Computational Graphs

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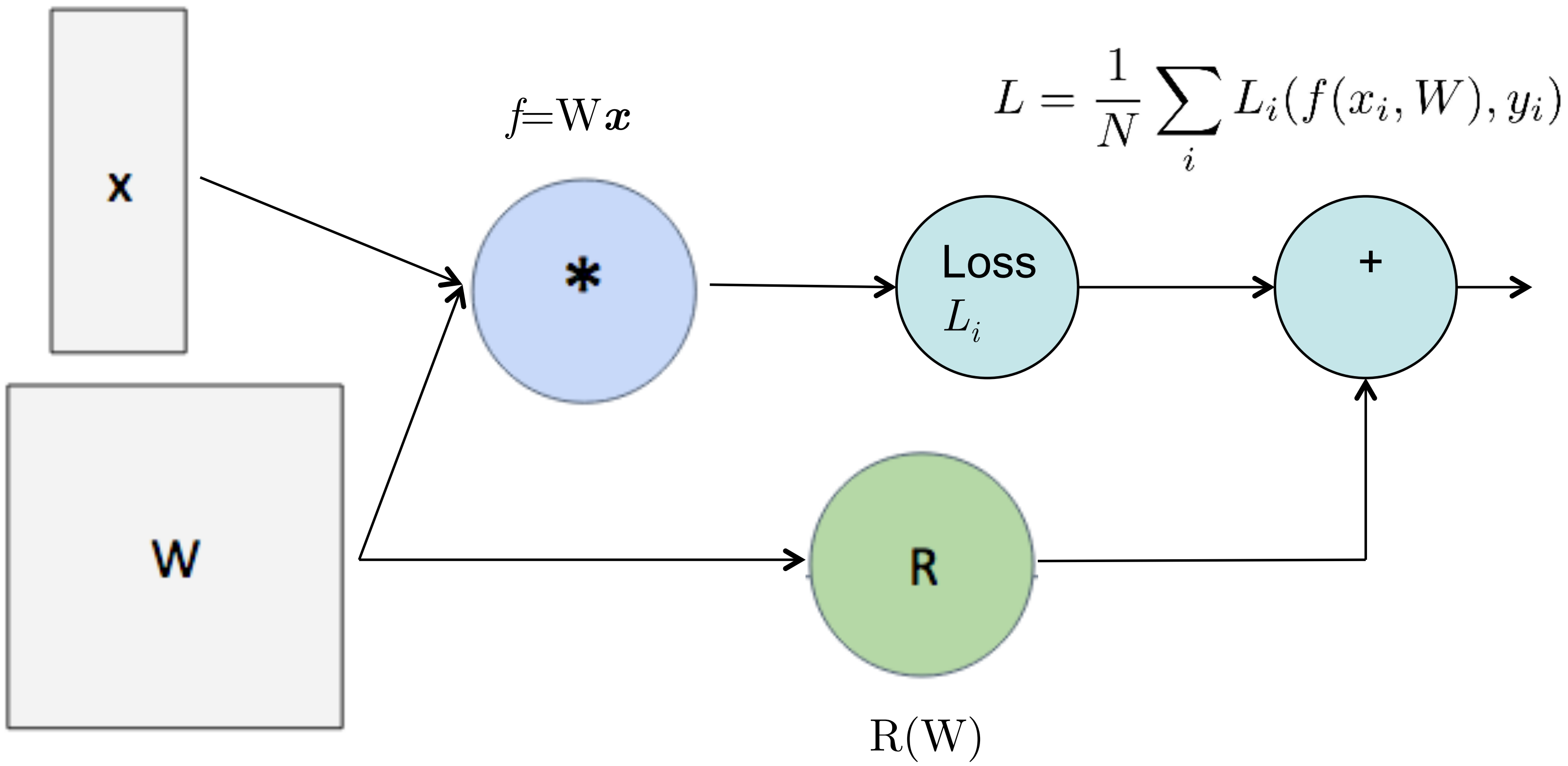
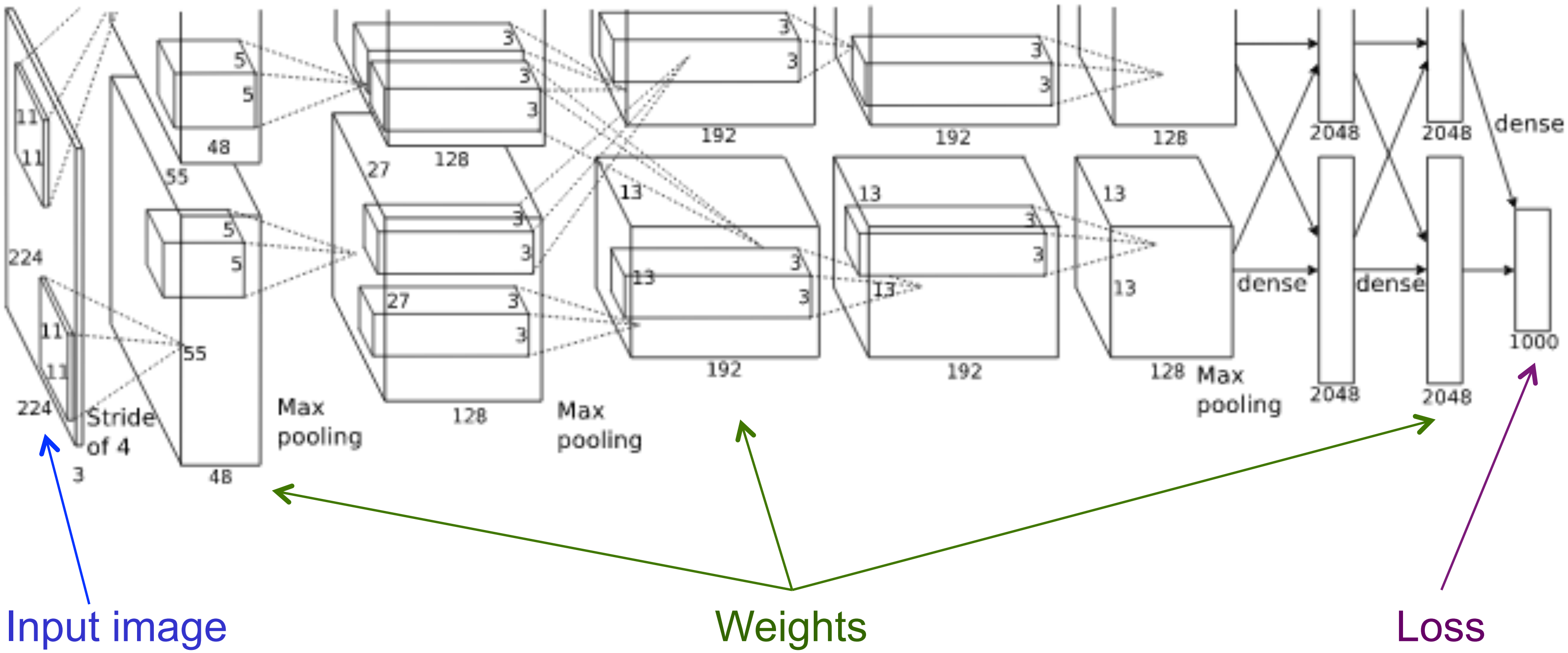
Topics

