CSE 176 Introduction to Machine Learning

Lecture 10: Back Propagation

Some slides from O. Veksler, Y. Boykov, A. Ng, Y. LeCun, G. Hinton, A. Ranzato, R. Fergus

Recap: Neural Unit

Output value

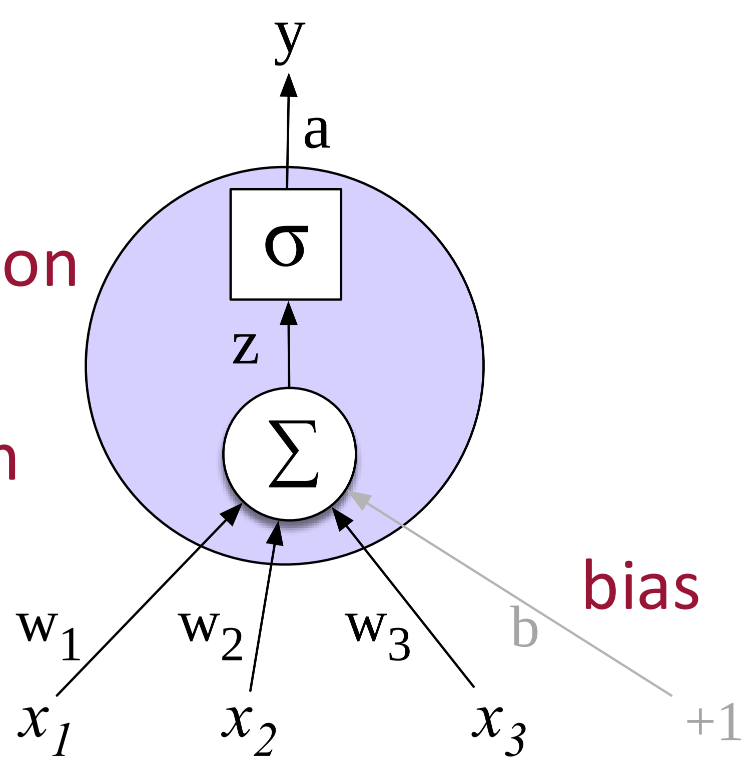
Non-linear activation function

Weighted sum

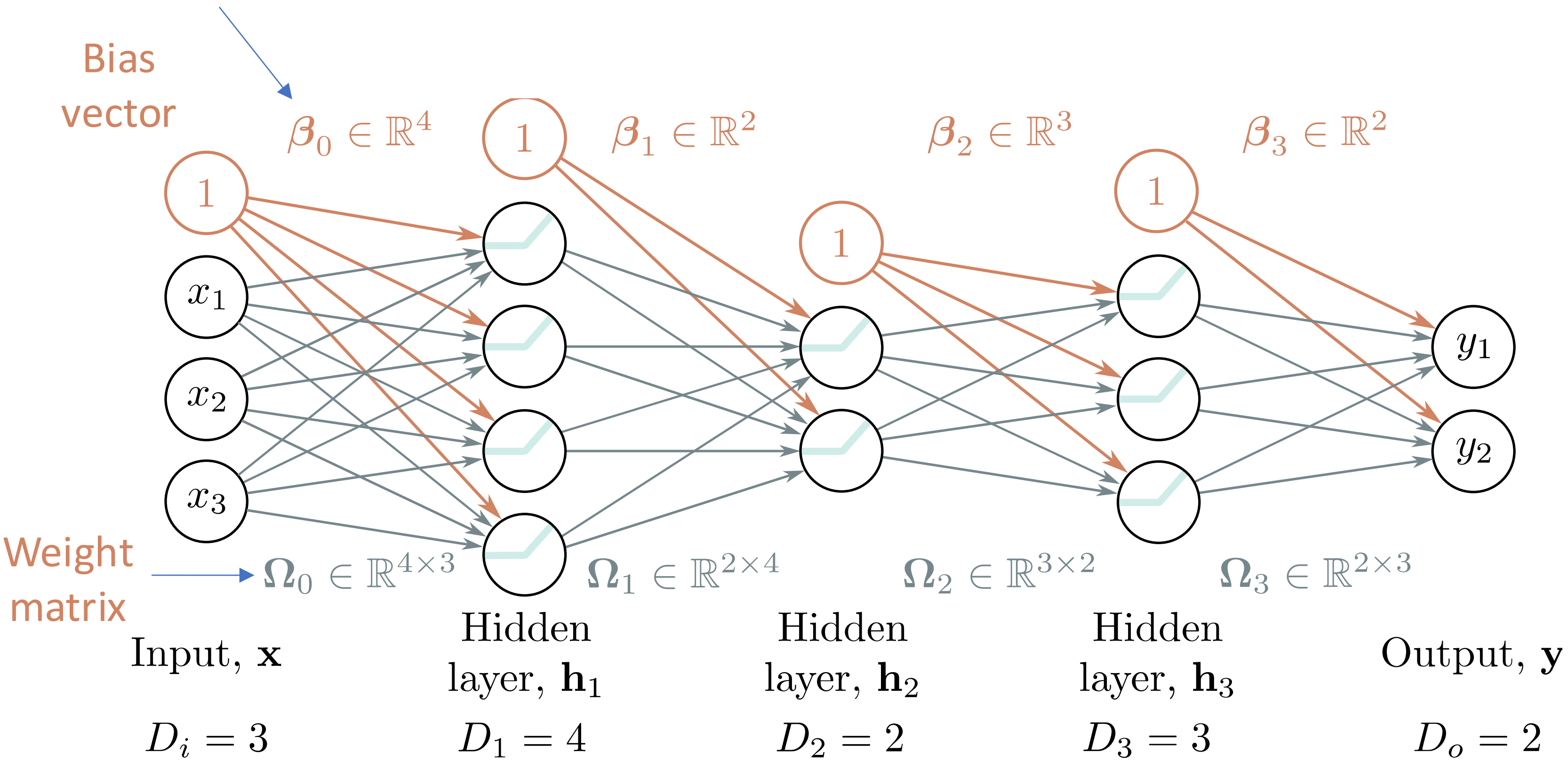
Weights

