

Mathematics for Machine Learning

— Vector Calculus: Gradients of Vector-Valued Functions and Matrices

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Credits for the resource

- The slides are based on the textbooks:
 - *Marc Peter Deisenroth, A. Aldo Faisal, and Cheng Soon Ong: Mathematics for Machine Learning. Cambridge University Press. 2020.*
 - *Howard Anton, Chris Rorres, Anton Kaul: Elementary Linear Algebra. Wiley. 2019.*
- We could partially refer to the monograph:
Francesco Orabona: A Modern Introduction to Online Learning.
<https://arxiv.org/abs/1912.13213>

Outline

1 Gradients of Vector-Valued Functions

2 Gradients of Matrices

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1 Gradients of Vector-Valued Functions

2 Gradients of Matrices

Our Focus

- Partial derivatives and gradients of functions $f : \mathbb{R}^n \mapsto \mathbb{R}^m$, for $n \geq 1, m > 1$.

Vector of Functions

Given

- $\mathbf{f} : \mathbb{R}^n \mapsto \mathbb{R}^m$.
- $\mathbf{x} = [x_1, \dots, x_n]^\top \in \mathbb{R}^n$.

The corresponding *vector of functions*:

$$\mathbf{f}[\mathbf{x}] = \begin{bmatrix} f_1(\mathbf{x}) \\ \vdots \\ f_m(\mathbf{x}) \end{bmatrix} \in \mathbb{R}^m.$$

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The corresponding *vector of functions*:

$$\mathbf{f}[\mathbf{x}] = \begin{bmatrix} f_1(\mathbf{x}) \\ \vdots \\ f_m(\mathbf{x}) \end{bmatrix} \in \mathbb{R}^m.$$

We can view \mathbf{f} as $[f_1, \dots, f_m]^\top$, such that $f_i : \mathbb{R}^n \mapsto \mathbb{R}$.

Therefore,

$$\frac{\partial \mathbf{f}}{\partial x_i} = \begin{bmatrix} \frac{\partial f_1}{\partial x_i} \\ \vdots \\ \frac{\partial f_m}{\partial x_i} \end{bmatrix} = \begin{bmatrix} \lim_{h \rightarrow 0} \frac{f_1(x_1, \dots, x_{i-1}, x_i + h, x_{i+1}, \dots, x_n) - f_1(\mathbf{x})}{h} \\ \vdots \\ \lim_{h \rightarrow 0} \frac{f_m(x_1, \dots, x_{i-1}, x_i + h, x_{i+1}, \dots, x_n) - f_m(\mathbf{x})}{h} \end{bmatrix} \in \mathbb{R}^m.$$

So,

$$\begin{aligned}\frac{d\mathbf{f}}{d\mathbf{x}} &= \left[\frac{\partial \mathbf{f}(\mathbf{x})}{\partial x_1} \quad \dots \quad \frac{\partial \mathbf{f}(\mathbf{x})}{\partial x_n} \right] \\ &= \begin{bmatrix} \frac{\partial f_1(\mathbf{x})}{\partial x_1} & \dots & \frac{\partial f_1(\mathbf{x})}{\partial x_n} \\ \vdots & & \vdots \\ \frac{\partial f_m(\mathbf{x})}{\partial x_1} & \dots & \frac{\partial f_m(\mathbf{x})}{\partial x_n} \end{bmatrix} \in \mathbb{R}^{m \times n}.\end{aligned}$$

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- We call this collection of all first-order partial derivatives of a vector-valued function \mathbf{f} the **Jacobian**.

So,

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- We call this collection of all first-order partial derivatives of a vector-valued function \mathbf{f} the **Jacobian**.

- ★ Denote by $\mathbf{J} = \nabla_{\mathbf{x}} \mathbf{f} = \frac{d\mathbf{f}(\mathbf{x})}{d\mathbf{x}}$
 - $J(i, j) = \frac{\partial f_i}{\partial x_j}$.

