17. Differentiation of Matrix Forms

There are no new 'calculus' results here. We merely have a few definitions so that we can take derivatives of functions expressed in matrix form.

Definitions

Given $y = f(x_1, x_2, ..., x_n)$, let $\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$, then define $\dfrac{\partial y}{\partial \mathbf{x}} = \begin{bmatrix} \partial y / \partial x_1 \\ \partial y / \partial x_2 \\ \vdots \\ \partial y / \partial x_n \end{bmatrix}$.

Example If $y = x_1^2 x_2^2 x_3$, then $\dfrac{\partial y}{\partial \mathbf{x}} = \begin{bmatrix} 2x_1 x_2^2 x_3 \\ 2x_1^2 x_2 x_3 \\ x_1^2 x_2^2 \end{bmatrix}$.

Example If $y = x_1 x_2 + x_3 x_4$, then $\dfrac{\partial y}{\partial \mathbf{x}} = \begin{bmatrix} x_2 \\ x_1 \\ x_4 \\ x_3 \end{bmatrix}$

Example Let $y = \det \begin{bmatrix} x_1 & x_2 \\ x_3 & x_4 \end{bmatrix} = x_1 x_4 - x_2 x_3$, then $\dfrac{\partial y}{\partial \mathbf{x}} = \begin{bmatrix} x_4 \\ -x_3 \\ -x_2 \\ x_1 \end{bmatrix}$

The case of linear functions and quadratic forms are particularly important. We have:

Example If $y = \mathbf{c}'\mathbf{x}$ where $\mathbf{c}$ and $\mathbf{x}$ are $(n \times 1)$, then $\dfrac{\partial y}{\partial \mathbf{x}} = \mathbf{c}$.

To see this, simply expand and differentiate: $y = \mathbf{c}'\mathbf{x} = c_1 x_1 + c_2 x_2 + ... + c_n x_n$, so

$$\frac{\partial y}{\partial \mathbf{x}} = \begin{bmatrix} \partial y / \partial x_1 \\ \partial y / \partial x_2 \\ \vdots \\ \partial y / \partial x_n \end{bmatrix} = \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \end{bmatrix} = \mathbf{c}$$

Example If $y = \mathbf{x}'\mathbf{A}\mathbf{x}$ where $\mathbf{x}$ is $(n \times 1)$ and $\mathbf{A}$ is $(n \times n)$, then

$$\frac{\partial y}{\partial \mathbf{x}} = (\mathbf{A}' + \mathbf{A})\mathbf{x}$$

This is easy to see this in the $n = 2$ case: let

$$\mathbf{A} = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix}$$

Then

$$y = \begin{bmatrix} x_1 & x_2 \end{bmatrix} \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = a_{11}x_1^2 + a_{12}x_1x_2 + a_{21}x_1x_2 + a_{22}x_2^2 .$$

Therefore

$$\frac{\partial y}{\partial \mathbf{x}} = \begin{bmatrix} \dfrac{\partial y}{\partial x_1} \\ \dfrac{\partial y}{\partial x_2} \end{bmatrix} = \begin{bmatrix} 2a_{11}x_1 + (a_{12} + a_{21})x_2 \\ (a_{12} + a_{21})x_1 + 2a_{22}x_2 \end{bmatrix} = \begin{bmatrix} 2a_{11} & a_{12} + a_{21} \\ a_{12} + a_{21} & 2a_{22} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix},$$

and it is easily seen that $\begin{bmatrix} 2a_{11} & a_{12} + a_{21} \\ a_{12} + a_{21} & 2a_{22} \end{bmatrix} = \mathbf{A} + \mathbf{A}'$.

You can easily extend this to the *n*-dimension case.

If $\mathbf{A}$ is symmetric, then $\mathbf{A} = \mathbf{A}'$, so

$$\frac{\partial y}{\partial \mathbf{x}} = 2\mathbf{Ax},$$

which bears considerable resemblance to the univariate case where $dy / dx = 2ax$ when $y = ax^2$. Remember that $\mathbf{x}'\mathbf{Ax}$ is the matrix version of the quadratic function.

The general principle is that the shape of the derivative matrix follows that of the denominator of the derivative, so that for $y = f(x_1, x_2, ..., x_n)$,

$$\frac{\partial y}{\partial \mathbf{x}'} = \begin{bmatrix} \dfrac{\partial y}{\partial x_1} & \dfrac{\partial y}{\partial x_2} & \cdots & \dfrac{\partial y}{\partial x_n} \end{bmatrix}$$

since $\mathbf{x} = \begin{bmatrix} x_1 & x_2 & \cdots & x_n \end{bmatrix}$.

Example If $y = \mathbf{c}'\mathbf{x}$ where $\mathbf{c}$ and $\mathbf{x}$ are $(n \times 1)$, then $\dfrac{\partial y}{\partial \mathbf{x}'} = \mathbf{c}'$.

