Derivative Computation from Cartesian Tensors

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Abstract

This note goes over taking a derivative by use of Cartesian tensors.

1 Preparation

Let $f(x, y, z)$ and $g(x, y, z)$ be scalar fields with continuous second partials on some open region R. Show that $\bigtriangledown \cdot (\bigtriangledown f \times \bigtriangledown g) = 0$ on R, where the symbol $\times$ means the cross product, $\bigtriangledown \cdot$ means the divergence, and $\bigtriangledown$ means the gradient.

Let's begin with some of the basics of Cartesian tensors. (For a more in depth presentation, please consult a more lengthy resource.) For vectors **A** and **B**, the dot product of **A** and **B** is given by

$$\mathbf{A} \cdot \mathbf{B} = \sum_{i=1}^{3} A_i B_i = A_i B_i \,, \tag{1}$$

where the last expression comes from using the Einstein convention of summing on the full range of an index if it appears repeated in a given expression.

Instead of asking the reader to accept (1) as a definition, I prefer to derive it from a more elementary definition. Let $\{\mathbf{e}_i\}$ $(i = 1, 2, 3)$ be an orthonormal basis for our vector space. Now, since the basis vectors constitute a set of orthonormal vectors, then by definition of orthonormality

$$\mathbf{e}_i \cdot \mathbf{e}_j = \delta_{ij} \,, \tag{2}$$

where δ_{ij} is the Kronecker delta, which is defined as follows

$$\delta_{ij} = \begin{cases} 1, & \text{if } i = j \,, \\ 0, & \text{otherwise.} \end{cases} \tag{3}$$

With $\mathbf{A} = A_i \mathbf{e}_i$ and $\mathbf{B} = B_j \mathbf{e}_j$, then

$$\mathbf{A} \cdot \mathbf{B} = (A_i \mathbf{e}_i) \cdot (B_j \mathbf{e}_j) = A_i B_j \mathbf{e}_i \cdot \mathbf{e}_j = A_i B_j \delta_{ij} = A_i B_i \,. \tag{4}$$

Definition: Now, for any $n \times n$ matrix M_{ij},

$$M_{jj} = M_{11} + M_{22} + \cdots M_{nn} = \operatorname{Tr} M \,, \tag{5}$$

where $\operatorname{Tr} M$ is called the *trace* of matrix M, that is, it's the sum of all the elements on the main diagonal of M.

Definition: A vector correspond to a tensor of *rank* 1. Let $\mathbf{F}$ be a vector and let F_i be its tensor representation, then

$$\mathbf{F} \Longleftrightarrow F_i \,, \tag{6}$$

where F_i are the components of $\mathbf{F}$. Now, let $\mathbf{G}$ be a vector and let G_j be its tensor representation, then

$$\mathbf{G} \Longleftrightarrow G_j \,, \tag{7}$$

By multiplying F_i and G_j together, we can form a rank 2 tensor

$$T_{ij} \equiv F_i G_j \,. \tag{8}$$

Finally, we can perform a *contraction* on the indices of T_{ij} by setting either i to j or j to i. Performing the former, we get a scalar T_{ii}, where summation is performed on i:

$$T_{ii} \equiv T_{11} + T_{22} + T_{33} = F_1 G_1 + F_2 G_2 + F_3 G_3 \,. \tag{9}$$

Clearly, T_{ii} is just the trace of matrix T_{ij}.

Now, to the cross product, which is a bit more difficult.

$$\mathbf{A} \times \mathbf{B} \equiv \epsilon_{jkm} \mathbf{e}_j A_k B_m \,, \tag{10}$$

where 1) we have taken the summation on repeated indices, 2) $\mathbf{e}_j$ is the jth member of the set of three orthonormal unit vectors, and 3) the symbol ϵ_{jkm} is the Levi-Civita symbol, which is defined as

$$\epsilon_{jkm} = \begin{cases} 1, & \text{if } jkm \text{ is an even permutation of } 123 \,, \\ -1, & \text{if } jkm \text{ is an odd permutation of } 123 \,, \\ 0, & \text{otherwise.} \end{cases} \tag{11}$$

We can grab the ith component of (10) by dotting through by $\mathbf{e}_i$, as follows

$$\begin{aligned} (\mathbf{A} \times \mathbf{B})_i &= \mathbf{e}_i \cdot (\mathbf{A} \times \mathbf{B}) \\ &= \epsilon_{jkm} (\mathbf{e}_i \cdot \mathbf{e}_j) A_k B_m \\ &= \epsilon_{jkm} \delta_{ij} A_k B_m \\ &= \epsilon_{ikm} A_k B_m \,. \end{aligned} \tag{12}$$

