QUY NHON UNIVERSITY
DEPARTMENT OF MATHEMATICS AND STATISTICS

Vector Caculus

Nguyen Quoc Duong

Master's Student, Department of Mathematics and Statistics, Quy Nhon University

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Roadmap

Summary

- Machine learning is about solving an optimization problem whose variables are the parameters of a given model.
- Solving optimization problems require gradient information.
- Central to this chapter is the concept of the function, which we often write

$$
\begin{aligned}
f : \mathbb{R}^D &\mapsto \mathbb{R} \\
\boldsymbol{x} &\mapsto f(\boldsymbol{x})
\end{aligned}
$$

Roadmap

(1) Differentiation of Univariate Functions

(2) Partial Differentiation and Gradients

(3) Gradients of Vector-Valued Functions

(4) Gradients of Matrices

(5) Useful Identities for Computing Gradients

(6) Backpropagation and Automatic Differentiation

(7) Higher-Order Derivatives

(8) Linearization and Multivariate Taylor Series

Difference Quotient and Derivative

- Difference Quotient. The average slope of f between x and $x + \partial x$

$$\frac{\partial y}{\partial x} := \frac{f(x + \partial x) - f(x)}{\partial x}$$

- Derivative. Pointing in the direction of steepest ascent of f.

$$\frac{\mathrm{d}f}{\mathrm{d}x} := \lim_{h \to 0} \frac{f(x + h) - f(x)}{h}$$

- Unless confusion arises, we often use $f' = \frac{\mathrm{d}f}{\mathrm{d}x}$.

Taylor Series

- Representation of a function as an infinite sum of terms, using derivatives of evaluated at x_0.

- Taylor polynomial. The Taylor polynomial of degree n of $f : \mathbb{R} \mapsto \mathbb{R}$ at x_0 is:

$$T_n(x) := \sum_{k=0}^{n} \frac{f^{(k)}(x_0)}{k!}(x - x_0)^k, \text{ where } f^{(k)}(x_0) \text{ is the } k\text{th derivative of } f$$

- Taylor Series. For a smooth function $f \in \mathcal{C}^\infty$, the Taylor series of f at x_0 is:

$$T_\infty(x) := \sum_{k=0}^{\infty} \frac{f^{(k)}(x_0)}{k!}(x - x_0)^k.$$

- If $f(x) = T_\infty(x)$, f is called analytic.

Differentiation Rules

- Product rule. $(f(x)g(x))' = f'(x)g(x) + f(x)g'(x)$
- Quotient rule. $\left(\frac{f(x)}{g(x)}\right)' = \frac{f'(x)g(x) - f(x)g'(x)}{(g(x))^2}$
- Sum rule. $(f(x) + g(x))' = f'(x) + g'(x)$
- Chain rule. $(g(f(x)))' = g'(f(x))f'(x)$

Roadmap

Gradient

- Now, $f : \mathbb{R}^n \mapsto \mathbb{R}$.
- Gradient of f w.r.t. $\boldsymbol{x}$ $\nabla_{\boldsymbol{x}} f$: Varying one variable at a time and keeping the others constant.

Partial Derivative. For $f : \mathbb{R}^n \mapsto \mathbb{R}$,

$$\frac{\partial f}{\partial x_1} = \lim_{h \to 0} \frac{f(x_1 + h, x_2, \ldots, x_n) - f(\boldsymbol{x})}{h}$$

$$\vdots$$

$$\frac{\partial f}{\partial x_n} = \lim_{h \to 0} \frac{f(x_1, x_2, \ldots, x_n + h) - f(\boldsymbol{x})}{h}$$

Gradient. Get the partial derivatives and collect them in the row vector.

$$\nabla_{\boldsymbol{x}} f = \frac{\mathrm{d} f}{\mathrm{d} \boldsymbol{x}} = \begin{pmatrix} \frac{\partial f(\boldsymbol{x})}{\partial x_1} & \cdots & \frac{\partial f(\boldsymbol{x})}{\partial x_n} \end{pmatrix} \in \mathbb{R}^{1 \times n}$$

Example

- Example. $f(x, y) = (x + 2y^3)^2$

$$\frac{\partial f(x,y)}{\partial x} = 2(x+2y^3)\frac{\partial x + 2y^3}{\partial x} = 2(x+2y^3)$$
$$\frac{\partial f(x,y)}{\partial y} = 2(x+2y^3)\frac{\partial x + 2y^3}{\partial y} = 12(x+2y^3)y^2$$

- Example. $f(x_1, x_2) = x_1^2 x_2 + x_1 x_2^3$

$$\nabla_{(x_1,x_2)} f = \frac{\mathrm{d}f}{\mathrm{d}x} = \begin{pmatrix} \frac{\partial f(x_1,x_2)}{\partial x_1} & \frac{\partial f(x_1,x_2)}{\partial x_2} \end{pmatrix} = \begin{pmatrix} 2x_1x_2 + x_2^3 & x_1^2 + 3x_1x_2^2 \end{pmatrix}$$