Input layer

bias

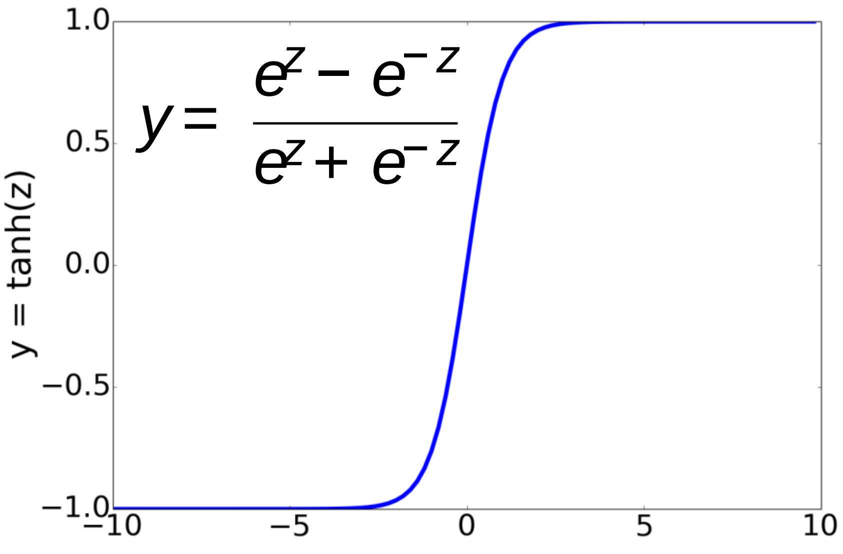


Recap: Multi-layer perceptron



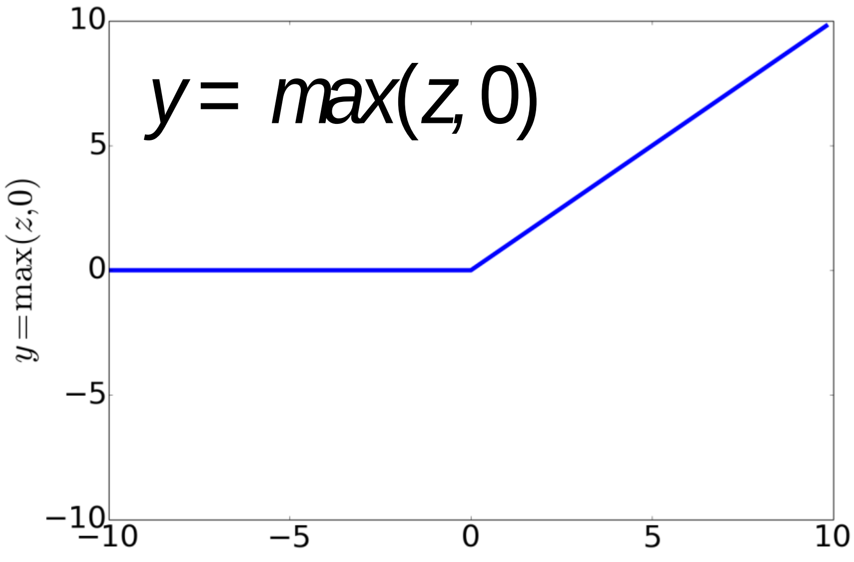
Example of Multi Layer Perceptron (MLP)

Recap: activation function



tanh

Most Common:



ReLU

Rectified Linear Unit

Which of the followings would you consider to be valid activation functions?