Example

Derivative of a Polynomial

Given $\mathbf{f}(\mathbf{x}) = \mathbf{A}\mathbf{x}$, $\mathbf{f}(\mathbf{x}) \in \mathbb{R}^M$, $\mathbf{A} \in \mathbb{R}^{M \times N}$, and $\mathbf{x} \in \mathbb{R}^N$. Compute

$$\frac{d\mathbf{f}}{d\mathbf{x}} = ?$$

Note:

- $\mathbf{f} : \mathbb{R}^N \mapsto \mathbb{R}^M$, so $\frac{d\mathbf{f}}{d\mathbf{x}} \in \mathbb{R}^{M \times N}$.
- $f_i(\mathbf{x}) =$

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Example: Gradient of a Least-Squared Loss in a Linear Model

Consider the linear model

$$\mathbf{y} = \Phi\boldsymbol{\theta},$$

where

- $\boldsymbol{\theta} \in \mathbb{R}^D$: a parameter vector
- $\Phi \in \mathbb{R}^{N \times D}$: input features
- $\mathbf{y} \in \mathbb{R}^N$: the corresponding observations.

We define that

$$L(\mathbf{e}) := \|\mathbf{e}\|^2.$$

$$\mathbf{e}(\boldsymbol{\theta}) := \mathbf{y} - \Phi\boldsymbol{\theta}.$$

Compute $\frac{\partial L}{\partial \boldsymbol{\theta}}$ (using the chain rule).

Example (2/3)

Note that

- $\frac{\partial L}{\partial \theta} \in \mathbb{R}^{1 \times D}$ ($\because L : \mathbb{R}^D \mapsto \mathbb{R}$).
- $\frac{\partial \mathbf{e}}{\partial \theta} \in \mathbb{R}^{N \times D}$ ($\because \mathbf{e} : \mathbb{R}^D \mapsto \mathbb{R}^N$).
- $\frac{\partial L}{\partial \mathbf{e}} \in \mathbb{R}^{1 \times N}$ ($\because L : \mathbb{R}^N \mapsto \mathbb{R}$).
- $\frac{\partial L}{\partial \theta} = \frac{\partial L}{\partial \mathbf{e}} \frac{\partial \mathbf{e}}{\partial \theta}$ (chain rule).

- The d th element:

$$\frac{\partial L}{\partial \theta}[1, d] = \sum_{i=1}^N \frac{\partial L}{\partial \mathbf{e}}[1, i] \frac{\partial \mathbf{e}}{\partial \theta}[i, d].$$

- $L = \|\mathbf{e}\|^2 = \mathbf{e}^\top \mathbf{e}$ and $\frac{\partial L}{\partial \mathbf{e}} = 2\mathbf{e}^\top \in \mathbb{R}^{1 \times N}$.
- $\frac{\partial \mathbf{e}}{\partial \theta} = -\Phi \in \mathbb{R}^{N \times D}$.

Example (3/3)

$$\frac{\partial L}{\partial \boldsymbol{\theta}} = -2\mathbf{e}^\top \boldsymbol{\Phi} = -2(\mathbf{y}^\top - \boldsymbol{\theta}^\top \boldsymbol{\Phi}^\top) \boldsymbol{\Phi} \in \mathbb{R}^{1 \times D}$$

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By the way, we can obtain the same result without using the chain rule:

$$L_2(\boldsymbol{\theta}) := \|\mathbf{y} - \boldsymbol{\Phi}\boldsymbol{\theta}\|^2 = (\mathbf{y} - \boldsymbol{\Phi}\boldsymbol{\theta})^\top (\mathbf{y} - \boldsymbol{\Phi}\boldsymbol{\theta}).$$

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$$\frac{\partial L}{\partial \boldsymbol{\theta}} = -2\mathbf{e}^\top \Phi = -2(\mathbf{y}^\top - \boldsymbol{\theta}^\top \Phi^\top) \Phi \in \mathbb{R}^{1 \times D}$$

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- It becomes impractical for deep function compositions.

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Motivations

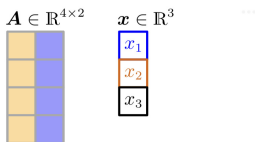
- There are scenarios that we need to take gradients of matrices w.r.t. vectors (or other matrices).
 - ⇒ This results in a multidimensional tensor.
 - Multidimensional array.
- Compute the gradient of an $m \times n$ matrix \mathbf{A} w.r.t. a $p \times q$ matrix \mathbf{B} :
 - The Jacobian \mathbf{J} would be $(m \times n) \times (p \times q)$ (4-dimensional tensor).
 - $J_{ijkl} = \frac{\partial A_{ij}}{\partial B_{kl}}$.
- Matrices \Leftrightarrow linear mappings, so

