Mathematical tools
M2. Tensor functions

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1. Tensor-valued functions of one variable

Example: Tensor depending on time $t \mapsto \mathbf{A}(t)$:

$$\mathbf{A}(t) = A^{ij}(t)\,\mathbf{g}_i \otimes \mathbf{g}_j \qquad \dot{\mathbf{A}}(t) = \frac{d}{dt}(\mathbf{A}(t)) = \dot{A}^{ij}(t)\,\mathbf{g}_i \otimes \mathbf{g}_j$$

in **fixed coordinate system** (when $\mathbf{g}_i$ independent of t).

Rules of differentiation:

$$\begin{aligned}
\frac{d}{dt}(\mathbf{A} \pm \mathbf{B}) &= \dot{\mathbf{A}} \pm \dot{\mathbf{B}} \\
\frac{d}{dt}(f(t)\mathbf{A}(t)) &= f'(t)\mathbf{A} + f(t)\dot{\mathbf{A}} \\
\frac{d}{dt}(\mathbf{A} \otimes \mathbf{B}) &= \dot{\mathbf{A}} \otimes \mathbf{B} + \mathbf{A} \otimes \dot{\mathbf{A}} \\
\frac{d}{dt}\left(\mathbf{A}^T\right) &= \left(\dot{\mathbf{A}}\right)^T \\
\frac{d}{dt}(\mathrm{tr}(\mathbf{A})) &= \mathrm{tr}(\dot{\mathbf{A}})
\end{aligned}$$

2. Scalar-valued functions of tensors

(Real) scalar-valued function of a tensor

$$\Phi(\mathbf{A}) : \mathbf{A} \mapsto \Phi(\mathbf{A}) \in \mathbb{R}$$

Gradient of $\Phi(\mathbf{A})$ with respect to $\mathbf{A}$: there exists a tensor $\frac{\partial \Phi(\mathbf{A})}{\partial \mathbf{A}}$ such that for all $d\mathbf{A}$ there is

$$\Phi(\mathbf{A} + d\mathbf{A}) = \Phi(\mathbf{A}) + \underbrace{\frac{\partial \Phi(\mathbf{A})}{\partial \mathbf{A}} : d\mathbf{A}}_{d\Phi} + o(d\mathbf{A})$$

(first-order Taylor's expansion around $\mathbf{A}$).

- $d\Phi$ is called the **total differential** in the direction $d\mathbf{A}$,
- $o(d\mathbf{A})$ is the **Landau order symbol** for a scalar error which tends to zero faster than $d\mathbf{A} \to \mathbf{0}$, ie.

$$\lim_{d\mathbf{A} \to \mathbf{0}} \frac{o(d\mathbf{A})}{|d\mathbf{A}|} = 0$$

2.1 Is gradient of Φ a tensor?

Example: Let $\mathbf{A}$ be a second-order tensor

$$\mathbf{A} = A^{ij}\, \mathbf{g}_i \otimes \mathbf{g}_j = A^i_{\ j}\, \mathbf{g}_i \otimes \mathbf{g}^j = A_{ij}\, \mathbf{g}^i \otimes \mathbf{g}^j$$

Take $\Phi(\mathbf{A}) = A_{ij} = \mathbf{g}_i \cdot (\mathbf{A}\mathbf{g}_j) = (\mathbf{g}_i \otimes \mathbf{g}_j) : \mathbf{A}$ and evaluate $\frac{\partial A_{ij}}{\partial \mathbf{A}}$ by using the definition:

$$\begin{aligned} \Phi(\mathbf{A} + d\mathbf{A}) &= \Phi(\mathbf{A}) + \frac{\partial \Phi(\mathbf{A})}{\partial \mathbf{A}} : d\mathbf{A} + o(d\mathbf{A}) \\ (\mathbf{g}_i \otimes \mathbf{g}_j) : (\mathbf{A} + d\mathbf{A}) &= (\mathbf{g}_i \otimes \mathbf{g}_j) : \mathbf{A} + (\mathbf{g}_i \otimes \mathbf{g}_j) : d\mathbf{A} \end{aligned}$$

