Math Diversion Problem 434: Structured Differentiation: Lesson Two

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> We discuss two types of partial derivatives which occur, e.g., in the Euler–Lagrange equations. To avoid confusion, a different notation ($\eth F/\eth x_\mu$) and a new name (whole-partial derivative) are suggested for what is usually written as $\partial F/\partial x_\mu$ but acts on both the explicit and implicit dependence of F upon the coordinate x_μ.
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> — K. R. Brownstein (from the abstract to his paper *The whole-partial derivative*, 1998)

1 Preface

Referring to the quote above, the issue that Brownstein seems to be addressing in his article is the same one SD wants to deal with, though SD does it differently. The math and physics communities have not found a way to deal with the generalization of the ordinary total derivative in a consistent and elegant way. In some sense, the partial derivative is meant to be that generalization, but its notations and interpretations are all over the place. It seems to me that Brownstein's 'whole-partial derivative' is equivalent to the SD total derivative.

In SD, the generalized total derivative is expressed as $\delta F/\delta x$, which is the sum of an implicit and explicit derivative, expressed as $\partial F/\partial x$ and $\not\partial F/\not\partial x$, respectively. Or

$$\frac{\delta F}{\delta x} = \frac{\partial F}{\partial x} + \frac{\not\partial F}{\not\partial x}\,. \tag{1}$$

Perhaps Brownstein has encountered the same opposition to employing a 'generalized total derivative' in much the same way that I have. People will argue back, "You can't declare $\delta F/\delta x$ to be the total derivative of F because it doesn't represent the total way that F can vary though its many dependencies." To such a silly reply I give my standard reply, "But it **is** the total way that F can vary through its dependencies by the variable x!" They either get it immediately or they don't. Further discussion on it is pointless.

2 Introduction

In this second article, we add new material on which the SD formalism can be applied. Let's get right to it.

Note 1: The first article in this series has the foundational material one needs to best follow the presentation here.

Note 2: In SD, the symbol $\dfrac{\partial \mathbf{F}}{\partial \mathbf{x}}$ represents a matrix, not a determinant. For example, if $\mathbf{F} = (F_1, F_2)^{\mathrm{T}}$ and $\mathbf{x} = (x_1, x_2)^{\mathrm{T}}$, then

$$\frac{\partial \mathbf{F}}{\partial \mathbf{x}} = \frac{\partial(F_1, F_2)}{\partial(x_1, x_2)} = \begin{bmatrix} \partial F_1/\partial x_1 & \partial F_1/\partial x_2 \\ \partial F_2/\partial x_1 & \partial F_2/\partial x_2 \end{bmatrix} . \tag{2}$$

This was a deliberate design decision I made about SD, which has to deal with both matrices and the determinants of $n \times n$ matrices. In the case of this last equation, its determinant is represented in the usual way:

$$\left|\frac{\partial \mathbf{F}}{\partial \mathbf{x}}\right| = \left|\frac{\partial(F_1, F_2)}{\partial(x_1, x_2)}\right| = \begin{vmatrix} \partial F_1/\partial x_1 & \partial F_1/\partial x_2 \\ \partial F_2/\partial x_1 & \partial F_2/\partial x_2 \end{vmatrix} . \tag{3}$$

Moving on.

There is perhaps no more difficult concept in this paper than that of convolution. A *convolution* is said to occur whenever a variable (or function) is functionally dependent on itself. (Our definition of convolution, however, has no direct connection to the convolution of the Laplace transform.) As we shall see later, the most efficient way to discovering the effects of making a change of fundamental variables in a given problem, is to make variables functionally dependent on themselves in a nontrivial way, i.e., through some intermediate variable.

3 Theory: 'Change of Variables'

Up to this point we have encountered functions that are dependent on variable $\mathbf{x}$ maybe both explicitly and implicitly, in which case by differentiation, we get

$$\frac{\delta \mathbf{f}}{\delta \mathbf{x}} = \frac{\partial \mathbf{f}}{\partial \mathbf{y}} \frac{\delta \mathbf{y}}{\delta \mathbf{x}} , \tag{4}$$

where $\mathbf{f} = \mathbf{f}(\mathbf{y})$ and $\mathbf{y}$ is the variant of $\mathbf{f}$, say. There are many situations that require us to extend our theory of SD to include problems in which the fundamental itself will change, that is, will be replaced by some other fundamental.