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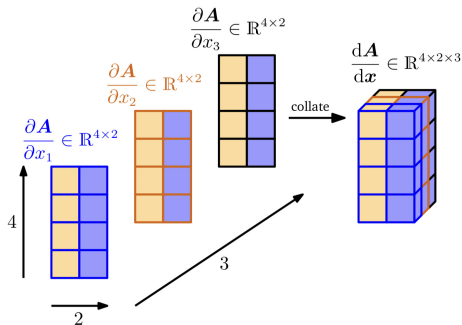
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 - $J_{ijkl} = \frac{\partial A_{ij}}{\partial B_{kl}}$.
- Matrices \Leftrightarrow linear mappings, so

There is a vector-space isomorphism (i.e., linear, invertible mapping) between the space $\mathbb{R}^{m \times n}$ of $m \times n$ matrices and the space \mathbb{R}^{mn} of mn vectors.

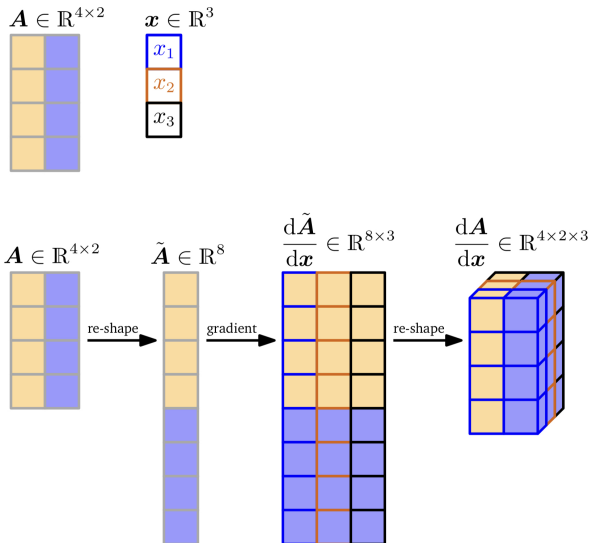
Visualization of Two Approaches for the Isomorphism

$$\mathbf{A} \in \mathbb{R}^{4 \times 2} \quad \mathbf{x} \in \mathbb{R}^3$$


Partial derivatives:



Visualization of Two Approaches for the Isomorphism



Example: Gradient of Vectors w.r.t. Matrices

Consider

$$\mathbf{f} = \mathbf{A}\mathbf{x}, \text{ where } \mathbf{f} \in \mathbb{R}^M, \mathbf{A} \in \mathbb{R}^{M \times N}, \mathbf{x} \in \mathbb{R}^N.$$

Goal: Compute the gradient $\frac{d\mathbf{f}}{d\mathbf{A}}$.

Note:

- $\frac{d\mathbf{f}}{d\mathbf{A}} \in$

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Goal: Compute the gradient $\frac{d\mathbf{f}}{d\mathbf{A}}$.

Note:

- $\frac{d\mathbf{f}}{d\mathbf{A}} \in \mathbb{R}^{M \times (M \times N)}.$

$$\frac{d\mathbf{f}}{d\mathbf{A}} =$$

$$\frac{d\mathbf{f}}{d\mathbf{A}} = \begin{bmatrix} \frac{\partial f_1}{\partial \mathbf{A}} \\ \vdots \\ \frac{\partial f_M}{\partial \mathbf{A}} \end{bmatrix},$$

$$\frac{d\mathbf{f}}{d\mathbf{A}} = \begin{bmatrix} \frac{\partial f_1}{\partial \mathbf{A}} \\ \vdots \\ \frac{\partial f_M}{\partial \mathbf{A}} \end{bmatrix}, \frac{\partial f_i}{\partial \mathbf{A}} \in \mathbb{R}^{1 \times (M \times N)}.$$

$$\frac{d\mathbf{f}}{d\mathbf{A}} = \begin{bmatrix} \frac{\partial f_1}{\partial \mathbf{A}} \\ \vdots \\ \frac{\partial f_M}{\partial \mathbf{A}} \end{bmatrix}, \quad \frac{\partial f_i}{\partial \mathbf{A}} \in \mathbb{R}^{1 \times (M \times N)}.$$

- We can explicitly expand $f_i = \sum_{j=1}^N A_{ij}x_j$, for $i = 1, \dots, M$.

