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

$$f : V \to W, \quad g : W \to X. \tag{1}$$

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

$$J_f \in W \otimes V^*, \quad J_g \in X \otimes W^*, \tag{2}$$

where V^* and W^* are the dual spaces of V and W, respectively. J_f is also a map $V \to W$; J_g is $W \to X$. 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

$$H_f \in W \otimes V^* \otimes V^*, \quad H_g \in X \otimes W^* \otimes W^*. \tag{3}$$

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

$$g \circ f : V \to X. \tag{4}$$

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

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

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

$$J_{g \circ f} = \mathrm{tr}_{23} \left(J_g \otimes J_f \right), \tag{6}$$

where

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

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

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

where

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

$$
\begin{aligned}
\left(H_g J_f\right) J_f &= \mathrm{tr}_{24}\left(\left(H_g J_f\right) \otimes J_f\right), \\
\mathrm{tr}_{24} &: (X \otimes W^* \otimes V^*) \otimes (W \otimes V^*) \to X \otimes V^* \otimes V^*,
\end{aligned}
\tag{10}
$$

$$
\begin{aligned}
J_g H_f &= \mathrm{tr}_{23}\left(J_g \otimes H_f\right), \\
J_g \otimes H_f &\in (X \otimes W^*) \otimes (W \otimes V^* \otimes V^*), \\
\mathrm{tr}_{23} &: (X \otimes W^*) \otimes (W \otimes V^* \otimes V^*) \to X \otimes V^* \otimes V^*,
\end{aligned}
\tag{11}
$$

Let T be a composite map of T_i

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

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

$$
J = \frac{\partial T}{\partial \boldsymbol{x}_0} = \prod_{k=0}^{m-1} \frac{\partial T_{m-1-k}}{\partial \boldsymbol{x}_{m-1-k}}. \tag{13}
$$

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

$$
J_{m-1} = \frac{\partial T_{m-1}}{\partial \boldsymbol{x}_{m-1}} J_{m-2}, \tag{14}
$$

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

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

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

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

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

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

where M is a state space, and $\boldsymbol{f}$ is a function such that $M \to \mathbb{R}^n$. We write the trajectory of the system (17) by $\boldsymbol{\varphi} : \mathbb{R} \times M \to M$, where $\boldsymbol{\varphi}(0, \boldsymbol{x}_0) = \boldsymbol{x}_0$ is the initial state and $\boldsymbol{\varphi}(t, \boldsymbol{x}_0)$ is the state at t. Let ∂M be an $n-1$ dimensional manifold defined by a conditional function $q : M \to \mathbb{R}$

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

Suppose that T_0 is a local map from $\boldsymbol{x}_0 \in M$ to a point in ∂M such that $M \to \partial M$. Then, the Jacobian matrix of T_0 is described by

$$J_{T_0} = \frac{\partial T_0}{\partial \boldsymbol{x}_0} = \left[I - \frac{1}{\frac{dq}{d\boldsymbol{x}} \boldsymbol{f}(\boldsymbol{x})} \boldsymbol{f}(\boldsymbol{x}) \frac{dq}{d\boldsymbol{x}} \right] \Bigg|_{\boldsymbol{x}=\boldsymbol{x}_1} \frac{\partial \boldsymbol{\varphi}}{\partial \boldsymbol{x}_0}(\tau) = B(\boldsymbol{x}_1) \frac{\partial \boldsymbol{\varphi}}{\partial \boldsymbol{x}_0}(\tau), \tag{19}$$

where τ is the spent time during the trajectory $\boldsymbol{\varphi}$ moves from $\boldsymbol{x}_0$ to the boundary ∂M, which only depends on $\boldsymbol{x}_0$, and $\boldsymbol{x}_1 = \boldsymbol{\varphi}(\tau, \boldsymbol{x}_0)$. The Hessian tensor of T_0 is

