Appendix A

Multivariable Calculus

A.1 Differentials

Consider an inclined plane in x-y-z coordinate space, as shown in Fig. 1. We can think of the plane as a meadow with the x axis pointed east and the y axis pointed north; the z coordinate is the elevation above sea level. Elevation is a state function of the east–north position in the field; we write $z(x, y)$. We seek the change of elevation (z) as we go from point i to point f in the meadow. This can be calculated by first traveling east, a distance Δx, ending up at point g. We indicate the easterly slope of the meadow as $(\Delta z/\Delta x)_y$. The subscript y indicates that the north–south position remains constant when measuring this slope. Our change in elevation upon arrival at point g is $\Delta z_1 = (\Delta z/\Delta x)_Y \Delta x$. We then complete our journey to point f by traveling in the northerly (y) direction. Our change in elevation in the second part of the trip is $\Delta z_2 = (\Delta z/\Delta y)_x \Delta y$. The change in elevation for the total trip is the sum of that in the first and the second parts of the trip:

$$\Delta z = \left(\frac{\Delta z}{\Delta x}\right)_y \Delta x + \left(\frac{\Delta z}{\Delta y}\right)_x \Delta y \tag{1}$$

What happens if the meadow is not planar? At a given point, we can approximate a nonplanar meadow with the plane that is tangent to the meadow at

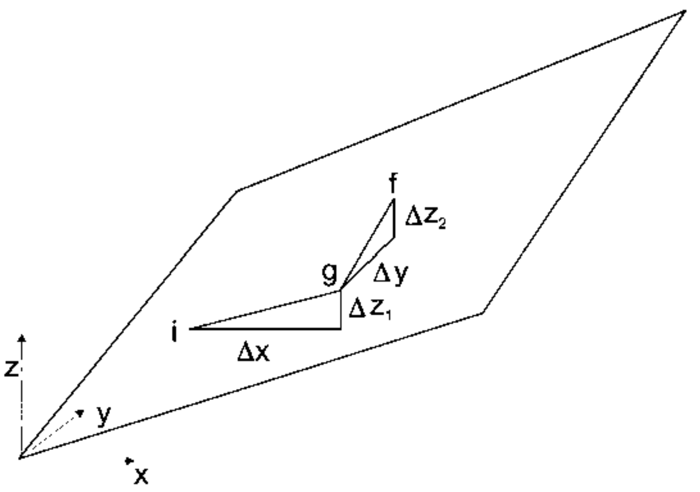

Figure 1 An inclined plane in the x-y-z coordinate space.

the point. If we stay very close to the original point, the tangent plane is a very good approximation to the meadow, and in the limit of infinitesimal displacement from the point, it is a perfect approximation and we can write

$$dz = \left(\frac{\partial z}{\partial x}\right)_y dx + \left(\frac{\partial z}{\partial y}\right)_x dy \tag{2}$$

where dz is called the *total differential* of the function $z(x, y)$. Quantities such as $(\partial z/\partial x)_y$, the *partial derivative of z with respect to x holding y constant*, are the slopes of the meadow in particular directions. Given a differential expression

$$dz = M(x, y)\, dx + N(x, y)\, dy \tag{3}$$

it must be identical to Eq. (2). Because dx and dy are arbitrary,

$$M(x, y) = \left(\frac{\partial z}{\partial x}\right)_y \quad \text{and} \quad N(x, y) = (\partial z/\partial y)_x \tag{4}$$

Example 1. If $z = x^3 \sin y$, what are $(\partial z/\partial x)_y$, $(\partial z/\partial y)_x$, and dz?

Solution: It is assumed that the reader can take ordinary derivatives of simple functions. In finding $(\partial z/\partial x)_y$, y is a constant, so z can be treated as Cx^3. Then,

$$\left(\frac{\partial z}{\partial x}\right)_y = 3x^2C = 3x^2 \ \sin\ y$$

For $(\partial z/\partial y)_x$, we write $z = C' \sin y$ and $(\partial z/\partial y)_x = C' \cos y = x^3 \cos y$. Finally, $dz = 3x^2(\sin y)\,dx + x^3(\cos y)\,dy$.

