then $A^c \in \mathcal{M}$.
- 3. If A_1, A_2, A_3, \ldots comprise a (countable) sequence of sets in \mathcal{M} , then the union should also be measurable:

$$\bigcup_{j=1}^{\infty} A_j \in \mathcal{M}.$$

The measure $\mu: \mathcal{M} \to [0, \infty]$ should have the following properties:

- 1. $\mu \phi = 0$.
- 2. If A_1, A_2, A_3, \ldots comprise a (countable) sequence of **pairwise disjoint** sets in \mathcal{M} , then

$$\mu \bigcup_{j=1}^{\infty} A_j = \sum_{j=1}^{\infty} \mu A_j.$$

The second property is called **countable additivity**.

Given a set X (with a metric and a measure) you can think of an integral as a limit

$$\int_X f = \lim_{\|\mathcal{P}\| \to 0} \sum_j f(x_j^*) \mu A_j$$

where $\mathcal{P} = \{A_j\}_{j=1}^{\infty}$ is a (finite) **partition** of X, that is

$$X = \bigcup_{j=1}^{k} A_j$$
 and $\mu(A_i \cap A_j) = 0$ for $i \neq j$,

and $\|\mathcal{P}\| = \max_i \operatorname{diam}(A_i)$.

Two important possibilities (for integration) are the following:

- 1. $X = \mathcal{U}$ is an open subset of \mathbb{R}^n with $\mu = \mathfrak{L}^n$ given by *n*-dimensional volume measure (or Lebesgue measure) and d the Euclidean metric. We call this **integration on flat space**.
- 2. $X = \partial \mathcal{U}$ is the smooth boundary of an open subset of \mathbb{R}^n with $\mu = \mathcal{H}^{n-1}$ given by (n-1)-dimensional Hausdorff measure on \mathbb{R}^n (and d again the Euclidean metric). These are examples of **integration** on manifolds.

If you do not know what it means for the boundary of an open subset of \mathbb{R}^n to be "smooth," (or what it means to be a "manifold") do not worry. We can give precise definitions later. You can just think of the boundary of the disk $\mathbb{S}^1 = \{(x,y) \in \mathbb{R}^2 : x^2 + y^2 = 1\}$ in the case n = 2 where you should have a pretty good idea of how one-dimensional Hausdorff measure \mathcal{H}^1 should work. You can also think of the boundary of the ball $\mathbb{S}^2 = \{(x,y,z) \in \mathbb{R}^3 : x^2 + y^2 + z^2 = 1\}$ in the case n = 3 on which one would use two-dimensional Hausdorff measure, that is area measure for surfaces in \mathbb{R}^3 .

In practice, computation of an integral on a higher dimensional flat space is often reduced to the computation of **iterated integrals** on lower dimensional spaces by some form of **Fubini's theorem**:

Theorem 10 (Fubini) If $f: X_1 \times X_2 \to \mathbb{R}$ is defined on the product $X_1 \times X_2 = \{(x_1, x_2) : x_j \in X_j, j = 1, 2\}$ of measurable metric spaces X_1 and X_2 , then

$$\int_{X_1 \times X_2} f = \int_{X_1} \left(\int_{X_2} f \right) = \int_{X_2} \left(\int_{X_1} f \right)$$

where the integrand of $\int_{X_2} f$ is taken to mean the function $g: X_2 \to \mathbb{R}$ given by $g(x) = f(x_1, x)$ for each (fixed) $x_1 \in X_1$, and the integrand of $\int_{X_1} f$ is interpreted similarly.

Integrals over manifolds are usually computed using a **parameterization** and a **change of variables** formula. To describe such a computation, in general terms, we change notation slightly: Let $\mathcal{U} \subset \mathbb{R}^n$ be a flat domain of integration and

$$X: \mathcal{U} \to \mathbb{R}^k$$
 an injection onto its image $M = X(\mathcal{U})$.

Here M is assumed to be a manifold (or a subset of a manifold) and the function X is a parameterization; this is almost the definition of a manifold. Then we seek a **change of variables formula** which looks like this:

$$\int_{M} f = \int_{\mathcal{U}} (f \circ X) \ \sigma.$$

In this formula:

1. $f: M \to \mathbb{R}$ is a real valued function on M, as expected,

2. $f \circ X : \mathcal{U} \to \mathbb{R}$ is the composition given by

$$f \circ X(\mathbf{p}) = f(X(\mathbf{p})),$$

and

3. σ is a scaling factor for the measures involved.

You can think of σ (roughly) according to the following description:

Using the measure μ on M, the measure of a set $A \subset M$ is

$$\mu A = \int_{A} 1 = \int_{X^{-1}(A)} \sigma \tag{22}$$

where $\sigma: \mathcal{U} \to \mathbb{R}$ is a (scaling) function allowing the computation of μA by integration on the corresponding (flat) preimage

$$X^{-1}(A) = \{ \mathbf{p} \in \mathcal{U} : X(\mathbf{p}) \in A \}.$$

The area scaling relation (22) is required to hold for all (measurable) sets A in such a way that the value of σ can be recovered by taking a limit

$$\sigma(p) = \lim_{A \to \{p\}} \frac{\mu A}{\mu_{\mathcal{U}}[X^{-1}(A)]}$$
 (23)

where $\mu_{\mathcal{U}}$ is the measure on \mathcal{U} and the limit is taken as A tends to $\{p\}$ as a set. You may recognize (23) as defining a kind of derivative of the measure μ .

Exercise 59 Consider the polar coordinates map $\Phi:(0,\infty)\times\mathbb{R}\to\mathbb{R}^2$. This function is a smooth bijection on any restriction to a half strip $(0,\infty)\times[\theta_0,\theta_0+2\pi)$. Let A be the image under Φ of a rectangle $R=[r_0,r_0+\epsilon]\times[\theta_0,\theta_0+\delta]$ for some $r_0>0$ and any θ_0 . That is,

$$A = \{ \Phi(r, \theta) : r_0 \le r \le r_0 + \epsilon, \ \theta_0 \le \theta \le \theta_0 + \delta \}.$$

Compute the area of A and the limit

$$\lim_{\epsilon,\delta\to 0} \frac{\mathfrak{L}^2 A}{\mathfrak{L}^2 R}$$

where \mathfrak{L}^2 denotes area measure in the plane, i.e., 2-dimensional Lebesgue measure.

Let's try to illustrate the notions of integration just introduced using an example. Say we want to integrate on the surface $M = \mathcal{S}$ shown in Figure 4.

