

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**.
 - $f : \mathbb{R}^D \mapsto \mathbb{R}$ (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

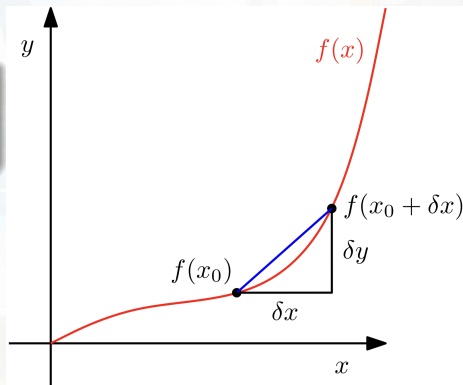
2 Partial Differentiation & Gradients

Derivative

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

Difference Quotient

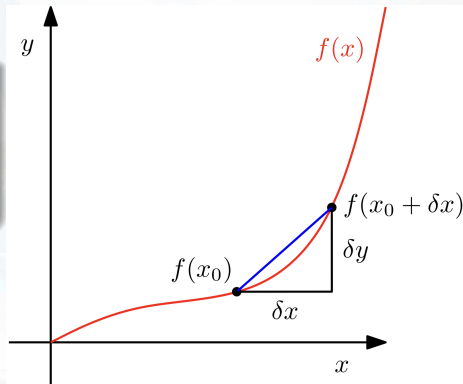
$$\frac{\delta y}{\delta x} := \frac{f(x + \delta x) - f(x)}{\delta x}.$$



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 $f : \mathbb{R} \mapsto \mathbb{R}$ 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 $f : \mathbb{R} \mapsto \mathbb{R}$, $f \in \mathcal{C}^\infty$, 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 $T_6(x) = f(x)$.

$$f'(x) =$$

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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

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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 $x_0 = 0$.

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

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

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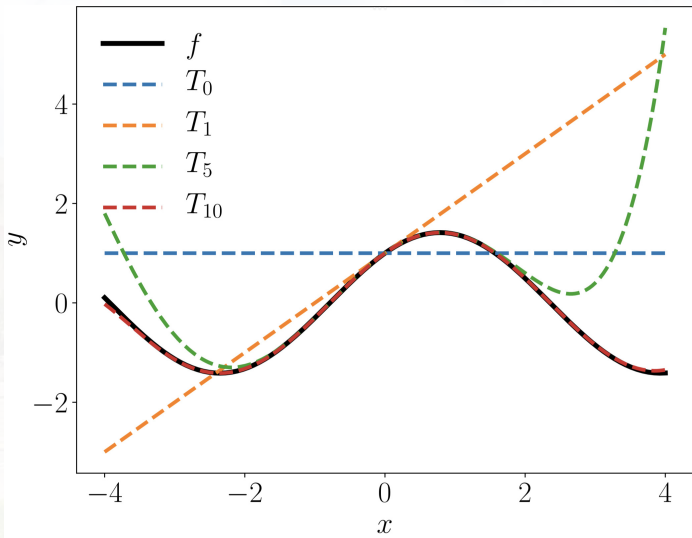
$$f''(0) = -\sin(0) - \cos(0) = -1$$

$$f^{(3)}(0) = -\cos(0) + \sin(0) = -1$$

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

$$\vdots$$

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



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

Outline

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Motivation

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

Partial Derivative

Partial Derivative

For a function $f : \mathbb{R}^n \mapsto \mathbb{R}$ 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 $f(x, y) = x_1^2 x_2 + x_1 x_2^3 \in \mathbb{R}$, compute $\frac{\partial f(x, y)}{\partial x}$, $\frac{\partial f(x, y)}{\partial y}$ 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 $f : \mathbb{R}^2 \mapsto \mathbb{R}$ of two variables x_1, x_2 .
 - $x_1(t), x_2(t) : \mathbb{R} \mapsto \mathbb{R}$.

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 $[x_1, x_2]^\top$ 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 $x_1, x_2 : \mathbb{R}^2 \mapsto \mathbb{R}$?

- Again, consider a function $f : \mathbb{R}^2 \mapsto \mathbb{R}$ of two variables x_1, x_2 .
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What if $x_1, x_2 : \mathbb{R}^2 \mapsto \mathbb{R}$?

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

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

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 $\boldsymbol{\theta} \in \mathbb{R}^2$.

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

$\frac{d\mathbf{x}}{d\boldsymbol{\theta}} : \mathbb{R}^2$ 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

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

Discussions