Natural Language Processing with Deep Learning

Lecture 2 — Gradient and backpropagation

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This lecture

- Refresher of supervised machine learning
- Refresher of derivatives
- Partial derivatives and gradient
- Backpropagation

Notation

Notation

Vectors in linear algebra are columns, for example $\mathbf{x} \in \mathbb{R}^3$

$$\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} \qquad \text{(bold face, lower case)}$$

We treat them as a row vector by transposing, for example $\mathbf{x}^\intercal = (x_1, x_2, x_3)$ — which is a matrix $\mathbb{R}^{1 \times 3}$

Caveat: 1-D array (a list of numbers) is sometimes considered a vector, so dealing with dimensions might be quite messy

Notation

Matrices are upper-case bold, for example $\mathbf{Z} \in \mathbb{R}^{2 \times 3}$

$$\mathbf{Z} = \begin{pmatrix} z_{1,1} & z_{1,2} & z_{1,3} \\ z_{2,1} & z_{2,2} & z_{2,3} \end{pmatrix}$$

Scalars are ordinary lower case letters, for example

$$a, b, c \in \mathbb{R}$$

Notation ambiguity

A dot $\cdot$ means multiple things, depending on context

Simple scalar multiplication, for example $a \cdot b$

$$\cdot : \mathbb{R} \times \mathbb{R} \to \mathbb{R}$$

Dot product $\mathbf{x} \cdot \mathbf{y} = \sum_{i=1}^{n} x_i y_i$

$$\cdot : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$$

Matrix-matrix (matrix-vector/vector-matrix) multiplication, for example $\mathbf{x} \cdot \mathbf{W}$ or $\mathbf{Y} \cdot \mathbf{Z}$

$$\cdot : \mathbb{R}^{m \times n} \times \mathbb{R}^{n \times p} \to \mathbb{R}^{m \times p}$$

Supervised ML basics

Supervised learning problem: Data

Dataset is a set of input-label tuples (labeled examples)

$$\{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n), \dots, (\mathbf{x}_N, y_N)\}$$

- Each input $\mathbf{x}_n$ is a D-dimensional vector of real numbers, which are called features, attributes, or covariates
- Label y_n associated with input vector $\mathbf{x}_n$

Models as functions

Predictor: a function from features to output

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

In classification we typically predict a probability distribution over categories, e.g.,

$$f : \mathbb{R}^D \to \mathbb{R}^{|C|}$$

$|C|$ — number of classes and arbitrary mapping, e.g.

$$C = \begin{cases} 0 & \text{Sport} \\ 1 & \text{Politics} \\ 2 & \text{Business} \end{cases}$$

Models as functions

For example

$$C = \begin{cases} 0 & \text{Sport} \\ 1 & \text{Politics} \\ 2 & \text{Business} \end{cases}$$

$$f(\mathbf{x}) \to \underbrace{(0.01, 0.82, 0.17)}_{\sum = 1.0}$$

Learning is finding 'the best' parameters θ

The goal of learning is to

- find a model and its corresponding parameters
- the resulting predictor should perform well on unseen data

Conceptually three distinct phases

1. Prediction or inference
2. Training or parameter estimation
3. Hyperparameter tuning or model selection

Loss function for training

What does it mean to fit the data "well"?

We need to specify a **loss function**

$$\ell(\underbrace{y_n}_{\text{True label}}, \underbrace{\hat{y}_n}_{\text{Predictor's output}}) \to \underbrace{\mathbb{R}^+}_{\text{"Loss"}}$$

representing 'how big' an error we made on this particular prediction

Loss example: Squared Loss

$$\ell(y_n, \hat{y_n}) = (y_n - \hat{y_n})^2$$

Minimizing so-called 'empirical risk'

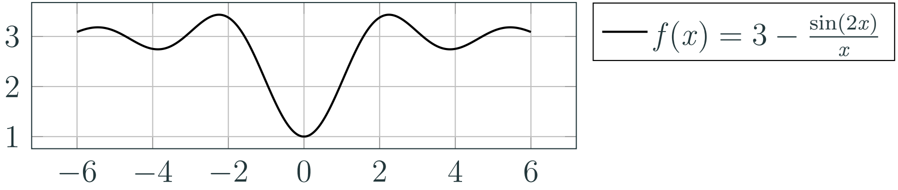
$$\min_{\theta} \frac{1}{N} \sum_{i=1}^{N} (y_i - f(\mathbf{x}, \theta))^2$$