- Typical computations in deep network learning
- Graph Language
  - Nodes as operations and inputs
  - Edges as values used in operations
- Composite functions as chains
- Derivatives in computational graphs
- Factoring paths
- Forward and Reverse Differentiation

Computing Loss in a typical network



Computational Graph of a CNN: Alexnet



1.2m high-res images in ImageNet with 1000 classes.

Eight layers with weights: first five are convolutional and remaining three fully-connected. Output of last fully-connected layer is fed to a 1000-way softmax which produces a distribution over the 1000 class labels

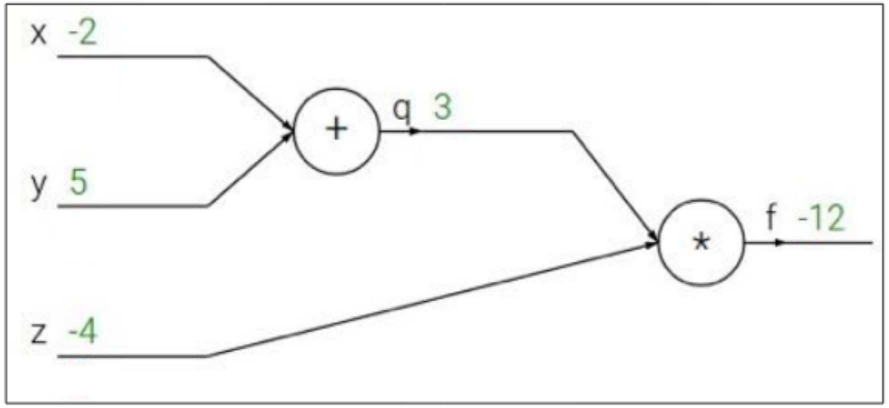
Example of Backprop Computation

$$f(x, y, z) = (x + y)z$$

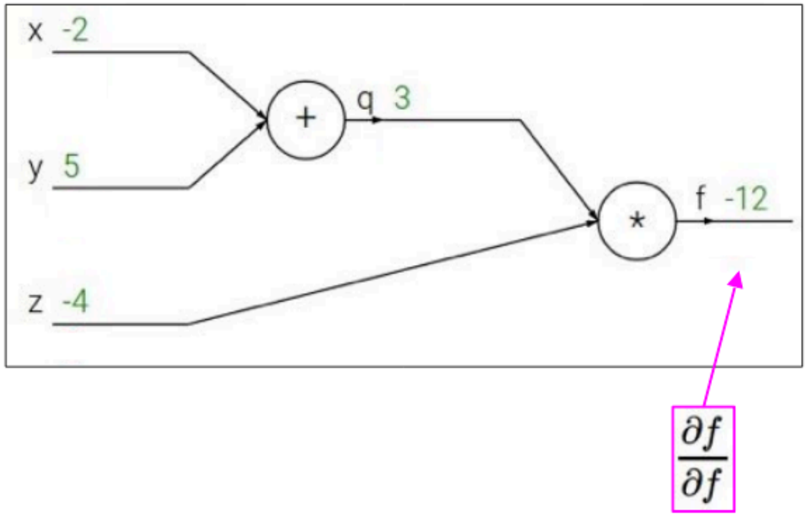
e.g. x = -2, y = 5, z = -4

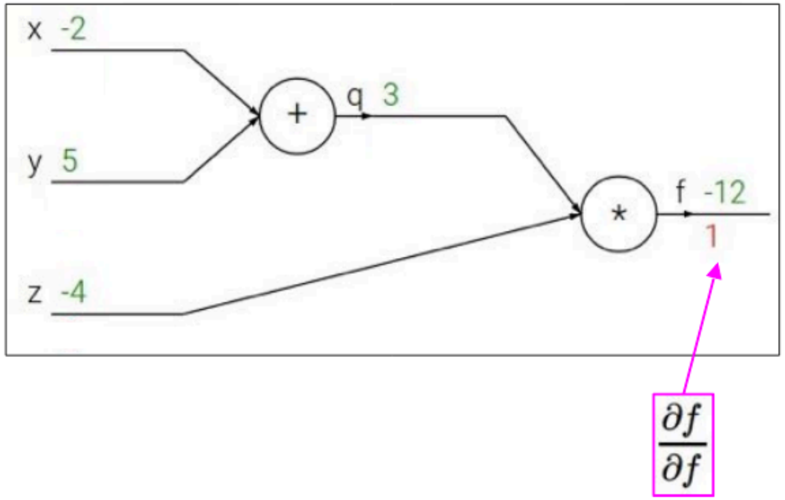
$$q = x + y \qquad \frac{\partial q}{\partial x} = 1, \frac{\partial q}{\partial y} = 1$$