If $z(x, y)$, then $x(y, z)$ and $y(z, x)$. Each of these functions permits the definition of two partial derivatives. What are the relationships between the six partial derivatives formed from three variables? If two partial derivatives hold the same variable constant, we only have two variables and can use the reciprocal rule from ordinary calculus:

$$\left(\frac{\partial z}{\partial x}\right)_y = \left(\frac{\partial x}{\partial z}\right)_y^{-1}, \qquad \left(\frac{\partial z}{\partial y}\right)_x = \left(\frac{\partial y}{\partial z}\right)_x^{-1}$$

and

$$\left(\frac{\partial y}{\partial x}\right)_z = \left(\frac{\partial x}{\partial y}\right)_z^{-1} \tag{5}$$

If z is held constant, we can set $dz = 0$ in Eq. (2):

$$0 = \left(\frac{\partial z}{\partial x}\right)_y dx_z + \left(\frac{\partial z}{\partial y}\right)_x dy_z \tag{6}$$

where we have placed a subscript on dx and dy to indicate that z is constant. Rearranging, we get

$$\frac{dy_z}{dx_z} \equiv \left(\frac{\partial y}{\partial x}\right)_z = -\left(\frac{\partial z}{\partial x}\right)_y \left(\frac{\partial z}{\partial y}\right)_x^{-1} = -\left(\frac{\partial y}{\partial z}\right)_x \left(\frac{\partial z}{\partial x}\right)_y \tag{7}$$

The last equation looks just like the chain rule for ordinary derivatives, except for the minus sign, which is often omitted by students. However, the need for the minus sign is fairly obvious. If z increases with x at constant y and with y at constant x, for z to remain constant, as we increase x, we must decrease y. We will call Eq. (7) the *chain rule for partial derivatives*.

If there is a relation among x, y, and z, any function of these variables can be written in terms of only two of the three variables, [e.g., $F(x, y)$ or $F(x, z)$]. If x, y, and z change, F will also change, and it will change the same amount whether we decide to consider it as a function of x and y or x and z.

$$dF(x, y) = \left(\frac{\partial F}{\partial x}\right)_y dx + \left(\frac{\partial F}{\partial y}\right)_x dy = dF(x, z) = \left(\frac{\partial F}{\partial x}\right)_z dx + \left(\frac{\partial F}{\partial z}\right)_x dz \tag{8}$$

We can apply Eq. (8) to a process at constant y $(dy = 0)$:

$$\left(\frac{\partial F}{\partial x}\right)_y dx_y = \left(\frac{\partial F}{\partial x}\right)_z dx_y + \left(\frac{\partial F}{\partial z}\right)_x dz_y \tag{9}$$

which gives

$$\left(\frac{\partial F}{\partial x}\right)_y = \left(\frac{\partial F}{\partial x}\right)_z + \left(\frac{\partial F}{\partial z}\right)_x \left(\frac{\partial z}{\partial x}\right)_y \tag{10}$$

Equation (10) shows how to change partial derivatives when changing the variable held constant.

We will also be interested in $dF(x, y)$ when $y = y(x)$. We have

$$dF = \left(\frac{\partial F}{\partial x}\right)_y dx + \left(\frac{\partial F}{\partial y}\right)_x dy = \left(\frac{\partial F}{\partial x}\right)_y dx + \left(\frac{\partial F}{\partial y}\right)_x \frac{dy}{dx}\, dx \tag{11}$$

This also gives

$$\frac{dF}{dx} = \left(\frac{\partial F}{\partial x}\right)_y + \left(\frac{\partial F}{\partial y}\right)_x \frac{dy}{dx} \tag{12}$$

To extend Eq. (2) to functions of more than two variables, the equation for the total derivative must include a term for each variable, with the partial derivative for that variable holding all other variables constant. For $h(x, y, z)$,

$$dh = \left(\frac{\partial h}{\partial x}\right)_{y,z} dx + \left(\frac{\partial h}{\partial y}\right)_{x,z} dy + \left(\frac{\partial h}{\partial z}\right)_{x,y} dz \tag{13}$$

which can be written as

$$dh = M(x, y, z)\, dx + N(x, y, z)\, dy + P(x, y, z)\, dz \tag{14}$$

A.2 Integrals

Integrals of the form $\int_{x_1}^{x_2} F(x)\, dx$ are completely determined, although the integration may not be trivial for complicated functions $F(x)$. Integrals of the form $\int_{x_1,y_1}^{x_2,y_2} G(y)\, dx$ or $\int_{x_1,y_1}^{x_2,y_2} G(x, y)\, dx$ are not determined until the relation between x and y, $x(y)$, is specified. They are called *path integrals*.

Example 2. Evaluate the integral $\int_{0,0}^{1,1} y\, dx$ for the following two paths: path A, $y = x$; path B, $y = 0 \to 1$, with $x = 0$, then $x = 0 \to 1$, with $y = 1$.

Solution:

Path A:

$$\int_0^1 x\, dx = \left.\frac{x^2}{2}\right|_0^1 = \frac{1}{2}$$

Path B:

$$0 + \int_0^1 1\, dx = 1$$

Clearly, these are not the same.

The integral of a total differential, however, is the difference between two values of a state function and, therefore, cannot depend on the path of the integral. This holds even if this difference is evaluated by means of partial derivatives.

$$\int_{x_1,y_1}^{x_2,y_2} dz = z(x_2, y_2) - z(x_1, y_1) = \int_{x_1,y_1}^{x_2,y_2} M(x, y)\, dx + \int_{x_1,y_1}^{x_2,y_2} N(x, y)\, dy \tag{15}$$

Example 3. Evaluate $\int_{0,0}^{1,1} dz$, where $z = xy$, both directly and using partial derivatives, with the paths used in Example 2.