Key approach to supervised learning

Finding a good parameter vector θ^* by **minimizing the average loss** on the set of N training examples

Minimizing functions

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

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

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

Function composition

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

$h = g \circ f$

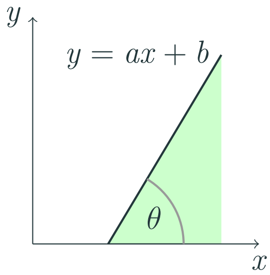
$h(x) = g(f(x))$ or $(g \circ f)(x) = g(f(x))$

Linear function in two dimensions

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

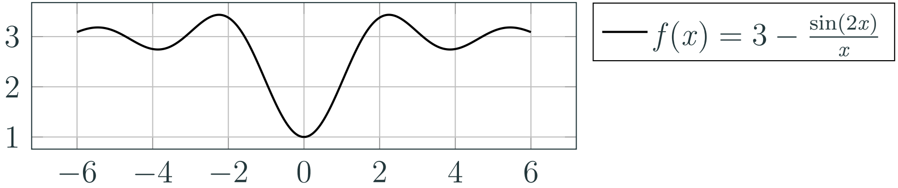
where w_1, w_2 and w_3 are fixed real numbers (called coefficients) such that w_1 and w_2 are not both zero.

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.

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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 $g'(f(x)) \cdot f'(x)$

Derivative of nested functions: The chain rule hammer

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

Derivative of nested functions: The chain rule hammer

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Let $h = g \circ f$. The derivative of h is $h' = (g \circ f)' = (g' \circ f) \cdot f'$

Variant 3 (Leibniz's notation)

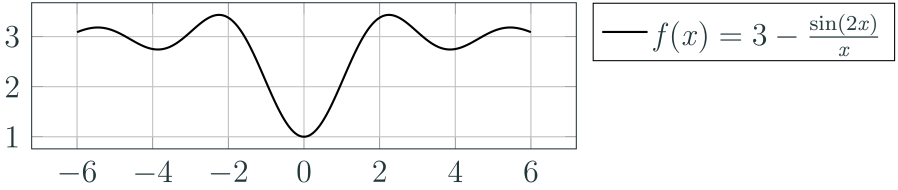
Call $h(x) = g(f(x))$. Then using $\frac{dh}{dx}$ for the derivative of h,
the chain rule for this would be $\frac{dh}{dx} = \frac{dh}{df} \frac{df}{dx}$

Gradient-based optimization: Find minimum of a function

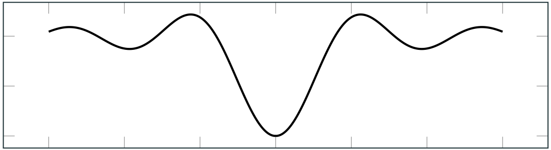
We want $\hat{x} = \operatorname{argmin}_x f(x)$

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



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

Minimizing multivariate functions

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

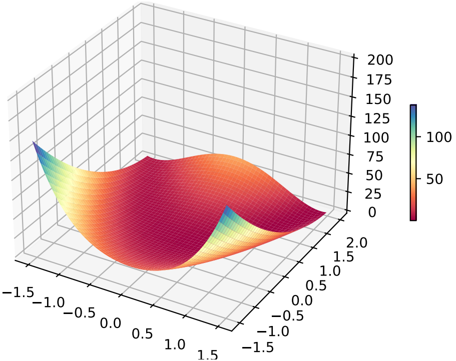


Figure 1: $f(x, y) = (a - x)^2 + b(y - x^2)^2$, $a = 1, b = 100$

`https://colab.research.google.com/drive/1mlZtxPXuk3mls56CQArmDzjdp5bLbrJC`

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

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

Chain rule for multivariate 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