Hence,

$$\frac{\partial f_i}{\partial A_{iq}} = x_q.$$

So we can derive

$$\frac{\partial f_i}{\partial A_{i,:}} = \mathbf{x}^\top$$

$$\frac{d\mathbf{f}}{d\mathbf{A}} = \begin{bmatrix} \frac{\partial f_1}{\partial \mathbf{A}} \\ \vdots \\ \frac{\partial f_M}{\partial \mathbf{A}} \end{bmatrix}, \quad \frac{\partial f_i}{\partial \mathbf{A}} \in \mathbb{R}^{1 \times (M \times N)}.$$

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$$\frac{\partial f_i}{\partial A_{i,:}} = \mathbf{x}^\top \in \mathbb{R}^{1 \times (1 \times N)} \quad \text{and} \quad \frac{\partial f_i}{\partial A_{k \neq i,:}} = \mathbf{0}^\top \in \mathbb{R}^{1 \times (1 \times N)}.$$

Stack the partial derivatives:

$$\frac{\partial f_i}{\partial \mathbf{A}} = \begin{bmatrix} \mathbf{0}^\top \\ \vdots \\ \mathbf{0}^\top \\ \mathbf{x}^\top \\ \mathbf{0}^\top \\ \vdots \\ \mathbf{0}^\top \end{bmatrix} \in \mathbb{R}^{1 \times (M \times N)}$$

Example: Gradient of **Matrices** w.r.t. Matrices

Consider a matrix $\mathbf{R} \in \mathbb{R}^{M \times N}$ and $\mathbf{f} : \mathbb{R}^{M \times N} \mapsto \mathbb{R}^{N \times N}$ with

$$\mathbf{f}(\mathbf{R}) = \mathbf{R}^\top \mathbf{R} := \mathbf{K} \in \mathbb{R}^{N \times N}$$

Goal: Compute the gradient $\frac{d\mathbf{K}}{d\mathbf{R}}$.

Note:

- $\frac{d\mathbf{K}}{d\mathbf{R}} \in$

Example: Gradient of **Matrices** w.r.t. Matrices

Consider a matrix $\mathbf{R} \in \mathbb{R}^{M \times N}$ and $\mathbf{f} : \mathbb{R}^{M \times N} \mapsto \mathbb{R}^{N \times N}$ with

$$\mathbf{f}(\mathbf{R}) = \mathbf{R}^\top \mathbf{R} := \mathbf{K} \in \mathbb{R}^{N \times N}$$

Goal: Compute the gradient $\frac{d\mathbf{K}}{d\mathbf{R}}$.

Note:

- $\frac{d\mathbf{K}}{d\mathbf{R}} \in \mathbb{R}^{(N \times N) \times (M \times N)}$.
- $\frac{dK_{pq}}{d\mathbf{R}} \in \mathbb{R}^{1 \times (M \times N)}$, for $p, q = 1, \dots, N$, K_{pq} : the (p, q) th entry of \mathbf{K} .

$$K_{pq} = \mathbf{r}_p^\top \mathbf{r}_q = \sum_{t=1}^M R_{tp} R_{tq}.$$

\mathbf{r}_i : the i th column of \mathbf{R} .

Example (2/2)

Compute $\frac{\partial K_{pq}}{\partial R_{ij}}$: (sum rule)

$$\frac{\partial K_{pq}}{\partial R_{ij}} = \sum_{t=1}^M \frac{\partial}{\partial R_{ij}} R_{tp} R_{tq} = \delta_{pqij},$$

where

$$\delta_{pqij} = \begin{cases} R_{iq} & \text{if } j = p, p \neq q \\ R_{ip} & \text{if } j = q, p \neq q \\ 2R_{iq} & \text{if } j = p, p = q \\ 0 & \text{otherwise} \end{cases}$$

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Hence, each entry of the desired gradient $\frac{d\mathbf{K}}{d\mathbf{R}} \in \mathbb{R}^{(N \times N) \times (M \times N)}$ is δ_{pqij} , for $p, q, j = 1, \dots, N$ and $i = 1, \dots, M$.