This surface is parameterized by

$$\Phi(r,\theta) = \frac{r}{4} \begin{pmatrix} (2+\sqrt{2})\cos\theta - (2-\sqrt{2})\sin\theta \\ (2+\sqrt{2})\sin\theta - (2-\sqrt{2})\cos\theta \\ 2(\cos\theta + \sin\theta) \end{pmatrix}$$

on the rectangle $\mathcal{U} = [1, 2] \times [0, \pi/2]$. A small square $[r_0, r_0 + \epsilon] \times [\theta_0, \theta_0 + \epsilon]$ in the rectangle \mathcal{U} has image approximated by the image of the linearization:

$$\Phi(r,\theta) \sim \Phi(r_0,\theta_0) + d\Phi_{(r_0,\theta_0)}(r - r_0,\theta - \theta_0).$$

The linear part $L = d\Phi_{(r_0,\theta_0)} : \mathbb{R}^2 \to \mathbb{R}^3$ is given by

$$L\mathbf{v} = D\Phi(r_0, \theta_0)\mathbf{v}$$

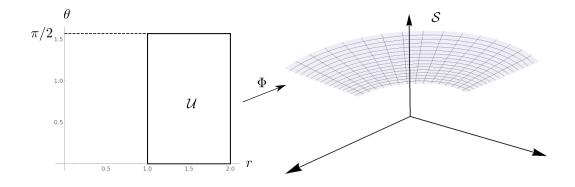


Figure 4: A parameterized surface and the associated scaling factor.

where $D\Phi$ is the total derivative matrix, in this case

$$D\Phi = \begin{pmatrix} \frac{\partial \Phi_1}{\partial r} & \frac{\partial \Phi_1}{\partial \theta} \\ \frac{\partial \Phi_2}{\partial r} & \frac{\partial \Phi_2}{\partial \theta} \\ \frac{\partial \Phi_3}{\partial r} & \frac{\partial \Phi_3}{\partial \theta} \end{pmatrix}$$

$$=\frac{1}{4}\left(\begin{array}{cc} (2+\sqrt{2})\cos\theta-(2-\sqrt{2})\sin\theta & -r[(2+\sqrt{2})\sin\theta+(2-\sqrt{2})\cos\theta \\ (2+\sqrt{2})\sin\theta-(2-\sqrt{2})\cos\theta & r[(2+\sqrt{2})\sin\theta+(2-\sqrt{2})\sin\theta] \\ \\ 2(\cos\theta+\sin\theta) & 2r(\cos\theta-\sin\theta) \end{array}\right).$$

The image $L([0,\epsilon]\times[0,\epsilon])$ is a parallelogram spanned by the vectors

$$\mathbf{w}_1 = \frac{\epsilon}{4} \begin{pmatrix} (2+\sqrt{2})\cos\theta_0 - (2-\sqrt{2})\sin\theta_0 \\ (2+\sqrt{2})\sin\theta_0 - (2-\sqrt{2})\cos\theta_0 \\ 2(\cos\theta_0 + \sin\theta_0) \end{pmatrix}$$

and

$$\mathbf{w}_{2} = \frac{\epsilon r_{0}}{4} \begin{pmatrix} -[(2+\sqrt{2})\sin\theta_{0} + (2-\sqrt{2})\cos\theta_{0}] \\ (2+\sqrt{2})\sin\theta_{0} + (2-\sqrt{2})\sin\theta_{0} \\ 2(\cos\theta_{0} - \sin\theta_{0}) \end{pmatrix}.$$

The area of this parallelogram is given by

$$|\mathbf{w}_1||\mathbf{w}_2|\sin A = |\mathbf{w}_1 \times \mathbf{w}_2|$$

where A is the angle between \mathbf{w}_1 and \mathbf{w}_2 with

$$\sin A = \frac{|\mathbf{w}_1 \times \mathbf{w}_2|}{|\mathbf{w}_1||\mathbf{w}_2|}.$$

Calculating, we find

$$|\mathbf{w}_1||\mathbf{w}_2|\sin A = |\mathbf{w}_1 \times \mathbf{w}_2| = \epsilon^2 r_0.$$

Thus, the linearization takes a square of area ϵ^2 (with corner at $(r_0, \theta_0) \in \mathcal{U}$ precisely onto a parallelogram of area $\epsilon^2 r_0$. Using this relation, we can decompose \mathcal{U} into many small squares \mathcal{U}_j (as indicated for example in Figure 5) with images $\Phi(\mathcal{U}_j)$ partitioning \mathcal{S} and observe

$$\sum_{j} f(q_{j}^{*}) \mu_{\mathcal{S}}[\Phi(\mathcal{U}_{j})] \sim \sum_{j} f(q_{j}^{*}) r_{j}^{*} \mu_{\mathcal{U}}[\mathcal{U}_{j}]$$

$$= \sum_{j} f(q_{j}^{*}) r_{j}^{*} \mathcal{L}^{2}[\mathcal{U}_{j}]$$

$$\sim \sum_{j} f \circ \Phi(p_{j}^{*}) r_{j}^{*} \mathcal{L}^{2}[\mathcal{U}_{j}]$$
(24)

where $p_j^* = (r_j^*, \theta_j^*) \in \mathcal{U}_j$ and we recall that \mathfrak{L}^2 denotes area measure, i.e., two-dimensional Lebesgue measure, in the plane. Taking the limit as the norms of our partitions tend to zero, we obtain the familiar change of variables formula

$$\int_{\mathcal{S}} f = \int_{\mathcal{U}} (f \circ \Phi) \, r.$$

Taking the special case $f \equiv 1$, we obtain (22) in the form

$$\mathcal{H}^2(A) = \int_{\Phi^{-1}(A)} r$$
 for subsets A of the surface \mathcal{S} .

We may continue with this calculation using Fubini's theorem to write the flat integral on the right in terms of iterated integrals:

$$\int_{\mathcal{S}} f = \int_{r \in [1,2]} r \left(\int_{\theta \in [0,\pi/2]} f \left(\frac{r}{4} \left(\frac{(2+\sqrt{2})\cos\theta - (2-\sqrt{2})\sin\theta}{(2+\sqrt{2})\sin\theta - (2-\sqrt{2})\cos\theta} \right) \right) \right)$$

on the rectangle $\mathcal{U} = [1, 2] \times [0, \pi/2]$.

Assuming f is a continuous (Riemann integrable) function, we can also write $\int_{\mathcal{S}} f$ in terms of familiar Riemann integrals:

$$\int_{\mathcal{S}} f = \int_{1}^{2} r \left(\int_{0}^{\pi/2} f \left(\frac{r}{4} \left(\frac{(2+\sqrt{2})\cos\theta - (2-\sqrt{2})\sin\theta}{(2+\sqrt{2})\sin\theta - (2-\sqrt{2})\cos\theta} \right) \right) d\theta \right) dr.$$

Exercise 60 Let $X: \mathcal{U} \to \mathbb{R}^k$ be a bijection onto the image manifold $M = X(\mathcal{U})$ where \mathcal{U} is a (flat) domain of integration in \mathbb{R}^n .

