Natural Language Processing with Deep Learning

Lecture 2 — Mathematical foundations of deep learning

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Natural Language Processing Group
Paderborn University
We focus on Trustworthy Human Language Technologies

www.trusthlt.org

Motivation

Quick poll

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1. Who of you knows stochastic gradient descent and backpropagation?
2. Who of you ever implemented it from scratch?

How does this lecture relate to the previous one and to entire course?

How deep will we go?

We won't cover

- Set theory: The assembler of mathematics
  - Sets $A = \{a, b, c\}$, $a \in A$, no ordering
  - Ordered tuples $(a, b) \neq (b, a)$
- Number theory
  - Set of natural numbers $\mathbb{N}_0 = \{0, 1, \ldots\}$
  - Set of real numbers $\mathbb{R}$, infinity
- Sequences and limits

$\mathbb{R}^2 = \mathbb{R} \times \mathbb{R}$ — tuples of reals, e.g., $(1.3, -44.67)$, also a two-dimensional vector

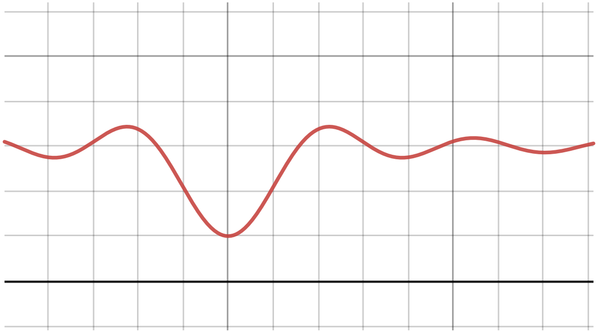
Problem 1: Minimize functions

Why is it important?

In supervised machine learning …

- We have some training data (e.g., for classification)
- We have a learning algorithm
- We want to minimize some kind of error (e.g., misclassification) of the learning algorithm on training data

Problem: Find minimum of any function



- For "easy" functions, closed-form solution (high school math)
- For complicated functions not trivial and cumbersome

Function of single variable

We typically use Euler's notation with arbitrary but somehow standard naming conventions (x, y, f)

$y = f(x) \qquad f : \mathbb{R} \to \mathbb{R}$

$f : A \to B$ where A is domain, B is co-domain

Function composition

$f : \mathbb{R} \to \mathbb{R} \quad g : \mathbb{R} \to \mathbb{R}$

$h = g \circ f$

$h(x) = g(f(x))$ or $(g \circ f)(x) = g(f(x))$

Lines in two dimensions

Lines in a Cartesian plane are characterized by linear equations.

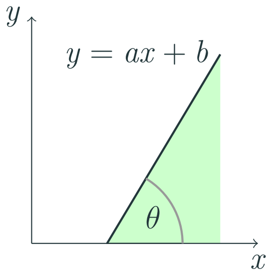
Every line L (including vertical lines) is the set of all points whose coordinates (x, y) satisfy a linear equation:

$$L = \{(x, y) \mid w_1 x + w_2 y = w_3\}$$

where w_1, w_2 and w_3 are fixed real numbers (called coefficients) such that w_1 and w_2 are not both zero.

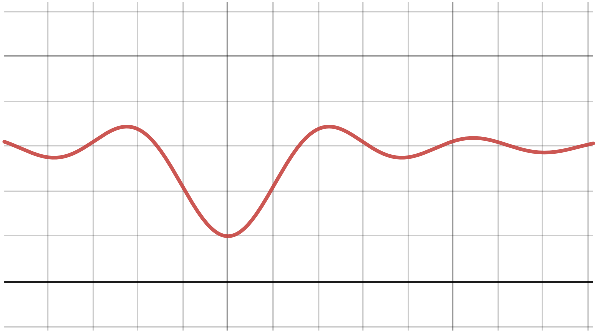
Linear function in two dimensions

Usually we use **slope-intercept** form $y = ax + b$



$\theta = \arctan(a) \qquad a = \tan(\theta)$

Approximate function by a line at point



"Steepness" at c?

$$f'(c) = \lim_{x \to c} \frac{f(x) - f(c)}{x - c}$$

The derivative of f at c

Derivative-computing function

We want a function D which, when given a differentiable function $f : \mathbb{R} \to \mathbb{R}$ as input, produces another function $g : \mathbb{R} \to \mathbb{R}$ output, such that $g(c) = f'(c)$ for every c.