Rules for Partial Differentiation

- Product rule

$$\frac{\partial}{\partial \boldsymbol{x}}\big(f(\boldsymbol{x})g(\boldsymbol{x})\big) = \frac{\partial f}{\partial \boldsymbol{x}}g(\boldsymbol{x}) + f(\boldsymbol{x})\frac{\partial g}{\partial \boldsymbol{x}}$$

- Sum rule

$$\frac{\partial}{\partial \boldsymbol{x}}\big(f(\boldsymbol{x}) + g(\boldsymbol{x})\big) = \frac{\partial f}{\partial \boldsymbol{x}} + \frac{\partial g}{\partial \boldsymbol{x}}$$

- Chain rule

$$\frac{\partial}{\partial \boldsymbol{x}}g\big(f(\boldsymbol{x})\big) = \frac{\partial g}{\partial f}\frac{\partial f}{\partial \boldsymbol{x}}$$

More about Chain Rule

- $f : \mathbb{R}^2 \mapsto \mathbb{R}$ of two variables x_1 and x_2. $x_1(t)$ and $x_2(t)$ are functions of t.

$$\frac{\mathrm{d}f}{\mathrm{d}t} = \begin{pmatrix} \frac{\partial f}{\partial x_1} & \frac{\partial f}{\partial x_2} \end{pmatrix} \begin{pmatrix} \frac{\partial x_1(t)}{\partial t} \\ \frac{\partial x_2(t)}{\partial t} \end{pmatrix} = \frac{\partial f}{\partial x_1}\frac{\partial x_1}{\partial t} + \frac{\partial f}{\partial x_2}\frac{\partial x_2}{\partial t}$$

- Example. $f(x_1, x_2) = x_1^2 + 2x_2$, where $x_1(t) = \sin(t)$, $x_2(t) = \cos(t)$

$$\frac{\mathrm{d}f}{\mathrm{d}t} = \frac{\partial f}{\partial x_1}\frac{\partial x_1}{\partial t} + \frac{\partial f}{\partial x_2}\frac{\partial x_2}{\partial t} = 2\sin(t)\cos(t) - 2\sin t = 2\sin(t)(\cos(t) - 1)$$

- $f : \mathbb{R}^2 \mapsto \mathbb{R}$ of two variables x_1 and x_2. $x_1(s,t)$ and $x_2(s,t)$ are functions of s, t.

$$\frac{\partial f}{\partial s} = \frac{\partial f}{\partial x_1}\frac{\partial x_1}{\partial s} + \frac{\partial f}{\partial x_2}\frac{\partial x_2}{\partial s}$$
$$\frac{\partial f}{\partial t} = \frac{\partial f}{\partial x_1}\frac{\partial x_1}{\partial t} + \frac{\partial f}{\partial x_2}\frac{\partial x_2}{\partial t}$$

$$\frac{\mathrm{d}f}{\mathrm{d}(s,t)} = \frac{\partial f}{\partial \mathbf{x}}\frac{\partial \mathbf{x}}{\partial (s,t)} = \begin{pmatrix} \frac{\partial f}{\partial x_1} & \frac{\partial f}{\partial x_2} \end{pmatrix} \begin{pmatrix} \frac{\partial x_1}{\partial s} & \frac{\partial x_1}{\partial t} \\ \frac{\partial x_2}{\partial s} & \frac{\partial x_2}{\partial t} \end{pmatrix}$$

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$\boldsymbol{f} : \mathbb{R}^n \mapsto \mathbb{R}^m$

- For a function $\boldsymbol{f} : \mathbb{R}^n \mapsto \mathbb{R}^m$ and vector $\boldsymbol{x} = \begin{pmatrix} x_1 & \dots & x_n \end{pmatrix}^\mathsf{T} \in \mathbb{R}^n$, the vector-valued function is:

$$\boldsymbol{f}(\boldsymbol{x}) = \begin{pmatrix} f_1(\boldsymbol{x}) \\ \vdots \\ f_m(\boldsymbol{x}) \end{pmatrix}$$

- Partial derivative w.r.t. x_i is a column vector: $\dfrac{\partial \boldsymbol{f}}{\partial x_i} = \begin{pmatrix} \frac{\partial f_1}{\partial x_i} \\ \vdots \\ \frac{\partial f_m}{\partial x_i} \end{pmatrix}$

