

Mathematics for Machine Learning

— Vector Calculus

Backpropagation & Automatic Differentiation

Joseph Chuang-Chieh Lin

Department of Computer Science & Engineering,
National Taiwan Ocean University

Fall 2025

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 Backpropagation
- 2 Automatic Differentiation

Outline

- 1 Backpropagation
- 2 Automatic Differentiation

Motivation

Consider the function

$$f(x) = \sqrt{x^2 + \exp(x^2)} + \cos(x^2 + \exp(x^2)).$$

Motivation

Consider the function

$$f(x) = \sqrt{x^2 + \exp(x^2)} + \cos(x^2 + \exp(x^2)).$$

Apply the chain rule, we can compute its gradient:

Motivation

Consider the function

$$f(x) = \sqrt{x^2 + \exp(x^2)} + \cos(x^2 + \exp(x^2)).$$

Apply the chain rule, we can compute its gradient:

$$\begin{aligned}\frac{df}{dx} &= \frac{2x + 2x \exp(x^2)}{2\sqrt{x^2 + \exp(x^2)}} - \sin(x^2 + \exp(x^2))(2x + 2x \exp(x^2)) \\ &= 2x \left(\frac{1}{2\sqrt{x^2 + \exp(x^2)}} - \sin(x^2 + \exp(x^2)) \right) (1 + \exp(x^2)).\end{aligned}$$

Motivation

Consider the function

$$f(x) = \sqrt{x^2 + \exp(x^2)} + \cos(x^2 + \exp(x^2)).$$

Apply the chain rule, we can compute its gradient:

$$\begin{aligned}\frac{df}{dx} &= \frac{2x + 2x \exp(x^2)}{2\sqrt{x^2 + \exp(x^2)}} - \sin(x^2 + \exp(x^2))(2x + 2x \exp(x^2)) \\ &= 2x \left(\frac{1}{2\sqrt{x^2 + \exp(x^2)}} - \sin(x^2 + \exp(x^2)) \right) (1 + \exp(x^2)).\end{aligned}$$

- Impractical to write it explicitly.
- The implementation of the gradient could be expensive.

Gradients in a Deep Network

$$\mathbf{y} = (f_k \circ f_{k-1} \circ \cdots \circ f_1)(\mathbf{x}) = f_k(f_{k-1}(\cdots(f_1(\mathbf{x}))\cdots)).$$

- \mathbf{x} : inputs (e.g., images).
- \mathbf{y} : observations (e.g., class labels).
- $f_i, i = 1, \dots, K$: functions with their own parameters.

Gradients in a Deep Network

$$\mathbf{y} = (f_k \circ f_{k-1} \circ \cdots \circ f_1)(\mathbf{x}) = f_k(f_{k-1}(\cdots(f_1(\mathbf{x}))\cdots)).$$

- \mathbf{x} : inputs (e.g., images).
- \mathbf{y} : observations (e.g., class labels).
- f_i , $i = 1, \dots, K$: functions with their own parameters.
 - $f_i(\mathbf{x}_{i-1}) = \sigma(\mathbf{A}_{i-1}\mathbf{x}_{i-1} + \mathbf{b}_{i-1})$, in the i th layer.
 - \mathbf{x}_{i-1} : the output of layer $i - 1$.
 - σ : **activation function** (e.g., $1/(1 + e^{-x})$, $\tanh(\mathbf{x})$, rectified linear unit (ReLU), etc.).
 - $\mathbf{f}_0 := \mathbf{x}$;
 $\mathbf{f}_i := \sigma_i(\mathbf{A}_{i-1}\mathbf{f}_{i-1} + \mathbf{b}_{i-1})$, $i = 1, \dots, K$.

Get the Gradients

- To obtain the gradients w.r.t. the parameter set θ :
 - $\theta = \{\mathbf{A}_0, \mathbf{b}_0, \dots, \mathbf{A}_{K-1}, \mathbf{b}_{K-1}\}$.
 - The squared loss: $L(\theta) = \|\mathbf{y} - \mathbf{f}_K(\theta, \mathbf{x})\|^2$.
 - $\theta_j = \{\mathbf{A}_j, \mathbf{b}_j\}$, for $j = 0, 1, \dots, K-1$.