This derivative-computing function D is often written as

$$\frac{d}{dx}$$

but this causes inconsistent notation like

$$\frac{d}{dx}(f), \qquad \frac{df}{dx}, \qquad \frac{dy}{dx}$$

and forces one to choose a variable name x or y

Derivative of nested functions: The chain rule hammer

Variant 1 (Lagrange's notation)

Let $f, g : \mathbb{R} \to \mathbb{R}$ be two functions which have derivatives. Then the derivative of $g(f(x))$ is $g'(f(x)) \cdot f'(x)$

Variant 2 (Function composition operator $\circ$)

Let $f, g : \mathbb{R} \to \mathbb{R}$ be two functions which have derivatives. Let $h = g \circ f$. The derivative of h is $h' = (g \circ f)' = (g' \circ f) \cdot f'$

Variant 3 (Leibnitz's notation)

Call $h(x) = g(f(x))$. Then using $\frac{dh}{dx}$ for the derivative of h, the chain rule for this would be $\frac{dh}{dx} = \frac{dh}{df}\frac{df}{dx}$

Chain rule example

Consider $y = e^{\sin(x^2)}$. Composite of three functions:

$$y = f(u) = e^u$$
$$u = g(v) = \sin v = \sin\left(x^2\right)$$
$$v = h(x) = x^2$$

Their derivatives are

$$\frac{dy}{du} = f'(u) = e^u = e^{\sin(x^2)}$$
$$\frac{du}{dv} = g'(v) = \cos v = \cos\left(x^2\right)$$
$$\frac{dv}{dx} = h'(x) = 2x$$

Chain rule example (cont.)

Consider $y = e^{\sin(x^2)}$. Composite of three functions:

$$y = f(u) = e^u, u = g(v) = \sin v = \sin\left(x^2\right), v = h(x) = x^2$$

Their derivatives are

$$\frac{dy}{du} = e^{\sin(x^2)}, \frac{du}{dv} = \cos\left(x^2\right), \frac{dv}{dx} = 2x$$

Derivative of their composite at the point $x = a$ is (in Leibniz notation)

$$\frac{dy}{dx} = \left.\frac{dy}{du}\right|_{u=g(h(a))} \cdot \left.\frac{du}{dv}\right|_{v=h(a)} \cdot \left.\frac{dv}{dx}\right|_{x=a}$$

Gradient-based optimization: Find minimum of a function

We want $\hat{x} = \operatorname{argmin}_x f(x)$

Pre-requisites:

- We can evaluate $y = f(x)$ for any x
- We can evaluate its derivative $f'(c)$ (or $\frac{dy}{dx}(c)$) for any c

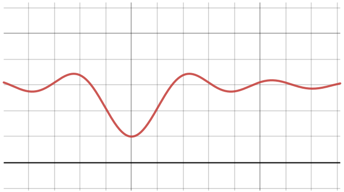
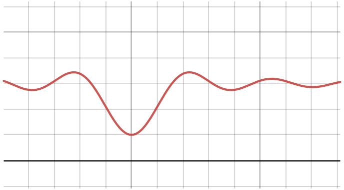


Figure 1: $3 - \frac{\sin(2x)}{x}$

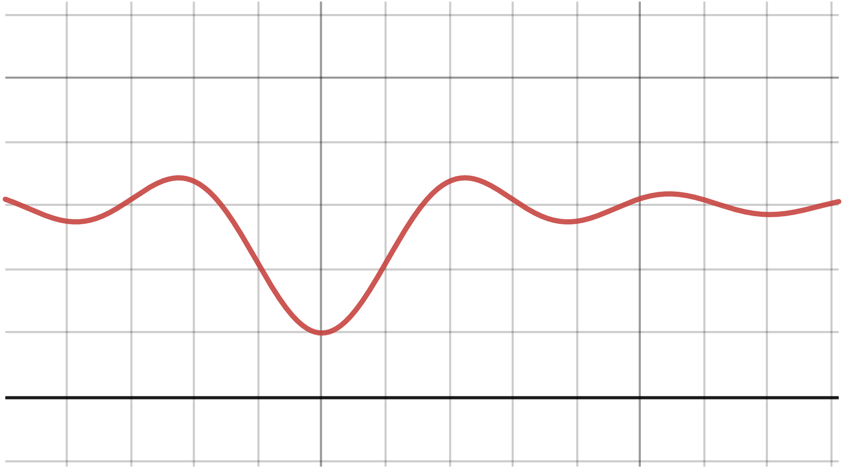
Gradient-based optimization: Find minimum of a function



1. Start with initial random value x_i
2. $u = f'(x_i)$ — direction and strength of change at x_i
3. Next value $x_{i+1} \leftarrow x_i - \eta \cdot u$
4. With small enough η (eta), $f(x_{i+1}) < f(x_i)$

Repeating 2 + 3 (with properly decreasing values of η) will find minimum point x_i

Gradient-based optimization: Workout example



Problem 2: Minimize multivariate functions

Multivariate functions

$f : \mathbb{R}^n \to \mathbb{R}$

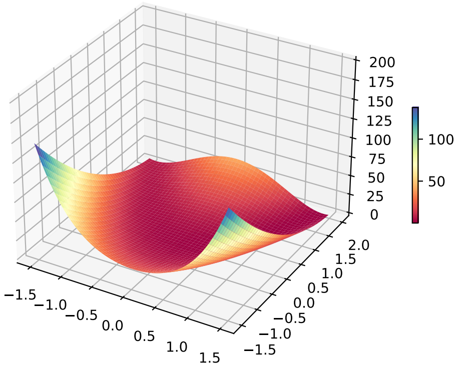


Figure 2: $f(x, y) = (a - x)^2 + b(y - x^2)^2$, $a = 1$, $b = 100$

Partial derivatives

Partial derivative: the directional derivative wrt. a single variable

$\frac{\partial f}{\partial x_2}$ — "the partial derivative of f with respect to x_2"