(a) $f(x) = -min(2, x)$

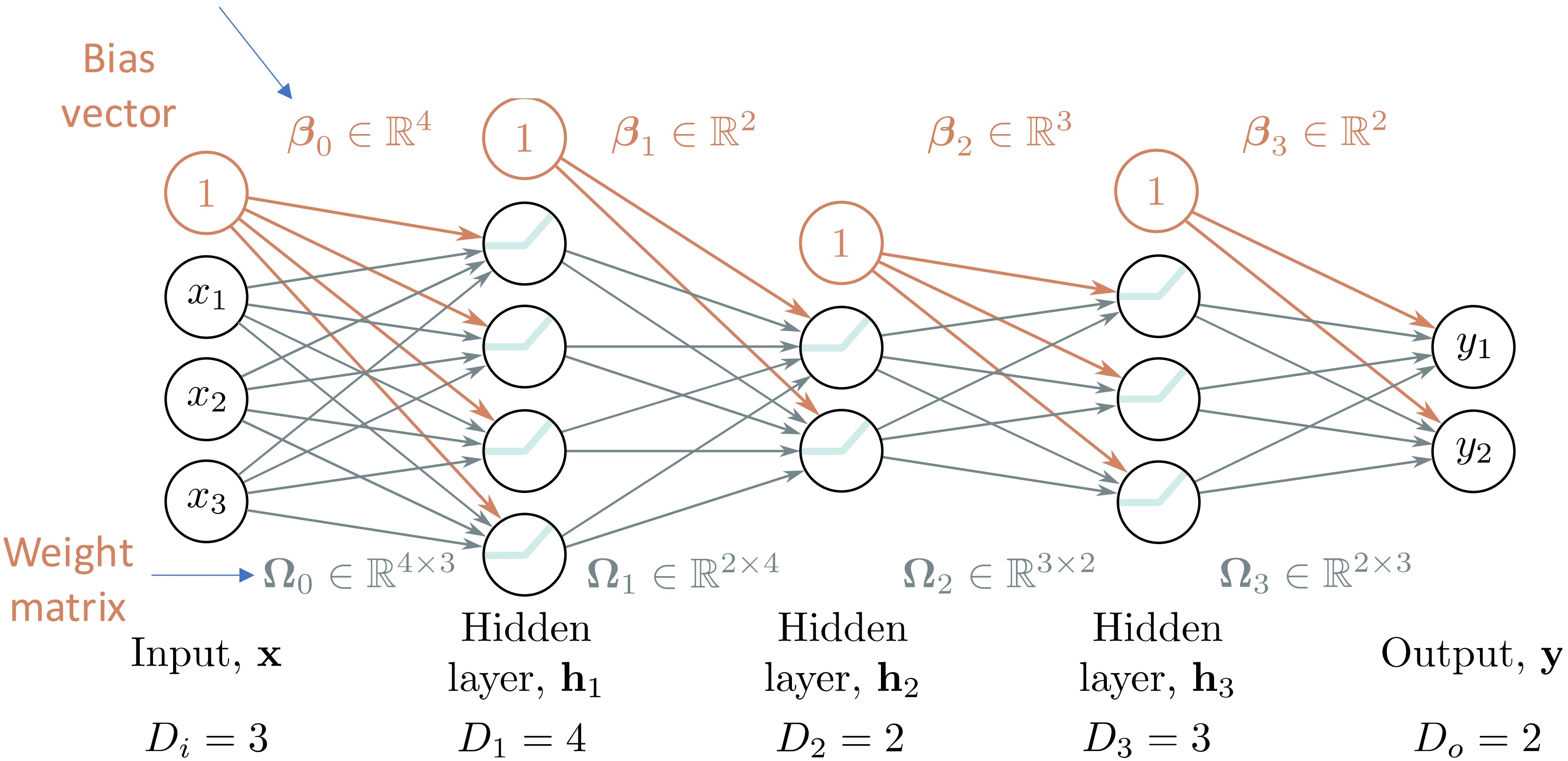
(b) $f(x) = 0.9x + 1$

(c) $f(x) = \begin{cases} min(x, 0.1x) \text{ if } x \geq 0 \\ min(x, 0.1x) \text{ if } x < 0 \end{cases}$

(d) $f(x) = \begin{cases} max(x, 0.1x) \text{ if } x \geq 0 \\ min(x, 0.1x) \text{ if } x < 0 \end{cases}$

How to train neural networks?

- Training == learning weight and bias



Example of Multi Layer Perceptron (MLP)