$$H_{T_0} = \left(\frac{\partial B}{\partial \boldsymbol{x}}(\boldsymbol{x}_1) \frac{\partial \boldsymbol{\varphi}}{\partial \boldsymbol{x}_0}(\tau) \right) \frac{\partial \boldsymbol{\varphi}}{\partial \boldsymbol{x}_0}(\tau) + \left(\frac{\partial B}{\partial \boldsymbol{x}}(\boldsymbol{x}_1) B \frac{\partial \boldsymbol{\varphi}}{\partial \boldsymbol{x}_0}(\tau) \right) \frac{\partial \boldsymbol{\varphi}}{\partial \boldsymbol{x}_0}(\tau) + B(\boldsymbol{x}_1) \frac{\partial^2 \boldsymbol{\varphi}}{\partial {\boldsymbol{x}_0}^2}(\tau), \tag{20}$$

where

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

since

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

Check if order “F” or “C”!

On the other hand,

$$\frac{d}{dt} \left(\frac{\partial \boldsymbol{\varphi}}{\partial \boldsymbol{x}_0} \right) = \frac{d\boldsymbol{f}}{d\boldsymbol{x}} \frac{\partial \boldsymbol{\varphi}}{\partial \boldsymbol{x}_0} \tag{23}$$

$$\frac{d}{dt} \left(\frac{\partial^2 \boldsymbol{\varphi}}{\partial {\boldsymbol{x}_0}^2} \right) = \left(\frac{d^2 \boldsymbol{f}}{d\boldsymbol{x}^2} \frac{\partial \boldsymbol{\varphi}}{\partial \boldsymbol{x}_0} \right) \frac{\partial \boldsymbol{\varphi}}{\partial \boldsymbol{x}_0} + \frac{d\boldsymbol{f}}{d\boldsymbol{x}} \frac{\partial^2 \boldsymbol{\varphi}}{\partial {\boldsymbol{x}_0}^2}, \tag{24}$$

where

$$\frac{d^2 \boldsymbol{f}}{d\boldsymbol{x}^2} \frac{\partial \boldsymbol{\varphi}}{\partial \boldsymbol{x}_0} = \mathrm{tr}_{34} \left(\frac{d^2 \boldsymbol{f}}{d\boldsymbol{x}^2} \otimes \frac{\partial \boldsymbol{\varphi}}{\partial \boldsymbol{x}_0} \right), \quad \frac{d\boldsymbol{f}}{d\boldsymbol{x}} \frac{\partial^2 \boldsymbol{\varphi}}{\partial {\boldsymbol{x}_0}^2} = \mathrm{tr}_{23} \left(\frac{d\boldsymbol{f}}{d\boldsymbol{x}} \otimes \frac{\partial^2 \boldsymbol{\varphi}}{\partial {\boldsymbol{x}_0}^2} \right). \tag{25}$$

