Math Diversion Problem 499: Use of Jacobians in Thermodynamics (E.T. Jaynes), Part 2

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In fields other than thermodynamics, one usually starts out by
stating explicitly what variables shall be considered the
independent ones, and then uses partial derivatives
without subscripts.....But in thermodynamics, one
never seems to be able to maintain a fixed set of
independent variables throughout a derivation,
and it becomes necessary to add one or more
subscripts to every derivative to indicate
what is being held constant.
— E.T. Jaynes

1 Introduction

This is my second of what I hope will be a series of articles explaining and demonstrating the revisions that physicist E.T. Jaynes[1] long ago proposed to the scientific community regarding how thermodynamics should be presented mathematically, especially with regard to partial derivatives and jacobians. I think it's probably necessary for the reader to have read and understood the first paper in this series to understand this paper.

Warning: I shall be using the techniques of structured differentiation (SD) throughout my explanations, to perform and explain what Jaynes has done in this section of his article. Some knowledge of calculus and matrices is assumed on the part of the reader.

Note: The paper on SD immediately preceding this one contains some results necessary to understand a section of this paper. But, in theory, you could just take those results at face value and you'd still get something out of it.

[1] Found in: "Use of Jacobians in Thermodynamics," available from on-line notes at https://bayes.wustl.edu/etj/thermo/stat.mech.2.pdf

Last time we established the identities found at the top of page 4, namely,

$$[AB] = -[BA], \qquad [AA] = 0\,, \tag{1a}$$
$$[A \pm B, C] = [AC] \pm [BC]\,, \tag{1b}$$
$$[AB, C] = [AC]B + A[BC]\,. \tag{1c}$$

The point of this article is bring the discussion to Eq. (2a).[2] We'll begin with these cyclic identities from page 4:

$$[AB]dC + [BC]dA + [CA]dB = 0\,, \tag{2a}$$
$$[A[B, C]] + [B[C, A]] + [C[A, B]] = 0\,, \tag{2b}$$
$$[AB][CX] + [BC][AX] + [CA][BX] = 0\,. \tag{2c}$$

Then Jaynes presented the 'theorem': If

$$dA = bdB + cdC\,. \tag{3}$$

then for all X,

$$[AX] = b[BX] + c[CX]\,. \tag{4}$$

2 Results Needed from My Last Paper on SD

Problem 1: Given a surface defined by $F(x, y, z) = 0$, we know that if $\partial F/\partial z \neq 0$ then, by the Implicit Function Theorem, $z = z(x, y)$. Show that the direction of the normal to the surface is given by the direction ratios

$$\frac{\partial z}{\partial x} \quad : \frac{\partial z}{\partial y} \quad : \quad -1\,. \tag{5}$$

Problem 2: Show that, under a change of independent variables to (u, v), i.e.,

$$\begin{cases} x = x(u, v) \\ y = y(u, v) \\ z = z(u, v) \end{cases}, \tag{6}$$

that the direction ratios of the normal can be given by

$$j_1 \quad : \quad j_2 \quad : \quad j_3 \tag{7}$$

where

$$j_1 = \left|\frac{\partial(y, z)}{\partial(u, v)}\right| \quad : \quad j_2 = \left|\frac{\partial(z, x)}{\partial(u, v)}\right| \quad : \quad j_3 = \left|\frac{\partial(x, y)}{\partial(u, v)}\right|\,. \tag{8}$$

[2] This is enough material for one article.

3 Getting Warmed Up

Jaynes's first equation of interest is the following:

$$\left(\frac{\partial A}{\partial B}\right)_C = \left(\frac{\partial A}{\partial B}\right)_D + \left(\frac{\partial A}{\partial D}\right)_B \left(\frac{\partial D}{\partial B}\right)_C . \tag{9}$$

If you're familiar with thermodynamics, you've probably seen similar equations. But how are we to interpret this?

For starters, in this article at least, we will consider problems with only two independent variables. I think I'll just provide my own interpretation of what's going on under the hood, and let the reader decide for him or herself how accurate they are.

Regrading (9), the independent (or **fundamental**) variables are B and C. In SD, one way to denote the **fundamental** of a variable is by double parentheses, like this:

$$A = A((B, C)), \quad D = D((B, C)) . \tag{10}$$

In SD, the ordered list of variables on which a function is explicitly dependent is referred to as its **variant**, although any one of them is also called a 'variant'. Context should clarify the distinction.

Now, the variant of a function is indicated in the usual way. For example, in (9), we can tease out the functional explicit dependencies as follows

$$A = A(B, D), \quad D = D(B, C) . \tag{11}$$

The function A is explicitly dependent on variables B and D, in that 'order'. So, the variant of A is (B, D). The variant of D is (B, C). In SD, a function whose variant is also its fundamental is said to be 'primitive'. Typically, these are the easiest functions to differentiate.