Optimization via Gradient Descent

Optimization of continuous differentiable functions

- How to minimize a function of a single variable

$$f(x) = (x-5)^2$$

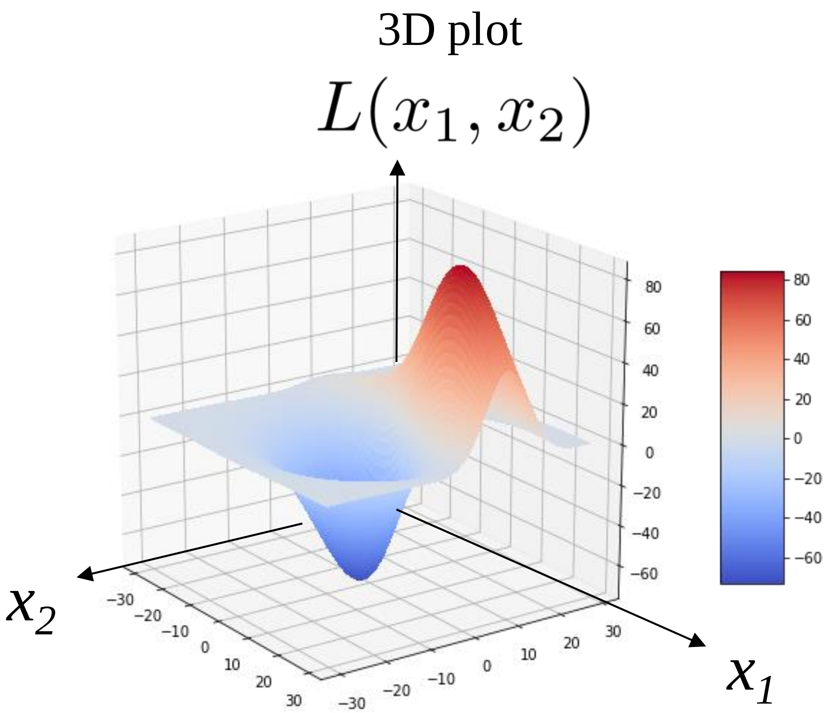
- Take derivative and set it to 0

$$\frac{d}{dx} f(x) = 0$$

- May find a closed form solution

$$\frac{d}{dx} f(x) \;=\; 2(x-5) \;=\; 0 \qquad \Rightarrow \qquad x = 5$$

Differentiation



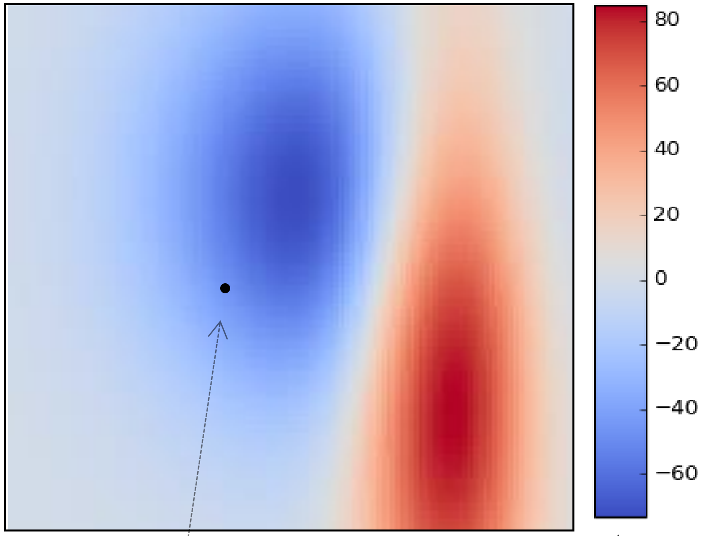
What is "**slope**" of $L(x_1,x_2)$ at a given point $\mathbf{x}=(x_1,x_2)$?

Differentiation

"heat-map" visualization of L

domain of $L(x_1,x_2)$ in R^2

x_2



x_1

range of $L(x_1,x_2)$

What is "**slope**" of $L(x_1,x_2)$ at a given point $\mathbf{x}=(x_1,x_2)$?

Differentiation

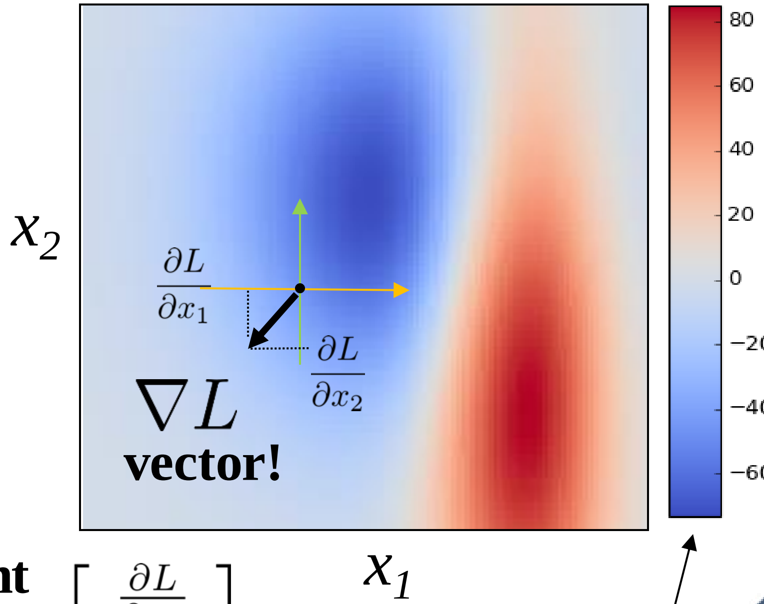
“heat-map” visualization of L

“partial” derivatives

$$\frac{\partial L}{\partial x_1} = \lim_{\epsilon \to 0} \left(\frac{L(x_1+\epsilon, x_2) - L(x_1, x_2)}{\epsilon} \right)$$

$$\frac{\partial L}{\partial x_2} = \lim_{\epsilon \to 0} \left(\frac{L(x_1, x_2+\epsilon) - L(x_1, x_2)}{\epsilon} \right)$$

domain of $L(x_1,x_2)$ in R^2



gradient

$$\nabla L = \begin{bmatrix} \frac{\partial L}{\partial x_1} \\ \frac{\partial L}{\partial x_2} \end{bmatrix}$$

range of $L(x_1,x_2)$

direction of the steepest ascent at point x=(x_1,x_2)