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

$$
\begin{aligned}
\frac{\partial^2 T_0}{\partial {\boldsymbol{x}_0}^2} &= \frac{\partial^2 \boldsymbol{\varphi}}{\partial {\boldsymbol{x}_0}^2} + \left(\frac{d\boldsymbol{f}}{d\boldsymbol{x}}\frac{\partial \boldsymbol{\varphi}}{\partial \boldsymbol{x}_0}\right)\otimes\frac{\partial \tau}{\partial \boldsymbol{x}_0} + \boldsymbol{f}(\boldsymbol{x}_1)\otimes\frac{\partial^2 \tau}{\partial {\boldsymbol{x}_0}^2} \\
\frac{\partial^2 \tau}{\partial {\boldsymbol{x}_0}^2} &= -\frac{1}{\left(\frac{dq}{d\boldsymbol{x}}\boldsymbol{f}(\boldsymbol{x}_1)\right)^2}\left[\frac{\partial}{\partial \boldsymbol{x}_0}\left(\frac{dq}{d\boldsymbol{x}}\frac{\partial \boldsymbol{\varphi}}{\partial \boldsymbol{x}_0}\right)\frac{dq}{d\boldsymbol{x}}\boldsymbol{f}(\boldsymbol{x}_1) - \left(\frac{dq}{d\boldsymbol{x}}\frac{\partial \boldsymbol{\varphi}}{\partial \boldsymbol{x}_0}\right)\otimes\frac{\partial}{\partial \boldsymbol{x}_0}\left(\frac{dq}{d\boldsymbol{x}}\boldsymbol{f}(\boldsymbol{x}_1)\right)\right] \\
&= -\frac{1}{\left(\frac{dq}{d\boldsymbol{x}}\boldsymbol{f}(\boldsymbol{x}_1)\right)^2}\left\{\left[\left(\frac{d^2q}{d\boldsymbol{x}^2}\frac{\partial \boldsymbol{\varphi}}{\partial \boldsymbol{x}_0}\right)\frac{\partial \boldsymbol{\varphi}}{\partial \boldsymbol{x}_0} + \frac{dq}{d\boldsymbol{x}}\frac{\partial^2 \boldsymbol{\varphi}}{\partial {\boldsymbol{x}_0}^2}\right]\frac{dq}{d\boldsymbol{x}}\boldsymbol{f}(\boldsymbol{x}_1) - \left(\frac{dq}{d\boldsymbol{x}}\frac{\partial \boldsymbol{\varphi}}{\partial \boldsymbol{x}_0}\right)\otimes\left[\left(\frac{d^2q}{d\boldsymbol{x}^2}\frac{\partial \boldsymbol{\varphi}}{\partial \boldsymbol{x}_0}\right)\boldsymbol{f}(\boldsymbol{x}_1) + \frac{dq}{d\boldsymbol{x}}\left(\frac{d\boldsymbol{f}}{d\boldsymbol{x}}\frac{\partial \boldsymbol{\varphi}}{\partial \boldsymbol{x}_0}\right)\right]\right\} \\
&= -\frac{1}{\frac{dq}{d\boldsymbol{x}}\boldsymbol{f}(\boldsymbol{x}_1)}\left[\left(\frac{d^2q}{d\boldsymbol{x}^2}\frac{\partial \boldsymbol{\varphi}}{\partial \boldsymbol{x}_0}\right)\frac{\partial \boldsymbol{\varphi}}{\partial \boldsymbol{x}_0} + \frac{dq}{d\boldsymbol{x}}\frac{\partial^2 \boldsymbol{\varphi}}{\partial {\boldsymbol{x}_0}^2}\right] + \frac{1}{\left(\frac{dq}{d\boldsymbol{x}}\boldsymbol{f}(\boldsymbol{x}_1)\right)^2}\left(\frac{dq}{d\boldsymbol{x}}\frac{\partial \boldsymbol{\varphi}}{\partial \boldsymbol{x}_0}\right)\otimes\left[\left(\frac{d^2q}{d\boldsymbol{x}^2}\frac{\partial \boldsymbol{\varphi}}{\partial \boldsymbol{x}_0}\right)\boldsymbol{f}(\boldsymbol{x}_1) + \frac{dq}{d\boldsymbol{x}}\left(\frac{d\boldsymbol{f}}{d\boldsymbol{x}}\frac{\partial \boldsymbol{\varphi}}{\partial \boldsymbol{x}_0}\right)\right] \\