Now for a note on terminology: There is only one free index in this last expression, namely i. The other two indices, being summed on, are referred to as *dummy indices.* We can replace these dummy indices, like this, if we want

$$\epsilon_{ikm} A_k B_m = \epsilon_{ipq} A_p B_q \,. \tag{13}$$

We can even swap the dummy indices if we include a minus sign:

$$\epsilon_{ikm} A_k B_m = -\epsilon_{imk} A_m B_k \,. \tag{14}$$

As a corollary to this last equation, we can let $\mathbf{A} \to \mathbf{e}_k$ and $\mathbf{B} \to \mathbf{e}_m$, to get,

$$\mathbf{e}_i \cdot (\mathbf{e}_k \times \mathbf{e}_m) = \epsilon_{ikm} \,. \tag{15}$$

Now, for the relationship of the Levi-Civita symbol to the determinant. Let $\mathbf{A}$, $\mathbf{B}$, and $\mathbf{C}$ be three vectors in Euclidean space. Then the volume of the parallepiped formed by the three vectors is given by

$$\mathbf{A} \cdot (\mathbf{B} \times \mathbf{C}) = \begin{vmatrix} A_1 & A_2 & A_3 \\ B_1 & B_2 & B_3 \\ C_1 & C_2 & C_3 \end{vmatrix} = \epsilon_{ijk} A_i B_j C_k \,. \tag{16}$$

We need two more properties of the Levi-Civita symbol. First, that the symbol changes sign under swapping of any two indices. Second, that

Lemma:

$$\epsilon_{jkm} S_{jk} = 0 \quad \text{for all } m \,, \tag{17}$$

where S_{jk} is any 3×3 symmetric matrix (i.e., $S_{jk} = S_{kj}$).

Proof: Fix m, say as 1. Then ϵ_{jk1} acts like the 3×3 antisymmetric matrix (where j is the row number and k is the column number, which can only take on the values of 2 or 3)

$$\epsilon_{jk1} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix} \,, \tag{18}$$

Since S_{jk} is a 3×3 symmetric matrix, we can write it as

$$S_{jk} = \begin{pmatrix} S_{11} & S_{12} & S_{13} \\ S_{12} & S_{22} & S_{23} \\ S_{13} & S_{23} & S_{33} \end{pmatrix} \,, \tag{19}$$

Let's begin with $\epsilon_{jk1} S_{k\ell}$: It's important to note that the index m above is *not* a free index. That is, its value is determined to be the leftover index from the index set $\{1, 2, 3\}$, once the values of both j and k have been chosen from this set, which must be distinct else $\epsilon_{jkm} = 0$. Hence,

$$\epsilon_{jk1} S_{k\ell} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix} \begin{pmatrix} S_{11} & S_{12} & S_{13} \\ S_{12} & S_{22} & S_{23} \\ S_{13} & S_{23} & S_{33} \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 \\ S_{13} & S_{23} & S_{33} \\ -S_{12} & -S_{22} & -S_{23} \end{pmatrix} \,. \tag{20}$$

Referring back to (17), we need to contract on indices j and ℓ, which has the effect of taking the trace:

$$\epsilon_{jk1}S_{kj} = \mathrm{Tr}\left[\begin{pmatrix} 0 & 0 & 0 \\ S_{13} & S_{23} & S_{33} \\ -S_{12} & -S_{22} & -S_{23} \end{pmatrix}\right] = 0 + S_{23} - S_{23} = 0\,. \tag{21}$$

For simplicity, let's rename $\epsilon_{jk1}S_{kj}$ to $M_{j\ell}$. Then, going back to (17):

$$\epsilon_{jkm}S_{jk} = \delta_{j\ell}\epsilon_{jkm}S_{k\ell} = \delta_{j\ell}M_{j\ell} = M_{jj} = 0\,. \tag{22}$$

Now, a similar calculation can be done, getting a similar result, for cases $m = 2$ and $m = 3$. To help out, for case $m = 2$:

$$\epsilon_{jk2} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix}\,, \tag{23}$$

and for case $m = 3$:

$$\epsilon_{jk3} = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}\,. \tag{24}$$

Thus, for each value of m the trace will be zero.

We can take a more abstract pathway to this proof. Let A_{jk} be an $n \times n$ antisymmetric matrix, and let $S_{k\ell}$ be an $n \times n$ symmetric matrix. Then

$$A_{jk}S_{kj} = A_{kj}S_{jk}\,, \tag{25}$$

where the dummy indices j and k were interchanged.[1] But, transposing j and k in each of A_{kj} and S_{jk}, yields

$$A_{kj}S_{jk} = -A_{jk}S_{kj}\,, \tag{26}$$

Thus, putting these last two equations together, gives us

$$A_{jk}S_{kj} = -A_{jk}S_{kj}\,, \tag{27}$$

Since $A_{jk}S_{kj}$ is a scalar, the only way that (27) can be true is if $A_{jk}S_{kj} = 0$, and we are finished.

