

Fundamentals on the package

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1 Derivatives of the composite map

Let V , W , and X be vector spaces over \mathbb{R} , and f and g be diffeomorphisms defined by

$$f : V \rightarrow W, \quad g : W \rightarrow X. \quad (1)$$

Then, the Jacobian matrix of f and g are elements of tensor products

$$J_f \in W \otimes V^*, \quad J_g \in X \otimes W^*, \quad (2)$$

where V^* and W^* are the dual spaces of V and W , respectively. J_f is also a map $V \rightarrow W$; J_g is $W \rightarrow X$. If J_f and J_g are differentiable in V and W , the Hessian tensors H_f and H_g are available as elements of another tensor products

$$H_f \in W \otimes V^* \otimes V^*, \quad H_g \in X \otimes W^* \otimes W^*. \quad (3)$$

On the other hand, a composite map $g \circ f$ is described as

$$g \circ f : V \rightarrow X. \quad (4)$$

From the chain-rule, the Jacobian matrix of $g \circ f$ is

$$J_{g \circ f} = J_g J_f \in X \otimes V^*. \quad (5)$$

In the context of the tensor, Eq. (5) is equivalent to the following contraction of the tensor product.

$$J_{g \circ f} = \text{tr}_{23} (J_g \otimes J_f), \quad (6)$$

where

$$\begin{aligned} J_g \otimes J_f &\in (X \otimes W^*) \otimes (W \otimes V^*), \\ \text{tr}_{23} : (X \otimes W^*) \otimes (W \otimes V^*) &\rightarrow X \otimes V^*. \end{aligned} \quad (7)$$

We write the (i, j) contraction of a tensor by tr_{ij} , which is a generalization of the trace. The Hessian tensor of $g \circ f$ is an element of $X \otimes V^* \otimes V^*$. From the chain-rule, we have

$$H_{g \circ f} = (H_g J_f) J_f + J_g H_f, \quad (8)$$

where

$$\begin{aligned} H_g J_f &= \text{tr}_{24} (H_g \otimes J_f) \quad (= \text{tr}_{34} (H_g \otimes J_f)), \\ H_g \otimes J_f &\in (X \otimes W^* \otimes W^*) \otimes (W \otimes V^*), \\ \text{tr}_{24} (= \text{tr}_{34}) : (X \otimes W^* \otimes W^*) \otimes (W \otimes V^*) &\rightarrow X \otimes W^* \otimes V^*, \end{aligned} \quad (9)$$

$$\begin{aligned} (H_g J_f) J_f &= \text{tr}_{24} ((H_g J_f) \otimes J_f), \\ \text{tr}_{24} : (X \otimes W^* \otimes V^*) \otimes (W \otimes V^*) &\rightarrow X \otimes V^* \otimes V^*, \end{aligned} \quad (10)$$

$$\begin{aligned} J_g H_f &= \text{tr}_{23} (J_g \otimes H_f), \\ J_g \otimes H_f &\in (X \otimes W^*) \otimes (W \otimes V^* \otimes V^*), \\ \text{tr}_{23} : (X \otimes W^*) \otimes (W \otimes V^* \otimes V^*) &\rightarrow X \otimes V^* \otimes V^*, \end{aligned} \quad (11)$$

Let T be a composite map of T_i

$$T = T_{m-1} \circ T_{m-2} \circ \cdots \circ T_1 \circ T_0, \quad T : M_0 \rightarrow M_{m-1} \quad (12)$$

where T_i is a C^∞ diffeomorphism $T_i : M_i \rightarrow M_{i+1}$ and $M_i \subset \mathbb{R}$. Given $\mathbf{x}_i \in M_i$, the Jacobian matrix of T is

$$J = \frac{\partial T}{\partial \mathbf{x}_0} = \prod_{k=0}^{m-1} \frac{\partial T_{m-1-k}}{\partial \mathbf{x}_{m-1-k}}. \quad (13)$$