$$f = qz \qquad \frac{\partial f}{\partial q} = z, \frac{\partial f}{\partial z} = q$$

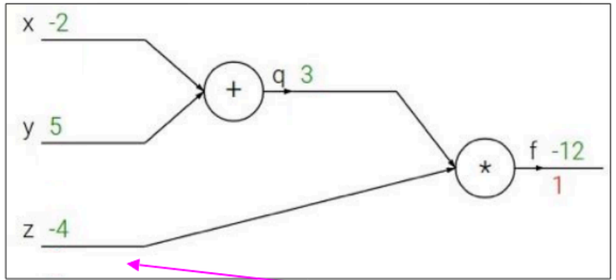


Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$

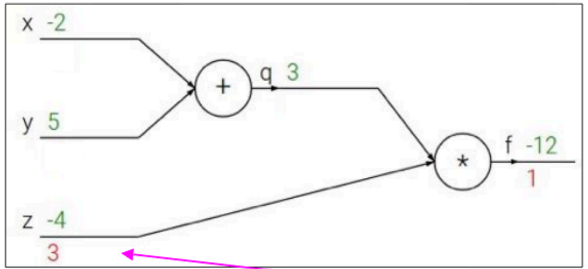




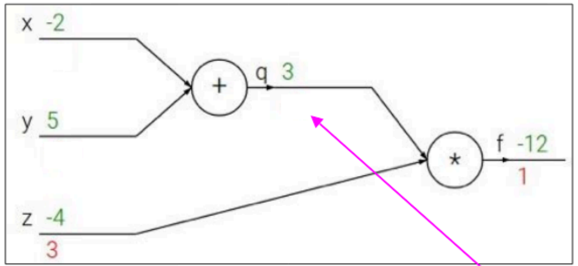
Steps in Backprop



$\frac{\partial f}{\partial z}$



$\frac{\partial f}{\partial z}$

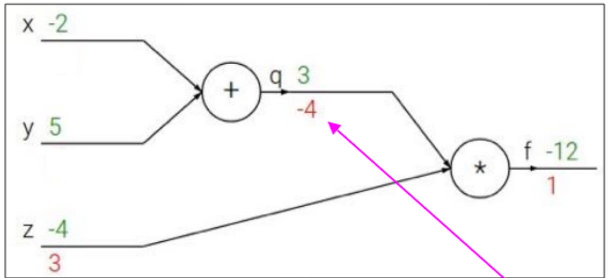


$\frac{\partial f}{\partial q}$

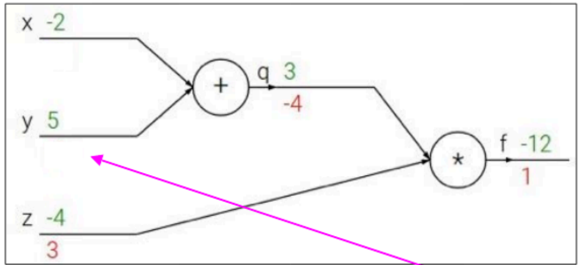
$q = x + y \qquad \frac{\partial q}{\partial x} = 1, \frac{\partial q}{\partial y} = 1$

$f = qz \qquad \frac{\partial f}{\partial q} = z, \frac{\partial f}{\partial z} = q$

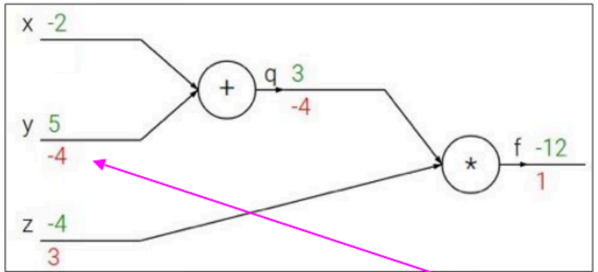
Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