Now, this is not a new concept even to a calculus student. Say we have the integral

$$I = \int A(x)\, dx \tag{5}$$

and we prefer to integrate with respect to some other variable, such as u. Then we recast this integral as

$$I = \int A(u)\,\frac{dx}{du}\,du\,. \tag{6}$$

This expression $\dfrac{dx}{du}$ is called the *Jacobian* of the transformation of variables from the old variable x to the new variable u. We will soon encounter problems where the old variables and the new variables both are treated as vectors in SD.

I will now present a couple definitions of SD on how to deal with derivatives resulting from a change of fundamental, which I cannot promise that all authors will use:

Definition of Jacobian matrix

The total derivative of the old fundamental with respect to the new fundamental shall be called the *Jacobian matrix* of the transformation of variables.[1] (Often, the total derivative can be reduced to the partial derivative.) The determinant of the Jacobian matrix is called the *Jacobian* of the transformation.

So, besides integration, where does this kind of change of variables come up? For one, when one wants to change coordinates, such from rectangular to polar or in 3D spherical polar coordinates, or back the other way. Another is in the transformation of variables in thermodynamics. We will soon see an example where a thermodynamic equation which is known for one pair of fundamental variables is to be converted to its equivalent for when a new couple of fundamental variables is chosen.

Now, a subtlety arises that hasn't to this point. We got by just fine with using $\frac{\partial \mathbf{f}}{\partial \mathbf{y}}$ in Eq. (4), but it may be safer to use a parallel to that which is done is ordinary chain rule. So, if $f(x) = f(u(x))$ then

$$\frac{df}{dx} = \frac{df}{du}\frac{du}{dx}\,. \tag{7}$$

Therefore, if $\mathbf{f}(\mathbf{x}) = \mathbf{f}(\mathbf{u}(\mathbf{x}))$, it may be safer (that is, more accurate) to write

$$\frac{\delta \mathbf{f}}{\delta \mathbf{x}} = \frac{\delta \mathbf{f}}{\delta \mathbf{u}}\frac{\delta \mathbf{u}}{\delta \mathbf{x}}\,, \tag{8}$$

and the utility of this convention should become obvious once we've done a couple problems in thermodynamics.

Rule 1) When one fundamental variable η_i is totally differentiated by a cofundamental variable η_j, the result is

$$\frac{\delta \eta_i}{\delta \eta_j} = \delta_{ij}\,, \tag{9}$$

[1] Of course, if both fundamentals are just scalars, then the Jacobian 'matrix' will be just a 1×1 matrix, or, a scalar.

where δ_{ij} is the Kronecker delta, meaning that when a fundamental variable is totally differentiated by itself, the result is unity, but when it is totally differentiated by a different cofundamental variable, the result is zero; hence, the notion of *variable independence* between different elements in a given fundamental is captured by this rule. Note: To remove ambiguity, any variable in a fundamental set is cofundamental to itself.[2]

Rule 2) In all other cases, i.e., when a new fundamental variable differentiates an old fundamental variable, or vice versa, the deltal derivative usually reduces to an explicit derivative. This is the standard thing to do in thermodynamics because, by default, we regard state variables as having no implicit dependence on other variables (at least this is my knowledge regarding them).[3]