\frac{\partial^2 T_0}{\partial {\boldsymbol{x}_0}^2} &= B(\boldsymbol{x}_1)\frac{\partial^2 \boldsymbol{\varphi}}{\partial {\boldsymbol{x}_0}^2} - \frac{1}{\frac{dq}{d\boldsymbol{x}}\boldsymbol{f}(\boldsymbol{x}_1)}\left[\left(\frac{d\boldsymbol{f}}{d\boldsymbol{x}}\frac{\partial \boldsymbol{\varphi}}{\partial \boldsymbol{x}_0}\right)\otimes\frac{dq}{d\boldsymbol{x}} + \boldsymbol{f}(\boldsymbol{x}_1)\otimes\left(\frac{d^2q}{d\boldsymbol{x}^2}\frac{\partial \boldsymbol{\varphi}}{\partial \boldsymbol{x}_0}\right)\right]\frac{\partial \boldsymbol{\varphi}}{\partial \boldsymbol{x}_0} \\
&\quad + \frac{1}{\left(\frac{dq}{d\boldsymbol{x}}\boldsymbol{f}(\boldsymbol{x}_1)\right)^2}\boldsymbol{f}(\boldsymbol{x}_1)\otimes\left(\frac{dq}{d\boldsymbol{x}}\frac{\partial \boldsymbol{\varphi}}{\partial \boldsymbol{x}_0}\right)\otimes\left[\left(\frac{d^2q}{d\boldsymbol{x}^2}\frac{\partial \boldsymbol{\varphi}}{\partial \boldsymbol{x}_0}\right)\boldsymbol{f}(\boldsymbol{x}_1) + \frac{dq}{d\boldsymbol{x}}\left(\frac{d\boldsymbol{f}}{d\boldsymbol{x}}\frac{\partial \boldsymbol{\varphi}}{\partial \boldsymbol{x}_0}\right)\right] \\
&= B(\boldsymbol{x}_1)\frac{\partial^2 \boldsymbol{\varphi}}{\partial {\boldsymbol{x}_0}^2} - \frac{1}{\frac{dq}{d\boldsymbol{x}}\boldsymbol{f}(\boldsymbol{x}_1)}\left[\left(\frac{d\boldsymbol{f}}{d\boldsymbol{x}}\otimes\frac{dq}{d\boldsymbol{x}} + \boldsymbol{f}(\boldsymbol{x}_1)\otimes\frac{d^2q}{d\boldsymbol{x}^2}\right)\frac{\partial \boldsymbol{\varphi}}{\partial \boldsymbol{x}_0}\right]\frac{\partial \boldsymbol{\varphi}}{\partial \boldsymbol{x}_0} \\
&\quad + \frac{1}{\left(\frac{dq}{d\boldsymbol{x}}\boldsymbol{f}(\boldsymbol{x}_1)\right)^2}\left(\boldsymbol{f}(\boldsymbol{x}_1)\frac{dq}{d\boldsymbol{x}}\right)\otimes\left[\left(\frac{d^2q}{d\boldsymbol{x}^2}\boldsymbol{f}(\boldsymbol{x}_1) + \frac{dq}{d\boldsymbol{x}}\frac{d\boldsymbol{f}}{d\boldsymbol{x}}\right)\frac{\partial \boldsymbol{\varphi}}{\partial \boldsymbol{x}_0}\right]\frac{\partial \boldsymbol{\varphi}}{\partial \boldsymbol{x}_0} \\
&= B(\boldsymbol{x}_1)\frac{\partial^2 \boldsymbol{\varphi}}{\partial {\boldsymbol{x}_0}^2} \\
&\quad - \frac{1}{\left(\frac{dq}{d\boldsymbol{x}}\boldsymbol{f}(\boldsymbol{x}_1)\right)^2}\left\{\left[\left(\frac{d\boldsymbol{f}}{d\boldsymbol{x}}\otimes\frac{dq}{d\boldsymbol{x}} + \boldsymbol{f}(\boldsymbol{x}_1)\otimes\frac{d^2q}{d\boldsymbol{x}^2}\right)\frac{dq}{d\boldsymbol{x}}\boldsymbol{f}(\boldsymbol{x}_1) - \left(\boldsymbol{f}(\boldsymbol{x}_1)\frac{dq}{d\boldsymbol{x}}\right)\otimes\left(\frac{d^2q}{d\boldsymbol{x}^2}\boldsymbol{f}(\boldsymbol{x}_1) + \frac{dq}{d\boldsymbol{x}}\frac{d\boldsymbol{f}}{d\boldsymbol{x}}\right)\right]\frac{\partial \boldsymbol{\varphi}}{\partial \boldsymbol{x}_0}\right\}\frac{\partial \boldsymbol{\varphi}}{\partial \boldsymbol{x}_0} \\
&= B(\boldsymbol{x}_1)\frac{\partial^2 \boldsymbol{\varphi}}{\partial {\boldsymbol{x}_0}^2} + \left(\frac{dB}{d\boldsymbol{x}}\frac{\partial \boldsymbol{\varphi}}{\partial \boldsymbol{x}_0}\right)\frac{\partial \boldsymbol{\varphi}}{\partial \boldsymbol{x}_0}
\end{aligned}
\tag{27}
$$