Let us denote the product in the right-hand of equation as J_{m-1} , and we have

$$J_{m-1} = \frac{\partial T_{m-1}}{\partial \mathbf{x}_{m-1}} J_{m-2}, \quad (14)$$

for $m \geq 2$. If J_k is Hessian tensor of T is available by differentiating Eq. (14),

$$H = \frac{\partial J}{\partial \mathbf{x}_0} = \left(\frac{\partial^2 T_{m-1}}{\partial \mathbf{x}_{m-1}^2} J_{m-2} \right) J_{m-2} + \frac{\partial T_{m-1}}{\partial \mathbf{x}_{m-1}} \frac{\partial J_{m-2}}{\partial \mathbf{x}_0}. \quad (15)$$

Rewriting the derivative of J_{m-1} by H_{m-1} , we get

$$H_{m-1} = \left(\frac{\partial^2 T_{m-1}}{\partial \mathbf{x}_{m-1}^2} J_{m-2} \right) J_{m-2} + \frac{\partial T_{m-1}}{\partial \mathbf{x}_{m-1}} H_{m-2} \quad (16)$$

Notice that $(J_{m-2} J_{m-2})$ is sometimes not J_{m-2}^2 because the dimensions of M_i and M_{i+1}^* are not necessarily equal.

2 Derivative of a map for the continuous-time systems

Consider a C^∞ autonomous dynamical system

$$\frac{dx}{dt} = f(x), \quad x \in M \subset \mathbb{R}^n, \quad t \in \mathbb{R}, \quad (17)$$

where M is a state space, and f is a function such that $M \rightarrow \mathbb{R}^n$. We write the trajectory of the system (17) by $\varphi : \mathbb{R} \times M \rightarrow M$, where $\varphi(0, x_0) = x_0$ is the initial state and $\varphi(t, x_0)$ is the state at t . Let ∂M be an $n - 1$ dimensional manifold defined by a conditional function $q : M \rightarrow \mathbb{R}$

$$\partial M = \{x \in M \mid q(x) = 0\} \quad (18)$$

Suppose that T_0 is a local map from $x_0 \in M$ to a point in ∂M such that $M \rightarrow \partial M$. Then, the Jacobian matrix of T_0 is described by

$$J_{T_0} = \frac{\partial T_0}{\partial x_0} = \left[I - \frac{1}{\frac{dq}{dx} f(x)} f(x) \frac{dq}{dx} \right] \bigg|_{x=x_1} \frac{\partial \varphi}{\partial x_0}(\tau) = B(x_1) \frac{\partial \varphi}{\partial x_0}(\tau), \quad (19)$$

where τ is the spent time during the trajectory φ moves from x_0 to the boundary ∂M , which only depends on x_0 , and $x_1 = \varphi(\tau, x_0)$. The Hessian tensor of T_0 is

$$\begin{aligned} H_{T_0} &= \left(\frac{\partial B}{\partial x}(x_1) J_{T_0} \right) \frac{\partial \varphi}{\partial x_0}(\tau) + B(x_1) \left[\frac{\partial^2 \varphi}{\partial x_0^2}(\tau) + \left(\frac{d}{dt} \frac{\partial \varphi}{\partial x_0}(\tau) \right) \otimes \frac{\partial \tau}{\partial x_0} \right], \\ &= \left(\frac{\partial B}{\partial x}(x_1) J_{T_0} \right) \frac{\partial \varphi}{\partial x_0}(\tau) + B(x_1) \left[\frac{\partial^2 \varphi}{\partial x_0^2}(\tau) - \frac{1}{\frac{dq}{dx} f(x_1)} \left(\frac{df}{dx} \frac{\partial \varphi}{\partial x_0}(\tau) \right) \otimes \left(\frac{dq}{dx} \frac{\partial \varphi}{\partial x_0}(\tau) \right) \right], \end{aligned} \quad (20)$$

where

$$\frac{\partial B}{\partial x} = - \frac{1}{\left(\frac{dq}{dx} f(x) \right)^2} \left\{ \left(\frac{df}{dx} \otimes \frac{dq}{dx} + f(x) \otimes \frac{d^2 q}{dx^2} \right) \frac{dq}{dx} f(x) - \left(f(x) \frac{dq}{dx} \right) \otimes \left(\frac{d^2 q}{dx^2} f(x) + \frac{dq}{dx} \frac{df}{dx} \right) \right\}, \quad (21)$$

since

$$\begin{aligned} B &\in X \otimes X^*, & \frac{\partial B}{\partial x} &\in X \otimes X^* \otimes X^*, \\ \frac{dq}{dx} &\in X^*, & \frac{d^2 q}{dx^2} &\in X^* \otimes X^*, \\ f(x) &\in X, & \frac{df}{dx} &\in X \otimes X^*. \end{aligned} \quad (22)$$