- Gradient (or Jacobian): $\dfrac{\mathrm{d}\boldsymbol{f}(\boldsymbol{x})}{\mathrm{d}\boldsymbol{x}} = \begin{pmatrix} \frac{\partial \boldsymbol{f}(\boldsymbol{x})}{\partial x_1} & \dots & \frac{\partial \boldsymbol{f}(\boldsymbol{x})}{\partial x_n} \end{pmatrix}$

Jacobian

$$
\begin{aligned}
\boldsymbol{J} = \nabla_{\boldsymbol{x}} \boldsymbol{f} = \frac{\mathrm{d}\boldsymbol{f}(\boldsymbol{x})}{\mathrm{d}\boldsymbol{x}} &= \begin{pmatrix} \frac{\partial \boldsymbol{f}(\boldsymbol{x})}{\partial x_1} & \cdots & \frac{\partial \boldsymbol{f}(\boldsymbol{x})}{\partial x_n} \end{pmatrix} \\
&= \begin{pmatrix} \frac{\partial f_1(\boldsymbol{x})}{\partial x_1} & \cdots & \frac{\partial f_1(\boldsymbol{x})}{\partial x_n} \\ \vdots & & \vdots \\ \frac{\partial f_m(\boldsymbol{x})}{\partial x_1} & \cdots & \frac{\partial f_m(\boldsymbol{x})}{\partial x_n} \end{pmatrix}
\end{aligned}
$$

- For a $\mathbb{R}^n \mapsto \mathbb{R}^m$ function, its Jacobian is a $m \times n$ matrix.

Example: Gradient of Vector-Valued Function

- $\boldsymbol{f}(\boldsymbol{x}) = \boldsymbol{A}\boldsymbol{x}$, $\boldsymbol{f} : \mathbb{R}^n \mapsto \mathbb{R}^m$, $\boldsymbol{A} \in \mathbb{R}^{m \times n}$, $\boldsymbol{x} \in \mathbb{R}^n$
- Partial derivatives: $f_i(\boldsymbol{x}) = \sum_{j=1}^{n} A_{ij} x_j \implies \dfrac{\partial f_i}{\partial x_j} = A_{ij}$
- Graident

$$\frac{\mathrm{d}\boldsymbol{f}}{\mathrm{d}\boldsymbol{x}} = \begin{pmatrix} \frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \vdots & & \vdots \\ \frac{\partial f_m}{\partial x_1} & \cdots & \frac{\partial f_m}{\partial x_n} \end{pmatrix} = \begin{pmatrix} A_{11} & \cdots & A_{1n} \\ \vdots & & \vdots \\ A_{m1} & \cdots & A_{mn} \end{pmatrix} = \boldsymbol{A}$$

Example: Chain Rule

- $h : \mathbb{R} \mapsto \mathbb{R},\ h(t) = (f \circ g)(t)$ with

$$f : \mathbb{R}^2 \mapsto \mathbb{R},\ \ f(\boldsymbol{x}) = \exp(x_1 x_2^2), \quad g : \mathbb{R} \mapsto \mathbb{R}^2,\ \ \boldsymbol{x} = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = g(t) = \begin{pmatrix} t\,\mathrm{co} \\ t\,\mathrm{si} \end{pmatrix}$$

- (Note) $\frac{\partial f}{\partial \boldsymbol{x}} \in \mathbb{R}^{1\times 2}$ and $\frac{\partial g}{\partial t} \in \mathbb{R}^{2\times 1}$
- Using the chain rule,

$$\begin{aligned} \frac{\mathrm{d}h}{\mathrm{d}t} = \frac{\partial f}{\partial \boldsymbol{x}} \frac{\partial \boldsymbol{x}}{\partial t} &= \begin{pmatrix} \frac{\partial f}{\partial x_1} & \frac{\partial f}{\partial x_2} \end{pmatrix} \begin{pmatrix} \frac{\partial x_1}{\partial t} \\ \frac{\partial x_2}{\partial t} \end{pmatrix} \\ &= \begin{pmatrix} \exp(x_1 x_2^2) x_2^2 & 2\exp(x_1 x_2^2) x_1 x_2 \end{pmatrix} \begin{pmatrix} \cos(t) - t\sin(t) \\ \sin(t) + t\cos(t) \end{pmatrix} \end{aligned}$$

Example: Least-Square Loss (1)

- A linear model: $\boldsymbol{y} = \boldsymbol{\Phi\theta}$
- $\boldsymbol{\theta} \in \mathbb{R}^D$: parameter vector
- $\boldsymbol{\Phi} \in \mathbb{R}^{N \times D}$: input features
- $\boldsymbol{y} \in \mathbb{R}^N$: observations
- Goal: Find a good parameter vector that provides the best-fit, formulated by minimizing the following loss $L : \mathbb{R}^D \mapsto \mathbb{R}$ over the parameter vector $\boldsymbol{\theta}$.