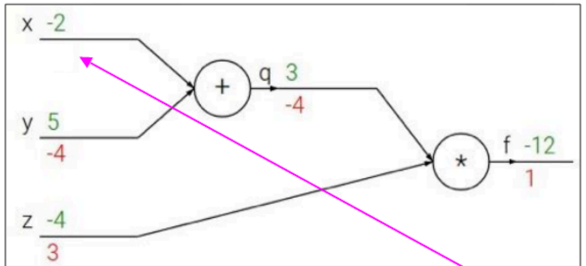
$\frac{\partial f}{\partial q}$



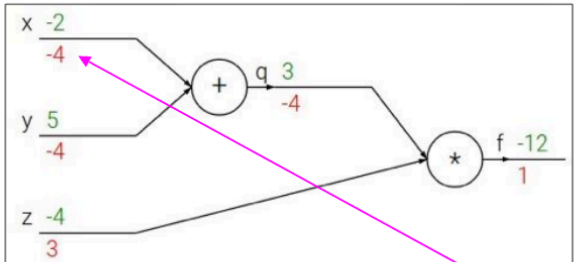
$\frac{\partial f}{\partial y}$



$\frac{\partial f}{\partial y}$



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

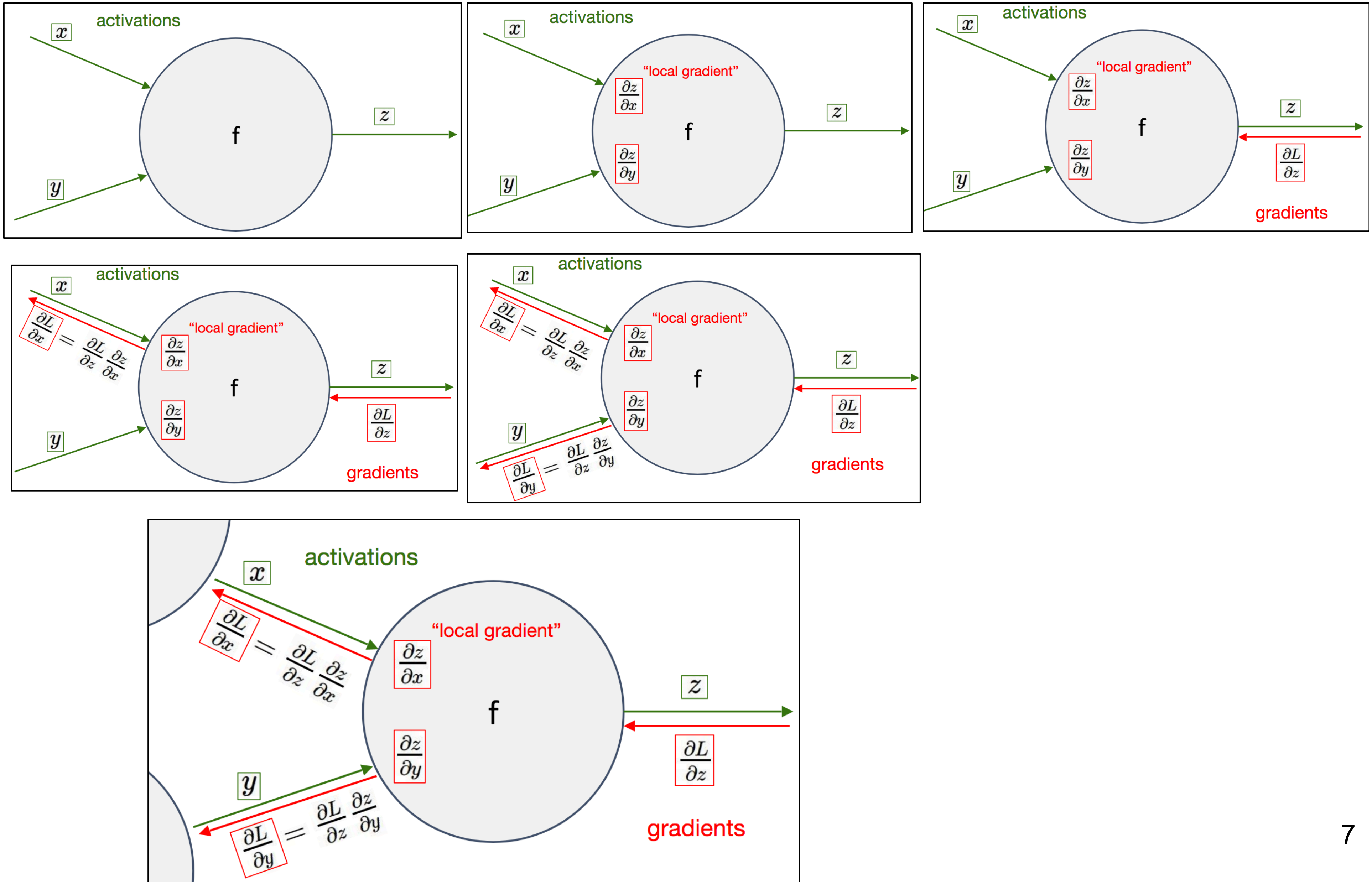


$\frac{\partial f}{\partial x}$

Chain rule:

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

Backprop for a neuron



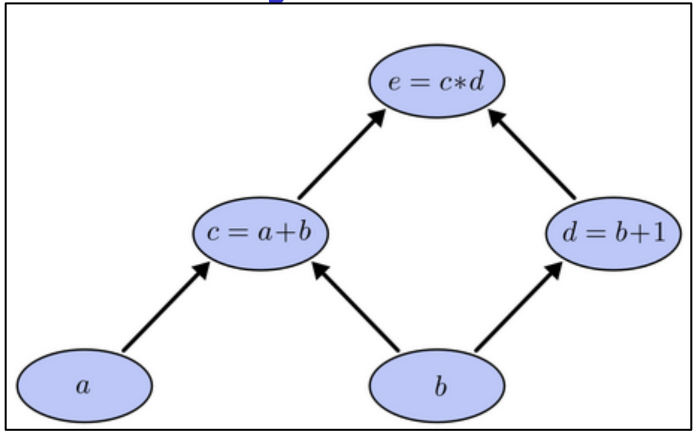
Graph of a math expression

- Computational graphs are a nice way to:
  - Think about math expressions
- Consider the expression

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

  - It has two adds, one multiply
  - Introduce a variable for result of each operation:

  $c=a+b$, $d=b+1$ and $e=c*d$

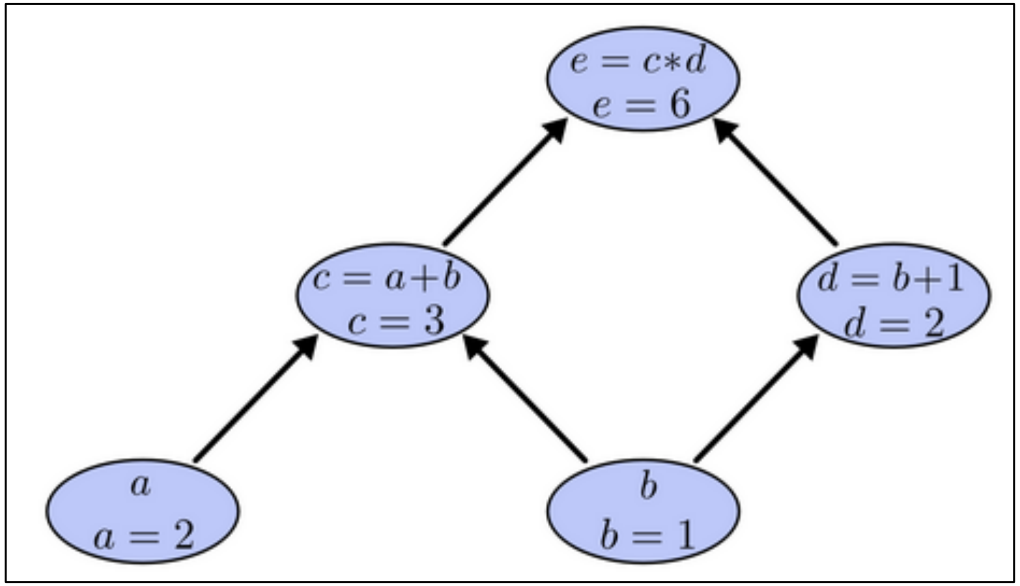


Such graphs are useful in CS especially functional programs. Core abstraction in deep learning using Theano

- To make a computational graph
  - Operations and inputs are nodes
  - Values used in operations are directed edges

Evaluating the expression

- Set the input variables to values and compute nodes up through the graph
- For $a=2$ and $b=1$



- Expression evaluates to 6

Computational Graph Language

- To describe backpropagation more precisely computational graph language is helpful
- Each node is either
  - a variable
    - Scalar, vector, matrix, tensor, or other type
  - Or an Operation
    - Simple function of one or more variables
    - Functions more complex than operations are obtained by composing operations
  - If variable y is computed by applying operation to variable x then draw directed edge from x to y

Composite Function

- Consider a composite function $f\,(g\,(h\,(x)))$
  - We have an outer function f, an inner function f and a final inner function $h(x)$
- Say $f\,(x) = e^{\sin(x**2)}$ we can decompose it as:

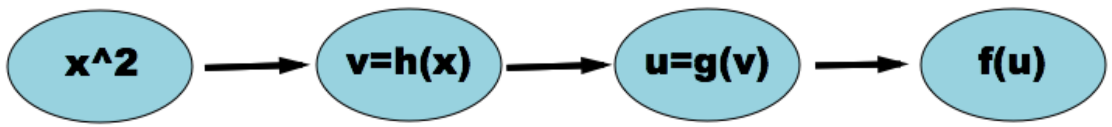
  $f\,(x) = e^{x}$

  $g(x) = sin\ x$ and

  $h(x) = x^{2}$ or

  $f\,(g(h(x))) = e^{\,g(h(x))}$

  - Its computational graph is



    - Every connection is an input, every node is a function or operation

Chain Rule for Composites

- Chain rule is the process we can use to analytically compute derivatives of composite functions.
- For example, $f\left(g\left(h\left(x\right)\right)\right)$ is a composite function
  - We have an outer function f, an inner function f and a final inner function $h(x)$
  - Say $f\left(x\right)= e^{\sin(x**2)}$ we can decompose it as:

    $f\left(x\right)=e^{x},\ g(x)=sin\ x$ and $h(x)=x^{2}$ or

    $f\left(g(h(x))\right)=e^{g(h(x))}$

Derivatives of Composite function

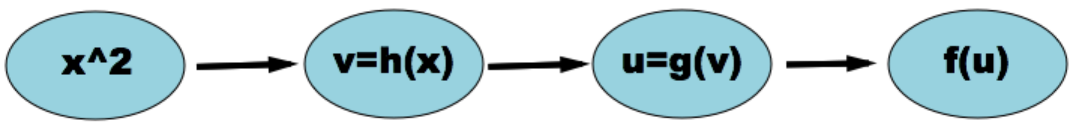
- To get derivatives of $f\,(g\,(h\,(x)))= e^{\,g(h(x))}$ wrt x
  1. We use the chain rule $\boxed{\frac{df}{dx}=\frac{df}{dg}\cdot\frac{dg}{dh}\cdot\frac{dh}{dx}}$ where

     $\boxed{\frac{df}{dg}=e^{g(h(x))}}$ since $f\,(g(h(x)))=e^{g(h(x))}$ & derivative of e^x is e

     $\boxed{\frac{dg}{dh}=\cos(h(x))}$ since $g(h(x))=sin\ h(x)$ & derivative $\sin$ is $\cos$

     $\boxed{\frac{dh}{dx}=2x}$ because $h(x)=x^2$ & its derivative is $2x$

     - Therefore $\boxed{\frac{df}{dx}=e^{g(h(x))}\cdot\cos\ h(x)\cdot 2x = e^{\sin x^{**}2}\cdot\cos x^2\cdot 2x}$
     - In each of these cases we pretend that the inner function is a single variable and derive it as such
  2. Another way to view it $f\,(x)=e^{\,\sin(x^{**}2)}$
     - Create temp variables $u=\sin\ v$, $v=x^2$, then $f\,(u)=e^u$ with computational graph