Differentiation

The most common optimization method for continuous differentiable (multi-variate) functions:

gradient descent

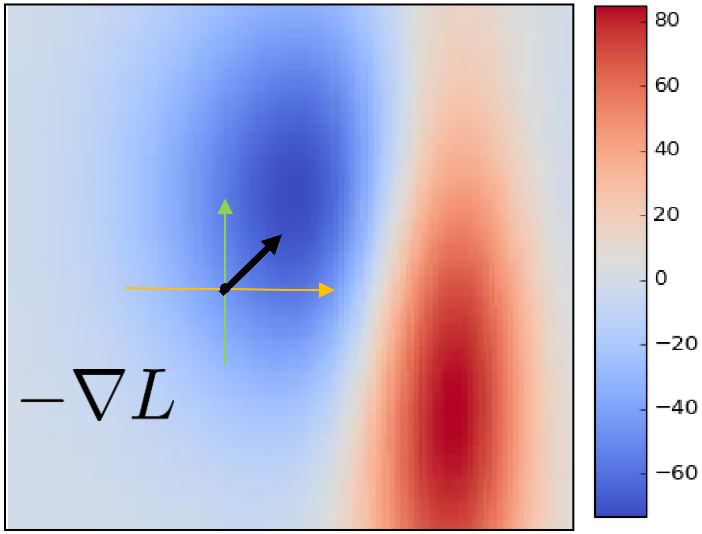
take a step $\mathbf{x}' = \mathbf{x} - \alpha \nabla L$

towards lower values of the function

"heat-map" visualization of L

domain of $L(x_1,x_2)$ in R^2

x_2



x_1

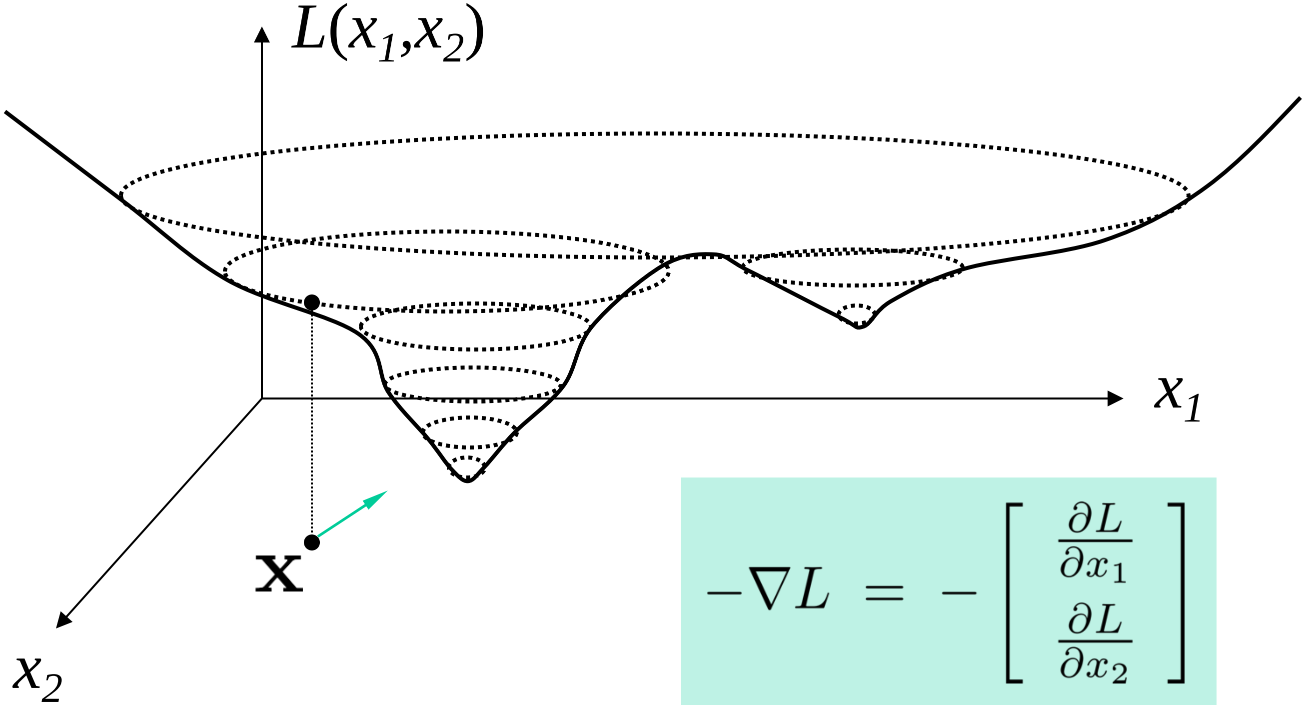
negative gradient

range of $L(x_1,x_2)$

direction of the steepest descent at point x=(x_1,x_2)