$$\boxed{L(\boldsymbol{e}) := \|\boldsymbol{e}\|^2, \quad \text{where } \boldsymbol{e}(\boldsymbol{\theta}) = \boldsymbol{y} - \boldsymbol{\Phi\theta}}$$

Example: Least-Square Loss (2)

- $\dfrac{\partial L}{\partial \boldsymbol{\theta}} = \dfrac{\partial L}{\partial \boldsymbol{e}} \dfrac{\partial \boldsymbol{e}}{\partial \boldsymbol{\theta}}$
- Note. $\dfrac{\partial L}{\partial \boldsymbol{\theta}} \in \mathbb{R}^{1 \times D}$, $\dfrac{\partial L}{\partial \boldsymbol{e}} \in \mathbb{R}^{1 \times N}$, $\dfrac{\partial \boldsymbol{e}}{\partial \boldsymbol{\theta}} \in \mathbb{R}^{N \times D}$
- Using that $\|\boldsymbol{e}\|^2 = \boldsymbol{e}^\top \boldsymbol{e}$, $\dfrac{\partial L}{\partial \boldsymbol{e}} = 2\boldsymbol{e}^\top \in \mathbb{R}^{1 \times N}$ and $\dfrac{\partial \boldsymbol{e}}{\partial \boldsymbol{\theta}} = -\boldsymbol{\Phi} \in \mathbb{R}^{N \times D}$

Finally, we get: $$\frac{\partial L}{\partial \boldsymbol{\theta}} = 2\boldsymbol{e}^\top(-\boldsymbol{\Phi}) = -\underbrace{2(\boldsymbol{y}^\top - \boldsymbol{\theta}^\top \boldsymbol{\Phi}^\top)}_{1 \times N} \underbrace{\boldsymbol{\Phi}}_{N \times D}$$

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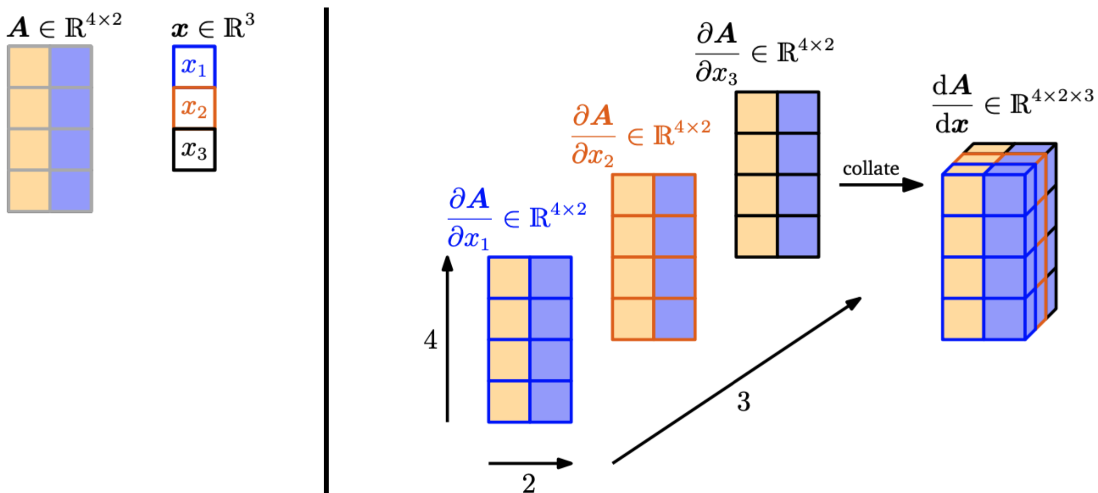
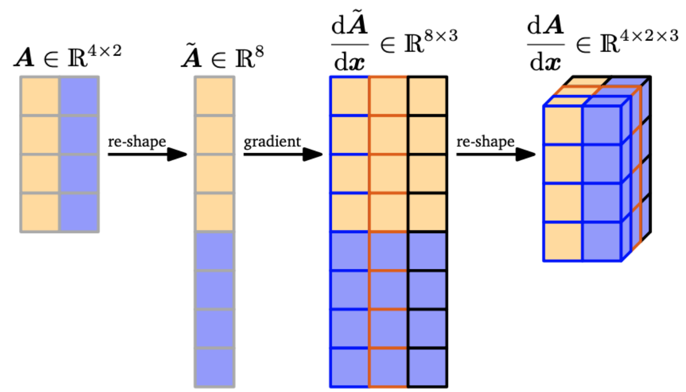
Gradients of matrices

- Gradient of matrix $\boldsymbol{A} \in \mathbb{R}^{m\times n}$ w.r.t. matrix $\boldsymbol{B} \in \mathbb{R}^{p\times q}$
- Jacobian: A four-dimensional tensor[1] $\boldsymbol{J} = \frac{\mathrm{d}\boldsymbol{A}}{\mathrm{d}\boldsymbol{B}} \in \mathbb{R}^{(m\times n)\times(p\times q)}$



(a) Approach 1: We compute the partial derivative $\frac{\partial \boldsymbol{A}}{\partial x_1}, \frac{\partial \boldsymbol{A}}{\partial x_2}, \frac{\partial \boldsymbol{A}}{\partial x_3}$, each of which is a 4×2 matrix, and collate them in a $4 \times 2 \times 3$ tensor.