- (a) Write down a measure scaling limit relation like (23) involving the measure μ on M and the measure \mathfrak{L}^n on \mathcal{U} .
- (b) Carefully justify the change of variables formula

$$\int_{M} f = \int_{\mathcal{U}} (f \circ X) \ \sigma$$

along the lines of (24).

Here are two change of variables formulas that cover many cases of interest:

Theorem 11 If \mathcal{U} and \mathcal{W} are open sets of \mathbb{R}^n and $\Phi: \mathcal{U} \to \mathcal{W}$ is a change of variables, i.e., a differentiable bijection (diffeomorphism), then

$$\int_{\mathcal{W}} f = \int_{\mathcal{U}} f \circ \Phi \mid \det D\Phi \mid.$$

The total derivative $D\Phi$ is an $n \times n$ matrix, and the scaling factor is

$$\sigma = |\det D\Phi|.$$

Theorem 12 If \mathcal{U} is an open subset of \mathbb{R}^n and $X: \mathcal{U} \to \mathbb{R}^k$ parameterizes a smooth manifold $M = X(\mathcal{U})$, then

$$\int_{M} f = \int_{\mathcal{U}} f \circ X \sqrt{\det(DX^{T} DX)}$$

where DX is the $k \times n$ matrix which is the total derivative of X and DX^T is the transpose of DX. The matrix DX^TDX is a $n \times n$, square, positive definite matrix with $\det(DX^TDX) > 0$. The scaling factor is

$$\sigma = \sqrt{\det(DX^T \, DX)}$$

Exercise 61 Apply Theorem 12 to the parameterization

$$\Phi(r,\theta) = \frac{r}{4} \begin{pmatrix} (2+\sqrt{2})\cos\theta - (2-\sqrt{2})\sin\theta \\ (2+\sqrt{2})\sin\theta - (2-\sqrt{2})\cos\theta \\ 2(\cos\theta + \sin\theta) \end{pmatrix}$$

to determine the scaling factor for integration on the surface S given above.

4.1 Special Integrands

The general theory of integration as presented above is not really complete in at least two respects. The major omission, perhaps, is that we have not discussed measures and the construction of specific measures in any detail. Closely related to this omission is the fact that we have not discussed conditions under which the limit in the Riemann style integral we have defined converges. It would also be natural to discuss alternatives to the Riemann style limit, but we will not include that discussion here. Hopefully it will be adequate for our purposes to know such questions can be addressed.

Say $\mathcal{U} \subset \mathbb{R}^n$ is an open subset of \mathbb{R}^n and $\partial \mathcal{U}$ is a smooth (n-1)-dimensional manifold upon which integration is possible and upon which there is a well-defined **outward unit normal field** N. Assume, furthermore, that $\mathbf{v} : \overline{\mathcal{U}} \to \mathbb{R}^n$ is a smooth vector field. Under these circumstances

$$\int_{\partial \mathcal{U}} \mathbf{v} \cdot N$$

is called the **outward flux integral** of v with respect to \mathcal{U} .

Exercise 62 Let \mathcal{U} be an open subset of \mathbb{R}^2 and consider a "window"

$$\underline{\mathcal{U}} = \{(x, y, z) \in \mathbb{R}^3 : (x, y) \in \mathcal{U}\}.$$

Let $\mathbf{v} = (0, 0, v)$ be a smooth vertical field on \mathbb{R}^3 with units given by

$$[v] = \frac{\text{mass}}{\text{area time}}$$

where $[\cdot]$ denotes the units of a quantity. A field in \mathbb{R}^3 with these units is called a **mass flow field**. If we take $N = \mathbf{e_3} = (0,0,1)$ what is the physical significance of

$$\int_{\underline{\mathcal{U}}} \mathbf{v} \cdot N?$$

Note: This integral is also called a flux integral.

Exercise 63 Let U be a rectangular "window"

$$\underline{\mathcal{U}} = \{(x, y, z) \in \mathbb{R}^3 : (x, y) \in [a, b] \times [c, d]\}$$

as described in the previous exercise. Let \mathbf{v} be a constant constant mass flow field on \mathbb{R}^3 with third component $v_3 > 0$. If we take $N = \mathbf{e}_3 = (0,0,1)$, explain the physical significance of

$$\int_{\underline{\mathcal{U}}} \mathbf{v} \cdot N$$

and draw a picture of this quantity in relation to a picture (you've drawn) of the mass which has passed through $\underline{\mathcal{U}}$ in one unit of time.

Exercise 64 If $\mathbf{v}: \mathbb{R}^3 \to \mathbb{R}^3$ denotes the identity (or outward radial) field on \mathbb{R}^3 given by $\mathbf{v}(\mathbf{x}) = \mathbf{x}$, compute the outward flux integral

$$\int_{\partial B_r(\mathbf{0})} \mathbf{v} \cdot N$$

for r > 0.

The Divergence

Let us assume again that \mathcal{U} is an open subset of \mathbb{R}^n with smooth boundary $\partial \mathcal{U}$ and outward unit normal field N. Also, we assume, as before that $\mathbf{v} : \overline{\mathcal{U}} \to \mathbb{R}^n$ is a smooth vector field. Taking a sequence of subdomains \mathcal{V} converging as sets to a singleton $\{\mathbf{p}\}$ with $p \in \mathcal{U}$, we define $\operatorname{div} \mathbf{v} : \mathcal{U} \to \mathbb{R}$ by

$$\operatorname{div} \mathbf{v}(\mathbf{p}) = \lim_{\mathcal{V} \to \{\mathbf{p}\}} \frac{1}{\mathfrak{L}^n} \int_{\partial \mathcal{V}} \mathbf{v} \cdot N.$$

Theorem 13 (divergence theorem)

$$\int_{\mathcal{U}} \operatorname{div} \mathbf{v} = \int_{\partial \mathcal{U}} \mathbf{v} \cdot N.$$

Outline of the proof: Partition \mathcal{U} into small pieces \mathcal{U}_j as indicated (in the two-dimensional case) in Figure 5. Call the partition \mathcal{P} . Then

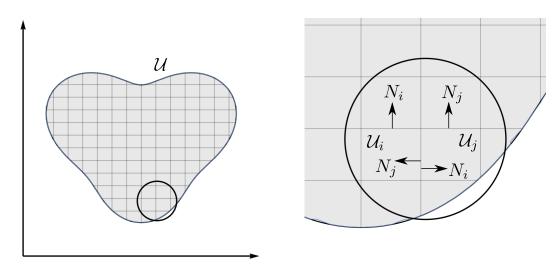


Figure 5: Proof of the divergence theorem in the plane; partitioning a region

$$\int_{\partial \mathcal{U}} \mathbf{v} \cdot N = \sum_{j} \int_{\partial \mathcal{U}_{j}} \mathbf{v} \cdot N$$

where $N = N_j$ is the outward unit normal to \mathcal{U}_j in the integrals on the right. Notice how the integrals over the intersections of adjacent pieces cancel one another. We can write this as

$$\int_{\partial \mathcal{U}} \mathbf{v} \cdot N = \sum_{j} \left(\frac{1}{\mu \mathcal{U}_{j}} \int_{\partial \mathcal{U}_{j}} \mathbf{v} \cdot N \right) \mu \mathcal{U}_{j} = \lim_{\|\mathcal{P}\| \to 0} \sum_{j} \left(\frac{1}{\mu \mathcal{U}_{j}} \int_{\partial \mathcal{U}_{j}} \mathbf{v} \cdot N \right) \mu \mathcal{U}_{j}.$$

