

# Mathematics for Machine Learning

## — Vector Calculus

Differentiation, Partial Differentiation & Gradients

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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 Differentiation of Univariate Functions
- 2 Partial Differentiation & Gradients

# Motivations

- Machine learning algorithms that optimize an objective function w.r.t. a set of model parameters.
- Examples:
  - Curve-fitting.
  - Neural networks (parameters as weights & biases of layers, repeatedly application of chain rule, etc.)
  - Gaussian mixture models (maximizing the likelihood of the model).
- We focus on **functions**.
  - $f : \mathbb{R}^D \rightarrow \mathbb{R}$  (i.e.,  $\mathbf{x} \mapsto f(\mathbf{x})$ ).

# Example

Get used to

$$f(\mathbf{x}) = \mathbf{x}^\top \mathbf{x}, \quad \mathbf{x} \in \mathbb{R}^2.$$

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$$\mathbf{x} \mapsto x_1^2 + x_2^2.$$

# Outline

## 1 Differentiation of Univariate Functions

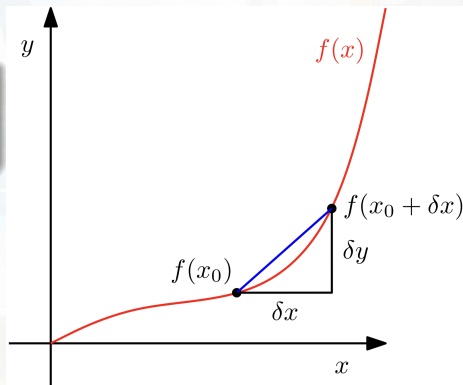
## 2 Partial Differentiation & Gradients

# Derivative

Consider a univariate function  $y = f(x)$ ,  $x, y \in \mathbb{R}$ .

## Difference Quotient

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

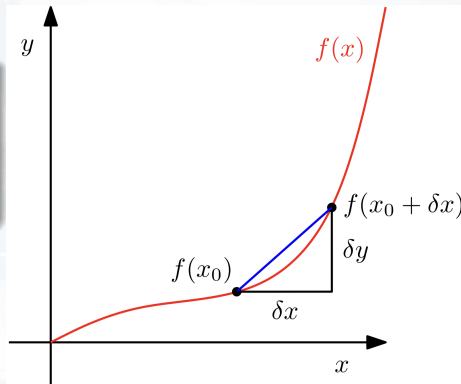




## Derivative

For  $h > 0$ , the derivative of  $f$  at  $x$ :

$$\frac{df}{dx} := \lim_{h \rightarrow 0} \frac{f(x+h) - f(x)}{h}.$$



# Example

## Derivative of a Polynomial

Given  $f(x) = x^n$ .

$$\begin{aligned}\frac{df}{dx} &= \lim_{h \rightarrow 0} \frac{f(x+h) - f(x)}{h} \\ &= \lim_{h \rightarrow 0} \frac{(x+h)^n - x^n}{h} \\ &= \lim_{h \rightarrow 0} \frac{\sum_{i=0}^n \binom{n}{i} x^{n-i} h^i - x^n}{h}\end{aligned}$$

Note that  $x^n = \binom{n}{0} x^{n-0} h^0$ .

# Example

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$$\begin{aligned}\frac{df}{dx} &= \lim_{h \rightarrow 0} \frac{\sum_{i=1}^n \binom{n}{i} x^{n-i} h^i}{h} \\&= \lim_{h \rightarrow 0} \sum_{i=1}^n \binom{n}{i} x^{n-i} h^{i-1} \\&= \lim_{h \rightarrow 0} \binom{n}{1} x^{n-1} + \lim_{h \rightarrow 0} \sum_{i=2}^n \binom{n}{i} x^{n-i} h^{i-1} \\&= nx^{n-1} + 0.\end{aligned}$$

# Taylor Series

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

$$T_n(x) = \sum_{k=0}^n \frac{f^{(k)}(x_0)}{k!} (x - x_0)^k$$

# Taylor Series

For a function  $f : \mathbb{R} \rightarrow \mathbb{R}$ ,  $f \in \mathcal{C}^\infty$ , the Taylor series  $f$  at  $x_0$  is:

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$f$  is **analytic**:  $f(x) = T_\infty(x)$ .



# Example

## Example

$f(x) = x^4$ . Seek the Taylor polynomial  $T_6$  evaluated at  $x_0 = 1$ .

Check if  $T_6(x) = f(x)$ .

$$f'(x) =$$

$$f'(x) = 4x^3,$$

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$$\begin{aligned} T_6(x) &= \sum_{k=0}^6 \frac{f^{(k)}(x_0)}{k!} (x - x_0)^k \\ &= 1 + 4(x - 1) + 6(x - 1)^2 + 4(x - 1)^3 + (x - 1)^4 + 0 \\ &= x^4. \end{aligned}$$

# Example

## Example

Given  $f(x) = \sin(x) + \cos(x)$ . We know  $f(x) \in \mathcal{C}^\infty$ . Seek the Taylor series  $T_\infty(x)$  evaluated at  $x_0 = 0$ .