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

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

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

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

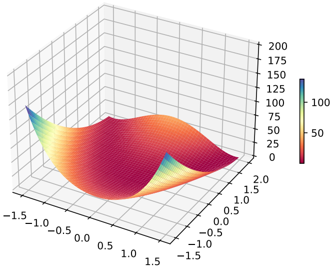
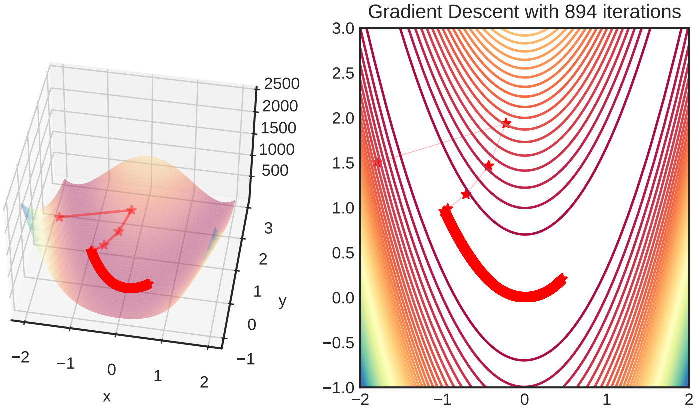


Figure 2: $f(x, y) = (a - x)^2 + b(y - x^2)^2$, $a = 1$, $b = 100$

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

Gradient for minimizing multivariate functions



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

https://colab.research.google.com/drive/1pTGjtbiQg3q08NGNkA7XgPMIQXf7uT76

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

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Example

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

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

$$\frac{\partial e}{\partial w_1} = \ldots$$

In reality we work with deeply composed functions

Example

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

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

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

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

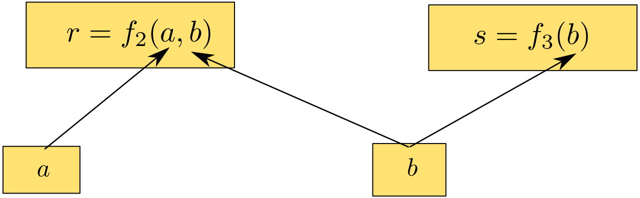
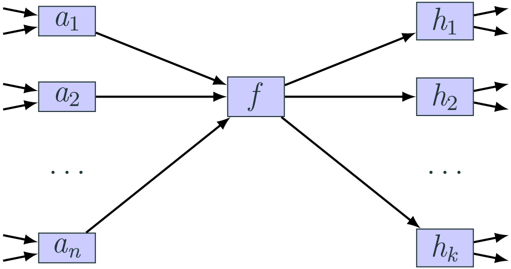


Figure 3: r, s are parents of b; a, b are children (arguments) of r

Generic node in a computational graph



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

Figure 4: 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.

When functions become heavily nested

Backpropagation

Working example

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

Compute gradient wrt. a and b

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

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

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

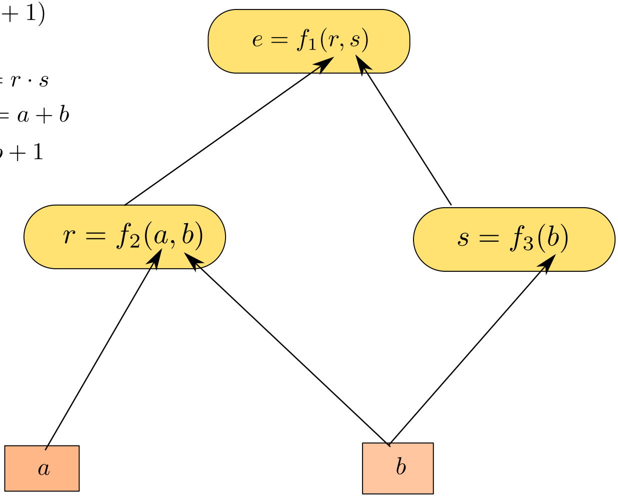
$$r = f_2(a, b) := a + b$$

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

Build computational graph and evaluate (forward step)