Example: $f(x_1, x_2, x_3) = (x_1)^2 x_2 + \cos(x_3)$

$$\frac{\partial f}{\partial x_1} = 2x_2x_1 \qquad \frac{\partial f}{\partial x_2} = (x_1)^2 \qquad \frac{\partial f}{\partial x_3} = -\sin(x_3)$$

Gradient

Example: $f(x_1, x_2, x_3) = (x_1)^2 x_2 + \cos(x_3)$

$$\frac{\partial f}{\partial x_1} = 2x_2x_1 \qquad \frac{\partial f}{\partial x_2} = (x_1)^2 \qquad \frac{\partial f}{\partial x_3} = -\sin(x_3)$$

The resulting total derivative matrix Df is called the **gradient** of f, denoted ∇f

Example: $f(x_1, x_2, x_3) = (x_1)^2 x_2 + \cos(x_3)$

$$\nabla f = \begin{pmatrix} \frac{\partial f}{\partial x_1} & \frac{\partial f}{\partial x_2} & \frac{\partial f}{\partial x_3} \end{pmatrix} = \begin{pmatrix} 2x_2x_1 & (x_1)^2 & -\sin(x_3) \end{pmatrix}$$

Gradient properties

Example: $f(x_1, x_2, x_3) = (x_1)^2 x_2 + \cos(x_3)$

$$\nabla f = \begin{pmatrix} \frac{\partial f}{\partial x_1} & \frac{\partial f}{\partial x_2} & \frac{\partial f}{\partial x_3} \end{pmatrix} = \begin{pmatrix} 2x_2 x_1 & (x_1)^2 & -\sin(x_3) \end{pmatrix}$$

J. Kun (2020). A Programmer's Introduction to Mathematics. 2nd ed., p. 252

For every differentiable function $f : \mathbb{R}^n \to \mathbb{R}$ and every point $\boldsymbol{x} \in \mathbb{R}^n$, the gradient $\nabla f(\boldsymbol{x})$ points in the direction of steepest ascent of f at $\boldsymbol{x}$.

Warning!

Sometimes we call gradient the function for computing concrete values for a given input (as above), sometimes the vector of concrete numbers computed for the given input

Gradient descent for minimizing multivariate functions

Given $f : \mathbb{R}^n \rightarrow \mathbb{R}$ we want to find

$$\hat{\boldsymbol{x}} = \underset{\boldsymbol{x}}{\operatorname{argmin}}\, f(\boldsymbol{x})$$

1. Start at some random position with a random value vector $\boldsymbol{x}_i = (x_1, \ldots, x_n)$
2. Compute the gradient and update the position

$$\boldsymbol{x}_{i+1} \leftarrow \boldsymbol{x}_i - \eta \cdot \nabla f(\boldsymbol{x}_i)$$

3. After enough iterations or some stopping criterion we have $\hat{\boldsymbol{x}}$

Gradient descent for minimizing multivariate functions

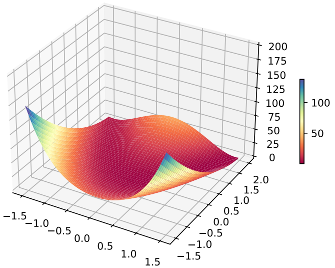
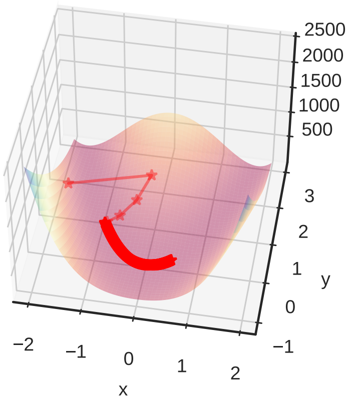
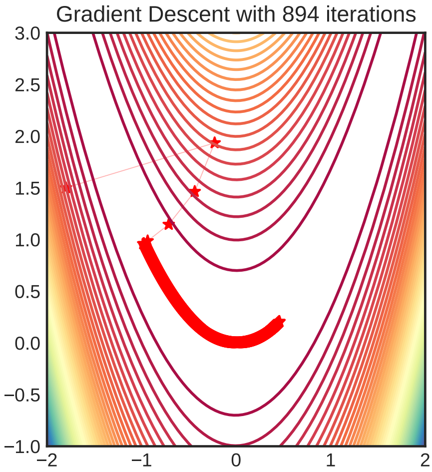


Figure 3: $f(x, y) = (a - x)^2 + b(y - x^2)^2, a = 1, b = 100$

$$\nabla f = \left(-400xy + 400x^3 + 2x - 2; \quad 200y - 200x^2\right)$$

Gradient for minimizing multivariate functions





Random starting point $(-1.8; 1.5)$, minimum at $(1; 1)$

Problem 3: When functions become heavily nested

In reality we work with deeply composed functions

Example

Minimize function e wrt. $w_0, w_1, \ldots, w_K$

$$e = -\frac{1}{N} \sum_{i=1}^{N} y_{[i]} \log \left(\frac{1}{1 + \exp\left(w_0 + \sum_{j=1}^{K} w_k \cdot \boldsymbol{x}_{[i][k]}\right)} \right)$$

Where $\boldsymbol{x}_{[1]}, \ldots, \boldsymbol{x}_{[N]}$, and $y_{[1]}, \ldots, y_{[N]}$ are constants

$$\nabla f = \left(\frac{\partial e}{\partial w_0}; \frac{\partial e}{\partial w_1}; \ldots; \frac{\partial e}{\partial w_K} \right)$$

$\frac{\partial e}{\partial w_1} = \ldots$ Good luck!