So, $\frac{\partial A_{ij}}{\partial \mathbf{A}} = \mathbf{g}_i \otimes \mathbf{g}_j$. Similarly, $\frac{\partial A^{ij}}{\partial \mathbf{A}} = \mathbf{g}^i \otimes \mathbf{g}^j$ and $\frac{\partial A^i_{\ j}}{\partial \mathbf{A}} = \mathbf{g}^i \otimes \mathbf{g}_j$.

For any smooth $\Phi(\mathbf{A})$: express Φ in terms of components A_{ij} of $\mathbf{A}$ in some basis $\mathcal{B} = \langle \mathbf{g}^1, \ldots, \mathbf{g}^n \rangle$:

$$\frac{\partial \Phi(\mathbf{A})}{\partial \mathbf{A}} = \frac{\partial \Phi(\mathbf{A})}{\partial A_{ij}} \frac{\partial A_{ij}}{\partial \mathbf{A}} = \frac{\partial \Phi(\mathbf{A})}{\partial A_{ij}}\, \mathbf{g}_i \otimes \mathbf{g}_j = \phi^{,ij}\, \mathbf{g}_i \otimes \mathbf{g}_j$$

Yes, $\frac{\partial \Phi(\mathbf{A})}{\partial \mathbf{A}}$ is a tensor. Derivatives of Φ with respect to covariant components A_{ij} give contravariant components of gradient!

2.2 Application of scalar invariants for $\frac{\partial \det(\mathbf{A})}{\partial \mathbf{A}}$

If a 2nd-order tensor A is invertible, then

$$\frac{\partial \det(\mathbf{A})}{\partial \mathbf{A}} = \det(\mathbf{A})\,\mathbf{A}^{-T}$$

Proof: by using the definition of $\frac{\partial \Phi}{\partial \mathbf{A}}$ and:

$$\det(\mathbf{A} + d\mathbf{A}) = \det\left[\mathbf{A}\left(\mathbf{I} + \mathbf{A}^{-1} d\mathbf{A}\right)\right] = \det(\mathbf{A})\,\det(\mathbf{I} + \mathbf{A}^{-1} d\mathbf{A})$$

Characteristic polynomial $p(\mathbf{M})$ of $\mathbf{M}$ in scalar invariants:

$$p_{\mathbf{M}}(\lambda) = \det(\mathbf{M} - \lambda\mathbf{I}) = -\left[\lambda^3 - I_1(\mathbf{M})\lambda^2 + I_2(\mathbf{M})\lambda - I_3(\mathbf{M})\right]$$

Hence, for $\mathbf{M} = \mathbf{A}^{-1}\, d\mathbf{A}$ and $\lambda = -1$ we get:

$$\begin{aligned} \det(\mathbf{I} + \mathbf{A}^{-1} d\mathbf{A}) &= 1 + I_1(\mathbf{A}^{-1} d\mathbf{A}) + I_2(\mathbf{A}^{-1} d\mathbf{A}) + I_3(\mathbf{A}^{-1} d\mathbf{A}) \\ &= 1 + \mathrm{tr}(\mathbf{A}^{-1}\, d\mathbf{A}) + o(d\mathbf{A}) \end{aligned}$$

because I_2 and I_3 are quadratic resp. cubic in $d\mathbf{A}$.