Get the Gradients

- To obtain the gradients w.r.t. the parameter set θ :

- $\theta = \{\mathbf{A}_0, \mathbf{b}_0, \dots, \mathbf{A}_{K-1}, \mathbf{b}_{K-1}\}$.
- The squared loss: $L(\theta) = \|\mathbf{y} - \mathbf{f}_K(\theta, \mathbf{x})\|^2$.
- $\theta_j = \{\mathbf{A}_j, \mathbf{b}_j\}$, for $j = 0, 1, \dots, K-1$.

- By the chain rule:

$$\frac{\partial L}{\partial \theta_{K-1}} = \frac{\partial L}{\partial \mathbf{f}_K} \frac{\partial \mathbf{f}_K}{\partial \theta_{K-1}}$$

Get the Gradients

- To obtain the gradients w.r.t. the parameter set θ :

- $\theta = \{\mathbf{A}_0, \mathbf{b}_0, \dots, \mathbf{A}_{K-1}, \mathbf{b}_{K-1}\}$.
- The squared loss: $L(\theta) = \|\mathbf{y} - \mathbf{f}_K(\theta, \mathbf{x})\|^2$.
- $\theta_j = \{\mathbf{A}_j, \mathbf{b}_j\}$, for $j = 0, 1, \dots, K-1$.

- By the chain rule:

$$\frac{\partial L}{\partial \theta_{K-1}} = \frac{\partial L}{\partial \mathbf{f}_K} \frac{\partial \mathbf{f}_K}{\partial \theta_{K-1}}$$

$$\frac{\partial L}{\partial \theta_{K-2}} = \frac{\partial L}{\partial \mathbf{f}_K} \frac{\partial \mathbf{f}_K}{\partial \mathbf{f}_{K-1}} \frac{\partial \mathbf{f}_{K-1}}{\partial \theta_{K-2}}$$

Get the Gradients

- To obtain the gradients w.r.t. the parameter set θ :

- $\theta = \{\mathbf{A}_0, \mathbf{b}_0, \dots, \mathbf{A}_{K-1}, \mathbf{b}_{K-1}\}$.
- The squared loss: $L(\theta) = \|\mathbf{y} - \mathbf{f}_K(\theta, \mathbf{x})\|^2$.
- $\theta_j = \{\mathbf{A}_j, \mathbf{b}_j\}$, for $j = 0, 1, \dots, K-1$.

- By the chain rule:

$$\begin{aligned}
 \frac{\partial L}{\partial \theta_{K-1}} &= \frac{\partial L}{\partial \mathbf{f}_K} \frac{\partial \mathbf{f}_K}{\partial \theta_{K-1}} \\
 \frac{\partial L}{\partial \theta_{K-2}} &= \frac{\partial L}{\partial \mathbf{f}_K} \frac{\partial \mathbf{f}_K}{\partial \theta_{K-1}} \frac{\partial \theta_{K-1}}{\partial \theta_{K-2}} \\
 \frac{\partial L}{\partial \theta_{K-3}} &= \frac{\partial L}{\partial \mathbf{f}_K} \frac{\partial \mathbf{f}_K}{\partial \theta_{K-1}} \frac{\partial \theta_{K-1}}{\partial \theta_{K-2}} \frac{\partial \theta_{K-2}}{\partial \theta_{K-3}} \\
 &\vdots
 \end{aligned}$$

Get the Gradients

- To obtain the gradients w.r.t. the parameter set θ :

- $\theta = \{\mathbf{A}_0, \mathbf{b}_0, \dots, \mathbf{A}_{K-1}, \mathbf{b}_{K-1}\}$.
- The squared loss: $L(\theta) = \|\mathbf{y} - \mathbf{f}_K(\theta, \mathbf{x})\|^2$.
- $\theta_j = \{\mathbf{A}_j, \mathbf{b}_j\}$, for $j = 0, 1, \dots, K-1$.

