Vector and Matrix Calculus

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1 Introduction

As explained in detail in [1], there unfortunately exists multiple competing notations concerning the layout of matrix derivatives. This can cause a lot of difficulty when consulting several sources, since different sources might use different conventions. Some sources, for example [2] (from which I use a lot of identities), even use a mixed layout (according to [1, Notes]). Identities for both the *numerator layout* (sometimes called the *Jacobian formulation*) and the *denominator layout* (sometimes called the *Hessian formulation*) is given in [1], so this makes it easy to check what layout a particular source uses. I will aim to stick to the denominator layout, which seems to be the most widely used in the field of statistics and pattern recognition (e.g. [3] and [4, pp. 327–332]). Other useful references concerning matrix calculus include [5] and [6]. In this document column vectors are assumed in all cases expect where specifically stated otherwise.

Table 1: Derivatives of scalars, vector functions and matrices [1, 6].

	scalar y	column vector $\mathbf{y} \in \mathbb{R}^m$	matrix $\mathbf{Y} \in \mathbb{R}^{m \times n}$
scalar x	scalar $\frac{\partial y}{\partial x}$	row vector $\frac{\partial \mathbf{y}}{\partial x} \in \mathbb{R}^m$	matrix $\frac{\partial \mathbf{Y}}{\partial x}$ (only numerator layout)
column vector $\mathbf{x} \in \mathbb{R}^n$	column vector $\frac{\partial y}{\partial \mathbf{x}} \in \mathbb{R}^n$	matrix $\frac{\partial \mathbf{y}}{\partial \mathbf{x}} \in \mathbb{R}^{n \times m}$	
matrix $\mathbf{X} \in \mathbb{R}^{p \times q}$	matrix $\frac{\partial y}{\partial \mathbf{X}} \in \mathbb{R}^{p \times q}$		

2 Definitions

Table 1 indicates the six possible kinds of derivatives when using the denominator layout. Using this layout notation consistently, we have the following definitions.

The derivative of a scalar function $f : \mathbb{R}^n \to \mathbb{R}$ with respect to vector $\mathbf{x} \in \mathbb{R}^n$ is

$$\frac{\partial f(\mathbf{x})}{\partial \mathbf{x}} \stackrel{\text{def}}{=} \begin{bmatrix} \frac{\partial f(\mathbf{x})}{\partial x_1} \\ \frac{\partial f(\mathbf{x})}{\partial x_2} \\ \vdots \\ \frac{\partial f(\mathbf{x})}{\partial x_n} \end{bmatrix} \tag{1}$$

This is the transpose of the gradient (some authors simply call this the gradient, irrespective of whether numerator or denominator layout is used).

The derivative of a vector function $\mathbf{f} : \mathbb{R}^n \rightarrow \mathbb{R}^m$, where $\mathbf{f}(\mathbf{x}) = \begin{bmatrix} f_1(\mathbf{x}) & f_2(\mathbf{x}) & \dots & f_m(\mathbf{x}) \end{bmatrix}^{\mathrm{T}}$ and $\mathbf{x} \in \mathbb{R}^n$, with respect to scalar x_i is

$$\frac{\partial \mathbf{f}(\mathbf{x})}{\partial x_i} \stackrel{\text{def}}{=} \begin{bmatrix} \frac{\partial f_1(x)}{\partial x_i} & \frac{\partial f_2(x)}{\partial x_i} & \dots & \frac{\partial f_m(x)}{\partial x_i} \end{bmatrix} \tag{2}$$

The derivative of a vector function $\mathbf{f} : \mathbb{R}^n \rightarrow \mathbb{R}^m$, where $\mathbf{f}(\mathbf{x}) = \begin{bmatrix} f_1(\mathbf{x}) & f_2(\mathbf{x}) & \dots & f_m(\mathbf{x}) \end{bmatrix}^{\mathrm{T}}$, with respect to vector $\mathbf{x} \in \mathbb{R}^n$ is