(b) Approach 2: We re-shape (flatten) $\boldsymbol{A} \in \mathbb{R}^{4\times 2}$ into a vector $\tilde{\boldsymbol{A}} \in \mathbb{R}^{8}$. Then, we compute the gradient $\frac{\mathrm{d}\tilde{\boldsymbol{A}}}{\mathrm{d}\boldsymbol{x}} \in \mathbb{R}^{8\times 3}$. We obtain the gradient tensor by re-shaping this gradient as illustrated above.

[1] A multidimensional array

Example: Gradient of Vectors for Matrices (1)

- $\boldsymbol{f}(\boldsymbol{x}) = \boldsymbol{A}\boldsymbol{x}$, $\boldsymbol{f} \in \mathbb{R}^m$, $\boldsymbol{A} \in \mathbb{R}^{m\times n}$, $\boldsymbol{x} \in \mathbb{R}^n$. What is $\frac{\mathrm{d}\boldsymbol{f}}{\mathrm{d}\boldsymbol{A}}$?
- Dimension: If we consider $\boldsymbol{f} : \mathbb{R}^{m\times n} \mapsto \mathbb{R}^m$, $\frac{\mathrm{d}\boldsymbol{f}}{\mathrm{d}\boldsymbol{A}} \in \mathbb{R}^{m\times(m\times n)}$
- Partial derivatives: $\frac{\partial f_i}{\partial \boldsymbol{A}} \in \mathbb{R}^{1\times(m\times n)}$, $\quad \frac{\mathrm{d}\boldsymbol{f}}{\mathrm{d}\boldsymbol{A}} = \begin{pmatrix} \frac{\partial f_1}{\partial \boldsymbol{A}} \\ \vdots \\ \frac{\partial f_m}{\partial \boldsymbol{A}} \end{pmatrix}$

$$f_i = \sum_{j=1}^{n} A_{ij} x_j, \ \ i = 1, \dots, m \implies \frac{\partial f_i}{\partial A_{iq}} = x_q,$$

$$\frac{\partial f_i}{\partial A_{i\cdot}} = \boldsymbol{x}^{\mathsf{T}} \in \mathbb{R}^{1\times 1\times n} \text{ (for } i\text{th row vector)}$$

$$\frac{\partial f_i}{\partial A_{k\neq i\cdot}} = 0^{\mathsf{T}} \in \mathbb{R}^{1\times 1\times n} \text{ (for } k\text{th row vector, } k \neq i)$$

$$\frac{\partial f_i}{\partial \boldsymbol{A}} = \begin{pmatrix} 0^{\mathsf{T}} \\ \vdots \\ 0^{\mathsf{T}} \\ \boldsymbol{x}^{\mathsf{T}} \\ 0^{\mathsf{T}} \\ \vdots \\ 0^{\mathsf{T}} \end{pmatrix} \in \mathbb{R}^{1\times(m\times n)}$$

Example: Gradient of Matrices for Matrices (2)

- $\boldsymbol{R} \in \mathbb{R}^{m \times n}$ and $\boldsymbol{f} : \mathbb{R}^{m \times n} \mapsto \mathbb{R}^{n \times n}$ with $\boldsymbol{f}(\boldsymbol{R}) = \boldsymbol{K} := \boldsymbol{R}^{\mathsf{T}}\boldsymbol{R} \in \mathbb{R}^{n \times n}$. What is $\frac{\mathrm{d}\boldsymbol{K}}{\mathrm{d}\boldsymbol{R}} \in \mathbb{R}^{(n \times n) \times (m \times n)}$?
- $\frac{\mathrm{d}K_{pq}}{\mathrm{d}\boldsymbol{R}} \in \mathbb{R}^{1 \times m \times n}$. Let $\boldsymbol{r}_i$ be the ith column of $\boldsymbol{R}$. Then $K_{pq} = \boldsymbol{r}_p{}^{\mathsf{T}}\boldsymbol{r}_q = \sum_{k=1}^{m} R_{kp}R_{kq}$.
- Partial derivative $\frac{\partial K_{pq}}{\partial R_{ij}}$

$$\frac{\partial K_{pq}}{\partial R_{ij}} = \sum_{k=1}^{m} \frac{\partial}{\partial R_{ij}} R_{kp}R_{kq} = \partial_{pqij}, \;\; \partial_{pqij} = \begin{cases} R_{iq} & \text{if } j = p, p \neq q \\ R_{ip} & \text{if } j = q, p \neq q \\ 2R_{iq} & \text{if } j = p, p = q \\ 0 & \text{otherwise} \end{cases}$$