Check if  $T_\infty(x) = f(x)$ .

# Example

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Given  $f(x) = \sin(x) + \cos(x)$ . We know  $f(x) \in \mathcal{C}^\infty$ . Seek the Taylor series  $T_\infty(x)$  evaluated at  $x_0 = 0$ .

Check if  $T_\infty(x) = f(x)$ .

- $\cos(x) = \sum_{k=0}^{\infty} (-1)^k \frac{1}{(2k)!} x^{2k}.$
- $\sin(x) = \sum_{k=0}^{\infty} (-1)^k \frac{1}{(2k+1)!} x^{2k+1}.$

$$f(0) = \sin(0) + \cos(0) = 1$$

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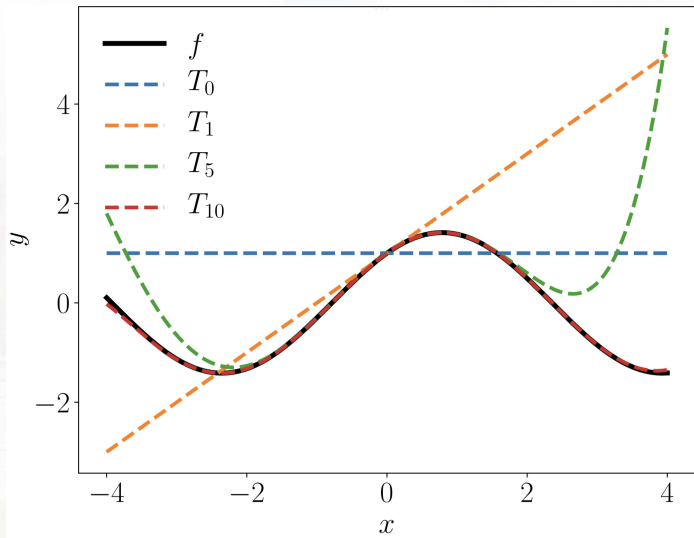
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$$f^{(4)}(0) = \sin(0) + \cos(0) = 1$$

$$\vdots$$

$$\begin{aligned} T_{\infty}(x) &= \sum_{k=0}^{\infty} \frac{f^{(k)}(x_0)}{k!} (x - x_0)^k \\ &= 1 + x - \frac{1}{2!}x^2 - \frac{1}{3!}x^3 + \frac{1}{4!}x^4 + \frac{1}{5!}x^5 - \dots \\ &= \cos(x) + \sin(x). \end{aligned}$$



# Differentiation Rules

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

- **Example:** Compute  $h'(x)$  where  $h(x) = (2x + 1)^4.$

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- Let  $f(x) = 2x + 1$ ,  $g(f) = f^4$ .
- $f'(x) = 2$ ,  $g'(f) = 4f^3$ .
- $h'(x) = g'(f)f'(x) = (4f^3) \cdot 2 = 4(2x + 1)^3 \cdot 2 = 8(2x + 1)^3$ .

# Outline

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- 2 Partial Differentiation & Gradients

# Motivation

- We consider a more general case:  $f : \mathbb{R}^n \rightarrow \mathbb{R}$ .
  - The derivative to functions of **several variables**  $\Rightarrow$  **gradient**.

# Partial Derivative

## Partial Derivative

For a function  $f : \mathbb{R}^n \rightarrow \mathbb{R}$  and  $\mathbf{x} \in \mathbb{R}^n$  of  $n$  variables  $x_1, \dots, x_n$ , the partial derivatives are:

$$\begin{aligned}\frac{\partial f}{\partial x_1} &= \lim_{h \rightarrow 0} \frac{f(\mathbf{x}_1 + h, x_2, \dots, x_n) - f(\mathbf{x})}{h} \\ &\vdots \\ \frac{\partial f}{\partial x_n} &= \lim_{h \rightarrow 0} \frac{f(x_1, \dots, x_{n-1}, \mathbf{x}_n + h) - f(\mathbf{x})}{h}\end{aligned}$$

We collect them in the **row vector**:

$$\nabla_{\mathbf{x}} f = \frac{df}{d\mathbf{x}} = \left[ \frac{\partial f(\mathbf{x})}{\partial x_1} \quad \frac{\partial f(\mathbf{x})}{\partial x_2} \quad \dots \quad \frac{\partial f(\mathbf{x})}{\partial x_n} \right]$$

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where  $\mathbf{x} = [x_1, \dots, x_n]^\top$ .

# Examples

## Example

Given  $f(x, y) = (x + 2y^3)^2$ , compute  $\frac{\partial f(x, y)}{\partial x}$  and  $\frac{\partial f(x, y)}{\partial y}$ .

## Example

Given  $f(x_1, x_2) = x_1^2 x_2 + x_1 x_2^3 \in \mathbb{R}$ , compute  $\frac{\partial f(x_1, x_2)}{\partial x_1}$ ,  $\frac{\partial f(x_1, x_2)}{\partial x_2}$  and  $\frac{df}{dx}$ .