On the other hand,

$$\frac{d}{dt} \left(\frac{\partial \varphi}{\partial x_0} \right) = \frac{df}{dx} \frac{\partial \varphi}{\partial x_0} \quad (23)$$

$$\frac{d}{dt} \left(\frac{\partial^2 \varphi}{\partial x_0^2} \right) = \left(\frac{d^2 f}{dx^2} \frac{\partial \varphi}{\partial x_0} \right) \frac{\partial \varphi}{\partial x_0} + \frac{df}{dx} \frac{\partial^2 \varphi}{\partial x_0^2}, \quad (24)$$

where

$$\frac{d^2 f}{dx^2} \frac{\partial \varphi}{\partial x_0} = \text{tr}_{34} \left(\frac{d^2 f}{dx^2} \otimes \frac{\partial \varphi}{\partial x_0} \right), \quad \frac{df}{dx} \frac{\partial^2 \varphi}{\partial x_0^2} = \text{tr}_{23} \left(\frac{df}{dx} \otimes \frac{\partial^2 \varphi}{\partial x_0^2} \right). \quad (25)$$

$$\begin{aligned}\frac{\partial T_0}{\partial \mathbf{x}_0} &= \frac{\partial \boldsymbol{\varphi}}{\partial \mathbf{x}_0} + \mathbf{f}(\mathbf{x}_1) \frac{\partial \tau}{\partial \mathbf{x}_0} \\ \frac{\partial \tau}{\partial \mathbf{x}_0} &= -\frac{1}{\frac{dq}{dx} \mathbf{f}(\mathbf{x}_1)} \frac{dq}{dx} \frac{\partial \boldsymbol{\varphi}}{\partial \mathbf{x}_0} \\ \frac{\partial T_0}{\partial \mathbf{x}_0} &= \left[I - \frac{1}{\frac{dq}{dx} \mathbf{f}(\mathbf{x}_1)} \mathbf{f}(\mathbf{x}_1) \frac{dq}{dx} \right] \frac{\partial \boldsymbol{\varphi}}{\partial \mathbf{x}_0} = B(\mathbf{x}_1) \frac{\partial \boldsymbol{\varphi}}{\partial \mathbf{x}_0}\end{aligned}\tag{26}$$