Chain Rule for Multivariable Functions

Suppose that $x = g(t)$ and $y = h(t)$ are differentiable functions of t and $z = f(x, y)$ is a differentiable function of x and y. Then $z = f(x(t), y(t))$ is a differentiable function of t and

$$\frac{\partial z}{\partial t} = \frac{\partial z}{\partial x} \cdot \frac{dx}{dt} + \frac{\partial z}{\partial y} \cdot \frac{dy}{dt}$$

where the ordinary derivatives are evaluated at t and the partial derivatives are evaluated at (x, y).

Be ready for possible notation madness

$$\frac{\partial f}{\partial t} = \frac{\partial f}{\partial g}\frac{\partial g}{\partial t} + \frac{\partial f}{\partial h}\frac{\partial h}{\partial t}$$

Chain rule for multivariable functions (two independent variables)

Suppose $x = g(u, v)$ and $y = h(u, v)$ are differentiable functions of u and v, and $z = f(x, y)$ is a differentiable function of x and y. Then, $z = f(g(u, v), h(u, v))$ is a differentiable function of u and v, and

$$\frac{\partial z}{\partial u} = \frac{\partial z}{\partial x}\frac{\partial x}{\partial u} + \frac{\partial z}{\partial y}\frac{\partial y}{\partial u}$$
$$\frac{\partial z}{\partial v} = \frac{\partial z}{\partial x}\frac{\partial x}{\partial v} + \frac{\partial z}{\partial y}\frac{\partial y}{\partial v}$$

Problem 3: When functions become heavily nested

Efficient computation of gradient

Working example

$$e = (a + b)(b + 1)$$

Compute gradient wrt. a and b

This one is easy by hand, but that's not the point

$$e = (a + b)(b + 1) = ab + a + b^2 + b$$

$$\frac{\partial e}{\partial a} = b + 1 \qquad \frac{\partial e}{\partial b} = a + 2b + 1$$

Add some intermediate variables and function names

$$e = (a + b)(b + 1)$$

$$e = f_1(r, s) := r \cdot s$$
$$r = f_2(a, b) := a + b$$
$$s = f_3(b) := b + 1$$

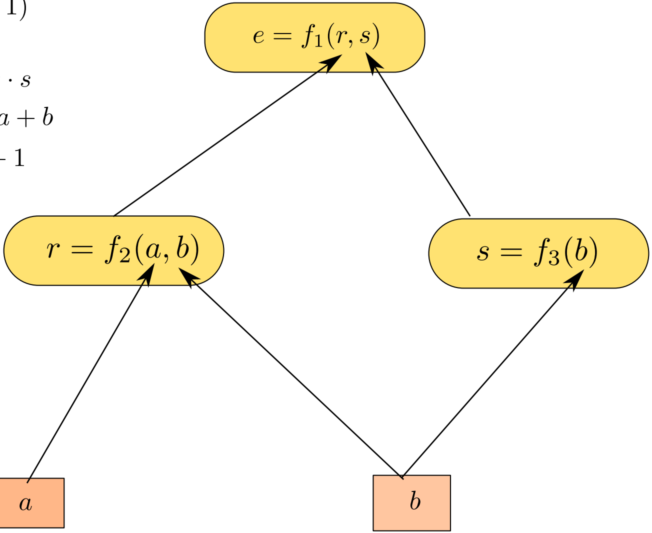
Build computational graph and evaluate (forward step)

$e = (a + b)(b + 1)$

$e = f_1(r, s) := r \cdot s$

$r = f_2(a, b) := a + b$

$s = f_3(b) := b + 1$



Important: a, b will be some concrete real numbers, therefore r, s, e will be concrete real numbers too!