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

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

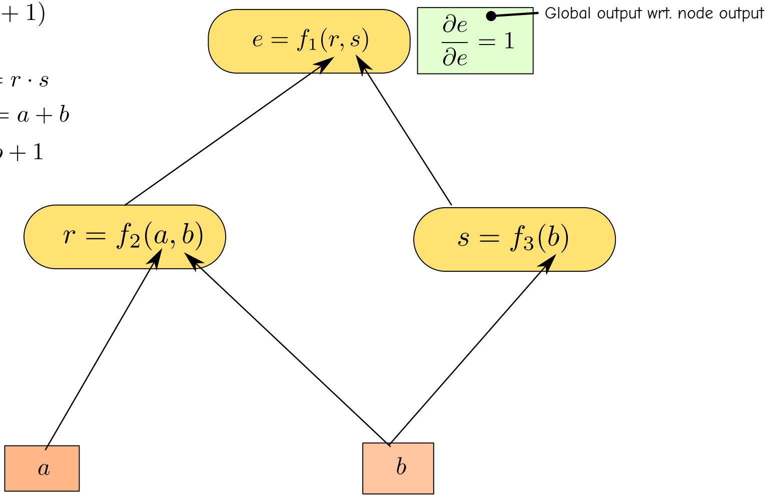


Important: a, b will be some concrete real numbers, therefore r, s, e will be concrete real numbers too!

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

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

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



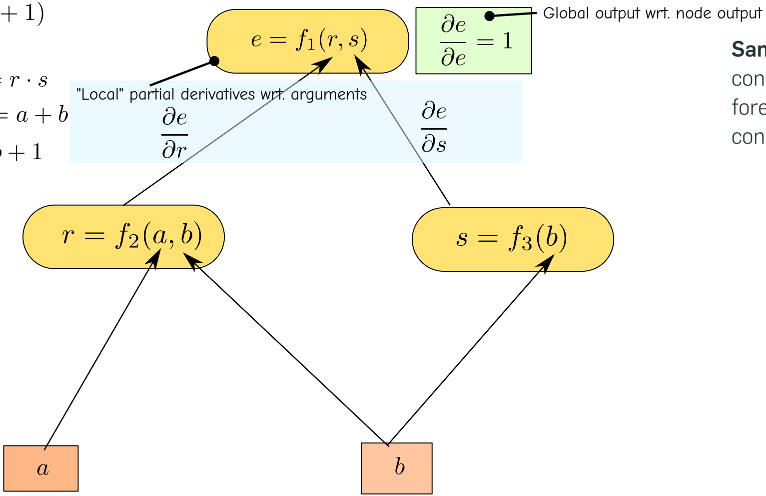
Since $e = r \cdot s$, partial derivatives are easy: $\frac{\partial e}{\partial r} = s$ and $\frac{\partial e}{\partial s} = r$

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

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

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

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



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!

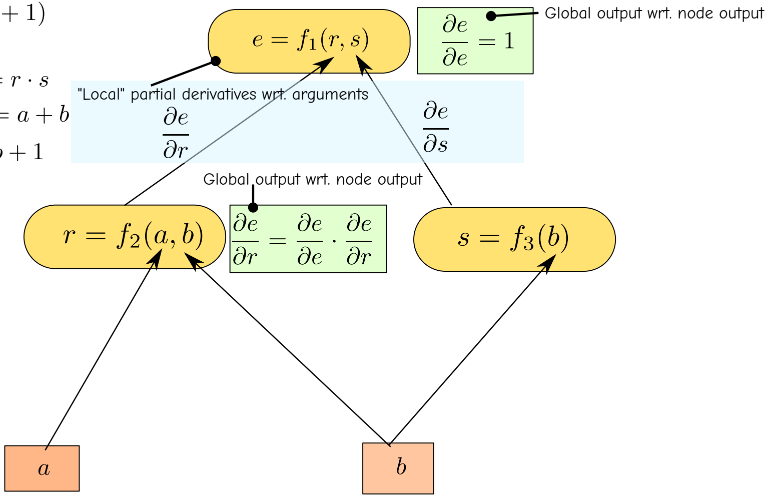
Proceed to next child r and compute $\frac{\partial e}{\partial r}$ – use chain rule!

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

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

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

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



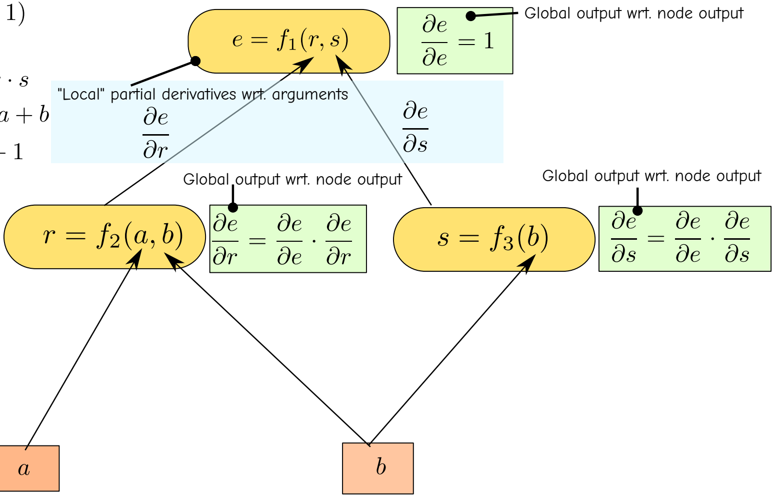
Proceed to next child s and compute $\frac{\partial e}{\partial s}$ – use chain rule!