# Basic Partial Differentiation Rules

- $\frac{\partial}{\partial \mathbf{x}}(f(\mathbf{x})g(\mathbf{x})) = \frac{\partial f}{\partial \mathbf{x}}g(\mathbf{x}) + f(\mathbf{x})\frac{\partial g}{\partial \mathbf{x}}.$
- $\frac{\partial}{\partial \mathbf{x}}(f(\mathbf{x}) + g(\mathbf{x})) = \frac{\partial f}{\partial \mathbf{x}} + \frac{\partial g}{\partial \mathbf{x}}.$
- $\frac{\partial}{\partial \mathbf{x}}(g \circ f)(\mathbf{x}) = \frac{\partial g}{\partial \mathbf{x}}(g(f(\mathbf{x}))) = \frac{\partial g}{\partial f} \frac{\partial f}{\partial \mathbf{x}}.$ 
  - Chain rule.

# Chain Rule (Partial Differentiation)

- Consider a function  $f : \mathbb{R}^2 \rightarrow \mathbb{R}$  of two variables  $x_1, x_2$ .
  - $x_1(t), x_2(t) : \mathbb{R} \rightarrow \mathbb{R}$ .

Then,

$$\frac{df}{dt} = \begin{bmatrix} \frac{\partial f}{\partial x_1} & \frac{\partial f}{\partial x_2} \end{bmatrix} \begin{bmatrix} \frac{\partial x_1(t)}{\partial t} \\ \frac{\partial x_2(t)}{\partial t} \end{bmatrix} = \frac{\partial f}{\partial x_1} \frac{\partial x_1}{\partial t} + \frac{\partial f}{\partial x_2} \frac{\partial x_2}{\partial t}.$$

Here 'd' denotes the **gradient** and '∂' denotes **partial derivatives**.

- Note:** Here the 't' in dt is in  $\mathbb{R}^1$ .
- Trick: View  $[x_1, x_2]^T$  as  $\mathbf{x} \in \mathbb{R}^2$ .

$$\frac{df}{d\mathbf{x}}: \mathbb{R} \text{ w.r.t. } \mathbb{R}^2.$$

$$\frac{d\mathbf{x}}{dt}: \mathbb{R}^2 \text{ w.r.t. } \mathbb{R}.$$



## Example

### Example

Consider  $f(x_1, x_2) = x_1^2 + 2x_2$ , where  $x_1 = \sin t$  and  $x_2 = \cos t$ . Calculate

$$\frac{df}{dt} = ?$$

# What if $x_1, x_2 : \mathbb{R}^2 \rightarrow \mathbb{R}$ ?

- Again, consider a function  $f : \mathbb{R}^2 \rightarrow \mathbb{R}$  of two variables  $x_1, x_2$ .  
However,

# What if $x_1, x_2 : \mathbb{R}^2 \rightarrow \mathbb{R}$ ?

- Again, consider a function  $f : \mathbb{R}^2 \rightarrow \mathbb{R}$  of two variables  $x_1, x_2$ . However,

- $x_1(s, t), x_2(s, t) : \mathbb{R}^2 \rightarrow \mathbb{R}$ .

Then,

$$\begin{aligned}\frac{\partial f}{\partial s} &= \frac{\partial f}{\partial x_1} \frac{\partial x_1}{\partial s} + \frac{\partial f}{\partial x_2} \frac{\partial x_2}{\partial s}, \\ \frac{\partial f}{\partial t} &= \frac{\partial f}{\partial x_1} \frac{\partial x_1}{\partial t} + \frac{\partial f}{\partial x_2} \frac{\partial x_2}{\partial t},\end{aligned}$$

- Trick: View  $[x_1, x_2]^\top$  as  $\mathbf{x} \in \mathbb{R}^2$  and  $[s, t]^\top$  as  $\boldsymbol{\theta} \in \mathbb{R}^2$ .

$$\frac{df}{d\mathbf{x}}: \mathbb{R} \text{ w.r.t. } \mathbb{R}^2.$$

$$\frac{d\mathbf{x}}{d\boldsymbol{\theta}}: \mathbb{R}^2 \text{ w.r.t. } \mathbb{R}^2.$$

$$\frac{df}{d\theta} = \frac{\partial f}{\partial \mathbf{x}} \frac{\partial \mathbf{x}}{\partial \theta} =$$

$$\frac{df}{d\boldsymbol{\theta}} = \frac{\partial f}{\partial \mathbf{x}} \frac{\partial \mathbf{x}}{\partial \boldsymbol{\theta}} = \begin{bmatrix} \frac{\partial f}{\partial x_1} & \frac{\partial f}{\partial x_2} \end{bmatrix}$$

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Somehow we can see why the gradient is defined as a row vector.

# Heads up

We will see that

- $f : \mathbb{R}^D \rightarrow \mathbb{R}$ : the gradient is a  $1 \times D$  **row** vector.
- $\mathbf{f} : \mathbb{R} \rightarrow \mathbb{R}^E$ : the gradient is a  $E \times 1$  **column** vector.
- $\mathbf{f} : \mathbb{R}^D \rightarrow \mathbb{R}^E$ : the gradient is a  $E \times D$  **matrix**.



# Discussions