Computational graph

- DAG — directed acyclic graph (not necessarily a tree!)
- Each node — a differentiable function with arguments
- Leaves — variables (e.g., a, b) or constants
- Arrows — Function composition

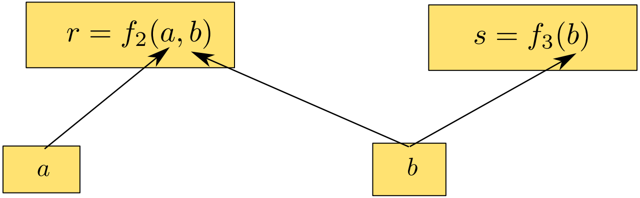


Figure 4: r, s are parents of b; a, b are children (arguments) of r

Goal: $\frac{\partial e}{\partial a}$ and $\frac{\partial e}{\partial b}$ (gradient), but let's do $\frac{\partial e}{\partial \star}$ for every node

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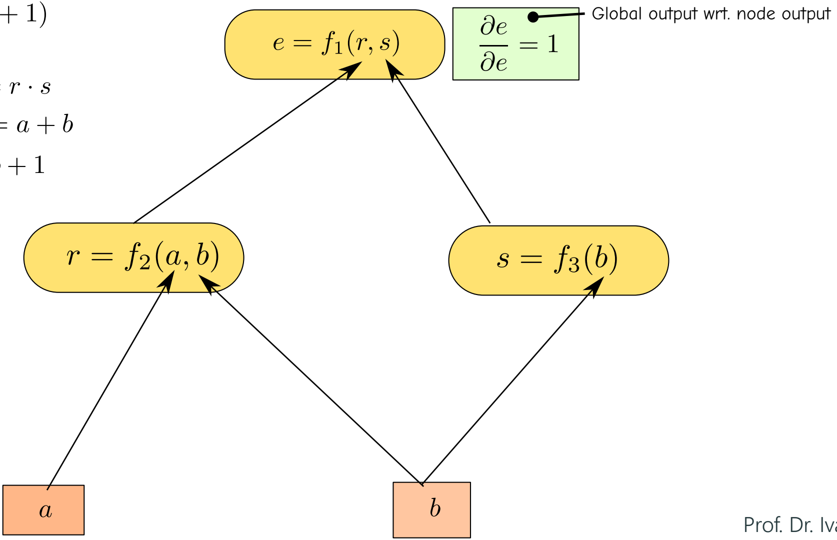
$$e = (a+b)(b+1)$$

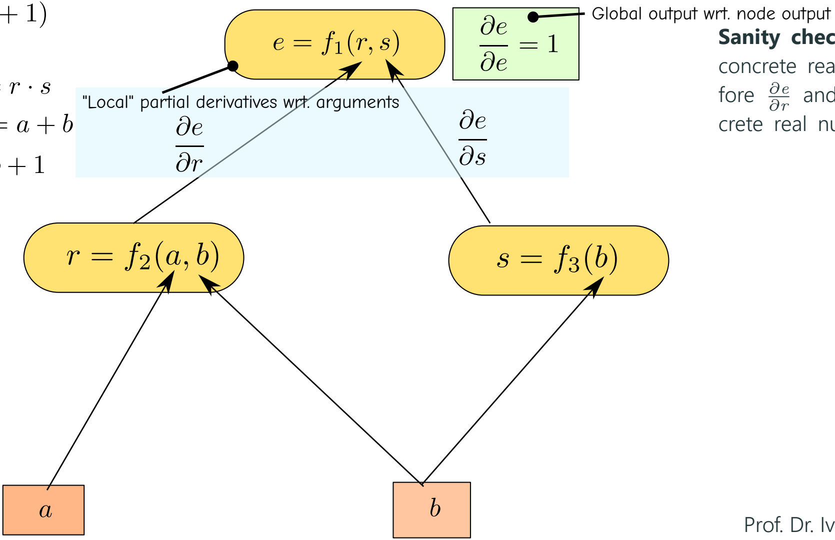
$$e = f_1(r,s) := r \cdot s$$
$$r = f_2(a,b) := a + b$$
$$s = f_3(b) := b + 1$$



Since $e = r \cdot s$, par. derivatives are easy: $\frac{\partial e}{\partial r} = s$ and $\frac{\partial e}{\partial s} = r$

$e = (a + b)(b + 1)$

$e = f_1(r, s) := r \cdot s$
$r = f_2(a, b) := a + b$
$s = f_3(b) := b + 1$



Sanity check: r, s are some concrete real numbers, therefore $\frac{\partial e}{\partial r}$ and $\frac{\partial e}{\partial s}$ will be concrete real numbers too!

Proceed to next child r and compute $\frac{\partial e}{\partial r}$ – use chain rule!

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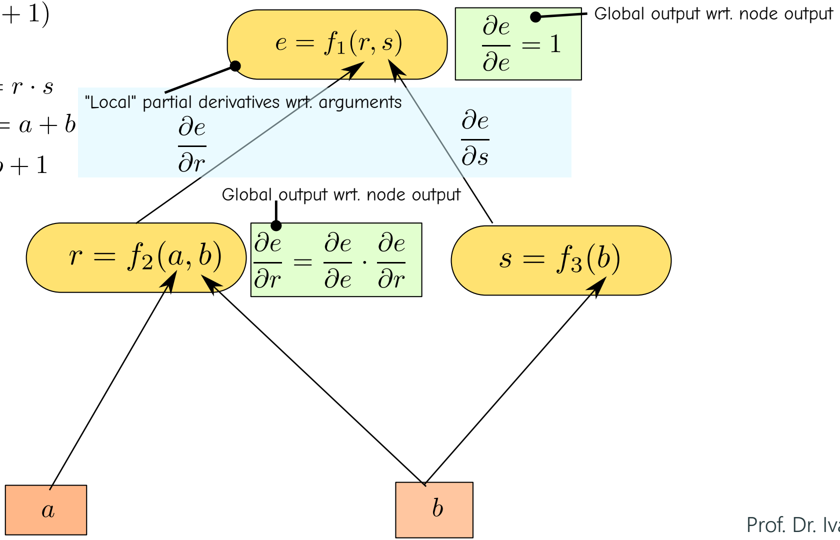
$$e = (a+b)(b+1)$$