The measure μ , in this case, is \mathfrak{L}^n . If $\|\mathcal{P}\|$ is small there is, for each j, some evaluation point $\mathbf{p}_j^* \in \mathcal{U}_j$ such that

 $\frac{1}{\mu \mathcal{U}_j} \int_{\partial \mathcal{U}_j} \mathbf{v} \cdot N \quad \text{is close to} \quad \operatorname{div} \mathbf{v}(\mathbf{p}_j^*).$

Naturally, we need the differences of these quantities to be uniformly small in j. Given that we can write

$$\int_{\partial \mathcal{U}} \mathbf{v} \cdot N = \lim_{\|\mathcal{P}\| \to 0} \sum_{j} \left(\operatorname{div} \mathbf{v}(\mathbf{p}_{k}^{*}) \right) \, \mu \mathcal{U}_{j} = \int_{\mathcal{U}} \operatorname{div} \mathbf{v}. \quad \Box$$

Exercise 65 Let $\mathcal{U} \subset \mathbb{R}^2$ be a set containing a rectangle

$$R = \{ \mathbf{p} + s(1,0) + t(0,1) : (s,t) \in [-\epsilon, \epsilon] \times [-\delta, \delta].$$

Assume $\mathbf{v}: \mathcal{U} \to \mathbb{R}^2$ is a C^1 vector field on \mathcal{U} .

(a) Use the mean value theorem to express the flux integral

$$\int_{\partial R} \mathbf{v} \cdot N$$

as a sum

$$2\delta \int_{-\epsilon}^{\epsilon} f_1(s) \, ds + 2\epsilon \int_{-\delta}^{\delta} f_2(t) \, dt$$

for appropriate functions f_1 and f_2 .

(b) Use your result to determine the value of

$$\operatorname{div} \mathbf{v}(\mathbf{p}) = \lim_{\epsilon, \delta \to 0} \frac{1}{\mu R} \int_{\partial R} \mathbf{v} \cdot N$$

in rectangular coordinates.

The divergence theorem is the version of integration by parts we need to find/derive partial differential equations as Euler-Lagrange equations in the calculus of variations. Such partial differential equations are called **variational PDE**.

Derivatives and the Gradient

Our proof of the divergence theorem relies heavily on the convergence of the limit in the definition of the divergence, which we have not shown. In fact, some (not so restrictive) conditions should be satisfied by the vector field \mathbf{v} and the regions $\mathcal{V} \subset \mathcal{U}$ with $\mathcal{V} \to \{\mathbf{p}\}$. We will show the limit exists for several different kinds of regions and for several different kinds of coordinates. It will be noted that the divergence is a differential expression (or a kind of derivative) though it was defined in terms of an integral expression/quantity. As

a consequence, filling in the deficiency of showing the divergence exists will benefit from some preliminary discussion of derivatives.

The starting point for essentially all derivatives is the limit of the diffence quotient

$$u'(x) = \lim_{h \to 0} \frac{u(x+h) - u(x)}{h} \tag{25}$$

for a real valued function $u:(a,b)\to\mathbb{R}$ of one variable, when this limit exists. This quantity is interpreted (physically) as the (instantaneous) rate of change of the quantity measured by u with respect to the change in the independent variable x and (geometrically) as the slope of the tangent line to the graph of u.

Exercise 66 Assume x = x(t) measures distance (length) and t measures time.

(a) Use the formula

$$average \ rate = \frac{total \ net \ distance}{total \ ellarsed \ time}$$

to find and expression for the average rate of change of x over a finite time interval [a, b].

(b) Interpret your answer geometrically in terms of points on the graph of the function $x:[a,b]\to\mathbb{R}$.

Given a function $u: \mathcal{U} \to \mathbb{R}$ of two or more variables defined on an open subset $\mathcal{U} \subset \mathbb{R}^n$, a natural generalization of (25) is the **directional derivative** given by

$$D_{\mathbf{v}}u(\mathbf{x}) = \lim_{h \to 0} \frac{u(\mathbf{x} + h\mathbf{v}) - u(\mathbf{x})}{h}$$
(26)

where \mathbf{v} is a (tangent) vector at $\mathbf{x} \in \mathcal{U}$. There are some differences between this kind of difference quotient and (25) and several remarks are in order. First of all, it will be remarked that to specialize (26) to the one-dimensional case and obtain the same derivative, one must make the particular choice $\mathbf{v} = 1 \in \mathbb{R}$. Thus, our generalization is not only a generalization in dimension but also in the generality of the notion considered. Illustrating this latter generalization, here are two special cases of note:

1. If \mathbf{v} is a unit vector, that is, $|\mathbf{v}| = 1$, then the value of $D_{\mathbf{v}}u(\mathbf{x})$ gives the instantaneous rate of change of the function u in the direction \mathbf{v} . Many authors restrict the definition (26) to only this case. In particular, in this case one may construct a "graph" over the line $\{\mathbf{x} + t\mathbf{v}\}$ given by taking some (small) $\epsilon > 0$ and considering

$$\mathcal{G} = \{(t, u(\mathbf{x} + t\mathbf{v})) : |t| < \epsilon\}.$$

The difference quotient (26) is then recognized as the slope of the secant line to the graph \mathcal{G} determined by the points $(h, u(\mathbf{x} + h\mathbf{v}))$ and $(0, u(\mathbf{x}))$ as indicated in Figure 6.

Exercise 67 In two dimensions, when $\mathcal{U} \subset \mathbb{R}^2$, the graph

$$\mathcal{G} = \{(x, y, u(x, y)) : (x, y) \in \mathcal{U}\}$$

of the function $u: \mathcal{U} \to \mathbb{R}$ is a surface, and the illustration of Figure 6 can be realized in a somewhat different form. Draw such an illustration and interpret the difference quotient in (26) in terms of your illustration.