Example If

$$y = \det \begin{bmatrix} x_1 & x_2 \\ x_3 & x_4 \end{bmatrix} = x_1x_4 - x_2x_3,$$

we have $\dfrac{\partial y}{\partial \mathbf{x}'} = \begin{bmatrix} \dfrac{\partial f}{\partial x_1} & \dfrac{\partial f}{\partial x_2} & \dfrac{\partial f}{\partial x_3} & \dfrac{\partial f}{\partial x_4} \end{bmatrix} = \begin{bmatrix} x_4 & -x_3 & -x_2 & x_1 \end{bmatrix}$.

This "row" form of the vector derivative is most often applied to situations where we are differentiating a vector of functions, i.e. when

$$\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{bmatrix} = \begin{bmatrix} f_1(x_1, x_2, \ldots, x_n) \\ f_2(x_1, x_2, \ldots, x_n) \\ \vdots \\ f_m(x_1, x_2, \ldots, x_n) \end{bmatrix},$$

in which case $\dfrac{\partial \mathbf{y}}{\partial \mathbf{x}'}$ is the application of the $\dfrac{\partial y}{\partial \mathbf{x}'} = \begin{bmatrix} \dfrac{\partial y}{\partial x_1} & \dfrac{\partial y}{\partial x_2} & \cdots & \dfrac{\partial y}{\partial x_n} \end{bmatrix}$ to each individual y_i to get

$$\frac{\partial \mathbf{y}}{\partial \mathbf{x}'} = \begin{bmatrix} \partial y_1/\partial x_1 & \partial y_1/\partial x_2 & \cdots & \partial y_1/\partial x_n \\ \partial y_2/\partial x_1 & \partial y_2/\partial x_2 & \cdots & \partial y_2/\partial x_n \\ \vdots & \vdots & \ddots & \vdots \\ \partial y_m/\partial x_1 & \partial y_m/\partial x_2 & \cdots & \partial y_m/\partial x_n \end{bmatrix}.$$

Example If $\mathbf{y} = \mathbf{A}\mathbf{x}$ where $\mathbf{A}$ is $(m \times n)$ and $\mathbf{x}$ is $(n \times 1)$, then $\dfrac{\partial \mathbf{y}}{\partial \mathbf{x}'} = \mathbf{A}$.

$$\mathbf{y} = \mathbf{A}\mathbf{x} = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} a_{11}x_1 + a_{12}x_2 + \cdots + a_{1n}x_n \\ a_{21}x_1 + a_{22}x_2 + \cdots + a_{2n}x_n \\ \vdots \\ a_{m1}x_1 + a_{m2}x_2 + \cdots + a_{mn}x_n \end{bmatrix}.$$

Then

$$\frac{\partial \mathbf{y}}{\partial \mathbf{x}'} = \begin{bmatrix} \partial y_1/\partial x_1 & \partial y_1/\partial x_2 & \cdots & \partial y_1/\partial x_n \\ \partial y_2/\partial x_1 & \partial y_2/\partial x_2 & \cdots & \partial y_2/\partial x_n \\ \vdots & \vdots & \ddots & \vdots \\ \partial y_m/\partial x_1 & \partial y_m/\partial x_2 & \cdots & \partial y_m/\partial x_n \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{bmatrix} = \mathbf{A}.$$

Another application is to get a matrix of second derivatives: if $y = f(x_1, x_2, \ldots, x_n)$, we have

$$\frac{\partial^2 y}{\partial \mathbf{x}\partial \mathbf{x}'} = \frac{\partial}{\partial \mathbf{x}'}\left(\frac{\partial y}{\partial \mathbf{x}}\right) = \begin{bmatrix} \dfrac{\partial^2 y}{\partial x_1^2} & \dfrac{\partial^2 y}{\partial x_1 \partial x_2} & \cdots & \dfrac{\partial^2 y}{\partial x_1 \partial x_n} \\ \dfrac{\partial^2 y}{\partial x_2 \partial x_1} & \dfrac{\partial^2 y}{\partial x_2^2} & \cdots & \dfrac{\partial^2 y}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \dfrac{\partial^2 y}{\partial x_n \partial x_1} & \dfrac{\partial^2 y}{\partial x_n \partial x_2} & \cdots & \dfrac{\partial^2 y}{\partial x_n^2} \end{bmatrix}.$$

This is called the Hessian of $f(\mathbf{x})$ and written $f''(\mathbf{x})$. Young's Theorem says that this will be a symmetric matrix.

Example If $y = \mathbf{x}'\mathbf{A}\mathbf{x}$ where $\mathbf{x}$ is $(n \times 1)$ and $\mathbf{A}$ is $(n \times n)$, then $\dfrac{\partial y}{\partial \mathbf{x}} = (\mathbf{A}' + \mathbf{A})\mathbf{x}$, and therefore

$$\frac{\partial^2 y}{\partial \mathbf{x}\partial \mathbf{x}'} = (\mathbf{A}' + \mathbf{A}), \; = 2\mathbf{A} \text{ if } \mathbf{A} \text{ is symmetric.}$$

This should remind you of the fact that $d^2y/dx^2 = 2a$ when $y = ax^2$.