4 Problem III. Example from Vector Analysis

Let $\mathbf{u}$ be a vector field defined on the open subset $\mathcal{D}$ of R^n, let $\mathbf{x}$ be a vector field defined on the open subset $\mathcal{D}'$ of R^n, and let T be a one-to-one, onto transformation which takes $\mathbf{u}$ to $\mathbf{x}$ by

$$\mathbf{x} = T(\mathbf{u}) = \mathbf{x}(\mathbf{u})\,. \tag{10}$$

Now T^{-1} exists on $\mathcal{D}'$ so that

$$\mathbf{u} = T^{-1}(\mathbf{x}) = \mathbf{u}(\mathbf{x})\,. \tag{11}$$

The *Jacobian matrix* of the transformation to be

$$\mathbf{J}_T = \frac{\partial T}{\partial \mathbf{u}} = \frac{\partial \mathbf{x}}{\partial \mathbf{u}}\,, \tag{12}$$

where $\mathbf{x}$ is the 'old' fundamental and $\mathbf{u}$ is the 'new' fundamental. Thus, the *Jacobian* of the transformation to be

$$J_T \equiv |\mathbf{J}_T|\,, \tag{13}$$

where $|\mathbf{J}_T|$ is the determinant of the Jacobian matrix. We will show that

$$\big(\mathbf{J}_T\big)^{-1} = \mathbf{J}_{T^{-1}} \tag{14}$$

and

$$\big(J_T\big)^{-1} = J_{T^{-1}}\,. \tag{15}$$

To prove this we take the convolution of $\mathbf{x}$ through $\mathbf{u}$ and get

$$\mathbf{x} = \mathbf{x}(\mathbf{u}(\mathbf{x}))\,. \tag{16}$$

[2]We will consider it axiomatic in SD that the total derivative of any variable with respect to itself is unity.

[3]When a state variable **does** have an implicit dependence on some variable, then we cannot just drop the implicit derivative as we have done in this case.

On taking the total derivative of (16) by $\mathbf{x}$ and simplifying we obtain

$$\mathbf{I} = \frac{\partial \mathbf{x}}{\partial \mathbf{u}} \frac{\partial \mathbf{u}}{\partial \mathbf{x}} \,. \tag{17}$$

But $\partial \mathbf{u}/\partial \mathbf{x} = \mathbf{J}_{T^{-1}}$; therefore, (17) establishes (14). To establish (15) we merely take the determinant of both sides of (17).

5 Problem IV. Transformation on Coordinates

Let

$$\left. \begin{aligned} x &= r \sin\theta \cos\phi \\ y &= r \sin\theta \sin\phi \\ z &= r \cos\theta \end{aligned} \right\} \tag{18}$$

Find ∇r, $\nabla\theta$, and $\nabla\phi$ where $\nabla = \partial/\partial\mathbf{x}$. One way to solve this problem is to solve for r, θ, ϕ in terms of x, y, z, then differentiate, but we will take another path.

The gradients we want are just the row vectors of the matrix $\partial\mathbf{u}/\partial\mathbf{x}$ where $\mathbf{u} = (r, \theta, \phi)$. Now, treating $\mathbf{x}$ as the old fundamental and $\mathbf{u}$ as the new fundamental, the Jacobian matrix is

$$\frac{\partial \mathbf{x}}{\partial \mathbf{u}} = \begin{bmatrix} \sin\theta\cos\phi & r\cos\theta\cos\phi & -r\sin\theta\sin\phi \\ \sin\theta\sin\phi & r\cos\theta\sin\phi & r\sin\theta\cos\phi \\ \cos\theta & -r\sin\theta & 0 \end{bmatrix} \tag{19}$$

and the Jacobian

$$\left| \frac{\partial \mathbf{x}}{\partial \mathbf{u}} \right| = r^2 \sin\theta \,. \tag{20}$$

Where the Jacobian is nonzero, we have from (17)

$$\frac{\partial \mathbf{u}}{\partial \mathbf{x}} = \left(\frac{\partial \mathbf{x}}{\partial \mathbf{u}} \right)^{-1} \,. \tag{21}$$

Therefore,

$$\frac{\partial \mathbf{u}}{\partial \mathbf{x}} = \begin{bmatrix} \nabla r \\ \nabla\theta \\ \nabla\phi \end{bmatrix} = \begin{bmatrix} \sin\theta\cos\phi & \sin\theta\sin\phi & \cos\theta \\ \dfrac{1}{r}\cos\theta\cos\phi & \dfrac{1}{r}\cos\theta\sin\phi & -\dfrac{1}{r}\sin\theta \\ -\dfrac{\sin\phi}{r\sin\theta} & \dfrac{\cos\phi}{r\sin\theta} & 0 \end{bmatrix} . \tag{22}$$