Gradient Descent

Example: for a function of two variables



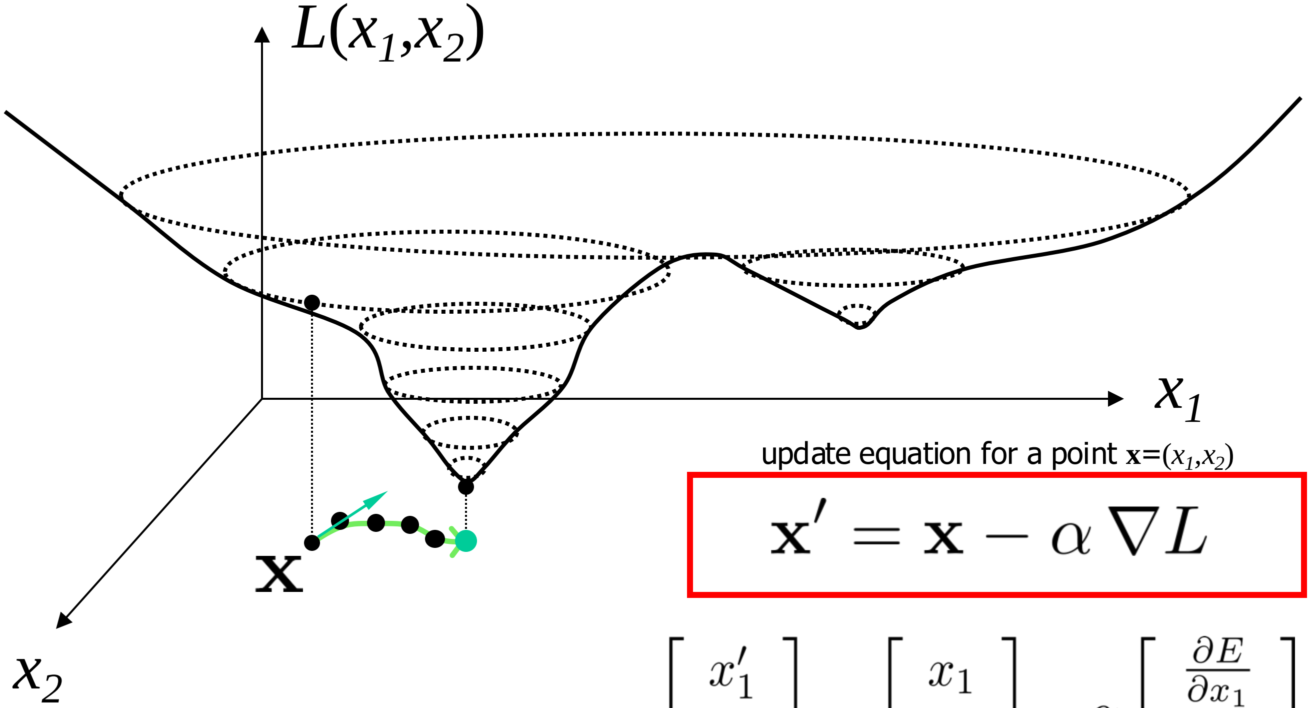
$$-\nabla L = -\begin{bmatrix} \frac{\partial L}{\partial x_1} \\ \frac{\partial L}{\partial x_2} \end{bmatrix}$$

- direction of (negative) gradient at point $\mathbf{x}=(x_1,x_2)$ is direction of the steepest descent towards lower values of function L

