Introduction to intelligent systems

Automatic differentiation

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Overview

1. Automatic differentiation
2. Dual numbers
3. PyTorch
4. Tasks

Feedback group

- Mathias Kræmer Eberhardt Sørensen
- Oskar Gotthardt Bak
- Christian Ludvig Meinert Sørensen
- Alexander Baumkirchner

Learning objectives

I Automatic differentiation: Forward and reverse accumulation.

II Computation graphs.

II Automatic differentiation in Pytorch.

II Implementation of neural networks in Pytorch.

I Understand the concepts and definitions, and know their application. Reason about the concepts in the context of an example. Use correct technical terminology.

II As above plus: Read, manipulate, and work with technical definitions and expressions (mathematical and Python code). Carry out practical computations. Interpret and evaluate results.

Automatic differentiation

Gradient descent

Initialize x_0
Repeat, $t = 0, 1, 2, \ldots$

$$\underbrace{x_{t+1}}_{\text{new parameter value}} = \underbrace{x_t}_{\text{old parameter value}} - \underbrace{\alpha}_{\text{step size}} \cdot \underbrace{\nabla f(x_t)}_{\text{gradient}}$$

until convergence

Definition of gradient

$$\nabla f(x, y, \ldots) = \begin{bmatrix} \dfrac{\partial f(x, y)}{\partial x} \\ \\ \dfrac{\partial f(x, y)}{\partial y} \\ \\ \vdots \end{bmatrix}$$

Symbolic, numerical, and automatic differentiation

Symbolic Automatic manipulation of mathematical expressions to get derivatives (e.g. Mathematical, Maple)

Numerical Approximation of derivatives by finite differences

Automatic Automatic computation of the derivative of a compound expression by applying the chain rule

Ryan Adams: You should be using automatic differentiation, https://www.youtube.com/watch?v=sq2gPzlrM0g&t=985s

The chain rule

Derivative of composition of functions, $z(x) = (f \circ g)(x) = f\big(g(x)\big)$

$$z' = (f \circ g)' = (f' \circ g) \cdot g'$$

In Leibnitz's notation

$$\frac{dz}{dx} = \frac{df}{dy} \cdot \frac{dy}{dx}$$

where $z = f(y)$ and $y = g(x)$

Chain rule for functions of multiple variables

Function of two variables $z(t) = f\big(x(t), y(t)\big)$

$$\frac{dz}{dt} = \frac{\partial f}{\partial x} \cdot \frac{dx}{dt} + \frac{\partial f}{\partial y} \cdot \frac{dy}{dt}$$

Exercise: Chain rule

Compute the derivative $\frac{dz}{dt}$ of the following function

$$z(t) = f(x, y) = xy + x^2$$

where

$$x(t) = \sin(t)$$
$$y(t) = t^2$$

Exercise: Chain rule

Compute the derivative $\frac{dz}{dt}$ of the following function

$$z(t) = f(x, y) = xy + x^2$$

where

$$\begin{aligned} x(t) &= \sin(t) \\ y(t) &= t^2 \end{aligned}$$

Solution

$$\begin{aligned} \frac{dz}{dt} &= \frac{\partial f}{\partial x} \cdot \frac{dx}{dt} + \frac{\partial f}{\partial y} \cdot \frac{dy}{dt} \\ &= (y + 2x) \cdot \cos(t) + x \cdot (2t) \end{aligned}$$

Computation graph

$$f(t) = \sin(t)t^2 + \sin^2(t)$$

Computation graph

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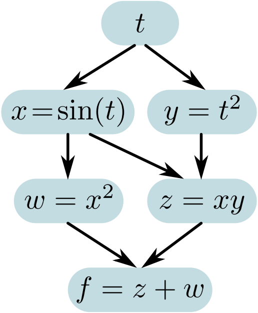