$$e = f_1(r, s) := r \cdot s$$

$$r = f_2(a, b) := a + b$$

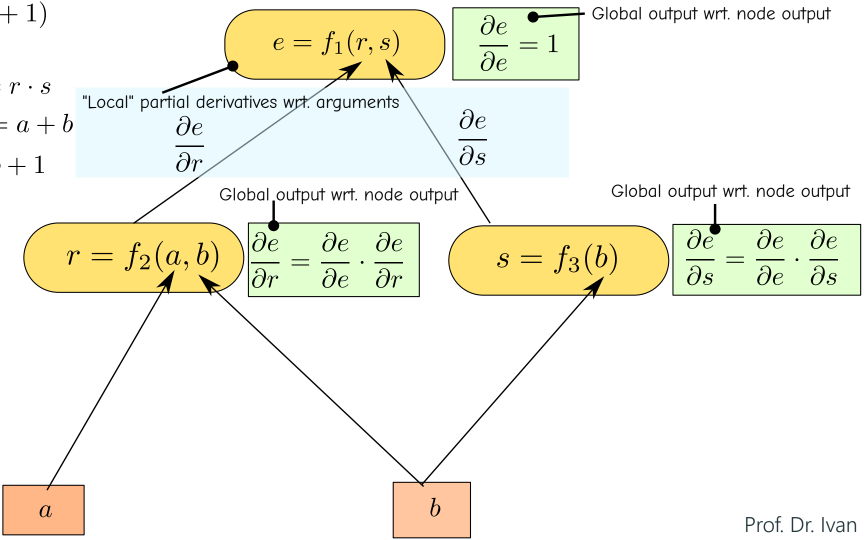
$$s = f_3(b) := b + 1$$



Proceed to next child s and compute $\frac{\partial e}{\partial s}$ – use chain rule!

$$e = (a + b)(b + 1)$$

$$e = f_1(r, s) := r \cdot s$$
$$r = f_2(a, b) := a + b$$
$$s = f_3(b) := b + 1$$



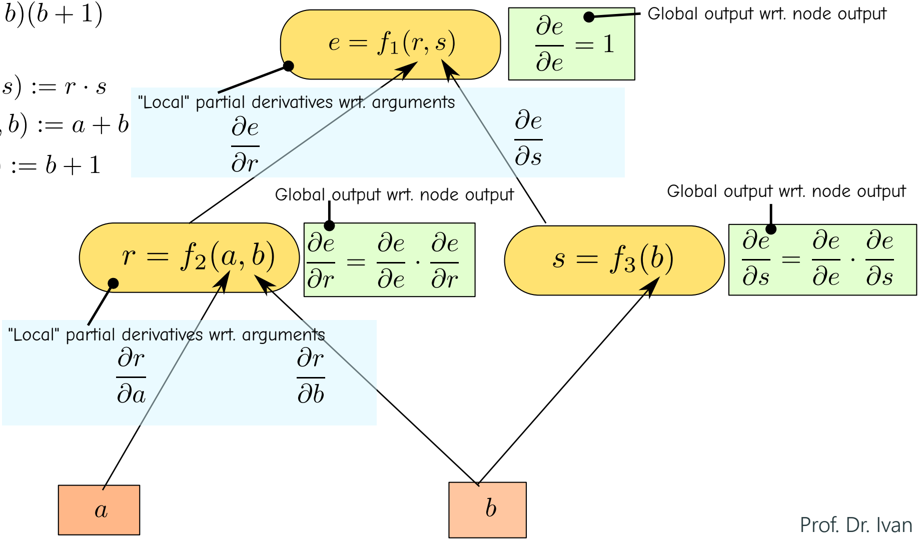
Since $r = a + b$, par. derivatives are easy: $\frac{\partial r}{\partial a} = 1$ and $\frac{\partial r}{\partial b} = 1$

