

Math Diversion Problem 495: Use of Jacobians in Thermodynamics (E.T. Jaynes), Part 1

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Many students find that thermodynamics, although mathematically almost trivial, is nevertheless one of the most difficult subjects in their program. A large part of the blame for this lies in the extremely cumbersome partial derivative notation.

— E.T. Jaynes

1 Introduction

This is my first of what I hope will be a series of articles explaining and demonstrating the revisions that physicist E.T. Jaynes¹ long ago proposed to the scientific community regarding how thermodynamics should be presented mathematically, especially with regard to partial derivatives and jacobians.

I'm planning that this series will continue for at least two more articles. My emphasis will be on explaining the calculus basis underlying jacobians, and that means addressing the transformations of $\mathbb{R}^m \rightarrow \mathbb{R}^n$, but without the technical talk. I'll be appealing to the reader's intuition on much of this, though it shouldn't be too difficult. The generalization of differentiating functions defined on $\mathbb{R}^1 \rightarrow \mathbb{R}^1$ is quite straightforward when we ignore the details one finds in advanced calculus books.

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: In SD, an expression like

$$\frac{\partial(W, X)}{\partial(Y, Z)} \tag{1}$$

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

is a matrix (the jacobian matrix), and the ‘jacobian’ derived from it as

$$\det \left[\frac{\partial(W, X)}{\partial(Y, Z)} \right] = \left| \frac{\partial(W, X)}{\partial(Y, Z)} \right|. \quad (2)$$

However, in conventional thermodynamics, an expression like (1) is a determinant already.

The point of this article is bring the discussion to the top of page 4, where we find the equations:

$$[AB] = -[BA], \quad [AA] = 0, \quad (3a)$$

$$[A \pm B, C] = [AC] \pm [BC], \quad (3b)$$

$$[AB, C] = [AC]B + A[BC]. \quad (3c)$$

By the way, if you’ve already read my previous two articles in this series, then perhaps you’ll recognize the above equations as enigmatic ‘muffin-top’ pseudo-equations, at least by the end of this article.

2 [2.1] Statement of the Problem

Jaynes’s first equation of interest is the following:

$$\left(\frac{\partial A}{\partial B} \right)_C = \left(\frac{\partial A}{\partial B} \right)_D + \left(\frac{\partial A}{\partial D} \right)_B \left(\frac{\partial D}{\partial B} \right)_C. \quad (4)$$

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 (4), 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:

$$A = A((B, C)), \quad D = D((B, C)). \quad (5)$$

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 (4), we can tease out the functional explicit dependencies as follows

$$A = A(B, D), \quad D = D(B, C). \quad (6)$$

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) . So, the equation that is being differentiated to obtain (4) is

$$A = A(B, D(B, C)). \quad (7)$$

Thus, we can interpret

$$\left(\frac{\partial A}{\partial B}\right)_C \tag{8}$$

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

$$\left(\frac{\partial A}{\partial B}\right)_D \tag{9}$$

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,

$$\left(\frac{\partial A}{\partial D}\right)_B \left(\frac{\partial D}{\partial B}\right)_C . \tag{10}$$

This is the **implicit** derivative of A by B going through variant D . Some authors express (4) in the following heuristic form

$$\left(\frac{\partial A}{\partial B}\right)_{\text{total}} = \left(\frac{\partial A}{\partial B}\right)_{\text{explicit}} + \left(\frac{\partial A}{\partial B}\right)_{\text{implicit}} . \tag{11}$$

3 [2.2] Formal Properties of Jacobians

It’s here that Jaynes introduces the formalism that he will use throughout the rest of this paper. What he referred to as a ‘condensed notation’. I’ll go over it, but in SD notation.

$$[A, B] \equiv \left| \frac{\partial(A, B)}{\partial(x, y)} \right| = \begin{vmatrix} \frac{\partial A}{\partial x} & \frac{\partial A}{\partial y} \\ \frac{\partial B}{\partial x} & \frac{\partial B}{\partial y} \end{vmatrix} . \tag{12}$$

One might ask where the variables x and y are present in the symbol $[A, B]$. They are implied, and by what symbols we choose to represent them is practically arbitrary—except that they must be capable of defining the physical system at hand.

Now, since we’ve introduced jacobians, perhaps we should defined what they are. For our present purposes, a jacobian is the determinant of an $n \times n$ matrix whose entries are first-order partial derivatives. The typical context that one usually finds jacobians is in a change of coordinate transformation, such as $|\partial(x, y)/\partial(x', y')|$.

Now we can go a level up by performing a change in the fundamental variable, from x, y to x', y' , as such

$$\left| \frac{\partial(A, B)}{\partial(x', y')} \right| = \left| \frac{\partial(A, B)}{\partial(x, y)} \right| \left| \frac{\partial(x, y)}{\partial(x', y')} \right|. \quad (13)$$

To someone new to all this, this last equation probably needs some explaining.