Useful Identities for Computing Gradients (1/2)

Reference: The Matrix Cookbook by Petersen and Pedersen, 2012.

$$\frac{\partial}{\partial \mathbf{X}} f(\mathbf{X})^\top = \left(\frac{\partial f(\mathbf{X})}{\partial \mathbf{X}} \right)^\top.$$

$$\frac{\partial}{\partial \mathbf{X}} \text{tr}(f(\mathbf{X})) = \text{tr} \left(\frac{\partial f(\mathbf{X})}{\partial \mathbf{X}} \right).$$

$$\frac{\partial}{\partial \mathbf{X}} \det(f(\mathbf{X})) = \det(f(\mathbf{X})) \text{tr} \left(f(\mathbf{X})^{-1} \frac{\partial f(\mathbf{X})}{\partial \mathbf{X}} \right)$$

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$$\frac{\partial}{\partial \mathbf{X}} \det(f(\mathbf{X})) = \det(f(\mathbf{X})) \text{tr} \left(f(\mathbf{X})^{-1} \frac{\partial f(\mathbf{X})}{\partial \mathbf{X}} \right) \Rightarrow \text{Jacobi's formula}$$

$$\frac{\partial}{\partial \mathbf{X}} f(\mathbf{X})^{-1} = -f(\mathbf{X})^{-1} \frac{\partial f(\mathbf{X})}{\partial \mathbf{X}} f(\mathbf{X})^{-1}$$

$$\frac{\partial \mathbf{a}^\top \mathbf{X}^{-1} \mathbf{b}}{\partial \mathbf{X}} = -(\mathbf{X}^{-1})^\top \mathbf{a} \mathbf{b}^\top (\mathbf{X}^{-1})^\top$$

Useful Identities for Computing Gradients (2/2)

$$\frac{\partial \mathbf{x}^\top \mathbf{a}}{\partial \mathbf{x}} = \mathbf{a}^\top$$

$$\frac{\partial \mathbf{a}^\top \mathbf{x}}{\partial \mathbf{x}} = \mathbf{a}^\top$$

$$\frac{\partial \mathbf{a}^\top \mathbf{X} \mathbf{b}}{\partial \mathbf{X}} = \mathbf{a} \mathbf{b}^\top$$

$$\frac{\partial \mathbf{x}^\top \mathbf{B} \mathbf{x}}{\partial \mathbf{x}} = \mathbf{x}^\top (\mathbf{B} + \mathbf{B}^\top)$$

$$\frac{\partial}{\partial \mathbf{s}} (\mathbf{x} - \mathbf{A} \mathbf{s})^\top \mathbf{W} (\mathbf{x} - \mathbf{A} \mathbf{s}) = -2(\mathbf{x} - \mathbf{A} \mathbf{s})^\top \mathbf{W} \mathbf{A} \text{ for symmetric } \mathbf{W}.$$

Clarification of some identities

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About the last formula

For symmetric \mathbf{W} ,

$$\frac{\partial}{\partial \mathbf{s}} (\mathbf{x} - \mathbf{A}\mathbf{s})^\top \mathbf{W} (\mathbf{x} - \mathbf{A}\mathbf{s}) = -2(\mathbf{x} - \mathbf{A}\mathbf{s})^\top \mathbf{W} \mathbf{A}.$$

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Let $\mathbf{z} = \mathbf{x} - \mathbf{A}\mathbf{s}$ and use

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Let $\mathbf{z} = \mathbf{x} - \mathbf{A}\mathbf{s}$ and use

$$\frac{\partial \mathbf{z}^\top \mathbf{W} \mathbf{z}}{\partial \mathbf{z}} = \mathbf{z}^\top (\mathbf{W} + \mathbf{W}^\top)$$

Then compute

$$\frac{\partial \mathbf{z}^\top \mathbf{W} \mathbf{z}}{\partial \mathbf{z}} \frac{\partial \mathbf{z}}{\partial \mathbf{s}}.$$

A sketch of Jacobi's formula

Reference: Wikipedia page.

$$\frac{\partial}{\partial \mathbf{X}} \det(f(\mathbf{X})) = \det(f(\mathbf{X})) \operatorname{tr} \left(f(\mathbf{X})^{-1} \frac{\partial f(\mathbf{X})}{\partial \mathbf{X}} \right)$$

- To simplify the discussion, let $\mathbf{M} := f(\mathbf{X})$ and denote the differential of \mathbf{M} by $d\mathbf{M}$. We omit the sizes of matrices if the context is clear.

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- To simplify the discussion, let $\mathbf{M} := f(\mathbf{X})$ and denote the differential of \mathbf{M} by $d\mathbf{M}$. We omit the sizes of matrices if the context is clear.