$$e = (a + b)(b + 1)$$

$$e = f_1(r, s) := r \cdot s$$

$$r = f_2(a, b) := a + b$$

$$s = f_3(b) := b + 1$$



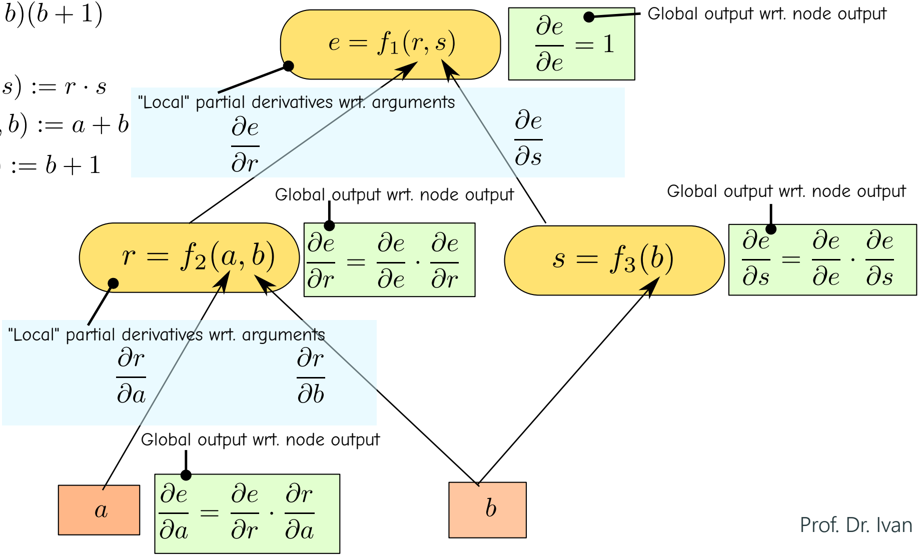
Proceed to next child a and compute $\frac{\partial e}{\partial a}$ – use chain rule!

$$e = (a+b)(b+1)$$

$$e = f_1(r, s) := r \cdot s$$

$$r = f_2(a, b) := a + b$$

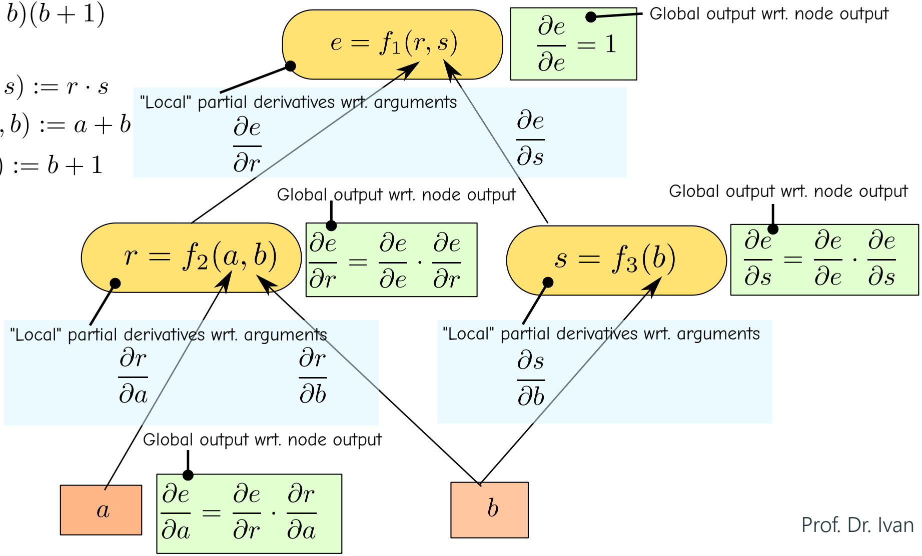
$$s = f_3(b) := b + 1$$



Since $s = b + 1$, par. derivatives are easy: $\frac{\partial s}{\partial b} = 1$

$$e = (a + b)(b + 1)$$

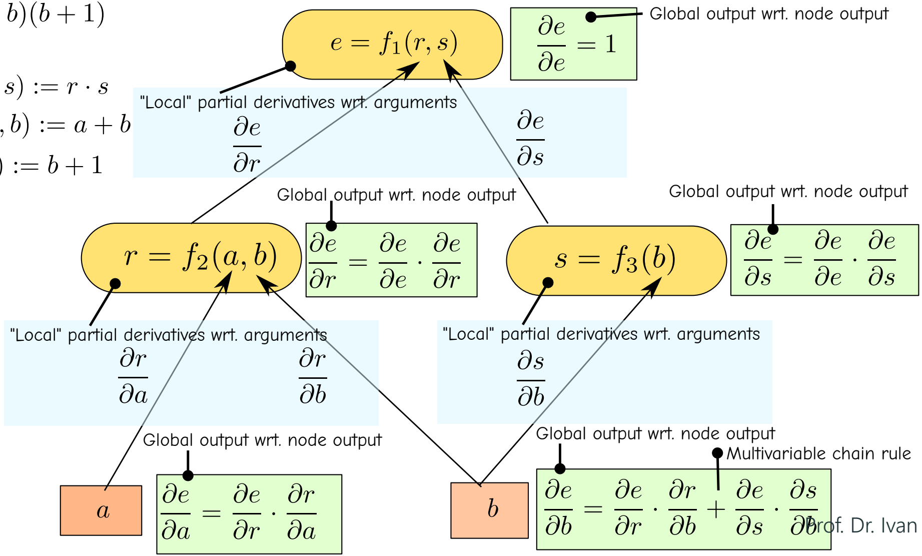
$$e = f_1(r, s) := r \cdot s$$
$$r = f_2(a, b) := a + b$$
$$s = f_3(b) := b + 1$$



Proceed to b and compute $\frac{\partial e}{\partial b}$ – use multivariate chain rule!