Useful Identities

$$\frac{\partial}{\partial \boldsymbol{X}} \boldsymbol{f}(\boldsymbol{X})^\top = \left(\frac{\partial \boldsymbol{f}(\boldsymbol{X})}{\partial \boldsymbol{X}}\right)^\top \tag{5.99}$$

$$\frac{\partial}{\partial \boldsymbol{X}} \mathrm{tr}(\boldsymbol{f}(\boldsymbol{X})) = \mathrm{tr}\left(\frac{\partial \boldsymbol{f}(\boldsymbol{X})}{\partial \boldsymbol{X}}\right) \tag{5.100}$$

$$\frac{\partial}{\partial \boldsymbol{X}} \det(\boldsymbol{f}(\boldsymbol{X})) = \det(\boldsymbol{f}(\boldsymbol{X}))\mathrm{tr}\left(\boldsymbol{f}(\boldsymbol{X})^{-1}\frac{\partial \boldsymbol{f}(\boldsymbol{X})}{\partial \boldsymbol{X}}\right) \tag{5.101}$$

$$\frac{\partial}{\partial \boldsymbol{X}} \boldsymbol{f}(\boldsymbol{X})^{-1} = -\boldsymbol{f}(\boldsymbol{X})^{-1}\frac{\partial \boldsymbol{f}(\boldsymbol{X})}{\partial \boldsymbol{X}}\boldsymbol{f}(\boldsymbol{X})^{-1} \tag{5.102}$$

$$\frac{\partial \boldsymbol{a}^\top \boldsymbol{X}^{-1}\boldsymbol{b}}{\partial \boldsymbol{X}} = -(\boldsymbol{X}^{-1})^\top \boldsymbol{a}\boldsymbol{b}^\top (\boldsymbol{X}^{-1})^\top \tag{5.103}$$

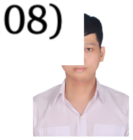
$$\frac{\partial \boldsymbol{x}^\top \boldsymbol{a}}{\partial \boldsymbol{x}} = \boldsymbol{a}^\top \tag{5.104}$$

$$\frac{\partial \boldsymbol{a}^\top \boldsymbol{x}}{\partial \boldsymbol{x}} = \boldsymbol{a}^\top \tag{5.105}$$

$$\frac{\partial \boldsymbol{a}^\top \boldsymbol{X}\boldsymbol{b}}{\partial \boldsymbol{X}} = \boldsymbol{a}\boldsymbol{b}^\top \tag{5.106}$$

$$\frac{\partial \boldsymbol{x}^\top \boldsymbol{B}\boldsymbol{x}}{\partial \boldsymbol{x}} = \boldsymbol{x}^\top(\boldsymbol{B}+\boldsymbol{B}^\top) \tag{5.107}$$

$$\frac{\partial}{\partial \boldsymbol{s}}(\boldsymbol{x}-\boldsymbol{A}\boldsymbol{s})^\top \boldsymbol{W}(\boldsymbol{x}-\boldsymbol{A}\boldsymbol{s}) = -2(\boldsymbol{x}-\boldsymbol{A}\boldsymbol{s})^\top \boldsymbol{W}\boldsymbol{A} \quad \text{for symmetric } \boldsymbol{W} \tag{5.108}$$



Roadmap

Motivation: Neural Networks with Many Layers (1)

- In a neural network with many layers, the function $\boldsymbol{y}$ is a many-level function compositions

$$\boldsymbol{y} = (f_K \circ f_{K-1} \circ \cdots \circ f_1)(\boldsymbol{x}),$$

where, for example,
  - $\boldsymbol{x}$: images as inputs, $\boldsymbol{y}$: class labels (e.g., cat or dog) as outputs
  - each f_i has its own parameters

- In neural networks, with the model parameters $\boldsymbol{\theta} = \{\boldsymbol{A}_0, \boldsymbol{b}_0, \ldots, \boldsymbol{A}_{K-1}, \boldsymbol{b}_{K-1}\}$

$$\begin{cases} \boldsymbol{f}_0 & := \boldsymbol{x} \\ \boldsymbol{f}_1 & := \sigma_1(\boldsymbol{A}_0 \boldsymbol{f}_0 + \boldsymbol{b}_0) \\ \vdots & \\ \boldsymbol{f}_K & := \sigma_K(\boldsymbol{A}_{K-1} \boldsymbol{f}_{K-1} + \boldsymbol{b}_{K-1}) \end{cases}$$