2. If \mathbf{v} is taken to be a **standard unit basis vector** \mathbf{e}_j , then the resulting directional derivative has a special name and notation. First of all, recall that the standard unit basis vector \mathbf{e}_j is the vector in \mathbb{R}^n with zeros in all entries except for the j-th entry, which is 1. The vector \mathbf{e}_j is also called the

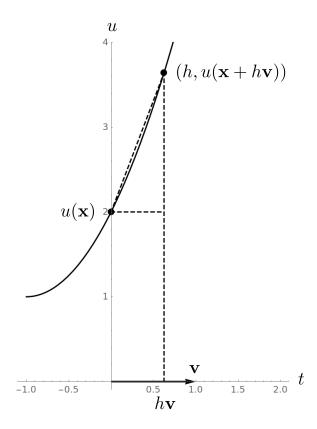


Figure 6: Difference quotient.

standard coordinate vector (with respect to a choice of rectangular coordinates). In this case we write

$$\frac{\partial u}{\partial x_j} = D_{\mathbf{e}_j} u$$

and call this quantity a partial derivative. The notations

$$D_{x_j}u, \quad D_ju, \quad u_{x_j}, \quad \text{and} \quad D^{\mathbf{e}_j}u$$
 (27)

are also used to denote this same quantity. In two dimensions $\mathbf{e}_1 = (1,0)$, $\mathbf{e}_2 = (0,1)$, and another usual notation is given by

$$\frac{\partial u}{\partial x_1} = \frac{\partial u}{\partial x}$$
 and $\frac{\partial u}{\partial x_2} = \frac{\partial u}{\partial y}$.

Similarly, in three dimensions one finds

$$\frac{\partial u}{\partial x_1} = \frac{\partial u}{\partial x}, \qquad \frac{\partial u}{\partial x_2} = \frac{\partial u}{\partial y} \quad \text{and} \quad \frac{\partial u}{\partial x_3} = \frac{\partial u}{\partial z}.$$

Each of the above notations, especially those in (27), should be considered carefully and compared to the meaning of this kind of derivative.

Exercise 68 How does your illustration and explanation from Exercise 67 change in the case $\mathbf{v} = \mathbf{e}_j$ is a standard unit basis vector in \mathbb{R}^2 ?

We have not followed other authors in restricting the directional derivative $D_{\mathbf{v}}u$ to unit vectors \mathbf{v} . As a consequence, $D_{\mathbf{v}}u(\mathbf{x})$ does not always give the instantaneous rate of change of the quantity u in the direction \mathbf{v} at \mathbf{x} , and we need (perhaps) to be a little careful. First notice $\mathbf{v} = \mathbf{0}$ implies $D_{\mathbf{v}}u = 0$, and this

quantity indicates nothing about the local behavior of u near \mathbf{x} . Nevertheless, we obtain a well-defined (zero) value in this case. If $\mathbf{v} \neq \mathbf{0}$, then

$$D_{\mathbf{v}}u(\mathbf{x}) = |\mathbf{v}| \lim_{h \to 0} \frac{u(\mathbf{x} + (h|\mathbf{v}|)(\mathbf{v}/|\mathbf{v}|)) - u(\mathbf{x})}{h|\mathbf{v}|} = |\mathbf{v}|D_{\mathbf{v}/|\mathbf{v}|}u$$

is the scaling of the rate of change of u in the unit direction $\mathbf{v}/|\mathbf{v}|$ by the factor $|\mathbf{v}|$. This can be recognized as a familiar form of the **chain rule** which says the derivative $(u \circ v)'(x)$ of a **composition** $u \circ v : (a, b) \to \mathbb{R}$ where $v : (a, b) \to (c, d)$ and $u : (c, d) \to \mathbb{R}$ is the product of the instantaneous rate of change of u at v(x) and the instantaneous rate of change of v at v(x)

$$(u \circ v)'(x) = u'(v(x)) \ v'(x),$$
 (28)

or (as it is often cryptically expressed)

$$\frac{du}{dx} = \frac{du}{dv} \, \frac{dv}{dx}.$$

In the multivariable case of $D_{\mathbf{v}}u$, the composition is one with u and the vector valued function $\alpha(t) = \mathbf{x} + t\mathbf{v}$ with velocity vector $\alpha' = \mathbf{v}$ is constant. To be explicit

$$\frac{d}{dt}u(\alpha(t))\Big|_{t=0} = D_{\mathbf{v}/|\mathbf{v}|}u(\alpha(0)) |\alpha'(0)|.$$
(29)

Exercise 69 Notice that in comparing the one-dimensional chain rule (28) with the chain rule we have derived/observed for directional derivatives (29) one contains a norm/absolute value which is conspicuously missing in the other.

- (a) If one applies the definition of a directional derivative (26) to a function $u:(a,b) \to \mathbb{R}$ of one variable using only unit vectors \mathbf{v} , what is the difference between $D_{\mathbf{v}}u$ and u'? Put another way, how many points are there in the boundary of the one-ball $B_r(0) = \{x \in \mathbb{R} : |x| = 1\}$?
- (b) Explain why there are no absolute values in (28).

In the context of higher dimensional directional derivatives defined by (26) certain additional constructions (often overlooked in 1-D calculus) are of interest. It may first be noted that the expression $D_{\mathbf{v}}u(\mathbf{x})$ has several possible quantities which can be considered as "arguments." Perhaps the simplest way to think about this quantity is with $u: \mathcal{U} \to \mathbb{R}$ and $\mathbf{v} \in \mathbb{R}^n$ fixed and argument $\mathbf{x} \in \mathcal{U}$. Thus, $D_{\mathbf{v}}u$ becomes a real valued function on \mathcal{U} . This naturally opens the door for repetition of the construction (directional differentiation) and consideration of **higher order** directional derivatives. Naturally, some regularity is required to compute derivatives as limits of difference quotients. The absolute value function is not differentiable at x = 0 in this sense, and we have already introduced the continuity/differentiability classes C^0 , C^1 , C^2 , ... in one dimension. We turn to partial derivatives for the analogue in higher dimensions:

Definition 10 A function $u: A \to \mathbb{R}$ defined on any subset $A \subset \mathbb{R}^n$ is continuous at $\mathbf{x}_0 \in A$ if for any $\epsilon > 0$, there is some $\delta > 0$ such that

$$|u(\mathbf{x}) - u(\mathbf{x}_0)| < \epsilon$$
 whenever $\mathbf{x} \in A$ and $|\mathbf{x} - \mathbf{x}_0| < \delta$.

The function $u: A \to \mathbb{R}$ is said to be **continuous on** A if u is continuous at each point $\mathbf{x}_0 \in A$.

Exercise 70 Show that if the domain of a function $u: \mathcal{U} \to \mathbb{R}$ is an open subset $\mathcal{U} \subset \mathbb{R}^n$, then the condtion $\mathbf{x} \in \mathcal{U}$ may be omitted from the definition. In other words, consider the alternative definition: u is continuous at $\mathbf{x}_0 \in \mathcal{U}$ if for any $\epsilon > 0$, there is some $\delta > 0$ such that

$$|u(\mathbf{x}) - u(\mathbf{x}_0)| < \epsilon$$
 whenever $|\mathbf{x} - \mathbf{x}_0| < \delta$.