We're almost there now.

$$\begin{aligned} \nabla \cdot Q &= (\mathbf{e}_i\partial_i).(Q_j\mathbf{e}_j) \\ &= (\mathbf{e}_i.\mathbf{e}_j)\partial_i Q_j \\ &= \delta_{ij}\partial_i Q_j \\ &= \partial_i Q_i \end{aligned} \tag{28}$$

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[1] By the way, this kind of product is referred to as the *Frobenius product*.

Just one more prior result to go. We are assuming that the functions f and g have continuous second partial derivatives everywhere they are defined. Thus, by Clairaut's theorem on equality of mixed partials

$$\begin{aligned}\partial_j\partial_k f &= \partial_k\partial_j f\,,\\ \partial_j\partial_k g &= \partial_k\partial_j g\,.\end{aligned} \tag{29}$$

2 Proof

Now we're ready.

$$\begin{aligned}\triangledown\cdot[(\triangledown f)\times(\triangledown g)] &= \mathbf{e}_i\partial_i\cdot[\mathbf{e}_j\epsilon_{jkm}(\partial_k f)(\partial_m g)]\\ &= \mathbf{e}_i\cdot\mathbf{e}_j\partial_i[\epsilon_{jkm}(\partial_k f)(\partial_m g)]\\ &= \delta_{ij}\partial_i[\epsilon_{jkm}(\partial_k f)(\partial_m g)]\\ &= \partial_j[\epsilon_{jkm}(\partial_k f)(\partial_m g)]\\ &= \epsilon_{jkm}\partial_j[(\partial_k f)(\partial_m g)\\ &= \epsilon_{jkm}\{[(\partial_j\partial_k f)(\partial_m g)]+[(\partial_k f)(\partial_j\partial_m g)]\}\\ &= [(\epsilon_{jkm}\partial_j\partial_k f)(\partial_m g)]+[(\partial_k f)(\epsilon_{jkm}\partial_j\partial_m g)]\\ &= 0\end{aligned} \tag{30}$$

Now here's why we got zero. Because both terms on the next-to-last line are zero. I'll prove this for the first term only, though. Because f and g have continuous second partials everywhere, the order of their partial derivatives is irrelevant. This means that the 3x3 matrix of derivatives of f, $[\partial_j\partial_k f]$, is symmetric. So, by the lemma above

$$\epsilon_{jkm}(\partial_j\partial_k f) = 0 \quad (\forall\, m = 1,2,3)\,. \tag{31}$$

Done. This proof employs just about every thing you'll need to know to use Cartesian tensors in advanced calculus.

There is a determinant approach to this theorem. Let $h_{,i}$ be the ith partial derivative of the function h. Then,

$$\triangledown\cdot(\triangledown f\times\triangledown g) = \begin{vmatrix}\partial_1 & \partial_2 & \partial_3\\ f_{,1} & f_{,2} & f_{,3}\\ g_{,1} & g_{,2} & g_{,3}\end{vmatrix}\,. \tag{32}$$

Now, just expand the determinant.

3 Appendix

Here, I want to return to the proof that the Frobenius product of a symmetric and an antisymmetric matrix (both $n\times n$) is zero.

Let A be antisymmetric and S be symmetric. Then, their Frobenius product is given as

$$\mathrm{Tr}\left(AS\right). \tag{33}$$

Our job is to prove that this quantity is zero. We will use three lemmas to do so:

Lemma 1: Let M and N be any $n \times n$ matrices. Then

$$\mathrm{Tr}\left(MN\right) = \mathrm{Tr}\left(NM\right). \tag{34}$$

Lemma 2: Let U be any $n \times n$ matrix, and let U^{T} be the transpose of U. Then

$$\mathrm{Tr}\left(U\right) = \mathrm{Tr}\left(U^{\mathrm{T}}\right). \tag{35}$$

Lemma 3: Let M and N be any $n \times n$ matrices. Then

$$\left(MN\right)^{\mathrm{T}} = N^{\mathrm{T}} M^{\mathrm{T}}. \tag{36}$$

My plan is to show that $\mathrm{Tr}\left(AS\right) = -\mathrm{Tr}\left(AS\right)$, which would force $\mathrm{Tr}\left(AS\right) = 0$. Now, by definition, $S^{\mathrm{T}} = S$ and $A^{\mathrm{T}} = -A$. Therefore,

$$\begin{aligned}
\mathrm{Tr}\left(AS\right) &= \mathrm{Tr}\left[(AS)^{\mathrm{T}}\right] \quad \text{(by Lemma 2)} \\
&= \mathrm{Tr}\left[S^{\mathrm{T}} A^{\mathrm{T}}\right] \quad \text{(by Lemma 3)} \\
&= \mathrm{Tr}\left[S(-A)\right] \\
&= -\mathrm{Tr}\left[SA\right] \\
&= -\mathrm{Tr}\left(AS\right) \quad \text{(by Lemma 1)}.
\end{aligned} \tag{37}$$

Therefore, $\mathrm{Tr}\left(AS\right) = 0$. And we're done.