- By the chain rule:

$$\begin{aligned} \frac{\partial L}{\partial \theta_{K-1}} &= \frac{\partial L}{\partial \mathbf{f}_K} \frac{\partial \mathbf{f}_K}{\partial \theta_{K-1}} \\ \frac{\partial L}{\partial \theta_{K-2}} &= \frac{\partial L}{\partial \mathbf{f}_K} \frac{\partial \mathbf{f}_K}{\partial \mathbf{f}_{K-1}} \frac{\partial \mathbf{f}_{K-1}}{\partial \theta_{K-2}} \\ \frac{\partial L}{\partial \theta_{K-3}} &= \frac{\partial L}{\partial \mathbf{f}_K} \frac{\partial \mathbf{f}_K}{\partial \mathbf{f}_{K-1}} \frac{\partial \mathbf{f}_{K-1}}{\partial \mathbf{f}_{K-2}} \frac{\partial \mathbf{f}_{K-2}}{\partial \theta_{K-3}} \\ &\vdots \end{aligned}$$

- Partial derivatives of the output of a layer w.r.t. (1) its **inputs** or (2) its **parameters**.

What have we learnt?

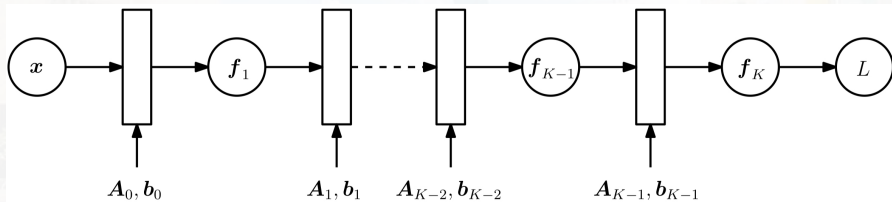
$$\begin{aligned}
 \frac{\partial L}{\partial \theta_{i+1}} &= \frac{\partial L}{\partial \mathbf{f}_K} \frac{\partial \mathbf{f}_K}{\partial \mathbf{f}_{K-1}} \cdots \frac{\partial \mathbf{f}_{i+3}}{\partial \mathbf{f}_{i+2}} \frac{\partial \mathbf{f}_{i+2}}{\partial \theta_{i+1}} \\
 \frac{\partial L}{\partial \theta_i} &= \frac{\partial L}{\partial \mathbf{f}_K} \frac{\partial \mathbf{f}_K}{\partial \mathbf{f}_{K-1}} \cdots \frac{\partial \mathbf{f}_{i+3}}{\partial \mathbf{f}_{i+2}} \underbrace{\frac{\partial \mathbf{f}_{i+2}}{\partial \mathbf{f}_{i+1}} \frac{\partial \mathbf{f}_{i+1}}{\partial \theta_i}}_{\text{not reused yet}}
 \end{aligned}$$

What have we learnt?

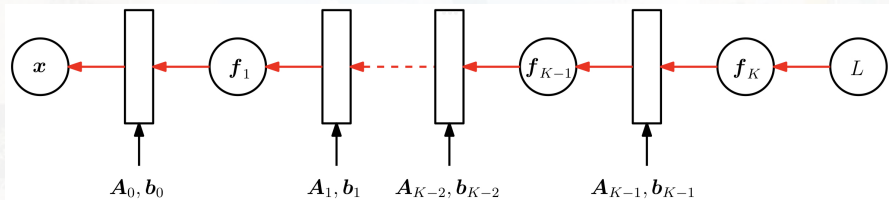
$$\begin{aligned}
 \frac{\partial L}{\partial \theta_{i+1}} &= \frac{\partial L}{\partial \mathbf{f}_K} \frac{\partial \mathbf{f}_K}{\partial \mathbf{f}_{K-1}} \cdots \frac{\partial \mathbf{f}_{i+3}}{\partial \mathbf{f}_{i+2}} \frac{\partial \mathbf{f}_{i+2}}{\partial \theta_{i+1}} \\
 \frac{\partial L}{\partial \theta_i} &= \frac{\partial L}{\partial \mathbf{f}_K} \frac{\partial \mathbf{f}_K}{\partial \mathbf{f}_{K-1}} \cdots \frac{\partial \mathbf{f}_{i+3}}{\partial \mathbf{f}_{i+2}} \underbrace{\frac{\partial \mathbf{f}_{i+2}}{\partial \mathbf{f}_{i+1}} \frac{\partial \mathbf{f}_{i+1}}{\partial \theta_i}}_{\text{not reused yet}}
 \end{aligned}$$

Hence the name *backpropagation*.