- magnitude of gradient at $\mathbf{x}=(x_1,x_2)$ gives the value of the slope

Gradient Descent

Example: for a function of two variables



update equation for a point $\mathbf{x}=(x_1,x_2)$

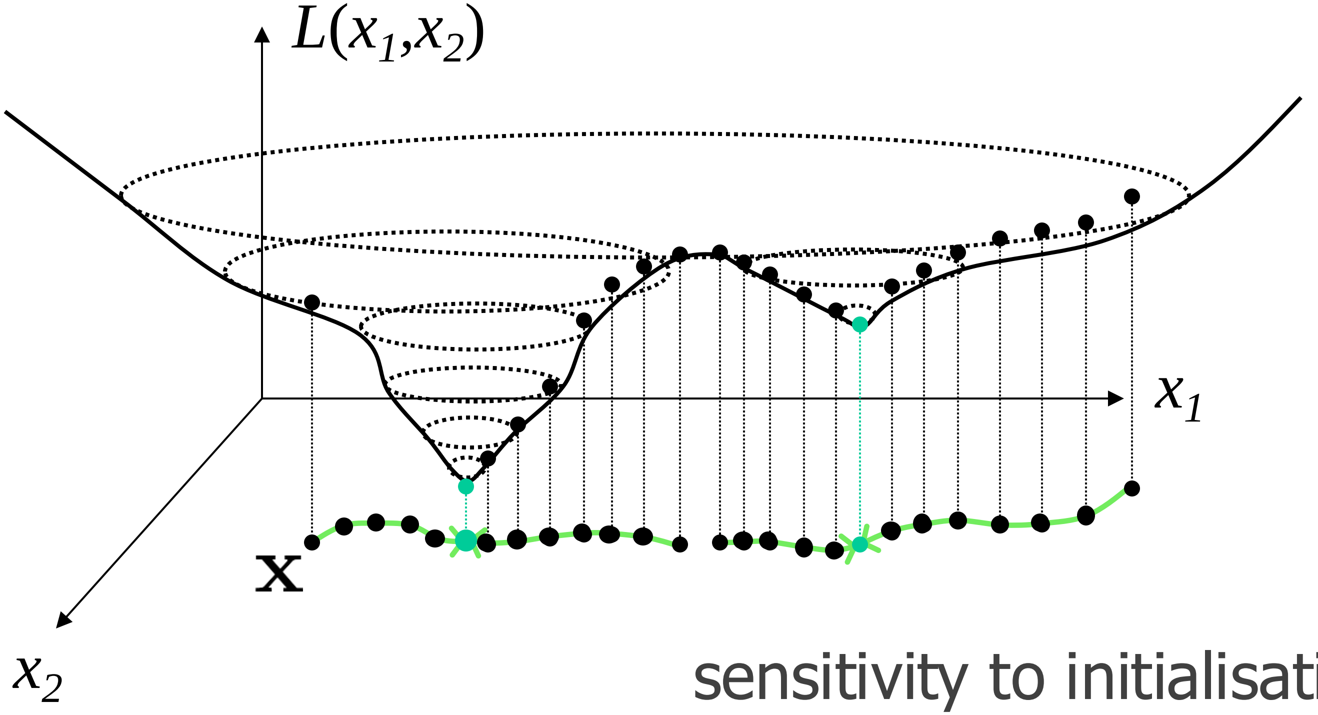
$$\boxed{\mathbf{x}' = \mathbf{x} - \alpha \nabla L}$$

$$\begin{bmatrix} x_1' \\ x_2' \end{bmatrix} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} - \alpha \begin{bmatrix} \frac{\partial E}{\partial x_1} \\ \frac{\partial E}{\partial x_2} \end{bmatrix}$$

Stop at a local minima where $\nabla L = \vec{0}$

Gradient Descent

Example: for a function of two variables

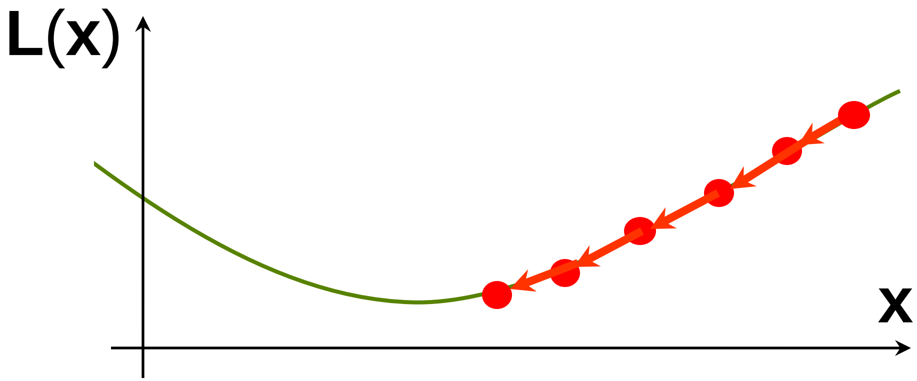


sensitivity to initialisation !!

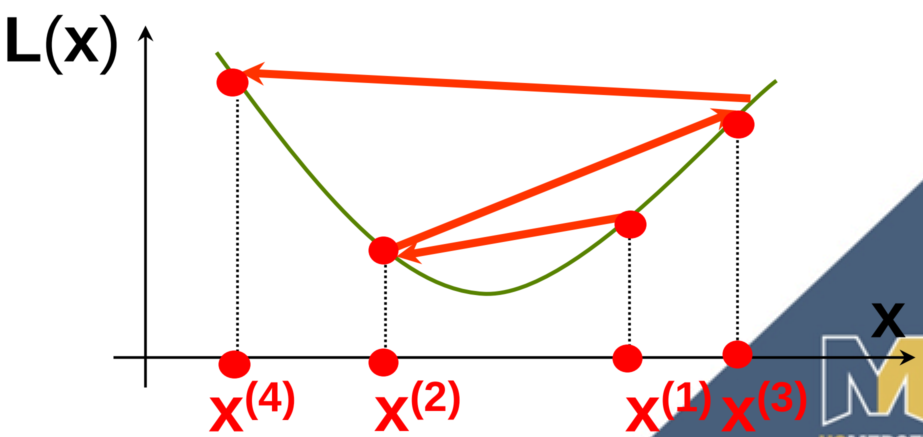
How to Set Learning Rate α?