Finally, we can use the principle that the shape of the derivative matrix follows that of the denominator of the derivative, to get derivatives with respect to matrices (as opposed to with respect to vectors):

Example If $\mathbf{X} = \begin{bmatrix} x_1 & x_2 \\ x_3 & x_4 \end{bmatrix}$, then

$$\frac{\partial \det(\mathbf{X})}{\partial \mathbf{X}} = \begin{bmatrix} \frac{\partial \det(\mathbf{X})}{\partial x_1} & \frac{\partial \det(\mathbf{X})}{\partial x_2} \\ \frac{\partial \det(\mathbf{X})}{\partial x_3} & \frac{\partial \det(\mathbf{X})}{\partial x_4} \end{bmatrix} = \begin{bmatrix} x_4 & -x_3 \\ -x_2 & x_1 \end{bmatrix}.$$

Taking this further, consider the derivative $\frac{\partial \ln(\det \mathbf{X})}{\partial \mathbf{X}}$. Applying the chain rule:

$$\frac{\partial \ln(\det \mathbf{X})}{\partial \mathbf{X}} = \frac{1}{\det \mathbf{X}} \begin{bmatrix} \frac{\partial \det \mathbf{X}}{\partial x_1} & \frac{\partial \det \mathbf{X}}{\partial x_2} \\ \frac{\partial \det \mathbf{X}}{\partial x_3} & \frac{\partial \det \mathbf{X}}{\partial x_4} \end{bmatrix} = \frac{1}{\det \mathbf{X}} \begin{bmatrix} x_4 & -x_3 \\ -x_2 & x_1 \end{bmatrix} = (\mathbf{X}^{-1})'$$

since $\mathbf{X}^{-1} = \frac{1}{\det \mathbf{X}} \begin{bmatrix} x_4 & -x_2 \\ -x_3 & x_1 \end{bmatrix}$.

This is true also for general $(n \times n)$ matrices. Note: to write down $\ln(\det \mathbf{X})$ we ought to have $\det \mathbf{X} > 0$, which is true if $\mathbf{X}$ is positive-definite. Furthermore, if $\mathbf{A}$ is symmetric, then the inverse is symmetric, and we do not require the transposition of the inverse.

As a final example, consider the quadratic form $y = \mathbf{x}'\mathbf{A}\mathbf{x}$, and consider differentiating it with respect to $\mathbf{A}$ (earlier we differentiated with respect to $\mathbf{x}$). To simplify the exposition, we again focus on the (2×2) case, where

$$y = \begin{bmatrix} x_1 & x_2 \end{bmatrix} \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = a_{11}x_1^2 + a_{12}x_1x_2 + a_{21}x_1x_2 + a_{22}x_2^2$$

We have

$$\frac{\partial\, \mathbf{x}'\mathbf{A}\mathbf{x}}{\partial \mathbf{A}} = \begin{bmatrix} \frac{\partial y}{\partial a_{11}} & \frac{\partial y}{\partial a_{12}} \\ \frac{\partial y}{\partial a_{21}} & \frac{\partial y}{\partial a_{22}} \end{bmatrix} = \begin{bmatrix} x_1^2 & x_1x_2 \\ x_1x_2 & x_2^2 \end{bmatrix} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \begin{bmatrix} x_1 & x_2 \end{bmatrix} = \mathbf{x}\mathbf{x}'$$

There are other important forms. These will do for now.

Summary

$$\frac{\partial\, \mathbf{c}'\mathbf{x}}{\partial \mathbf{x}} = \mathbf{c}\,.$$

$$\frac{\partial \mathbf{x}'\mathbf{A}\mathbf{x}}{\partial \mathbf{x}} = (\mathbf{A}' + \mathbf{A})\mathbf{x}\,,\ = 2\mathbf{A}\mathbf{x} \text{ if } \mathbf{A} \text{ is symmetric.}$$

$$\frac{\partial^2 y}{\partial \mathbf{x}\partial \mathbf{x}'} = \begin{bmatrix} \frac{\partial^2 y}{\partial x_1{}^2} & \frac{\partial^2 y}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 y}{\partial x_1 \partial x_n} \\ \frac{\partial^2 y}{\partial x_2 \partial x_1} & \frac{\partial^2 y}{\partial x_2{}^2} & \cdots & \frac{\partial^2 y}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 y}{\partial x_n \partial x_1} & \frac{\partial^2 y}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 y}{\partial x_n{}^2} \end{bmatrix}, \quad \frac{\partial \mathbf{x}'\mathbf{A}\mathbf{x}}{\partial \mathbf{x}\partial \mathbf{x}'} = (\mathbf{A}' + \mathbf{A})\,,\ = 2\mathbf{A} \text{ if } \mathbf{A} \text{ is symmetric.}$$

$$\frac{\partial \mathbf{A}\mathbf{x}}{\partial \mathbf{x}'} = \mathbf{A}\,, \qquad \frac{\partial \ln(\det \mathbf{X})}{\partial \mathbf{X}} = (\mathbf{X}^{-1})', \qquad \frac{\partial\, \mathbf{x}'\mathbf{A}\mathbf{x}}{\partial \mathbf{A}} = \mathbf{x}\mathbf{x}'\,.$$