Exercise: Computation graph

Draw the computation graph for the function

$$f(x_1, x_2) = x_1^2 + x_1 \cdot x_2$$

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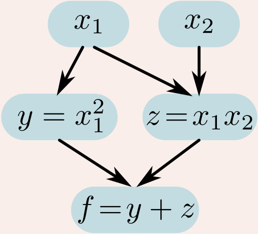
Solution

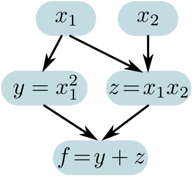


Forward accumulation

Function and derivatives

$$f(x_1, x_2) = x_1^2 + x_1 \cdot x_2$$

$$\frac{\partial f}{\partial x_1} = 2x_1 + x_2, \quad \frac{\partial f}{\partial x_2} = x_1, \quad \nabla f(3,4) = \begin{bmatrix} 10 \\ 3 \end{bmatrix}$$



Evaluate $f(3,4)$

$$\begin{aligned} x_1 &= 3 \\ x_2 &= 4 \\ y &= x_1^2 \\ z &= x_1 x_2 \\ f &= y + z \end{aligned}$$

Forward accumulation

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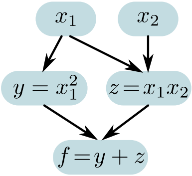

Evaluate $f(3,4)$

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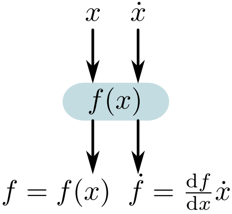
Evaluate $\nabla_{x_1} f(3,4)$

$$\begin{aligned} \dot{x}_1 &= \frac{\partial x_1}{\partial x_1} = 1 \\ \dot{x}_2 &= \frac{\partial x_2}{\partial x_1} = 0 \\ \dot{y} &= \frac{\partial y}{\partial x_1}\dot{x}_1 = 2x_1 \cdot \dot{x}_1 = 2 \cdot 3 \cdot 1 = 6 \\ \dot{z} &= \frac{\partial z}{\partial x_1}\dot{x}_1 + \frac{\partial z}{\partial x_2}\dot{x}_2 = x_2 \cdot \dot{x}_1 + x_1 \cdot \dot{x}_2 = 4 \cdot 1 + 3 \cdot 0 = 4 \\ \dot{f} &= \frac{\partial f}{\partial y}\dot{y} + \frac{\partial f}{\partial z}\dot{z} = 1 \cdot \dot{y} + 1 \cdot \dot{z} = 1 \cdot 6 + 1 \cdot 4 = \underline{10} \end{aligned}$$

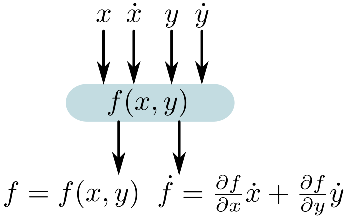
Forward accumulation

Function of one variable



Forward accumulation

Function of multiple variables



Forward accumulation

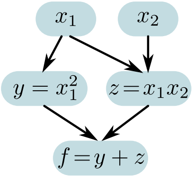
- Direct application of chain rule (going from input to output)
- Computation involves one forward pass through the graph per derivative
- Computationally expensive with many inputs

Reverse accumulation

Function and derivatives

$$f(x_1, x_2) = x_1^2 + x_1 \cdot x_2$$

$$\frac{\partial f}{\partial x_1} = 2x_1 + x_2, \quad \frac{\partial f}{\partial x_2} = x_1, \quad \nabla f(3,4) = \begin{bmatrix} 10 \\ 3 \end{bmatrix}$$



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Reverse accumulation

Function and derivatives

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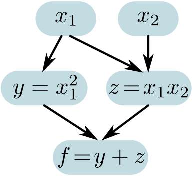


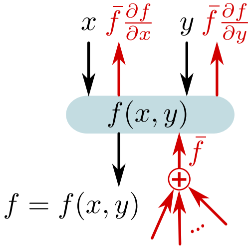
Evaluate $f(3,4)$

$$\begin{aligned} x_1 &= 3 \\ x_2 &= 4 \\ y &= x_1^2 \\ z &= x_1 x_2 \\ f &= y + z \end{aligned}$$