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

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

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

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



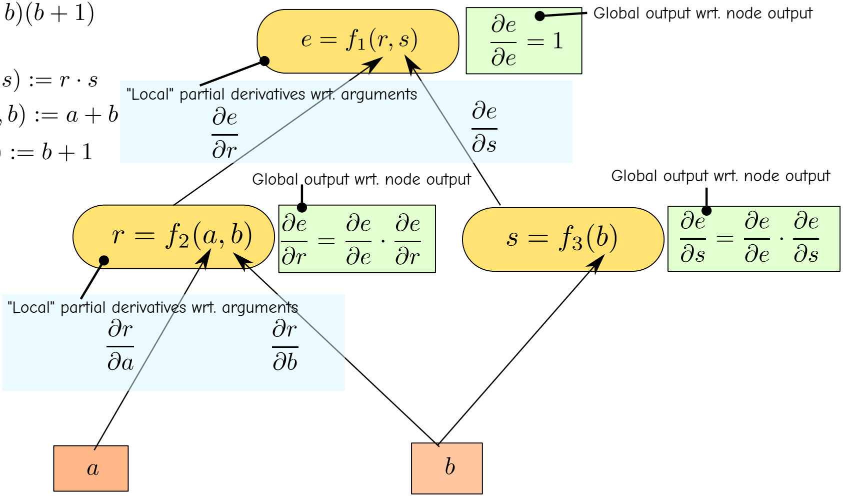
Since $r = a + b$, partial derivatives are easy: $\frac{\partial r}{\partial a} = 1$ and $\frac{\partial r}{\partial b} = 1$

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

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

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

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



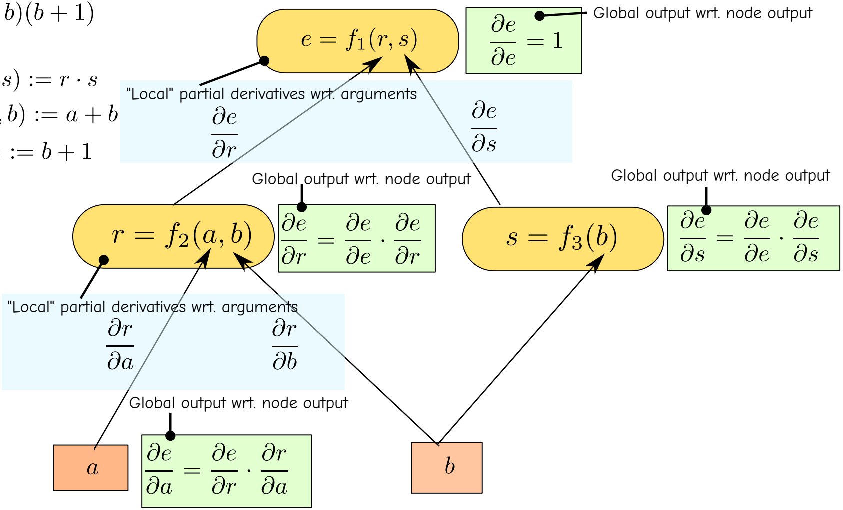
Proceed to next child a and compute $\frac{\partial e}{\partial a}$ – use chain rule!