◦ σ_i is called the activation function at i-th layer

◦ Minimizing the loss function over $\boldsymbol{\theta}$:

$$\min_{\boldsymbol{\theta}} L(\boldsymbol{\theta}),$$

where

$$L(\boldsymbol{\theta}) = \|\boldsymbol{y} - \boldsymbol{f}_K(\boldsymbol{\theta}, \boldsymbol{x})\|^2$$

Motivation: Neural Networks with Many Layers (2)

- In neural networks, with the model parameters $\boldsymbol{\theta} = \{\boldsymbol{A}_0, \boldsymbol{b}_0, \ldots, \boldsymbol{A}_{K-1}, \boldsymbol{b}_{K-1}\}$

$$\begin{cases} \boldsymbol{f}_0 & := \boldsymbol{x} \\ \boldsymbol{f}_1 & := \sigma_1(\boldsymbol{A}_0 \boldsymbol{f}_0 + \boldsymbol{b}_0) \\ \vdots & \\ \boldsymbol{f}_K & := \sigma_K(\boldsymbol{A}_{K-1} \boldsymbol{f}_{K-1} + \boldsymbol{b}_{K-1}) \end{cases}$$

◦ σ_i is called the activation function at i-th layer

◦ Minimizing the loss function over $\boldsymbol{\theta}$:

$$\min_{\boldsymbol{\theta}} L(\boldsymbol{\theta}),$$

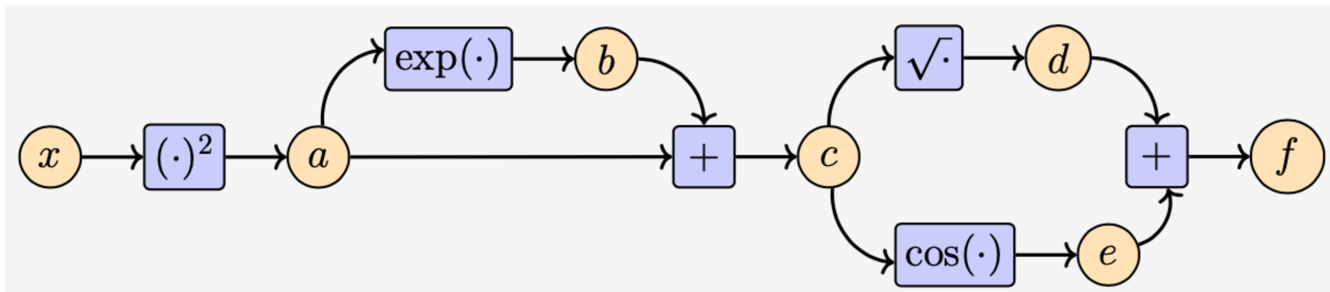
where

$$L(\boldsymbol{\theta}) = \left\| \boldsymbol{y} - \boldsymbol{f}_K(\boldsymbol{\theta}, \boldsymbol{x}) \right\|^2$$

- Question. How can we efficiently compute $\dfrac{\mathrm{d}L}{\mathrm{d}\boldsymbol{\theta}}$ in computers?

Backpropagatin: Example (1)

- $f(x) = \sqrt{x^2 + \exp(x^2)} + \cos\left(x^2 + \exp(x^2)\right)$
- Computation graph: Connect via "elementary" operations



$$\color{blue}{a} = x^2,\ \color{blue}{b} = \exp(a),\ \color{blue}{c} = a + b,\ \color{blue}{d} = \sqrt{c},\ \color{blue}{e} = \cos(c),\ \color{blue}{f} = d + e$$

- Automatic Differentiation
  - A set of techniques to numerically (not symbolically) evaluate the gradient of a function by working with intermediate variables and applying the chain rule.

Backpropagation: Example (2)

- $a = x^2,\ b = \exp(a),\ c = a + b,\ d = \sqrt{c},\ e = \cos(c),\ f = d + e$
- Derivatives of the intermediate variables with their inputs

$$\frac{\partial a}{\partial x} = 2x,\ \frac{\partial b}{\partial a} = \exp(a),\ \frac{\partial c}{\partial a} = 1 = \frac{\partial c}{\partial b},\ \frac{\partial d}{\partial c} = \frac{1}{2\sqrt{c}},\ \frac{\partial e}{\partial c} = -\sin(c),\ \frac{\partial f}{\partial d}$$