$$e = (a+b)(b+1)$$

$$e = f_1(r, s) := r \cdot s$$
$$r = f_2(a, b) := a + b$$
$$s = f_3(b) := b + 1$$



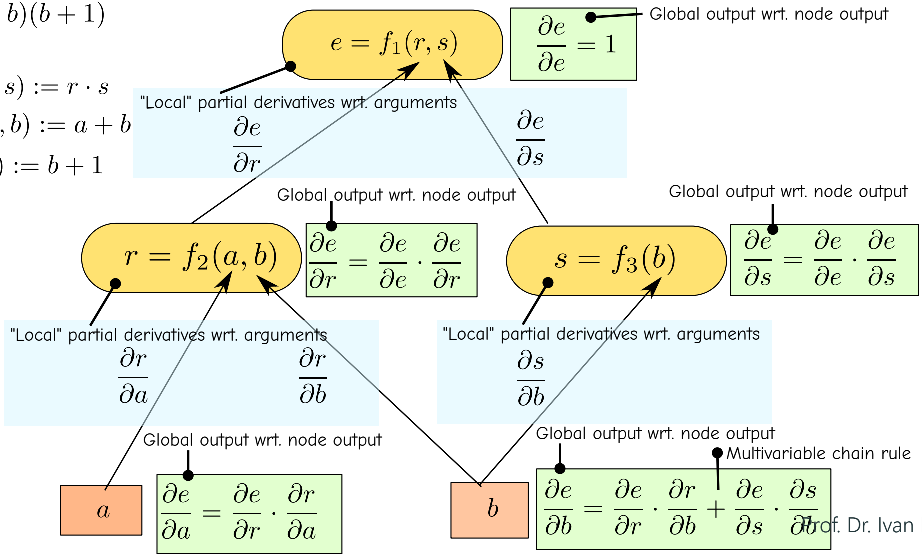
Goal: $\nabla e = \left(\frac{\partial e}{\partial a}; \frac{\partial e}{\partial b}\right)$ — we computed it for concrete a and b

$e = (a + b)(b + 1)$

$e = f_1(r, s) := r \cdot s$

$r = f_2(a, b) := a + b$

$s = f_3(b) := b + 1$



Generic node in a computational graph

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Adapted from J. Kun (2020). A Programmer's Introduction to Mathematics. 2nd ed., p. 265

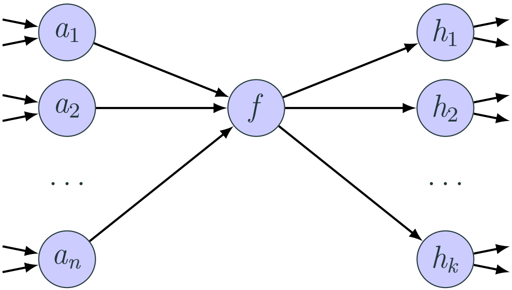
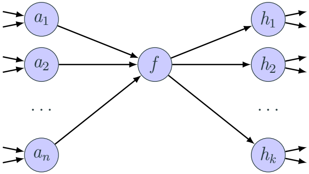


Figure 5: A generic node of a computation graph. Node f has many inputs, its output feeds into many nodes, and each of its inputs and outputs may also have many inputs and outputs.

Generic node in a computational graph $f(a_1, \ldots, a_n)$



Assuming the graph is a function $e = g(\ldots)$, we compute

$$\frac{\partial e}{\partial f} = \sum_{i=1}^{k} \frac{\partial e}{\partial h_i} \cdot \frac{\partial h_i}{\partial f}$$

and

$$\frac{\partial f}{\partial a_i} \quad \text{for } a_i, \ldots, a_n$$

What each node must implement?

For example a function $s = f(a, b, c, d)$

- How to compute the output value s (given the parameters a, b, c, d)
- How to compute partial derivatives wrt. the parameters, i.e. $\frac{\partial s}{\partial a}, \frac{\partial s}{\partial b}, \frac{\partial s}{\partial c}, \frac{\partial s}{\partial d}$

Backpropagation

- Forward computation: Compute all nodes' output (and cache it)
- Backward computation (Backprop): Compute the overall function's partial derivative with respect to each node

Ordering of the computations? Recursively or build a graph's topology upfront and iterate

Backpropagation: Recap

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- We can express any arbitrarily complicated function $f : \mathbb{R}^n \to \mathbb{R}$ as a computational graph
- For computing the gradient ∇f at a concrete point $(x_1, x_2, \ldots, x_n)$ we run the forward pass and backprop
- When caching each node's intermediate output and partial derivatives, we avoid repeating computations $\to$ efficient algorithm

Recap

Motivation

Problem 1: Minimize functions

Problem 2: Minimize multivariate functions

Problem 3: When functions become heavily nested

  Efficient computation of gradient

Take aways

- We can quite efficiently find a minimum of any differentiable nested multivariate function
  - Iterative gradient descent takes the most promising direction
  - Backpropagation utilizes computational graphs and caching $\rightarrow$ computes gradients efficiently
- We have not touched neural networks yet at all!

License and credits

Credits

Ivan Habernal