Show a function continuous according to this definition is continuous with respect to the "official" definition above.

Definition 11 Given an open set $\mathcal{U} \subset \mathbb{R}^n$, the set $C^1(\mathcal{U})$ consists of the real valued functions $u : \mathcal{U} \to \mathbb{R}$ for which the partial derivatives satisfy

$$\frac{\partial u}{\partial x_1}, \frac{\partial u}{\partial x_2}, \dots, \frac{\partial u}{\partial x_n} \in C^0(\mathcal{U}).$$

Exercise 71 Show that $u \in C^1(\mathcal{U})$ implies $u \in C^0(\mathcal{U})$.

Definition 12 Given an open subset $\mathcal{U} \subset \mathbb{R}^n$ and a natural number $k \geq 2$, the set $C^k(\mathcal{U})$ consists of the real valued functions $u : \mathcal{U} \to \mathbb{R}$ for which the partial derivatives satisfy

$$\frac{\partial u}{\partial x_1}, \frac{\partial u}{\partial x_2}, \dots, \frac{\partial u}{\partial x_n} \in C^{k-1}(\mathcal{U}).$$

Exercise 72 If \mathcal{U} is an open subset of \mathbb{R}^n and $u \in C^2(\mathcal{U})$, then (show)

$$D_{\mathbf{v}}D_{\mathbf{w}}u = D_{\mathbf{w}}D_{\mathbf{v}}u$$
 for any vectors $\mathbf{v}, \mathbf{w} \in \mathbb{R}^n$.

Definition 13 If A is any subset of \mathbb{R}^n and k is a natural number with $k \geq 1$, then $C^k(A)$ consists of those functions $u: A \to \mathbb{R}$ for which the following holds: There exists an open set $\mathcal{U} \subset \mathbb{R}^n$ and an extension $\overline{u} \in C^k(\mathcal{U})$ for which

- 1. $A \subset \mathcal{U}$, and
- 2. the restriction of \overline{u} to A is u:

$$\overline{u}_{|_{A}} = u.$$

Exercise 73 If $u \in C^0(A)$, then does there (necessarily) exist an extension $\overline{u} : \mathcal{U} \to \mathbb{R}$ with \mathcal{U} some open subset satisfying

- 1. $A \subset \mathcal{U}$, and
- 2. the restriction of \overline{u} to A is u:

$$\overline{u}_{|_{\Lambda}} = u,$$

and $u \in C^0(\mathcal{U})$?

Returning to the possible arguments of $D_{\mathbf{v}}u(\mathbf{x})$, in addition to $D_{\mathbf{v}}u:\mathcal{U}\to\mathbb{R}$, we may consider u and \mathbf{x} fixed, so that $D_{\mathbf{v}}u(\mathbf{x})$ is considered a function of \mathbf{v} . This point of view brings to light a distinction which is usually lost (or ignored) in calculus that the collection of vectors \mathbf{v} is ususally distinct from the set of arguments $\mathbf{x}\in\mathcal{U}\subset\mathbb{R}^n$ for the function u. Technically, the directions \mathbf{v} available for computing $D_{\mathbf{v}}u(\mathbf{x})$ include all vectors in the **tangent space to the domain** \mathcal{U} at \mathbf{x} which is $T_{\mathbf{x}}\mathcal{U}=\mathbb{R}^n$. When the value of the directional derivative is considered as a function of the direction of differentiation \mathbf{v} in this way, the result is called the **differential** of u at \mathbf{x} and is denoted by

$$du_{\mathbf{x}}: \mathbb{R}^n \to \mathbb{R}.$$

While $u: \mathcal{U} \to \mathbb{R}$, we have a collection of differential functions (one for each $\mathbf{x} \in \mathcal{U}$) with $du_{\mathbf{x}}: \mathbb{R}^n \to \mathbb{R}$. In addition to having the distinction of having all of \mathbb{R}^n for domain, we have given an argument above showing homogeneity with respect to scaling along the following lines:

Exercise 74 Show that the differential $du_{\mathbf{x}}: \mathbb{R}^n \to \mathbb{R}$, as we have defined it, satisfies

$$du_{\mathbf{x}}(a\mathbf{v}) = a \ du_{\mathbf{x}}(\mathbf{v})$$
 for each $\mathbf{v} \in \mathbb{R}^n$ and $a \in \mathbb{R}$.

This suggests, at the very least, we should consider the possibility that the functions $du_{\mathbf{x}}$ might be **linear**. It follows from Exercise 74, in fact, that in the case n=1 the differential map is linear. At this point it should be confessed that I have again departed, to a certain extent, from standard usage in not making the linearity of a differential an apriori requirement. As I now examine this point in more detail, let me start by recalling that in 1-D calculus the functions in $\mathrm{Diff}(a,b)$, considered as a special case of functions $u:\mathcal{U}\to\mathbb{R}$ where \mathcal{U} might be a higher dimensional domain, are both the functions that are **differentiable** at each point and the functions that have all partial derivatives (of which there is only one) existing at each point, and

$$C^0(a,b) \supseteq \text{Diff}(a,b) \supseteq C^1(a,b).$$
 (30)

In higher dimensions it is customary to make a distinction so that the **differentiable functions** on a domain \mathcal{U} in a higher dimensional space and those with **all first order partial derivatives existing** at each point \mathbf{x} in \mathcal{U} are **not** the same thing. With this in mind, we introduce the set of functions $u: \mathcal{U} \to \mathbb{R}$ with all first order partial derivatives existing at every point \mathbf{x} in an open subset $\mathcal{U} \subset \mathbb{R}^n$ and call it pDiff(\mathcal{U}). These may be informally called the collection of **partially differentiable functions** on \mathcal{U} , and we can also write for (30)

$$C^0(a,b) \supseteq \text{Diff}(a,b) = \text{pDiff}(a,b) \supseteq C^1(a,b).$$

For $\mathcal{U} \subset \mathbb{R}^n$ (any n) and $u \in \mathrm{pDiff}(\mathcal{U})$, there is a linear function $L_{\mathbf{x}} : \mathbb{R}^n \to \mathbb{R}$ associated to u at the point \mathbf{x} with values given by

$$L_{\mathbf{x}}(\mathbf{v}) = Du(\mathbf{x}) \cdot \mathbf{v} = \langle Du(\mathbf{x}), \mathbf{v} \rangle_{\mathbb{R}^n}$$

where $Du: \mathcal{U} \to \mathbb{R}^n$ represents the vector field on \mathcal{U} given in standard coordinates by

$$Du = \left(\frac{\partial u}{\partial x_1}, \frac{\partial u}{\partial x_2}, \dots, \frac{\partial u}{\partial x_n}\right).$$

This vector of first partial derivatives is also called the **total derivative** of u or the **gradient vector**. It should be noted that this is a coordinate dependent expression for the gradient, and we will discuss an important coordinate free version of the gradient vector below. For now, however, we have a linear function $L_{\mathbf{x}}$ at each point $\mathbf{x} \in \mathcal{U}$ associated with each function u in

$$\operatorname{pDiff}(\mathcal{U}) \supseteq C^1(\mathcal{U}).$$

The difference between the one dimensional case and the higher dimensional cases starts to become apparent now since there is no simple inclusion relating pDiff(\mathcal{U}) and $C^0(\mathcal{U})$ when $\mathcal{U} \subset \mathbb{R}^n$ and n > 1.