Derivative using Computational Graph

- All we need to do is get the derivative of each node wrt each of its inputs

With $u=\sin\ v,\ v=x^2,\ f\,(u)=e^u$

$$\frac{dh}{dx} = 2x \qquad \frac{dg}{dh} = \cos(h(x)) \qquad \frac{df}{dg} = e^{g(h(x))}$$

- We can get whichever derivative we want by multiplying the ‘connection’ derivatives

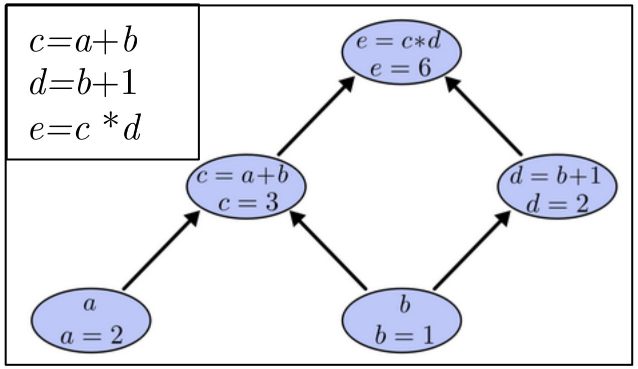
$$\frac{df}{dx} = \frac{df}{dg} \cdot \frac{dg}{dh} \cdot \frac{dh}{dx}$$

$$\frac{df}{dx} = e^{g(h(x))} \cdot \cos\ \ h(x) \cdot 2x$$
$$= e^{\sin x^2} \cdot \cos x^2 \cdot 2x$$

Since $f\,(x)=e^x,\ g(x)=sin\ x$ and $h(x)=x^2$

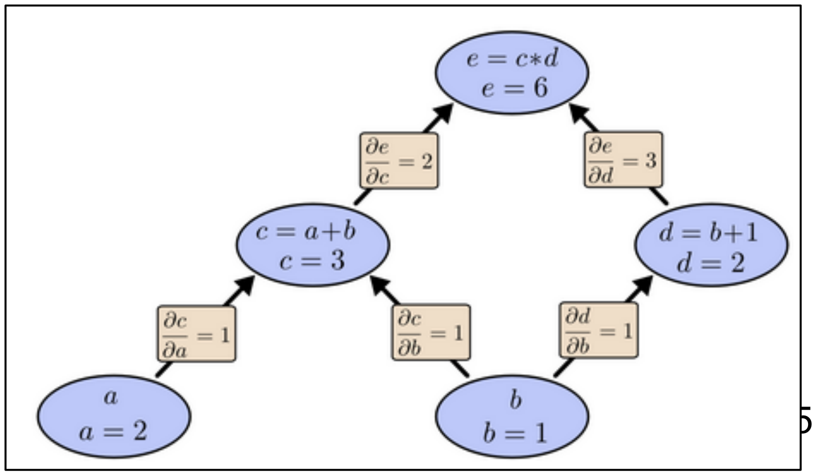
Derivatives for $e=(a+b)*\ (b+1)$

- Computational graph
  - for $e=(a+b)*\ (b+1)$



- Need derivatives on the edges
  - If a directly affects $c=a+b$, then we want to know how it affects c.
  - This is called *partial derivative* of c wrt a.
    - For partial derivatives of e we need sum & product rules of calculus

$$\frac{\partial}{\partial a}(a+b) = \frac{\partial a}{\partial a} + \frac{\partial b}{\partial a} = 1$$
$$\frac{\partial}{\partial u}uv = u\frac{\partial v}{\partial u} + v\frac{\partial u}{\partial u} = v$$



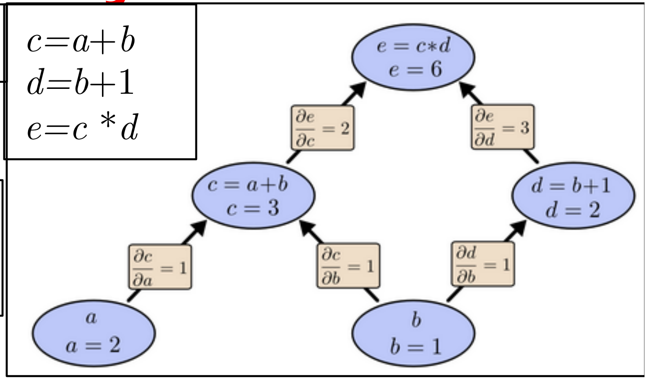
    - Derivative on edge: labeled

Derivative wrt variables indirectly connected

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

$c=a+b$
$d=b+1$
$e=c*d$

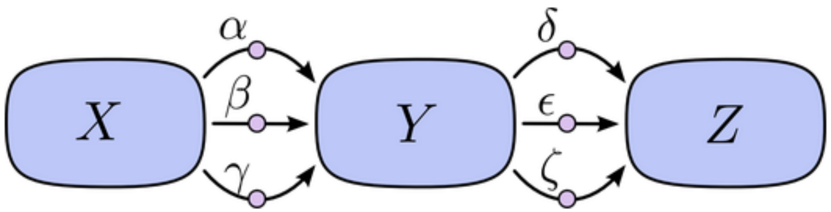
$a=2$ and $b=1$



- Effect of indirect connection:
  - How is e affected by a?
    - Since $\frac{\partial c}{\partial a}=\frac{\partial}{\partial a}(a+b)=1+0=1$
      - If we change a at a speed of 1, c changes by speed of 1
    - Since $\frac{\partial e}{\partial c}=\frac{\partial}{\partial c}(c*d)=d=b+1=1+1=2$
      - If we change c by a speed of 1, e changes by speed of 2
    - So e changes by a speed of $1*2=2$ wrt a
    - Equivalent to chain rule: $\frac{\partial e}{\partial a}=\frac{\partial c}{\partial a}\cdot\frac{\partial e}{\partial c}$
- The general rule (with multiple paths) is:
  - Sum over all possible paths from one node to the other while multiplying derivatives on each path
    - E.g., to get derivative of e wrt b $\frac{\partial e}{\partial b}=1*2+1*3=5$