2.2 Application of scalar invariants for $\frac{\partial \det(\mathbf{A})}{\partial \mathbf{A}}$

Hence:

$$\begin{aligned} \det(\mathbf{A} + d\mathbf{A}) &= \det(\mathbf{A})\,\det(\mathbf{I} + \mathbf{A}^{-1} d\mathbf{A}) \\ &= \det(\mathbf{A}) + \det(\mathbf{A})\,\mathrm{tr}(\mathbf{A}^{-1}\, d\mathbf{A}) + o(d\mathbf{A}) \\ &= \det(\mathbf{A}) + \mathrm{tr}(\det(\mathbf{A})\,\mathbf{A}^{-1}\, d\mathbf{A}) + o(d\mathbf{A}) \\ &= \det(\mathbf{A}) + \det(\mathbf{A})\,\mathbf{A}^{-T} : d\mathbf{A} + o(d\mathbf{A}) \end{aligned}$$

And by comparing with the definition of gradient:

$$\Phi(\mathbf{A} + d\mathbf{A}) = \Phi(\mathbf{A}) + \frac{\partial \Phi(\mathbf{A})}{\partial \mathbf{A}} : d\mathbf{A} + o(d\mathbf{A})$$

we get

$$\frac{\partial \det(\mathbf{A})}{\partial \mathbf{A}} = \det(\mathbf{A})\,\mathbf{A}^{-T}$$

3. Gradient of tensor-valued functions of tensors

(Real) tensor-valued function of a tensor

$$\mathbf{A}(\mathbf{B}) : \mathbf{B} \mapsto \mathbf{A}(\mathbf{B})$$

Gradient of $\mathbf{A}(\mathbf{B})$ with respect to $\mathbf{B}$: there exists a tensor $\frac{\partial \mathbf{A}(\mathbf{B})}{\partial \mathbf{B}}$ such that for all $d\mathbf{B}$ there is

$$\mathbf{A}(\mathbf{B}+d\mathbf{B}) = \mathbf{A}(\mathbf{B}) + \underbrace{\frac{\partial \mathbf{A}(\mathbf{B})}{\partial \mathbf{B}} : d\mathbf{B}}_{d\mathbf{A}} + o(d\mathbf{B})$$

(first-order Taylor's expansion around $\mathbf{B}$).

- order of the tensor $\frac{\partial \mathbf{A}(\mathbf{B})}{\partial \mathbf{B}}$: sum of orders of $\mathbf{A}$ and of $\mathbf{B}$.
- special case: for $\mathbf{A}$ second-order tensor, $\frac{\partial \mathbf{A}}{\partial \mathbf{A}} = \mathbb{I}$, a fourth-order identity tensor (defined by $\mathbf{A} = \mathbb{I} : \mathbf{A}$).
  Component-wise (in some basis): $\frac{\partial A_{ij}}{\partial A_{k\ell}} = \delta_i^k \cdot \delta_j^\ell$.

3.1 Derivative of $\mathbf{A}^{-1}$ with respect to $\mathbf{A}$

If a 2nd-order tensor A is invertible, then

$$\left(\frac{\partial \mathbf{A}^{-1}}{\partial \mathbf{A}}\right)_{ij,k\ell} = \frac{\partial A^{-1}_{\ \ ij}}{\partial A^{k\ell}} = -A^{-1}_{\ \ ik}\, A^{-1}_{\ \ \ell j}$$

component-wise (in some basis).

Proof:

$$0 = \frac{\partial(\delta_i^k)}{\partial A^{mn}} = \frac{\partial (A^{-1}_{\ \ ij} A^{jk})}{\partial A^{mn}} = \frac{\partial A^{-1}_{\ \ ij}}{\partial A^{mn}} A^{jk} + A^{-1}_{\ \ ij} \underbrace{\frac{\partial A^{jk}}{\partial A^{mn}}}_{\delta_m^j \delta_n^k}$$

Hence, multiplied by $A^{-1}_{\ \ k\ell}$ and re-arranged:

$$\frac{\partial A^{-1}_{\ \ i\ell}}{\partial A^{mn}} = \frac{\partial A^{-1}_{\ \ ij}}{\partial A^{mn}} \delta_\ell^j = \frac{\partial A^{-1}_{\ \ ij}}{\partial A^{mn}} A^{jk} A^{-1}_{\ \ k\ell} = -A^{-1}_{\ \ im} A^{-1}_{\ \ n\ell}$$