So, the equation that is being differentiated to obtain (9) is

$$A = A(B, D(B, C)) . \tag{12}$$

Thus, we can interpret

$$\left(\frac{\partial A}{\partial B}\right)_C \tag{13}$$

as the **total derivative** of A by B, which manifests as the sum of an explicit derivative and an implicit derivative. All the subscript C does is to clarify what the other independent variable is at the time this derivative was 'first' calculated. This is necessary in thermodynamics because in this subject the list of independent variables can change faster than a street light.

Next, the derivative

$$\left(\frac{\partial A}{\partial B}\right)_D \tag{14}$$

is the **explicit** derivative of A by B. It ignores how A changes due to B through the variable D; that effect is entailed in the last term, namely,

$$\left(\frac{\partial A}{\partial D}\right)_B \left(\frac{\partial D}{\partial B}\right)_C . \tag{15}$$

This is the **implicit** derivative of A by B going through variant D. Some authors express (9) in the following heuristic form

$$\left(\frac{\partial A}{\partial B}\right)_{\text{total}} = \left(\frac{\partial A}{\partial B}\right)_{\text{explicit}} + \left(\frac{\partial A}{\partial B}\right)_{\text{implicit}} . \tag{16}$$

4 Making Sense of (2a)

Jaynes regard this identity as nearly trivial. Well, I'm going to try to make sense of this relation, obtaining one of two possible results. First, I could be totally wrong in my interpretation. Second, my interpretation could be right, but my proof faulty.

Okay, the relation is the following:

$$[AB]\,dC + [BC]\,dA + [CA]\,dB = 0 . \tag{17}$$

Using Jaynes's notation (and SD conventions), this becomes

$$\left|\frac{\partial(A,B)}{\partial(x,y)}\right| dC + \left|\frac{\partial(B,C)}{\partial(x,y)}\right| dA + \left|\frac{\partial(C,A)}{\partial(x,y)}\right| dB = 0 . \tag{18}$$

This result looks like an inner product to me, namely,

$$\left[\left|\frac{\partial(A,B)}{\partial(x,y)}\right|, \left|\frac{\partial(B,C)}{\partial(x,y)}\right|, \left|\frac{\partial(C,A)}{\partial(x,y)}\right|\right] \begin{bmatrix} dC \\ dA \\ dB \end{bmatrix} = 0 . \tag{19}$$

So, it looked to me that I could use (8), but before that, I'd have to use (5). Okay, I'm looking for some way to get an inner product in x, y, z equal to zero, which I'll do next.

We begin with fundamental variables x, y and accept that $z = z(x, y)$, and, using the results from the last paper (noted above), we add to that

$$dz = \frac{\partial z}{\partial x} dx + \frac{\partial z}{\partial y} dy . \tag{20}$$

It's easy to show that

$$\left[\frac{\partial z}{\partial x}, \frac{\partial z}{\partial y}, -1\right] \begin{bmatrix} dx \\ dy \\ dz \end{bmatrix} = 0 . \tag{21}$$

On multiplying this out on the LHS, we have that

$$\frac{\partial z}{\partial x}\,dx + \frac{\partial z}{\partial y}\,dy - dz\,. \tag{22}$$

But by (20), this is equal to zero. And we are getting closer.

Now, since the vector $(\partial z/\partial x, \partial z/\partial y, -1)$ differs from the following vector by only a scalar factor,

$$\left(\left|\frac{\partial(y,z)}{\partial(u,v)}\right|, \left|\frac{\partial(z,x)}{\partial(u,v)}\right|, \left|\frac{\partial(x,y)}{\partial(u,v)}\right| \right)\,, \tag{23}$$

we can replace the former by the latter in (21), to get

$$\left(\left|\frac{\partial(y,z)}{\partial(u,v)}\right|, \left|\frac{\partial(z,x)}{\partial(u,v)}\right|, \left|\frac{\partial(x,y)}{\partial(u,v)}\right| \right) \begin{bmatrix} dx \\ dy \\ dz \end{bmatrix} = 0\,, \tag{24}$$

which multiplies out to

$$\left|\frac{\partial(y,z)}{\partial(u,v)}\right|\,dx + \left|\frac{\partial(z,x)}{\partial(u,v)}\right|\,dy + \left|\frac{\partial(x,y)}{\partial(u,v)}\right|\,dz = 0\,. \tag{25}$$

Now, we make the crucial identifications:

$$x \to C\,, \qquad y \to A\,, \qquad z \to B\,, \tag{26}$$

and now (25) becomes

$$\left|\frac{\partial(A,B)}{\partial(u,v)}\right|\,dC + \left|\frac{\partial(B,C)}{\partial(u,v)}\right|\,dA + \left|\frac{\partial(C,A)}{\partial(u,v)}\right|\,dB = 0\,. \tag{27}$$

At this point, we can treat u, v as dummy variables, and write

$$[AB]\,dC + [BC]\,dA + [CA]\,dB = 0\,. \tag{28}$$

And this is the same as (2a).