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

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

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

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



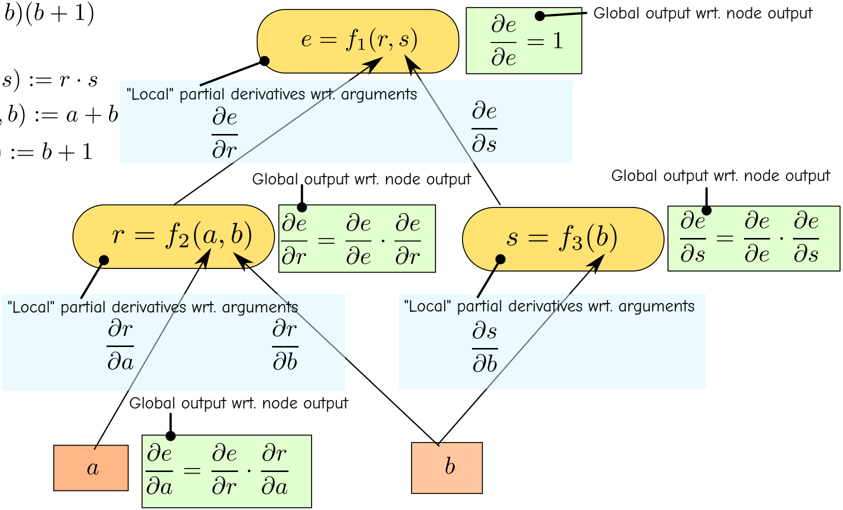
Since $s = b + 1$, partial derivatives are easy: $\frac{\partial s}{\partial b} = 1$

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

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

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

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



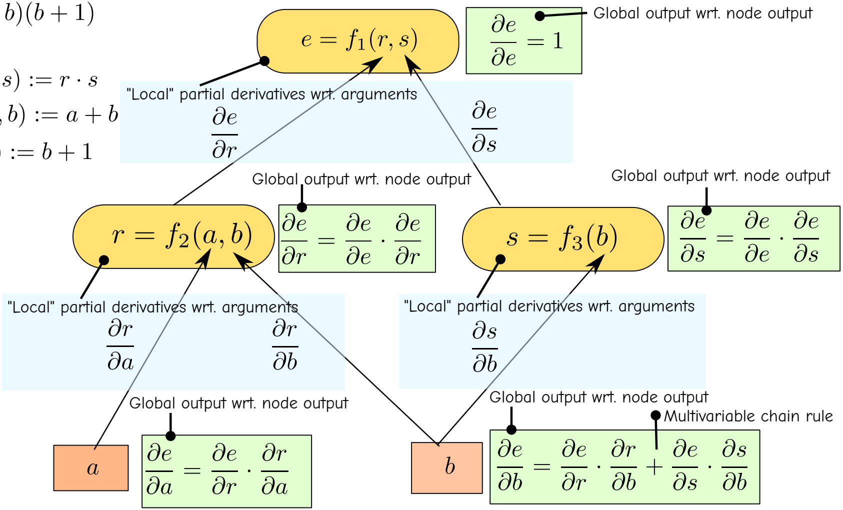
Proceed to b and compute $\frac{\partial e}{\partial b}$ – use multivariate chain rule!

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

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

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

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



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

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

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

$e = f_1(r,s)$

$\frac{\partial e}{\partial e} = 1$ — Global output wrt. node output

"Local" partial derivatives wrt. arguments $\frac{\partial e}{\partial r}$ $\frac{\partial e}{\partial s}$

$r = f_2(a,b)$

Global output wrt. node output: $\frac{\partial e}{\partial r} = \frac{\partial e}{\partial e} \cdot \frac{\partial e}{\partial r}$

$s = f_3(b)$

Global output wrt. node output: $\frac{\partial e}{\partial s} = \frac{\partial e}{\partial e} \cdot \frac{\partial e}{\partial s}$

"Local" partial derivatives wrt. arguments $\frac{\partial r}{\partial a}$ $\frac{\partial r}{\partial b}$

"Local" partial derivatives wrt. arguments $\frac{\partial s}{\partial b}$

a

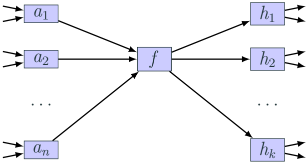
Global output wrt. node output: $\frac{\partial e}{\partial a} = \frac{\partial e}{\partial r} \cdot \frac{\partial r}{\partial a}$

b

Global output wrt. node output: $\frac{\partial e}{\partial b} = \frac{\partial e}{\partial r} \cdot \frac{\partial r}{\partial b} + \frac{\partial e}{\partial s} \cdot \frac{\partial s}{\partial b}$

Multivariable chain rule

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

- 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

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!

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Credits

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Chain rule example

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

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

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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

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

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)

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