Factoring Paths

- Summing over paths leads to combinatorial explosion



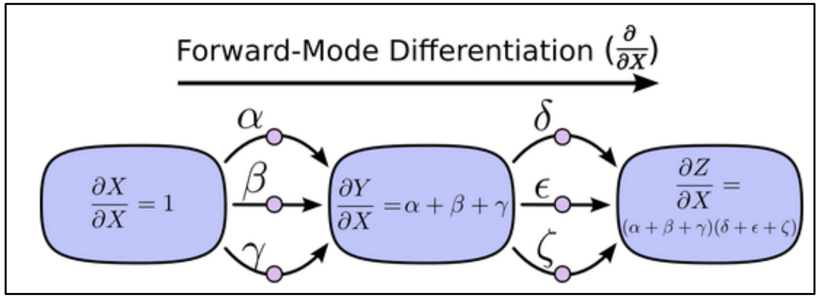
- If we want to get derivative $\frac{\partial Z}{\partial X}$ we need to sum over $3*3=9$ paths: $\frac{\partial Z}{\partial X} = \alpha\delta + \alpha\varepsilon + \alpha\zeta + \beta\delta + \beta\varepsilon + \beta\zeta + \gamma\delta + \gamma\varepsilon + \gamma\zeta$
  - It will grow exponentially
  - Instead we could factor the paths as:

$$\frac{\partial Z}{\partial X} = (\alpha + \beta + \gamma)(\delta + \varepsilon + \zeta)$$

- This is where *forward-mode* and *reverse-mode* differentiation come in

Forward- and Reverse-Mode Differentiation

- Forward mode differentiation tracks how one input affects every node
  - Applies $\boxed{\frac{\partial}{\partial X}}$ to every node



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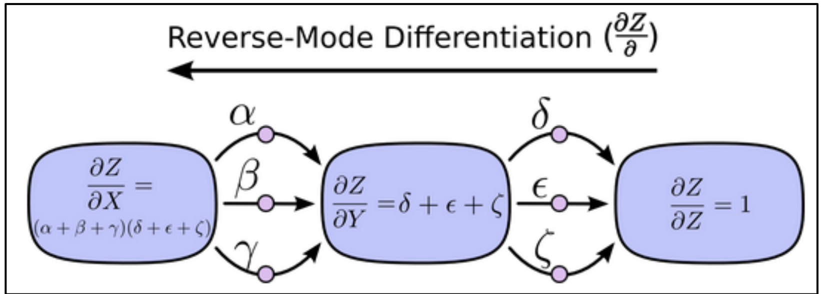
- Reverse mode differentiation tracks how every node affects one output
  - Applies $\boxed{\frac{\partial Z}{\partial}}$ to every node



Reverse Mode Differentiation

Reverse-mode differentiation from e down

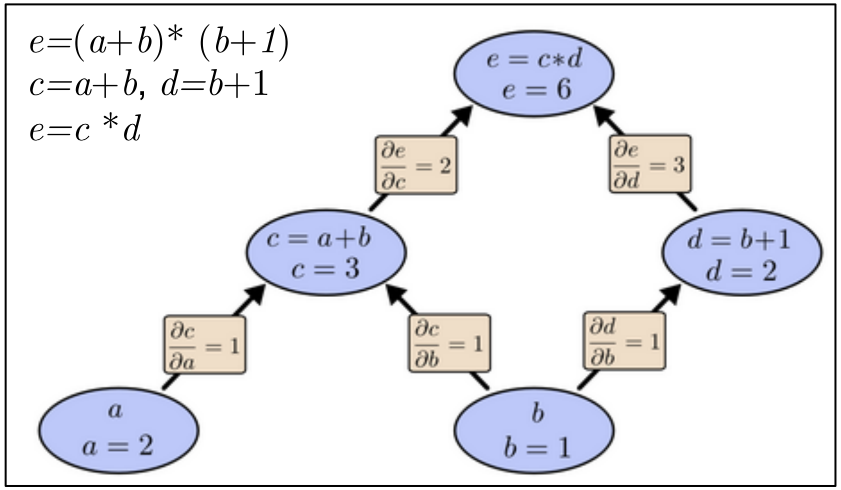
- Apply $\boxed{\frac{\partial e}{\partial}}$ to every node