- Compute $\dfrac{\partial f}{\partial x}$ by working backward from the output

$$\frac{\partial f}{\partial c} = \frac{\partial f}{\partial d}\frac{\partial d}{\partial c} + \frac{\partial f}{\partial e}\frac{\partial e}{\partial c},\quad \frac{\partial f}{\partial b} = \frac{\partial f}{\partial c}\frac{\partial c}{\partial b}$$

$$\frac{\partial f}{\partial a} = \frac{\partial f}{\partial b}\frac{\partial b}{\partial a} + \frac{\partial f}{\partial c}\frac{\partial c}{\partial a},\quad \boxed{\frac{\partial f}{\partial x}} = \frac{\partial f}{\partial a}\frac{\partial a}{\partial x}$$

$$\frac{\partial f}{\partial c} = 1 \cdot \frac{1}{2\sqrt{c}} + 1 \cdot (-\sin(c))$$

$$\frac{\partial f}{\partial b} = \frac{\partial f}{\partial c} \cdot 1,\quad \frac{\partial f}{\partial a} = \frac{\partial f}{\partial b}\exp(a) + \frac{\partial f}{\partial c} \cdot 1$$

$$\boxed{\frac{\partial f}{\partial x}} = \frac{\partial f}{\partial a} \cdot 2x$$

Backpropagation

- Implementation of gradients can be very expensive, unless we are careful.
- Using the idea of automatic differentiation, the whole gradient computation is decomposed into a set of gradients of elementary functions and application of the chain rule.
- Why backward?
  - In neural networks, the input dimensionality is often much higher than the dimensionality of labels.
  - In this case, the backward computation (than the forward computation) is much cheaper.
- Works if the target is expressed as a computation graph whose elementary functions are differentiable. If not, some care needs to be taken.

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Higher-Order Derivatives

- Some optimization algorithms (e.g., Newton's method) require second-order derivatives, if they exist.
- (Truncated) Taylor series is often used as an approximation of a function.
- For $f : \mathbb{R}^n \mapsto \mathbb{R}$ of variable $\boldsymbol{x} \in \mathbb{R}^n$,
  $\nabla_{\boldsymbol{x}} f = \frac{\mathrm{d}f}{\mathrm{d}\boldsymbol{x}} = \begin{pmatrix} \frac{\partial f(\boldsymbol{x})}{\partial x_1} & \cdots & \frac{\partial f(\boldsymbol{x})}{\partial x_n} \end{pmatrix} \in \mathbb{R}^{1\times n}$
  - If f is twice-differentiable, the order doesn't matter.

$$\mathrm{H}_{\boldsymbol{x}} f = \begin{pmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \vdots & & & \vdots \\ \frac{\partial^2 f}{\partial x_1 \partial x_n} & \frac{\partial^2 f}{\partial x_2 \partial x_n} & \cdots & \frac{\partial^2 f}{\partial x_n \partial x_n} \end{pmatrix}$$

- For $f : \mathbb{R}^n \mapsto \mathbb{R}^m$, $\nabla_{\boldsymbol{x}} f \in \mathbb{R}^{m\times n}$
  - Thus, $\mathrm{H}_{\boldsymbol{x}} f \in \mathbb{R}^{m\times n\times n}$ (a tensor)

Function Approximation: Linearization and More

- First-order approximation of $f(\boldsymbol{x})$ (i.e., linearization by taking the first two terms of Taylor Series)

$$f(\boldsymbol{x}) \approx f(\boldsymbol{x}_0) + (\nabla_{\boldsymbol{x}} f)(\boldsymbol{x}_0)(\boldsymbol{x} - \boldsymbol{x}_0)$$

- Multivariate Talyer Series for $f : \mathbb{R}^D \mapsto \mathbb{R}$ at $\boldsymbol{x}_0$

$$f(\boldsymbol{x}) = \sum_{k=0}^{\infty} \frac{D_{\boldsymbol{x}}^k f(\boldsymbol{x}_0)}{k!} \boldsymbol{\delta}^k,$$

  where $D_{\boldsymbol{x}}^k f(\boldsymbol{x}_0)$ is the kth derivative of f w.r.t. $\boldsymbol{x}$, evaluated at $\boldsymbol{x}_0$, and $\boldsymbol{\delta} := \boldsymbol{x} - \boldsymbol{x}_0$.
  - Partial sum up to, say n, can be an approximation of $f(\boldsymbol{x})$.
  - $D_{\boldsymbol{x}}^k f(\boldsymbol{x}_0)$ and $\boldsymbol{\delta}^k$ are kth order tensors, i.e., k-dimensional array.
  - $\boldsymbol{\delta}^k$ is a k-fold outer product $\otimes$. For example, $\boldsymbol{\delta}^2 = \boldsymbol{\delta} \otimes \boldsymbol{\delta} = \boldsymbol{\delta}\boldsymbol{\delta}^\mathsf{T}$. $\boldsymbol{\delta}^3 = \boldsymbol{\delta} \otimes \boldsymbol{\delta} \otimes \boldsymbol{\delta}$.

THANKS FOR YOUR ATTENTION

Discussions