Evaluate $\nabla f(3,4)$

$$\begin{aligned} \bar{f} &= \frac{\partial f}{\partial f} = 1 \\ \bar{y} &= \bar{f}\frac{\partial f}{\partial y} = \bar{f} \cdot 1 = 1 \cdot 1 = 1 \\ \bar{z} &= \bar{f}\frac{\partial f}{\partial z} = \bar{f} \cdot 1 = 1 \cdot 1 = 1 \\ \bar{x}_1 &= \bar{y}\frac{\partial y}{\partial x_1} + \bar{z}\frac{\partial z}{\partial x_1} = \bar{y} \cdot 2 \cdot x_1 + \bar{z} \cdot x_2 = 1 \cdot 2 \cdot 3 + 1 \cdot 4 = 10 \\ \bar{x}_2 &= \bar{z}\frac{\partial z}{\partial x_2} = \bar{x}_2 + \bar{z} \cdot x_1 = 0 + 1 \cdot 3 = 3 \end{aligned}$$

Reverse accumulation



Reverse accumulation

- Direct application of chain rule (going from output to input)
- Computation involves one backward pass through the graph to compute all derivatives
- Requires a bit more “book-keeping” to keep track of dependencies and trace the graph backwards

Dual numbers

Complex and dual numbers

$\mathbb{C}$: *Complex numbers*

$$a + ib$$
$$i^2 = -1$$

Addition

$$(a + ib) + (c + id) = a + c + i(b + d)$$

Multiplication

$$\begin{aligned}(a + ib)(c + id) &= ac + iad + ibc + i^2 bd \\ &= (ac - bd) + i(ad + bc)\end{aligned}$$

$\mathbb{D}$: *Dual numbers*

$$a + \epsilon b$$
$$\epsilon^2 = 0$$

Addition

$$(a + \epsilon b) + (c + \epsilon d) = a + c + \epsilon(b + d)$$

Multiplication

$$\begin{aligned}(a + \epsilon b)(c + \epsilon d) &= ac + \epsilon ad + \epsilon bc + \epsilon^2 bd \\ &= ac + \epsilon(ad + bc)\end{aligned}$$

Example: $f(x) = x^2$

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Evaluating $f(x)$ on $x = a + \epsilon$ we get

$$f(a+\epsilon) = (a+\epsilon)^2 = a^2 + 2a\epsilon + \epsilon^2 = \underbrace{a^2}_{f(a)} + \epsilon \underbrace{2a}_{f'(a)}$$

The dual part happens to be $f'(a) = 2a$. Coincidence?

Exercise: $f(x) = Ax^2 + Bx + C$

Consider the function

$$f(x) = Ax^2 + Bx + C$$

Evaluate the function on $x = a + \epsilon$

Exercise: $f(x) = Ax^2 + Bx + C$

Consider the function

$$f(x) = Ax^2 + Bx + C$$

Evaluate the function on $x = a + \epsilon$

Solution

$$\begin{aligned} f(a+\epsilon) &= A(a+\epsilon)^2 + B(a+\epsilon) + C \\ &= A(a^2 + 2a\epsilon + \epsilon^2) + B(a+\epsilon) + C \\ &= \underbrace{(Aa^2 + Ba + C)}_{f(a)} + \epsilon \underbrace{(2Aa + B)}_{f'(a)} \end{aligned}$$

Taylor series

Taylor series around a

$$f(x) = f(a) + \frac{f'(a)}{1!}(x - a) + \frac{f''(a)}{2!}(x - a)^2 + \frac{f'''(a)}{3!}(x - a)^3 + \cdots$$

Taylor series

Taylor series around a

$$f(x) = f(a) + \frac{f'(a)}{1!}(x - a) + \frac{f''(a)}{2!}(x - a)^2 + \frac{f'''(a)}{3!}(x - a)^3 + \cdots$$

