Differentiation

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Contents

1 introduction

When differentiating an arbitrary-shaped (scalar, vector, matrix or higher rank tensor) function f w.r.t. a scalar (e.t. t, the time), the result ($\partial f/\partial t$, the Jacobian) has the same shape as the function.

When differentiating a scalar function w.r.t. x (scalar, vector or matrix), the result has the same shape as x^T, i.e., the transpose of x.

Combining the 2 above, let's say for example that $f(x)$ is an n-vector, and x is an m-vector. Then $\partial f(x)/\partial x$ is an n-by-m matrix. This can be generalized with tensors.

2 scalar functions

2.1 differentiation w.r.t. a vector

1. Let $\mathbf{a} \in \mathbb{R}^n$ be a constant vector, $\mathbf{x} \in \mathbb{R}^n$. Then

$$\frac{d}{d\mathbf{x}}(\mathbf{x}^T\mathbf{a}) = \frac{d}{d\mathbf{x}}(\mathbf{a}^T\mathbf{x}) = \mathbf{a}^{\mathbf{T}} \tag{1}$$

2. Let $\mathbf{A} \in \mathbb{R}^{nxn}$ be a constant matrix, $\mathbf{x} \in \mathbb{R}^n$ Then

$$\frac{d}{d\mathbf{x}}(\mathbf{x}^T\mathbf{A}\mathbf{x}) = \mathbf{x}^T(\mathbf{A}^T + \mathbf{A}) \tag{2}$$

We can derive this as follows:

$$\begin{aligned}
\frac{d}{d\mathbf{x}}(\mathbf{x}^T\mathbf{A}\mathbf{x}) =& \frac{d}{d\mathbf{y}}(\mathbf{y}^T\mathbf{A}\mathbf{x}) + \frac{d}{d\mathbf{y}}(\mathbf{x}^T\mathbf{A}\mathbf{y}) \\
=& \frac{d}{d\mathbf{y}}(\mathbf{x}^T\mathbf{A}^T\mathbf{y}) + \frac{d}{d\mathbf{y}}(\mathbf{x}^T\mathbf{A}\mathbf{y}) \\
=& \mathbf{x}^T\mathbf{A}^T + \mathbf{x}^T\mathbf{A} \\
=& \mathbf{x}^T(\mathbf{A}^T + \mathbf{A})
\end{aligned}$$

2.2 differentiation w.r.t. a matrix

1. Let $\mathbf{A} \in \mathbb{R}^{m\times n}$, $\mathbf{X} \in \mathbb{R}^{m\times n}$. Then

$$\frac{d}{d\mathbf{X}}\mathrm{Tr}(\mathbf{A}^{\mathbf{T}}\mathbf{X}) = \frac{d}{d\mathbf{X}}\mathrm{Tr}(\mathbf{X}^{\mathbf{T}}\mathbf{A}) = \mathbf{A} \tag{3}$$

2. Let $\mathbf{A} \in \mathbb{R}^{m\times m}$, $\mathbf{X} \in \mathbb{R}^{m\times n}$. Then

$$\frac{d}{d\mathbf{X}}\mathrm{Tr}(\mathbf{X}^T\mathbf{A}\mathbf{X}) = (\mathbf{A}+\mathbf{A}^T)\mathbf{X} \tag{4}$$

We can derive it as follows:

$$\begin{aligned}\frac{d}{d\mathbf{X}}\mathrm{Tr}(\mathbf{X}^T\mathbf{A}\mathbf{X}) =& \frac{d}{d\mathbf{Y}}\mathrm{Tr}(\mathbf{Y}^T\mathbf{A}\mathbf{X}) + \frac{d}{d\mathbf{Y}}\mathrm{Tr}(\mathbf{X}^T\mathbf{A}\mathbf{Y})\\ =& \mathbf{X}^T\mathbf{A}^T + \mathbf{X}^T\mathbf{A}\\ =& \mathbf{X}^T(\mathbf{A}^T+\mathbf{A})\end{aligned}$$

Example. Consider now this example.

$$f(\mathbf{X}) = \mathrm{Tr}(\mathbf{X}^T\mathbf{A}\mathbf{X}\mathbf{B}\mathbf{X}^T\mathbf{C})$$

where $\mathbf{X} \in \mathbb{R}^{n\times m}$, $\mathbf{A} \in \mathbb{R}^{n\times n}$, $\mathbf{B} \in \mathbb{R}^{m\times m}$, $\mathbf{C} \in \mathbb{R}^{n\times m}$.

$$\begin{aligned}\frac{d}{d\mathbf{X}}f(\mathbf{X}) =& \frac{d}{d\mathbf{Y}}\mathrm{Tr}(\mathbf{Y}^T\mathbf{A}\mathbf{X}\mathbf{B}\mathbf{X}^T\mathbf{C})\\ &+\frac{d}{d\mathbf{Y}}\mathrm{Tr}(\mathbf{X}^T\mathbf{A}\mathbf{Y}\mathbf{B}\mathbf{X}^T\mathbf{C})\\ &+\frac{d}{d\mathbf{Y}}\mathrm{Tr}(\mathbf{X}^T\mathbf{A}\mathbf{X}\mathbf{B}\mathbf{Y}^T\mathbf{C})\end{aligned}$$

Calculating these:

$$\frac{d}{d\mathbf{Y}}\mathrm{Tr}(\mathbf{Y}^T\mathbf{A}\mathbf{X}\mathbf{B}\mathbf{X}^T\mathbf{C}) = (\mathbf{A}\mathbf{X}\mathbf{B}\mathbf{X}^T\mathbf{C})^T = \mathbf{C}^T\mathbf{X}\mathbf{B}^T\mathbf{X}^T\mathbf{A}^T$$

$$\begin{aligned}\frac{d}{d\mathbf{Y}}\mathrm{Tr}(\mathbf{X}^T\mathbf{A}\mathbf{Y}\mathbf{B}\mathbf{X}^T\mathbf{C}) =& \frac{d}{d\mathbf{Y}}\mathrm{Tr}(\mathbf{Y}\mathbf{B}\mathbf{X}^T\mathbf{C}\mathbf{X}^T\mathbf{A})\\ =& \mathbf{B}\mathbf{X}^T\mathbf{C}\mathbf{X}^T\mathbf{A}\end{aligned}$$

$$\begin{aligned}\frac{d}{d\mathbf{Y}}\mathrm{Tr}(\mathbf{X}^T\mathbf{A}\mathbf{X}\mathbf{B}\mathbf{Y}^T\mathbf{C}) &= \frac{d}{d\mathbf{Y}}\mathrm{Tr}(\mathbf{Y}^T\mathbf{C}\mathbf{X}^T\mathbf{A}\mathbf{X}\mathbf{B})\\ &= (\mathbf{C}\mathbf{X}^T\mathbf{A}\mathbf{X}\mathbf{B})^T = \mathbf{B}^T\mathbf{X}^T\mathbf{A}^T\mathbf{X}\mathbf{C}^T\end{aligned}$$

So the result is:

$$\frac{d}{d\mathbf{X}}\mathrm{Tr}(\mathbf{X}^T\mathbf{A}\mathbf{X}\mathbf{B}\mathbf{X}^T\mathbf{C}) = \mathbf{C}^T\mathbf{X}\mathbf{B}^T\mathbf{X}^T\mathbf{A}^T + \mathbf{B}\mathbf{X}^T\mathbf{C}\mathbf{X}^T\mathbf{A} + \mathbf{B}^T\mathbf{X}^T\mathbf{A}^T\mathbf{X}\mathbf{C}^T$$