Forward Pass



Backward Pass



Outline

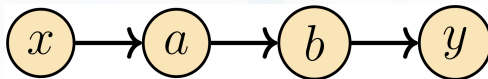
- 1 Backpropagation
- 2 Automatic Differentiation

Automatic Differentiation

- A set of techniques to *numerically* evaluate the “exact” (up to machine precision) gradient of a function.
 - By intermediate variables & chain rule.
- Complicated functions can be computed automatically(?).

Forward Mode & Reverse Mode

- Input: x ; Output: y ; Intermediate variables a, b .



Reverse Mode:

$$\frac{dy}{dx} = \left(\frac{dy}{db} \frac{db}{da} \right) \frac{da}{dx}$$

Forward Mode:

$$\frac{dy}{dx} = \frac{dy}{db} \left(\frac{db}{da} \frac{da}{dx} \right)$$

Example

Example (Reverse Mode)

Consider the function

$$f(x) = \sqrt{x^2 + \exp(x^2)} + \cos(x^2 + \exp(x^2)).$$

Introducing intermediate variables:

$$a = x^2$$

$$b = \exp(a)$$

$$c = a + b$$

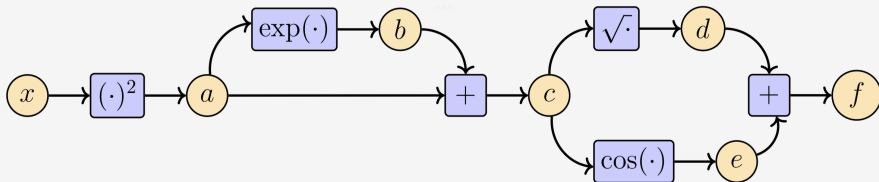
$$d = \sqrt{c}$$

$$e = \cos(c)$$

$$f = d + e.$$

Example

$$f(x) = \sqrt{x^2 + \exp(x^2)} + \cos(x^2 + \exp(x^2)).$$



$$\begin{aligned}a &= x^2 \\b &= \exp(a) \\c &= a + b \\d &= \sqrt{c} \\e &= \cos(c) \\f &= d + e.\end{aligned}$$

$$\begin{aligned}\frac{\partial a}{\partial x} &= 2x \\ \frac{\partial b}{\partial a} &= \exp(a) \\ \frac{\partial c}{\partial a} &= 1 = \frac{\partial c}{\partial b} \\ \frac{\partial d}{\partial c} &= \frac{1}{\sqrt{c}} \\ \frac{\partial e}{\partial c} &= -\sin(c) \\ \frac{\partial f}{\partial d} &= 1 = \frac{\partial f}{\partial e}.\end{aligned}$$

Compute $\frac{\partial f}{\partial x}$

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

$$\frac{\partial f}{\partial b} = \frac{\partial f}{\partial c} \frac{\partial c}{\partial b}$$

$$\frac{\partial f}{\partial a} = \frac{\partial f}{\partial b} \frac{\partial b}{\partial a} + \frac{\partial f}{\partial c} \frac{\partial c}{\partial a}$$

$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial a} \frac{\partial a}{\partial x}$$

Compute $\frac{\partial f}{\partial x}$

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

$$\frac{\partial f}{\partial b} = \frac{\partial f}{\partial c} \frac{\partial c}{\partial b} = \frac{\partial f}{\partial c} \cdot 1$$

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

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

Automatic Differentiation in General

Automatic Differentiation in General

- x_1, \dots, x_d : input variables
- x_{d+1}, \dots, x_{D-1} : intermediate variables
- x_D : the output variable

The **computation graph** can be expressed as

$$\text{For } i = d + 1, \dots, D : \quad x_i = g_i(x_{\text{pa}(x_i)}),$$

where $g_i(\cdot)$ are (elementary) functions, $x_{\text{pa}(x_i)}$ are parent nodes of x_i .