Inserting $x = a + \epsilon$

$$\begin{aligned} f(a + \epsilon) &= f(a) + \frac{f'(a)}{1!}\epsilon + \frac{f''(a)}{2!}\epsilon^2 + \frac{f'''(a)}{3!}\epsilon^3 + \cdots \\ &= f(a) + \epsilon f'(a) \end{aligned}$$

PyTorch

PyTorch

Demonstration

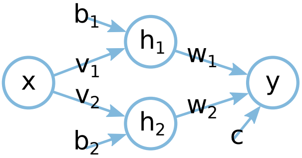
Demo: PyTorch

```
>>> import torch
>>> x1 = torch.tensor(3., requires_grad=True)
>>> x2 = torch.tensor(4., requires_grad=True)
>>> f = x1**2+x1*x2
>>> f.backward()
>>> x1.grad
tensor(10.)
>>> x2.grad
tensor(3.)
```

Neural network notebook

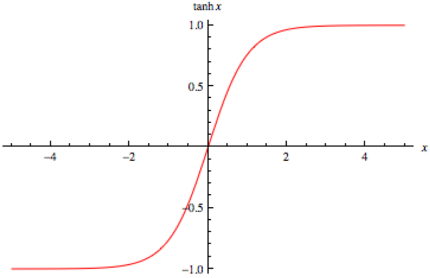
Cost function

$$E = \sum_{n=1}^{N} \big(y(n) - \hat{y}(n)\big)^2$$



Network structure

$$\begin{aligned} \hat{y}(n) &= w_1 h_1(n) + w_2 h_2(n) + c \\ h_1(n) &= \tanh\left(v_1 x(n) + b_1\right) \\ h_2(n) &= \tanh\left(v_2 x(n) + b_2\right) \end{aligned}$$



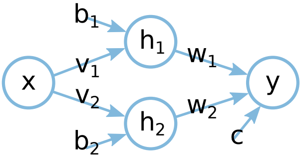
Model parameters

$$c,\ w_1,\ w_2,\ v_1,\ v_2,\ b_1,\ b_2$$

Neural network notebook

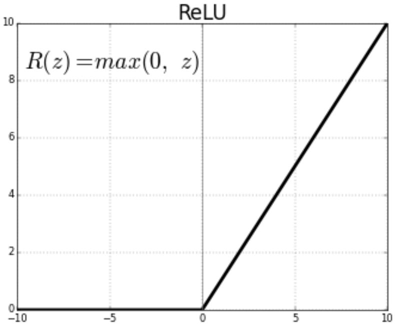
Cost function

$$E = \sum_{n=1}^{N} \left(y(n) - \hat{y}(n)\right)^2$$



Network structure

$$\hat{y}(n) = w_1 h_1(n) + w_2 h_2(n) + c$$
$$h_1(n) = \text{ReLU}\left(v_1 x(n) + b_1\right)$$
$$h_2(n) = \text{ReLU}\left(v_2 x(n) + b_2\right)$$



Model parameters

$$c,\ w_1,\ w_2,\ v_1,\ v_2,\ b_1,\ b_2$$

Tasks

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1. Work through introduction to PyTorch notebooks
   See `09-PyTorchTutorial1.ipynb` and `09-PyTorchTutorial2.ipynb` on the fileshare
2. Work through introduction to PyTorch notebooks
   See `09-TwoLayerNet-x.ipynb` on the fileshare
3. Experiment with the neural network challenge notebook
   See `09-NeuralNetworkChallenge.ipynb` on the fileshare
4. Today's feedback group
   - Mathias Kræmer Eberhardt Sørensen
   - Oskar Gotthardt Bak
   - Christian Ludvig Meinert Sørensen
   - Alexander Baumkirchner

Lab report

- Lab 4: Neural networks (Deadline: Thursday 9 November 20:00)