Let $\mathbf{A} = (A, B)$, $\mathbf{x} = (x, y)$, and $\mathbf{x}' = (x', y')$. Then, in more or less physics notation, we can write:

$$\mathbf{A}(\mathbf{x}') = \mathbf{A}(\mathbf{x}(\mathbf{x}')). \quad (14)$$

Now, on taking the total derivative of this by \mathbf{x}' , we get,

$$\frac{\delta \mathbf{A}}{\delta \mathbf{x}'} = \frac{\delta \mathbf{A}}{\delta \mathbf{x}} \frac{\delta \mathbf{x}}{\delta \mathbf{x}'}, \quad (15)$$

and we recognize this as an application of the chain rule. Now, because of the restricted way that functional dependencies are defined in (14), it's generally safe to demote total derivatives to partial derivatives, yielding,

$$\frac{\partial \mathbf{A}}{\partial \mathbf{x}'} = \frac{\partial \mathbf{A}}{\partial \mathbf{x}} \frac{\partial \mathbf{x}}{\partial \mathbf{x}'}. \quad (16)$$

Next, we just take the determinant across this equation, leaving us with

$$\det \left[\frac{\partial \mathbf{A}}{\partial \mathbf{x}'} \right] = \det \left[\frac{\partial \mathbf{A}}{\partial \mathbf{x}} \right] \det \left[\frac{\partial \mathbf{x}}{\partial \mathbf{x}'} \right], \quad (17)$$

or more simply as

$$\left| \frac{\partial \mathbf{A}}{\partial \mathbf{x}'} \right| = \left| \frac{\partial \mathbf{A}}{\partial \mathbf{x}} \right| \left| \frac{\partial \mathbf{x}}{\partial \mathbf{x}'} \right|. \quad (18)$$

On dividing through by $\left| \frac{\partial \mathbf{x}}{\partial \mathbf{x}'} \right|$ and then flipping sides, we get

$$\left| \frac{\partial \mathbf{A}}{\partial \mathbf{x}} \right| = \left| \frac{\partial \mathbf{A}}{\partial \mathbf{x}'} \right| / \left| \frac{\partial \mathbf{x}}{\partial \mathbf{x}'} \right| = \frac{|\partial \mathbf{A} / \partial \mathbf{x}'|}{|\partial \mathbf{x} / \partial \mathbf{x}'|}. \quad (19)$$

Then, on putting in the components, we have that

$$\left| \frac{\partial(A, B)}{\partial(x, y)} \right| = \frac{|\partial(A, B) / \partial(x', y')|}{|\partial(x, y) / \partial(x', y')|}. \quad (20)$$

Anyway, Eq. (18) is the same as (13).

Jaynes then introduces the 'condensed notation' for (13):

$$[A, B]' = [A, B][x, y]'. \quad (21)$$

By the way, SD is perfectly capable of receiving Jaynes's 'condensed notation' as is. Once one understands what's going on 'under the hood' of an equation like (21), it makes perfect sense.

4 The Relations of Antisymmetry, Linearity, and Composition

$$[AB] = -[BA], \quad [AA] = 0, \quad (22a)$$

$$[A \pm B, C] = [AC] \pm [BC], \quad (22b)$$

$$[AB, C] = [AC]B + A[BC]. \quad (22c)$$

So now Jaynes even drops the middle comma whenever we can get away with it. And we have to be able to put it back in for clarity's sake.

That $[AB] = -[BA]$ is a simple fact that the determinant of a matrix changes sign whenever two rows are interchanged. That $[AA] = 0$ is a general consequence of every antisymmetric relation over a field. The only way that the real numbers $[AA]$ and $-[AA]$ can be equal is if $[AA] = 0$. In our specific case, the determinant of a square matrix with two equal rows is identically zero.²

Next we move to Eq. (22b). I'll work it out for the '+' sign only.

$$\begin{aligned} [A + B, C] &= \begin{vmatrix} \frac{\partial(A+B)}{\partial x} & \frac{\partial(A+B)}{\partial y} \\ \frac{\partial C}{\partial x} & \frac{\partial C}{\partial y} \end{vmatrix} \\ &= \frac{\partial(A+B)}{\partial x} \frac{\partial C}{\partial y} - \frac{\partial(A+B)}{\partial y} \frac{\partial C}{\partial x} \\ &= \frac{\partial A}{\partial x} \frac{\partial C}{\partial y} + \frac{\partial B}{\partial x} \frac{\partial C}{\partial y} - \left[\frac{\partial A}{\partial y} \frac{\partial C}{\partial x} + \frac{\partial B}{\partial y} \frac{\partial C}{\partial x} \right] \\ &= \left[\frac{\partial A}{\partial x} \frac{\partial C}{\partial y} - \frac{\partial A}{\partial y} \frac{\partial C}{\partial x} \right] + \left[\frac{\partial B}{\partial x} \frac{\partial C}{\partial y} - \frac{\partial B}{\partial y} \frac{\partial C}{\partial x} \right] \\ &= [A, C] + [B, C]. \end{aligned} \quad (23)$$

This last proof is just the warm-up for the next one in (22c). It's not hard, but it's got a lot of moving parts.

$$[AB, C] = [[A, B], C] = \begin{vmatrix} \frac{\partial[A, B]}{\partial x} & \frac{\partial[A, B]}{\partial y} \\ \frac{\partial C}{\partial x} & \frac{\partial C}{\partial y} \end{vmatrix}. \quad (24)$$

Now,

$$[A, B] = \frac{\partial A}{\partial x} \frac{\partial B}{\partial y} - \frac{\partial A}{\partial y} \frac{\partial B}{\partial x}. \quad (25)$$

²More generally, the determinant of a square matrix with linearly-dependent rows is zero.