Automatic Differentiation in General

Automatic Differentiation in General

- x_1, \dots, x_d : input variables
- x_{d+1}, \dots, x_{D-1} : intermediate variables
- x_D : the output variable

The **computation graph** can be expressed as

For $i = d + 1, \dots, D$: $x_i = g_i(x_{\text{pa}(x_i)})$, (forward propagation)

where $g_i(\cdot)$ are (elementary) functions, $x_{\text{pa}(x_i)}$ are parent nodes of x_i .

$$f = x_D \implies \frac{\partial f}{\partial x_D} = 1.$$

Automatic Differentiation in General

Automatic Differentiation in General

- x_1, \dots, x_d : input variables
- x_{d+1}, \dots, x_{D-1} : intermediate variables
- x_D : the output variable

The **computation graph** can be expressed as

For $i = d + 1, \dots, D$: $x_i = g_i(x_{\text{pa}(x_i)})$, (forward propagation)

where $g_i(\cdot)$ are (elementary) functions, $x_{\text{pa}(x_i)}$ are parent nodes of x_i .

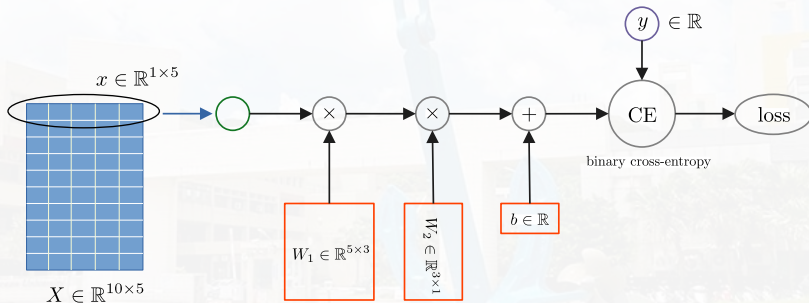
$$f = x_D \implies \frac{\partial f}{\partial x_D} = 1.$$

$$\frac{\partial f}{\partial x_i} = \sum_{x_j: x_i \in \text{pa}(x_j)} \frac{\partial f}{\partial x_j} \frac{\partial x_j}{\partial x_i} = \sum_{x_j: x_i \in \text{pa}(x_j)} \frac{\partial f}{\partial x_j} \frac{\partial g_j}{\partial x_i}. \text{ (backpropagation)}$$

Automatic Differentiation

- A set of techniques to *numerically* evaluate the “exact” (up to machine precision) gradient of a function.
 - By intermediate variables & chain rule.
- Complicated functions can be computed automatically, **whenever it can be expressed as a computation graph and the elementary functions are differentiable**.
- Programming structures, such as for **loops** and **if** statements, require more care as well.

Example



$$\text{CE} \approx -y \cdot \log \sigma(z) + (1 - y) \cdot \log(1 - \sigma(z))$$

$$z = \mathbf{x} \mathbf{W}_1 \mathbf{W}_2 + b$$

$$\sigma(z) = \frac{1}{1 + e^{-z}}$$

Example

```

1  #-*- coding: utf-8 -*-
2  """
3  Created on Wed Nov 1 09:20:33 2023
4
5  @author: jcclin
6  """
7
8  import torch
9
10 x = torch.randn(10, 5) # input tensor
11 y = torch.zeros(10, 1) # expected output
12 w1 = torch.randn(5, 3, requires_grad=True)
13 w2 = torch.randn(3, 1, requires_grad=True)
14 b = torch.randn(1, requires_grad=True)
15 z = torch.matmul(x, w1)
16 r = torch.matmul(z, w2) + b
17
18 loss = torch.nn.functional.binary_cross_entropy_with_logits(r, y)
19
20 print(f'Gradient function for z = {z.grad_fn}')
21 print(f'Gradient function for loss = {loss.grad_fn}')
22
23 loss.backward()
24 print(w1.grad)
25 print(w2.grad)
26 print(b.grad)

```

```

In [33]: runfile('E:/Research/ElectionGame/untitled0.py', wdir='E:/Research/ElectionGame')
Gradient function for z = <MmBackward0 object at 0x000001ECA98E5370>
Gradient function for loss = <BinaryCrossEntropyWithLogitsBackward0 object at 0x000001ECA98E5280>
tensor([[ 0.3135, 0.2991, 0.0587],
        [ 0.3177, 0.3031, 0.0595],
        [ 0.3489, 0.3328, 0.0653],
        [-0.1449, -0.1382, -0.0271],
        [-0.3144, -0.2999, -0.0588]])
tensor([[ -0.3156],
        [ 1.0223],
        [ 0.5931]])
tensor([0.8936])

```

In [34]:

Discussions