6 Problem V. First Example from Thermodynamics

A certain thermodynamic state can be represented by the differential equation of state

$$\frac{\partial U}{\partial V} - T\frac{\partial P}{\partial T} + P = 0 \,, \tag{23}$$

where V and T are the fundamental variables. What, then, is the appropriate form that (23) takes when U and P replace V and T as the fundamental variables? The current problem is from Buck [7], prob. 18, pg. 146.

Let the old fundamental be represented by

$$\boldsymbol{\eta} = (V, T)^t \,, \tag{24}$$

and the new fundamental by

$$\boldsymbol{\eta}' = (U, P)^t \,. \tag{25}$$

For convenience, we also define the state vector

$$\psi = (U, P, V, T)^t \,. \tag{26}$$

Then

$$\psi'(\boldsymbol{\eta}') = \psi(\boldsymbol{\eta}(\boldsymbol{\eta}')) \,. \tag{27}$$

Differentiating this by $\boldsymbol{\eta}'$, we get

$$\frac{\delta \psi'}{\delta \boldsymbol{\eta}'} = \frac{\delta \psi}{\delta \boldsymbol{\eta}} \frac{\delta \boldsymbol{\eta}}{\delta \boldsymbol{\eta}'} \,, \tag{28}$$

and simplifying, we have

$$\begin{bmatrix} 1 & 0 \\ 0 & 1 \\ \partial V/\partial U & \partial V/\partial P \\ \partial T/\partial U & \partial T/\partial P \end{bmatrix} = \begin{bmatrix} \partial U/\partial V & \partial U/\partial T \\ \partial P/\partial V & \partial P/\partial T \\ 1 & 0 \\ 0 & 1 \end{bmatrix} \mathbf{J} \tag{29}$$

where $\mathbf{J} = \partial \boldsymbol{\eta}/\partial \boldsymbol{\eta}'$.

The relations we want can be extracted from (29) by inspection, yielding

$$\frac{\partial T}{\partial P} = \frac{\partial U}{\partial V} J \tag{30a}$$

and

$$\frac{\partial V}{\partial U} = \frac{\partial P}{\partial T} J \,. \tag{30b}$$

Solving these for $\partial U/\partial V$, $\partial P/\partial T$ and then substituting the results into (23) yields

$$\frac{\partial T}{\partial P} - T \frac{\partial V}{\partial U} + PJ = 0 \,. \tag{31}$$

The technique used to derive (30a) and (30b) from (29) we refer to as *decomposition*, which we describe in brief. From the first and fourth rows of (29), we may write the 2×2 matrix equation

$$\begin{bmatrix} 1 & 0 \\ \partial T/\partial U & \partial T/\partial P \end{bmatrix} = \begin{bmatrix} \partial U/\partial V & \partial U/\partial T \\ 0 & 1 \end{bmatrix} \mathbf{J} \,, \tag{32}$$

and from the second and third rows, we may similarly write

$$\begin{bmatrix} 0 & 1 \\ \partial V/\partial U & \partial V/\partial P \end{bmatrix} = \begin{bmatrix} \partial P/\partial V & \partial P/\partial T \\ 1 & 0 \end{bmatrix} \mathbf{J}\,. \tag{33}$$

Equations (30a) and (30b) follow by taking the determinant of these last two matrix equations, employing the fact that the determinant of a product is the product of the determinants.

References

[1] J. Hubbard and B. Hubbard. *Vector Calculus, Linear Algebra, and Differential Forms*. Prentice Hall NJ. (2002).

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[6] A. Taylor and W.R. Mann. *Advanced Calculus,* 2ed. John Wiley & Sons. New York (1972).

[7] R.C. Buck. *Advanced Calculus*, 3ed. McGraw-Hill Book Co. (1984).