$$\begin{aligned}
\frac{\partial^2 T_0}{\partial x_0^2} &= \frac{\partial^2 \varphi}{\partial x_0^2} + \left(\frac{df}{dx} \frac{\partial \varphi}{\partial x_0} \right) \otimes \frac{\partial \tau}{\partial x_0} + f(x_1) \otimes \frac{\partial^2 \tau}{\partial x_0^2} \\
\frac{\partial^2 \tau}{\partial x_0^2} &= -\frac{1}{\left(\frac{dq}{dx} f(x_1) \right)^2} \left[\frac{\partial}{\partial x_0} \left(\frac{dq}{dx} \frac{\partial \varphi}{\partial x_0} \right) \frac{dq}{dx} f(x_1) - \left(\frac{dq}{dx} \frac{\partial \varphi}{\partial x_0} \right) \otimes \frac{\partial}{\partial x_0} \left(\frac{dq}{dx} f(x_1) \right) \right] \\
&= -\frac{1}{\left(\frac{dq}{dx} f(x_1) \right)^2} \left\{ \left[\left(\frac{d^2 q}{dx^2} \frac{\partial \varphi}{\partial x_0} \right) \frac{\partial \varphi}{\partial x_0} + \frac{dq}{dx} \frac{\partial^2 \varphi}{\partial x_0^2} \right] \frac{dq}{dx} f(x_1) - \left(\frac{dq}{dx} \frac{\partial \varphi}{\partial x_0} \right) \otimes \left[\left(\frac{d^2 q}{dx^2} \frac{\partial \varphi}{\partial x_0} \right) f(x_1) + \frac{dq}{dx} \left(\frac{df}{dx} \frac{\partial \varphi}{\partial x_0} \right) \right] \right\} \\
&= -\frac{1}{\frac{dq}{dx} f(x_1)} \left[\left(\frac{d^2 q}{dx^2} \frac{\partial \varphi}{\partial x_0} \right) \frac{\partial \varphi}{\partial x_0} + \frac{dq}{dx} \frac{\partial^2 \varphi}{\partial x_0^2} \right] + \frac{1}{\left(\frac{dq}{dx} f(x_1) \right)^2} \left(\frac{dq}{dx} \frac{\partial \varphi}{\partial x_0} \right) \otimes \left[\left(\frac{d^2 q}{dx^2} \frac{\partial \varphi}{\partial x_0} \right) f(x_1) + \frac{dq}{dx} \left(\frac{df}{dx} \frac{\partial \varphi}{\partial x_0} \right) \right] \\
\frac{\partial^2 T_0}{\partial x_0^2} &= B(x_1) \frac{\partial^2 \varphi}{\partial x_0^2} - \frac{1}{\frac{dq}{dx} f(x_1)} \left[\left(\frac{df}{dx} \frac{\partial \varphi}{\partial x_0} \right) \otimes \frac{dq}{dx} + f(x_1) \otimes \left(\frac{d^2 q}{dx^2} \frac{\partial \varphi}{\partial x_0} \right) \right] \frac{\partial \varphi}{\partial x_0} \\
&\quad + \frac{1}{\left(\frac{dq}{dx} f(x_1) \right)^2} f(x_1) \otimes \left(\frac{dq}{dx} \frac{\partial \varphi}{\partial x_0} \right) \otimes \left[\left(\frac{d^2 q}{dx^2} \frac{\partial \varphi}{\partial x_0} \right) f(x_1) + \frac{dq}{dx} \left(\frac{df}{dx} \frac{\partial \varphi}{\partial x_0} \right) \right] \\
&= B(x_1) \frac{\partial^2 \varphi}{\partial x_0^2} - \frac{1}{\frac{dq}{dx} f(x_1)} \left[\left(\frac{df}{dx} \otimes \frac{dq}{dx} + f(x_1) \otimes \frac{d^2 q}{dx^2} \right) \frac{\partial \varphi}{\partial x_0} \right] \frac{\partial \varphi}{\partial x_0} \\
&\quad + \frac{1}{\left(\frac{dq}{dx} f(x_1) \right)^2} \left(f(x_1) \frac{dq}{dx} \right) \otimes \left[\left(\frac{d^2 q}{dx^2} f(x_1) + \frac{dq}{dx} \frac{df}{dx} \right) \frac{\partial \varphi}{\partial x_0} \right] \frac{\partial \varphi}{\partial x_0} \\
&= B(x_1) \frac{\partial^2 \varphi}{\partial x_0^2} \\
&\quad - \frac{1}{\left(\frac{dq}{dx} f(x_1) \right)^2} \left\{ \left[\left(\frac{df}{dx} \otimes \frac{dq}{dx} + f(x_1) \otimes \frac{d^2 q}{dx^2} \right) \frac{dq}{dx} f(x_1) - \left(f(x_1) \frac{dq}{dx} \right) \otimes \left(\frac{d^2 q}{dx^2} f(x_1) + \frac{dq}{dx} \frac{df}{dx} \right) \right] \frac{\partial \varphi}{\partial x_0} \right\} \frac{\partial \varphi}{\partial x_0} \\
&= B(x_1) \frac{\partial^2 \varphi}{\partial x_0^2} + \left(\frac{dB}{dx} \frac{\partial \varphi}{\partial x_0} \right) \frac{\partial \varphi}{\partial x_0}
\end{aligned}$$