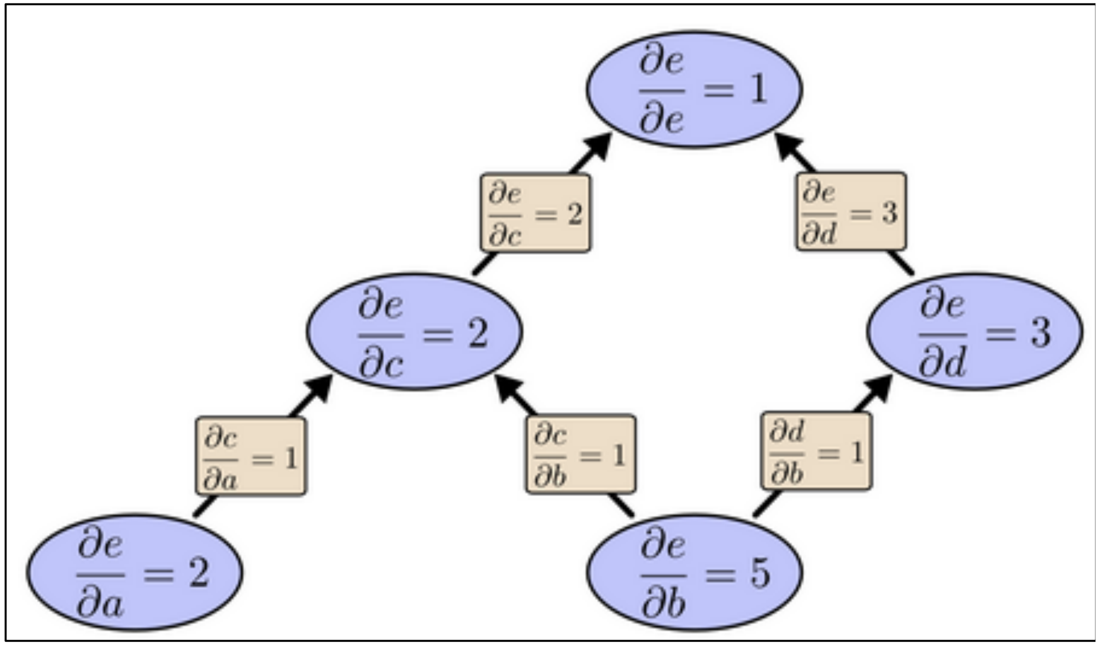
$$\boxed{\frac{\partial e}{\partial c} = \frac{\partial (c*d)}{\partial c} = d = b+1 = 1+1 = 2}$$

$$\boxed{\frac{\partial e}{\partial a} = \frac{\partial (c*d)}{\partial a} = \frac{\partial ((a+b)*(b+1))}{\partial a} = b+1 = 2}$$

- Gives derivative of e wrt every node
- We get both $\boxed{\frac{\partial e}{\partial a}}$ and $\boxed{\frac{\partial e}{\partial b}}$

$a=2$ and $b=1$





Combining the two modes

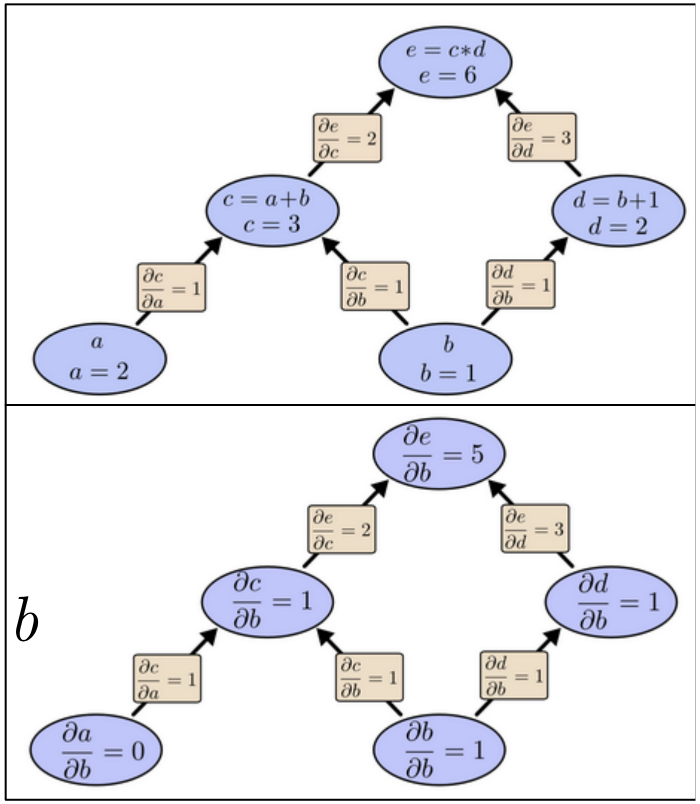
- Why reverse mode?

Consider Original example

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

$$c=a+b,\ d=b+1$$

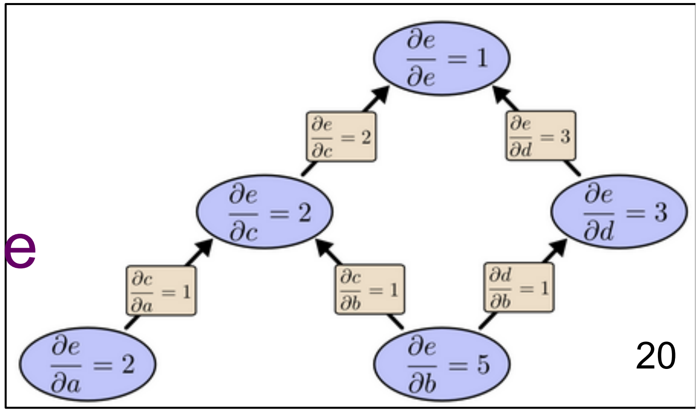
$$e=c*d$$



Forward differentiation from b up

- Gives derivative of every node wrt b
- *i.e.*, wrt a single input
- We get $\boxed{\frac{\partial e}{\partial b}}$

Reverse-mode diff from e down



- Gives derivative of e wrt every node
- We get both $\boxed{\frac{\partial e}{\partial a}}$ and $\boxed{\frac{\partial e}{\partial b}}$

References

- colah.github, outlace.com/Computational-Graphs