That is,

$$d \det(\mathbf{M}) = \det(\mathbf{M}) \operatorname{tr}(\mathbf{M}^{-1} d\mathbf{M}).$$

Fact

$$\sum_i \sum_j \mathbf{A}_{ij} \mathbf{B}_{ij} = \operatorname{tr}(\mathbf{A}^\top \mathbf{B}) \text{ for any square matrices } \mathbf{A}, \mathbf{B}.$$

A sketch of Jacobi's formula (2/4)

By the cofactor expansion, we have

$$\det(\mathbf{M}) = \sum_j \mathbf{M}_{ij} \operatorname{adj}^\top(\mathbf{M})_{ij}$$

and recall that

$$\mathbf{M} \operatorname{adj}^\top(\mathbf{M}) = \det(\mathbf{M}) \mathbf{I},$$

A sketch of Jacobi's formula (2/4)

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which means

$$\mathbf{M}^{-1} = \frac{1}{\det(\mathbf{M})} \operatorname{adj}^\top(\mathbf{M}).$$

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Thus, we are actually proving

$$\mathrm{d} \det(\mathbf{M}) = \det(\mathbf{M}) \operatorname{tr}(\mathbf{M}^{-1} \mathrm{d}\mathbf{M}) = \operatorname{tr}(\operatorname{adj}^\top(\mathbf{M}) \mathrm{d}\mathbf{M}).$$

Note

- Assume $\det \mathbf{M} = F(\mathbf{M}_{11}, \mathbf{M}_{12}, \dots, \mathbf{M}_{nn})$ is a function of $\mathbf{M}_{11}, \mathbf{M}_{12}, \dots, \mathbf{M}_{nn}$ and $\mathbf{M}_{ij} := \mathbf{M}_{ij}(t)$. Then,

$$\frac{d}{dt} \det(\mathbf{M}) = \sum_i \sum_j \frac{\partial F}{\partial \mathbf{M}_{ij}} \frac{d\mathbf{M}_{ij}}{dt}.$$

That is,

$$d \det(\mathbf{M}) = \sum_i \sum_j \frac{\partial F}{\partial \mathbf{M}_{ij}} d\mathbf{M}_{ij}.$$

A sketch of Jacobi's formula (3/4)

Differential of the cofactor expansion:

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$$\frac{\partial \det(\mathbf{M})}{\partial \mathbf{M}_{ij}} = \frac{\partial \sum_k \mathbf{M}_{ik} \text{adj}^\top(\mathbf{M})_{ik}}{\partial \mathbf{M}_{ij}} = \sum_k \frac{\partial \mathbf{M}_{ik} \text{adj}^\top(\mathbf{M})_{ik}}{\partial \mathbf{M}_{ij}}$$

Applying the product rule we can derive

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Applying the product rule we can derive

$$\begin{aligned} \frac{\partial \det(\mathbf{M})}{\partial \mathbf{M}_{ij}} &= \sum_k \frac{\partial \mathbf{M}_{ik}}{\partial \mathbf{M}_{ij}} \operatorname{adj}^\top(\mathbf{M})_{ik} + \sum_k \mathbf{M}_{ik} \frac{\partial \operatorname{adj}^\top(\mathbf{M})_{ik}}{\partial \mathbf{M}_{ij}} \\ &= \sum_k \frac{\partial \mathbf{M}_{ik}}{\partial \mathbf{M}_{ij}} \operatorname{adj}^\top(\mathbf{M})_{ik}. \end{aligned}$$

A sketch of Jacobi's formula (4/4)

Note that

$$\frac{\partial \mathbf{M}_{ik}}{\partial \mathbf{M}_{ij}} = \delta_{jk}$$

where $\delta_{jk} = 1$ if $j = k$ and 0 otherwise. So,

A sketch of Jacobi's formula (4/4)

Note that

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$$\frac{\partial \det(\mathbf{M})}{\partial \mathbf{M}_{ij}} = \sum_k \delta_{jk} \operatorname{adj}^\top(\mathbf{M})_{ik} = \operatorname{adj}^\top(\mathbf{M})_{ij}.$$

Thus,

$$\mathrm{d} \det(\mathbf{M}) = \sum_i \sum_j \operatorname{adj}^\top(\mathbf{M})_{ij} \mathrm{d} \mathbf{M}_{ij} = \operatorname{tr}(\operatorname{adj}(\mathbf{M}) \mathrm{d} \mathbf{M}).$$

Discussions