$$\frac{\partial \mathbf{f}(\mathbf{x})}{\partial \mathbf{x}} \stackrel{\text{def}}{=} \begin{bmatrix} \frac{\partial \mathbf{f}(\mathbf{x})}{\partial x_1} \\ \frac{\partial \mathbf{f}(\mathbf{x})}{\partial x_2} \\ \vdots \\ \frac{\partial \mathbf{f}(\mathbf{x})}{\partial x_n} \end{bmatrix} = \begin{bmatrix} \frac{\partial f_1(\mathbf{x})}{\partial x_1} & \frac{\partial f_2(\mathbf{x})}{\partial x_1} & \dots & \frac{\partial f_m(\mathbf{x})}{\partial x_1} \\ \frac{\partial f_1(\mathbf{x})}{\partial x_2} & \frac{\partial f_2(\mathbf{x})}{\partial x_2} & \dots & \frac{\partial f_m(\mathbf{x})}{\partial x_2} \\ \vdots & \vdots & \vdots & \vdots \\ \frac{\partial f_1(\mathbf{x})}{\partial x_n} & \frac{\partial f_2(\mathbf{x})}{\partial x_n} & \dots & \frac{\partial f_m(\mathbf{x})}{\partial x_n} \end{bmatrix} \tag{3}$$

This is just the transpose of the Jacobian matrix.

The derivative of a scalar function $f : \mathbb{R}^{m \times n} \rightarrow \mathbb{R}$ with respect to matrix $\mathbf{X} \in \mathbb{R}^{m \times n}$ is

$$\frac{\partial f(\mathbf{X})}{\partial \mathbf{X}} \stackrel{\text{def}}{=} \begin{bmatrix} \frac{\partial f(\mathbf{X})}{\partial X_{11}} & \frac{\partial f(\mathbf{X})}{\partial X_{12}} & \dots & \frac{\partial f(\mathbf{X})}{\partial X_{1n}} \\ \frac{\partial f(\mathbf{X})}{\partial X_{21}} & \frac{\partial f(\mathbf{X})}{\partial X_{22}} & \dots & \frac{\partial f(\mathbf{X})}{\partial X_{2n}} \\ \vdots & \vdots & \vdots & \vdots \\ \frac{\partial f(\mathbf{X})}{\partial X_{m1}} & \frac{\partial f(\mathbf{X})}{\partial X_{m2}} & \dots & \frac{\partial f(\mathbf{X})}{\partial X_{mn}} \end{bmatrix} \tag{4}$$

Observe that the (1) is just a special case of (4) for column vectors. Often (as in [3]) the gradient notation is used as an alternative to the notation used above, for example:

$$\nabla_{\mathbf{x}} f(\mathbf{x}) = \frac{\partial f(\mathbf{x})}{\partial \mathbf{x}} \tag{5}$$

$$\nabla_{\mathbf{X}} f(\mathbf{X}) = \frac{\partial f(\mathbf{X})}{\partial \mathbf{X}} \tag{6}$$

3 Identities

3.1 Scalar-by-vector product rule

If $\mathbf{a} \in \mathbb{R}^m$, $\mathbf{b} \in \mathbb{R}^n$ and $\mathbf{C} \in \mathbb{R}^{m \times n}$ then

$$\mathbf{a}^{\mathrm{T}}\mathbf{C}\mathbf{b} = \sum_{i=1}^{m} a_i (\mathbf{C}\mathbf{b})_i = \sum_{i=1}^{m} a_i \left(\sum_{j=1}^{n} C_{ij} b_j \right) = \sum_{i=1}^{m} \sum_{j=1}^{n} C_{ij} a_i b_j \tag{7}$$

Now assume we have vector functions $\mathbf{u} : \mathbb{R}^m \rightarrow \mathbb{R}^m$, $\mathbf{v} = \mathbb{R}^n \rightarrow \mathbb{R}^n$ and $\mathbf{A} \in \mathbb{R}^{m \times n}$. The vector functions $\mathbf{u}$ and $\mathbf{v}$ are functions of $\mathbf{x} \in \mathbb{R}^q$, but $\mathbf{A}$ is not. We want to find an identity for

$$\frac{\partial \mathbf{u}^{\mathrm{T}}\mathbf{A}\mathbf{v}}{\partial \mathbf{x}} \tag{8}$$