Exercise 75 Find a function $u \in pDiff(\mathcal{U}) \setminus C^0(\mathcal{U})$. Find a function $u \in C^0(\mathcal{U}) \setminus pDiff(\mathcal{U})$.

The notion of differentiability in higher dimensions involves another linear function, potentially different from both $L_{\mathbf{x}}$ and $du_{\mathbf{x}}$ mentioned above, and more explicitly based on first order approximation:

Definition 14 Given an open subset $\mathcal{U} \subset \mathbb{R}^n$, a function $u : \mathcal{U} \to \mathbb{R}$ is differentiable at $\mathbf{x} \in \mathcal{U}$ if there exists a linear function $\ell : \mathbb{R}^n \to \mathbb{R}$ for which

$$\lim_{\mathbf{v}\to\mathbf{0}}\frac{u(\mathbf{x}+\mathbf{v})-u(\mathbf{x})-\ell(\mathbf{v})}{|\mathbf{v}|}=0.$$

The collection of functions $u: \mathcal{U} \to \mathbb{R}$ which are differentiable at each point $\mathbf{x} \in \mathcal{U}$ is denoted by Diff(\mathcal{U}).

Exercise 76 Show that the definition of Diff(\mathcal{U}) in the special case n = 1, with \mathcal{U} an interval (a, b), is consistent with the previous definition of Diff(a, b) based on the limit of the difference quotient.

It is, thus, with this notion we obtain a higher dimensional version of (30):

$$C^0(\mathcal{U}) \supseteq \text{Diff}(\mathcal{U}) \supseteq C^1(\mathcal{U}).$$

In order to verify the inclusion on the right we recall the **mean value theorem** for functions of one variable:

Theorem 14 Given $u \in C^0[a,b] \cap C^1(a,b)$, there exists some $x_* \in (a,b)$ with

$$u'(x_*) = \frac{u(b) - u(a)}{b - a}. (31)$$

In the special case $u \in C^1[a, b]$ there is a simple proof of (31) using (mainly) the fundamental theorem of calculus and the chain rule. The construction is useful in many contexts, so we present it:

$$u(b) - u(a) = \int_0^1 \frac{d}{dt} u((1-t)a + tb) dt = \int_0^1 u'((1-t)b + ta)(b-a) dt.$$

The quantity

$$\int_0^1 u'((1-t)b+ta)\,dt$$

is the average value of the integrand u'((1-t)b+ta) which is a continuous function of t, and it follows that for some $t_* \in (0,1)$

$$\int_0^1 u'((1-t)b+ta) dt = u((1-t^*)b+t^*a).$$

Now, in the case $u \in C^1(\mathcal{U})$, we claim the linear function $L_{\mathbf{x}}$ given by the Euclidean inner product with the vector of partial derivatives $Du(\mathbf{x})$ gives the linear approximation required by the definition of differentiability. To see this, let $\mathbf{v} = (v_1, v_2, \dots, v_n)$ and note that by the mean value theorem

$$u(\mathbf{x} + v_1 \mathbf{e}_1) - u(\mathbf{x}) = D_{\mathbf{e}_1} u(\mathbf{x}_1^*) v_1$$

where $\mathbf{x}_1^* = \mathbf{x} + v_1^* \mathbf{e}_1$ and v_1^* is between 0 and v_1 . Similarly,

$$u(\mathbf{x} + v_2\mathbf{e}_2 + v_1\mathbf{e}_1) - u(\mathbf{x} + v_1\mathbf{e}_1) = D_{\mathbf{e}_2}u(\mathbf{x}_2^*)v_2$$

where $\mathbf{x}_2^* = \mathbf{x} + v_2^* \mathbf{e}_2 + v_1 \mathbf{e}_1$ and v_2^* is between 0 and v_2 . Repeating this application of the mean value theorem along the remaining standard coordinate directions, we obtain

$$u(\mathbf{x} + \mathbf{v}) - u(\mathbf{x}) = \sum_{k=2}^{n} \left[u \left(\mathbf{x} + \sum_{j=1}^{k} v_j \mathbf{e}_j \right) - u \left(\mathbf{x} + \sum_{j=1}^{k-1} v_j \mathbf{e}_j \right) \right] + u(\mathbf{x} + v_1 \mathbf{e}_1) - u(\mathbf{x})$$
$$= \sum_{j=1}^{n} D_{\mathbf{e}_j} u(\mathbf{x}_j^*) v_j$$

for points $\mathbf{x}_1^*, \mathbf{x}_2^*, \dots, \mathbf{x}_n^*$ tending to \mathbf{x} as \mathbf{v} tends to $\mathbf{0}$. This can be written as

$$u(\mathbf{x} + \mathbf{v}) - u(\mathbf{x}) = \langle D^* u, \mathbf{v} \rangle_{\mathbb{R}^n}$$

where $D^*u = (D_{\mathbf{e}_1}u(\mathbf{x}_1^*), D_{\mathbf{e}_2}u(\mathbf{x}_2^*), \dots, D_{\mathbf{e}_n}u(\mathbf{x}_n^*))$. Therefore,

$$u(\mathbf{x} + \mathbf{v}) - u(\mathbf{x}) - L_{\mathbf{x}}(\mathbf{v}) = \langle (D^*u - Du(\mathbf{x}), \mathbf{v})_{\mathbb{R}^n} .$$

The Cauchy-Schwarz inequality says that for any vectors \mathbf{v} and \mathbf{w} in \mathbb{R}^n , we have

$$|\langle \mathbf{v}, \mathbf{w} \rangle_{\mathbb{R}^n}| \le |\mathbf{v}||\mathbf{w}|.$$

Applying this inequality we have

$$|u(\mathbf{x} + \mathbf{v}) - u(\mathbf{x}) - L_{\mathbf{x}}(\mathbf{v})| \le |D^*u - Du(\mathbf{x})||\mathbf{v}||$$

and

$$\left| \frac{u(\mathbf{x} + \mathbf{v}) - u(\mathbf{x}) - L_{\mathbf{x}}(\mathbf{v})}{|\mathbf{v}|} \right| = \frac{|u(\mathbf{x} + \mathbf{v}) - u(\mathbf{x}) - L_{\mathbf{x}}(\mathbf{v})|}{|\mathbf{v}|} \le |D^*u - Du(\mathbf{x})|.$$

By the continuity of the partial derivatives

$$\lim_{\mathbf{v}\to\mathbf{0}} |D^*u - Du(\mathbf{x})| = 0$$

since

$$D_{\mathbf{e}_k} u(\mathbf{x}_k^*) = \frac{\partial u}{\partial x_k} \left(\mathbf{x} + v_k^* \mathbf{e}_k + \sum_{j \neq k} v_j \mathbf{e}_j \right)$$

and v_k^* is between 0 and v_k .