Solution: Directly, $\int_{0,0}^{1,1} dz = (1 \times 1) - (0 \times 0) = 1$.
Path A, $x = y$:

$$\int_{0,0}^{1,1} dz = \int_{0,0}^{1,1} y\, dx + \int_{0,0}^{1,1} x\, dy = \int_0^1 x\, dx + \int_0^1 y\, dy = \frac{1}{2} + \frac{1}{2} = 1$$

Path B, $y = 0 \rightarrow 1$, with $x = 0$, then $x = 0 \rightarrow 1$, with $y = 1$:

$$\int_{0,0}^{1,1} dz = \int_{\text{path}} y\, dx + \int_{\text{path}} x\, dy = [0 + 1] + [0 + 0] = 1$$

The direct method and the two paths give the same value.

An integral over one cycle of a cyclic process in indicated by $\oint$. If the integrand is a total differential,

$$\oint dz = z(x_1, y_1) - z(x_1, y_1) = 0 \tag{16}$$

A.3 Second Derivatives

There are four second partial derivatives of the function $z(x, y)$. These are

$$\left(\frac{\partial^2 z}{\partial x^2}\right)_y, \qquad \left(\frac{\partial^2 z}{\partial y^2}\right)_x,$$

$$\left(\frac{\partial^2 z}{\partial x\, \partial y}\right) \equiv \left(\frac{\partial}{\partial x}\left(\frac{\partial z}{\partial y}\right)_x\right)_y$$

and

$$\left(\frac{\partial^2 z}{\partial y\,\partial x}\right) \equiv \left(\frac{\partial}{\partial y}\left(\frac{\partial z}{\partial x}\right)_y\right)_x$$

The latter two derivatives are known as *cross-derivatives*, and for any well-behaved function of x and y, they are equal[1]:

$$\left(\frac{\partial^2 z}{\partial x\,\partial y}\right) = \left(\frac{\partial^2 z}{\partial y\,\partial x}\right) \tag{17}$$

Example 4. Find the four second derivatives of the function $z = x^3 \sin y$. Compare the two cross-second-derivatives.

Solution:

$$\left(\frac{\partial z}{\partial x}\right)_y = 3x^2\ \sin\ y \quad \text{and} \quad \left(\frac{\partial z}{\partial y}\right)_x = x^3\ \cos\ y$$

$$\left(\frac{\partial^2 z}{\partial x^2}\right)_y = 6x\ \sin\ y, \qquad \left(\frac{\partial^2 z}{\partial y^2}\right)_x = -x^3\ \sin\ y$$

$$\left(\frac{\partial^2 z}{\partial y\,\partial x}\right) = 3x^2\ \cos\ y \quad \text{and} \quad \left(\frac{\partial^2 z}{\partial x\,\partial y}\right) = 3x^2 \cos\ y$$

The latter two derivatives are equal as stated.

For a total differential of the form of Eq. (3), Eq. (17) requires

$$\left(\frac{\partial M}{\partial y}\right)_x = \left(\frac{\partial N}{\partial x}\right)_y \tag{18}$$

This useful equation is known as the cross-derivative rule. There are nine second partial derivatives of a function $h(x, y, z)$ of three variables. Calculating derivatives for a few of these functions can convince the reader that the cross-derivative rule also holds for such functions. Thus, using the notation of Eq. (14),

$$\begin{gathered}\left(\frac{\partial M}{\partial y}\right)_{x,z} = \left(\frac{\partial N}{\partial x}\right)_{y,z}, \qquad \left(\frac{\partial M}{\partial z}\right)_{x,y} = \left(\frac{\partial P}{\partial x}\right)_{x,y} \\ \left(\frac{\partial N}{\partial z}\right)_{y,x} = \left(\frac{\partial P}{\partial y}\right)_{z,x}\end{gathered} \tag{19}$$

Problems

1. For further justification of the chain rule for partial derivatives, consider the following example: Let z equal the money in your checking account, x be the number of times you go shopping for clothes in a month, and y the number of times you eat out in a month. What

are the signs of $(\partial z/\partial x)_y$ and $(\partial z/\partial y)_x$? What is the significance of $(\partial y/\partial x)_z$ and what is its sign (from your experience)? Are the signs of these three partial derivatives in agreement with the chain rule for partial derivatives?

2. Demonstrate Eq. (17) for the function

$$F = 3xy^2z + 2z \sin y + 4x \cos y.$$

Note

1. A proof of this can be found in most textbooks on multivariable calculus. Alternatively, the reader can just pick a few functions of two variables and compare the cross-second-derivatives, as is done in Example 4. The latter procedure has the advantage of providing some practice in taking partial derivatives.