From (7), we have:

$$\begin{aligned}
\left[\frac{\partial \mathbf{u}^{\mathrm{T}}\mathbf{A}\mathbf{v}}{\partial \mathbf{x}}\right]_l = \frac{\partial \mathbf{u}^{\mathrm{T}}\mathbf{A}\mathbf{v}}{\partial x_l} &= \frac{\partial}{\partial x_l}\sum_{i=1}^{m}\sum_{j=1}^{n} A_{ij}u_i v_j \\
&= \sum_{i=1}^{m}\sum_{j=1}^{n} A_{ij}\frac{\partial}{\partial x_l}u_i v_j \\
&= \sum_{i=1}^{m}\sum_{j=1}^{n} A_{ij}\left[v_j\frac{\partial u_i}{\partial x_l} + u_i\frac{\partial v_j}{\partial x_l}\right] \\
&= \sum_{i=1}^{m}\sum_{j=1}^{n} A_{ij}v_j\frac{\partial u_i}{\partial x_l} + \sum_{i=1}^{m}\sum_{j=1}^{n} A_{ij}u_i\frac{\partial v_j}{\partial x_l}
\end{aligned} \tag{9}$$

Now we can show (by writing out the elements [Notebook, 2012-05-22]) that:

$$\begin{aligned}
\left[\frac{\partial \mathbf{u}}{\partial \mathbf{x}}\mathbf{A}\mathbf{v} + \frac{\partial \mathbf{v}}{\partial \mathbf{x}}\mathbf{A}^{\mathrm{T}}\mathbf{u}\right]_l &= \sum_{i=1}^{m}\sum_{j=1}^{n} A_{ij}v_j\frac{\partial u_i}{\partial x_l} + \sum_{i=1}^{m}\sum_{j=1}^{n} (\mathbf{A}^{\mathrm{T}})_{ji}u_i\frac{\partial v_j}{\partial x_l} \\
&= \sum_{i=1}^{m}\sum_{j=1}^{n} A_{ij}v_j\frac{\partial u_i}{\partial x_l} + \sum_{i=1}^{m}\sum_{j=1}^{n} A_{ij}u_i\frac{\partial v_j}{\partial x_l}
\end{aligned} \tag{10}$$

A comparison of (9) and (10) completes the proof that

$$\boxed{\frac{\partial \mathbf{u}^{\mathrm{T}}\mathbf{A}\mathbf{v}}{\partial \mathbf{x}} = \frac{\partial \mathbf{u}}{\partial \mathbf{x}}\mathbf{A}\mathbf{v} + \frac{\partial \mathbf{v}}{\partial \mathbf{x}}\mathbf{A}^{\mathrm{T}}\mathbf{u}} \tag{11}$$

3.2 Useful identities from scalar-by-vector product rule

From (11) it follows, with vectors and matrices $\mathbf{b} \in \mathbb{R}^m$, $\mathbf{d} \in \mathbb{R}^q$, $\mathbf{x} \in \mathbb{R}^n$, $\mathbf{B} \in \mathbb{R}^{m\times n}$, $\mathbf{C} \in \mathbb{R}^{m\times q}$, $\mathbf{D} \in \mathbb{R}^{q\times n}$, that

$$\frac{\partial(\mathbf{B}\mathbf{x}+\mathbf{b})^{\mathrm{T}}\mathbf{C}(\mathbf{D}\mathbf{x}+\mathbf{d})}{\partial \mathbf{x}} = \frac{\partial(\mathbf{B}\mathbf{x}+\mathbf{b})}{\partial \mathbf{x}}\mathbf{C}(\mathbf{D}\mathbf{x}+\mathbf{d}) + \frac{\partial(\mathbf{D}\mathbf{x}+\mathbf{d})^{\mathrm{T}}}{\partial \mathbf{x}}\mathbf{C}^{\mathrm{T}}(\mathbf{B}\mathbf{x}+\mathbf{b}) \tag{12}$$

resulting in the identity:

$$\boxed{\frac{\partial(\mathbf{B}\mathbf{x}+\mathbf{b})^{\mathrm{T}}\mathbf{C}(\mathbf{D}\mathbf{x}+\mathbf{d})}{\partial \mathbf{x}} = \mathbf{B}^{\mathrm{T}}\mathbf{C}(\mathbf{D}\mathbf{x}+\mathbf{d}) + \mathbf{D}^{\mathrm{T}}\mathbf{C}^{\mathrm{T}}(\mathbf{B}\mathbf{x}+\mathbf{b})} \tag{13}$$

by using the easily verifiable identities:

$$\boxed{\frac{\partial(\mathbf{u}(\mathbf{x})+\mathbf{v}(\mathbf{x}))}{\partial \mathbf{x}} = \frac{\partial \mathbf{u}(\mathbf{x})}{\partial \mathbf{x}} + \frac{\partial \mathbf{v}(\mathbf{x})}{\partial \mathbf{x}}} \tag{14}$$

$$\boxed{\frac{\partial \mathbf{A}\mathbf{x}}{\partial \mathbf{x}} = \mathbf{A}^{\mathrm{T}}} \tag{15}$$

$$\boxed{\frac{\partial \mathbf{a}}{\partial \mathbf{x}} = \mathbf{0}} \tag{16}$$

Some other useful special cases of (11):

$$\boxed{\frac{\partial \mathbf{x}^{\mathrm{T}}\mathbf{A}\mathbf{b}}{\partial \mathbf{x}} = \mathbf{A}\mathbf{b}} \tag{17}$$

$$\boxed{\frac{\partial \mathbf{x}^{\mathrm{T}}\mathbf{A}\mathbf{x}}{\partial \mathbf{x}} = (\mathbf{A}+\mathbf{A}^{\mathrm{T}})\mathbf{x}} \tag{18}$$

$$\boxed{\frac{\partial \mathbf{x}^{\mathrm{T}}\mathbf{A}\mathbf{x}}{\partial \mathbf{x}} = 2\mathbf{A}\mathbf{x} \text{ if } \mathbf{A} \text{ is symmetric}} \tag{19}$$

3.3 Derivatives of determinant

See [7, p. 374] for definition of cofactors. Also see [Notebook, 2012-05-22].

We can write the determinant of matrix $\mathbf{X} \in \mathbb{R}^{n\times n}$ as

$$|\mathbf{X}| = X_{i1}C_{i1} + X_{i2}C_{i2} + \ldots + X_{in}C_{in} = \sum_{j=1}^{n} X_{ij}C_{ij+} \tag{20}$$

Thus the derivative will be

$$\begin{aligned}
\left[\frac{\partial|\mathbf{X}|}{\partial \mathbf{X}}\right]_{kl} &= \frac{\partial}{\partial X_{kl}}\{X_{i1}C_{i1} + X_{i2}C_{i2} + \ldots + X_{in}C_{in}\} \\
&= \frac{\partial}{\partial X_{kl}}\{X_{k1}C_{k1} + X_{k2}C_{k2} + \ldots + X_{kn}C_{kn}\} \\
&\qquad\qquad \text{(can choose } i \text{ any number, so choose } i = k) \\
&= C_{kl} \qquad (21)
\end{aligned}$$

Thus (see [7, p. 386])

$$\frac{\partial|\mathbf{X}|}{\partial \mathbf{X}} = \operatorname{cofactor}\mathbf{X} = (\operatorname{adj}\mathbf{X})^{\mathrm{T}} \tag{22}$$

But we know that the inverse of $\mathbf{X}$ is given by [7, p. 387]

$$\mathbf{X}^{-1} = \frac{1}{|\mathbf{X}|}\operatorname{adj}\mathbf{X} \tag{23}$$

thus

$$\operatorname{adj}\mathbf{X} = |\mathbf{X}|\mathbf{X}^{-1} \tag{24}$$

which, when substituted into (22), results in the identity

$$\boxed{\frac{\partial|\mathbf{X}|}{\partial \mathbf{X}} = |\mathbf{X}|(\mathbf{X}^{-1})^{\mathrm{T}}} \tag{25}$$

From (25) we can also write

$$\left[\frac{\partial \ln|\mathbf{X}|}{\partial \mathbf{X}}\right]_{kl} = \frac{\partial \ln|\mathbf{X}|}{\partial X_{kl}} = \frac{1}{|\mathbf{X}|}\frac{\partial|\mathbf{X}|}{\partial \mathbf{X}} = \frac{1}{|\mathbf{X}|}|\mathbf{X}|(\mathbf{X}^{-1})^{\mathrm{T}} \tag{26}$$

giving the identity

$$\boxed{\frac{\partial \ln|\mathbf{X}|}{\partial \mathbf{X}} = (\mathbf{X}^{-1})^{\mathrm{T}}} \tag{27}$$

References

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