The argument above not only shows that $u \in C^1(\mathcal{U})$ is differentiable, but the approximating linear function ℓ in the definition of differentiability can be taken to be the particular linear function $L_{\mathbf{x}}$ obtained using the inner product with the total derivative/gradient vector $Du(\mathbf{x})$.

A multivariable chain rule

Let $u \in C^1(\mathcal{U})$ where \mathcal{U} is an open subset of \mathbb{R}^2 .

4.2 Coordinates and inner product spaces

The relation of vectors and other mathematical constructions to coordinates is often first encountered (and usually not fully appreciated) in a course on linear algebra. The basic idea is also operative in elementary geometry where a circle with a given radius and center can be considered without coordinates and, yet, if one wishes to make certain computations introducing coordinates for the center of a circle is seemingly unavoidable. A similar situation prevails with vectors, linear transformations, and other mathematical constructions. Two such constructions we wish to consider here are the gradient of a real valued function (of several variables) and the divergence of a vector field. It will be noted that in the first case, we have used coordinates to define the gradient:

$$Du = \left(\frac{\partial u}{\partial x_1}, \frac{\partial u}{\partial x_2}, \dots, \frac{\partial u}{\partial x_n}\right).$$

The divergence, on the other hand, we have defined in a manner that did not use coordinates:

$$\div \mathbf{v}(\mathbf{x}) = \lim_{\mathcal{V} \to \{\mathbf{x}\}} \frac{1}{\mathfrak{L}^n(\mathcal{V})} \int_{\mathcal{V}} \mathbf{v} \cdot \mathbf{n}.$$

Technically, the dot product appearing in this definition involves coordinates if by $\mathbf{v} \cdot \mathbf{n}$ we mean

$$\mathbf{v} \cdot \mathbf{n} = \sum_{j=1}^{n} v_j n_j.$$

The dot product itself, however, can be considered without coordinates, and this distinction may be indicated by the use of a different notation.

Definition 15 An inner product space is a vector space V equipped with a function $\langle \cdot, \cdot \rangle : V \times V \to \mathbb{R}$ having the following properties:

- (i) $\langle \mathbf{v}, \mathbf{w} \rangle = \langle \mathbf{w}, \mathbf{v} \rangle$ for all $\mathbf{v}, \mathbf{w} \in V$. (symmetric)
- (ii) $\langle a\mathbf{v} + b\mathbf{w}, \mathbf{z} \rangle = a\langle \mathbf{v}, \mathbf{z} \rangle + b\langle \mathbf{w}, \mathbf{z} \rangle$ for all $a, b \in \mathbb{R}$ and $\mathbf{v}, \mathbf{w}, \mathbf{z} \in V$. (bilinear)
- (iii) $\langle \mathbf{v}, \mathbf{v} \rangle \geq 0$ with equality if and only if $\mathbf{v} = \mathbf{0}$. (positive definite)

Multi-index notation

The last notation for a partial derivative given in (27) deserves special notice. Though $D^{\mathbf{e}_j}u$ bears a strong superficial resemblance to the standard notation $D_{\mathbf{e}_j}u$ for a partial derivative, something quite different is in mind. Though not immediately of interest in regard to our present discussion of **first order** partial derivatives, the multi-index notation is quite useful in certain applications, most notably for writing down higher order Taylor approximations in several variables, so let us briefly explain it in passing. The superscript vector in $D^{\beta}u$ can not only be taken as one of the standard unit basis vectors to indicate a single directional derivative in that direction, but β denotes a multi-index which is an element in the set

$$\mathbb{N}_0^n = \{ (\beta_1, \beta_2, \dots, \beta_n) : \beta_j \in \mathbb{N}_0 \text{ for } j = 1, 2, \dots, n \}$$

and $\mathbb{N}_0 = \{0, 1, 2, \ldots\}$ denotes the nonnegative integers. In words, $D^{\beta}u$ indicates the result of taking β_j partial derivatives of u with respect to \mathbf{e}_j for $j = 1, 2, \ldots, n$. It is assumed, when this notation is used, that u is continuously (partial) differentiable $\beta_1 + \beta_2 + \cdots + \beta_n$ times in any combination of standard directions. In this context, the sum $\sum \beta_j$ is denoted $\|\beta\|$ and called the **norm of the multi-index** β , and a function with this regularity on an open subset $\mathcal{U} \subset \mathbb{R}^n$ is said to be in $C^{\|\beta\|}(\mathcal{U})$. It can then be proved that the order of application of the partial derivatives does not effect the result, so we can write

$$D^{\beta}u = \frac{\partial^{\|\beta\|}u}{\partial^{\beta_1}x_1\partial^{\beta_2}x_2\cdots\partial^{\beta_n}x_n}.$$
 (32)

This may seem complicated, but consider the simplicity and economy of notation obtained in (32). Returning to $D_{\mathbf{e}_j}u$ and $D^{\mathbf{e}_j}u$, the former denotes taking a directional derivative in the direction of the vector \mathbf{e}_j , which happens to be a partial derivative. Thus, $D_{\mathbf{e}_j}u$ is simply a special case of $D_{\mathbf{v}}u$ as explained above. The expression $D^{\mathbf{e}_j}u$ on the other hand means "one partial derivative with respect to the variable x_i " where $D^{\beta}u$ has the more general meaning " β_j derivatives with respect to x_j for $j = 1, 2, \ldots, n$."

Definition 16 Given an open subset $\mathcal{U} \subset \mathbb{R}^n$ and a natural number $k \geq 1$, the set $C^k(\overline{\mathcal{U}})$ consists of all functions $u \in C^k(\mathcal{U})$ such that each partial derivative $D^{\beta}u$ with $|\beta| \leq k$ has a continuous extension $v_{\beta} \in C^0(\overline{\mathcal{U}})$ to the closure of \mathcal{U} :

$$v_{\beta}|_{\mathcal{U}} = D^{\beta}u.$$

Exercise 77 Definition 13 and Definition 16 overlap when $A = \overline{\mathcal{U}}$ is the closure of an open subset of \mathbb{R}^n . Are they consistent with one another in this case?