So,

$$\frac{\partial}{\partial x}[A, B] = \frac{\partial^2 A}{\partial x^2} \frac{\partial B}{\partial y} - \frac{\partial^2 A}{\partial x \partial y} \frac{\partial B}{\partial x} + \frac{\partial A}{\partial x} \frac{\partial^2 B}{\partial x \partial y} - \frac{\partial A}{\partial y} \frac{\partial^2 B}{\partial x^2}. \quad (26)$$

Now tack on $\frac{\partial C}{\partial y}$:

$$\frac{\partial}{\partial x}[A, B] \frac{\partial C}{\partial y} = \left[\frac{\partial^2 A}{\partial x^2} \frac{\partial B}{\partial y} - \frac{\partial^2 A}{\partial x \partial y} \frac{\partial B}{\partial x} + \frac{\partial A}{\partial x} \frac{\partial^2 B}{\partial x \partial y} - \frac{\partial A}{\partial y} \frac{\partial^2 B}{\partial x^2} \right] \frac{\partial C}{\partial y}. \quad (27)$$

Now, switch x and y :

$$\frac{\partial}{\partial y}[A, B] \frac{\partial C}{\partial x} = \left[\frac{\partial^2 A}{\partial y^2} \frac{\partial B}{\partial x} - \frac{\partial^2 A}{\partial y \partial x} \frac{\partial B}{\partial y} + \frac{\partial A}{\partial y} \frac{\partial^2 B}{\partial y \partial x} - \frac{\partial A}{\partial x} \frac{\partial^2 B}{\partial y^2} \right] \frac{\partial C}{\partial x}. \quad (28)$$

Therefore,

$$\begin{aligned} [AB, C] &= \frac{\partial}{\partial x}[A, B] \frac{\partial C}{\partial y} - \frac{\partial}{\partial y}[A, B] \frac{\partial C}{\partial x} \\ &= \left[\frac{\partial^2 A}{\partial x^2} \frac{\partial B}{\partial y} - \frac{\partial^2 A}{\partial x \partial y} \frac{\partial B}{\partial x} + \frac{\partial A}{\partial x} \frac{\partial^2 B}{\partial x \partial y} - \frac{\partial A}{\partial y} \frac{\partial^2 B}{\partial x^2} \right] \frac{\partial C}{\partial y} \\ &\quad - \left[\frac{\partial^2 A}{\partial y^2} \frac{\partial B}{\partial x} - \frac{\partial^2 A}{\partial y \partial x} \frac{\partial B}{\partial y} + \frac{\partial A}{\partial y} \frac{\partial^2 B}{\partial y \partial x} - \frac{\partial A}{\partial x} \frac{\partial^2 B}{\partial y^2} \right] \frac{\partial C}{\partial x}. \end{aligned} \quad (29)$$

Now, just as I had to interpret the LHS of (22c), I also have to interpret its RHS. So, what does $[AC]B$ mean in this context? This is my guess:

$$[AC]B = [[A, C], B]. \quad (30)$$

Hence,

$$\begin{aligned} [AC]B = [[A, C], B] &= \frac{\partial}{\partial x} \left[\frac{\partial A}{\partial x} \frac{\partial C}{\partial y} - \frac{\partial A}{\partial y} \frac{\partial C}{\partial x} \right] \frac{\partial B}{\partial y} \\ &\quad - \frac{\partial}{\partial y} \left[\frac{\partial A}{\partial x} \frac{\partial C}{\partial y} - \frac{\partial A}{\partial y} \frac{\partial C}{\partial x} \right] \frac{\partial B}{\partial x}. \end{aligned} \quad (31)$$

Then,

$$\begin{aligned} A[BC] = [A, [B, C]] &= \frac{\partial A}{\partial x} \frac{\partial [B, C]}{\partial y} - \frac{\partial A}{\partial y} \frac{\partial [B, C]}{\partial x} \\ &= \frac{\partial A}{\partial x} \frac{\partial}{\partial y} \left[\frac{\partial B}{\partial x} \frac{\partial C}{\partial y} - \frac{\partial B}{\partial y} \frac{\partial C}{\partial x} \right] \\ &\quad - \frac{\partial A}{\partial y} \frac{\partial}{\partial x} \left[\frac{\partial B}{\partial x} \frac{\partial C}{\partial y} - \frac{\partial B}{\partial y} \frac{\partial C}{\partial x} \right]. \end{aligned} \quad (32)$$

Now, if we add these last two equations together, distribute the derivatives, cancel opposite terms, and then simplify, we'll get $[AB, C]$, and thus we establish (22c).

And this is as far as I want to go in this first review of Jaynes's paper.