$$\boxed{\mathbf{x}' = \mathbf{x} - \alpha \nabla L}$$

- If α too small, too many iterations to converge



- If α too large, may overshoot the local minimum and possibly never even converge



Variable Learning Rate

If desired, can change learning rate α at each iteration

$\mathbf{k} = 1$

$\mathbf{x}^{(1)}$ = any initial guess

choose α, ε

while $\alpha \|\nabla \mathbf{L}(\mathbf{x}^{(k)})\| > \varepsilon$

  $\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - \alpha \nabla \mathbf{L}(\mathbf{x}^{(k)})$

  $\mathbf{k} = \mathbf{k} + 1$

fixed α
gradient descent

$\mathbf{k} = 1$

$\mathbf{x}^{(1)}$ = any initial guess

choose ε

while $\alpha \|\nabla \mathbf{L}(\mathbf{x}^{(k)})\| > \varepsilon$

  choose $\alpha^{(k)}$

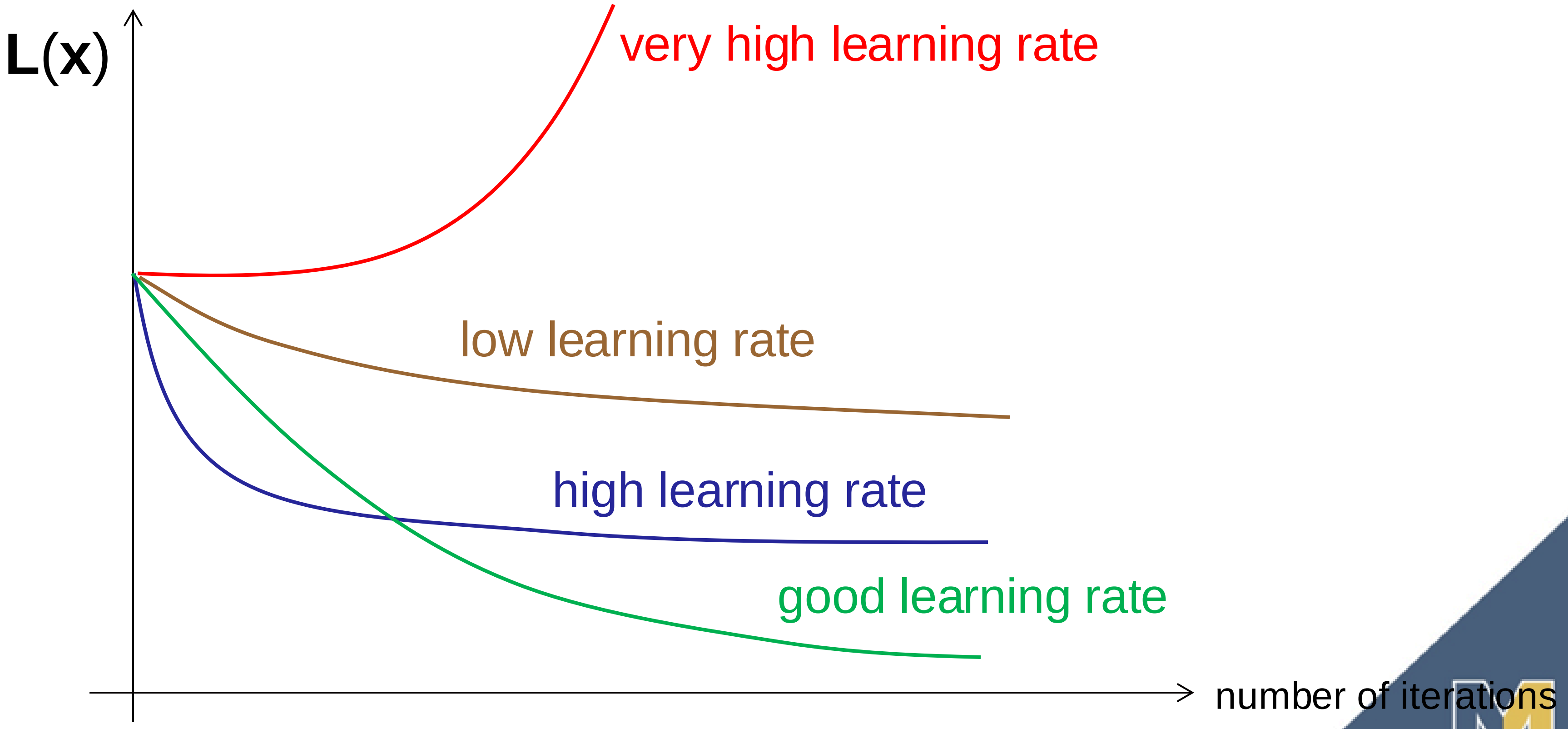
  $\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - \alpha^{(k)} \nabla \mathbf{L}(\mathbf{x}^{(k)})$

  $\mathbf{k} = \mathbf{k} + 1$

variable α
gradient descent

Learning Rate

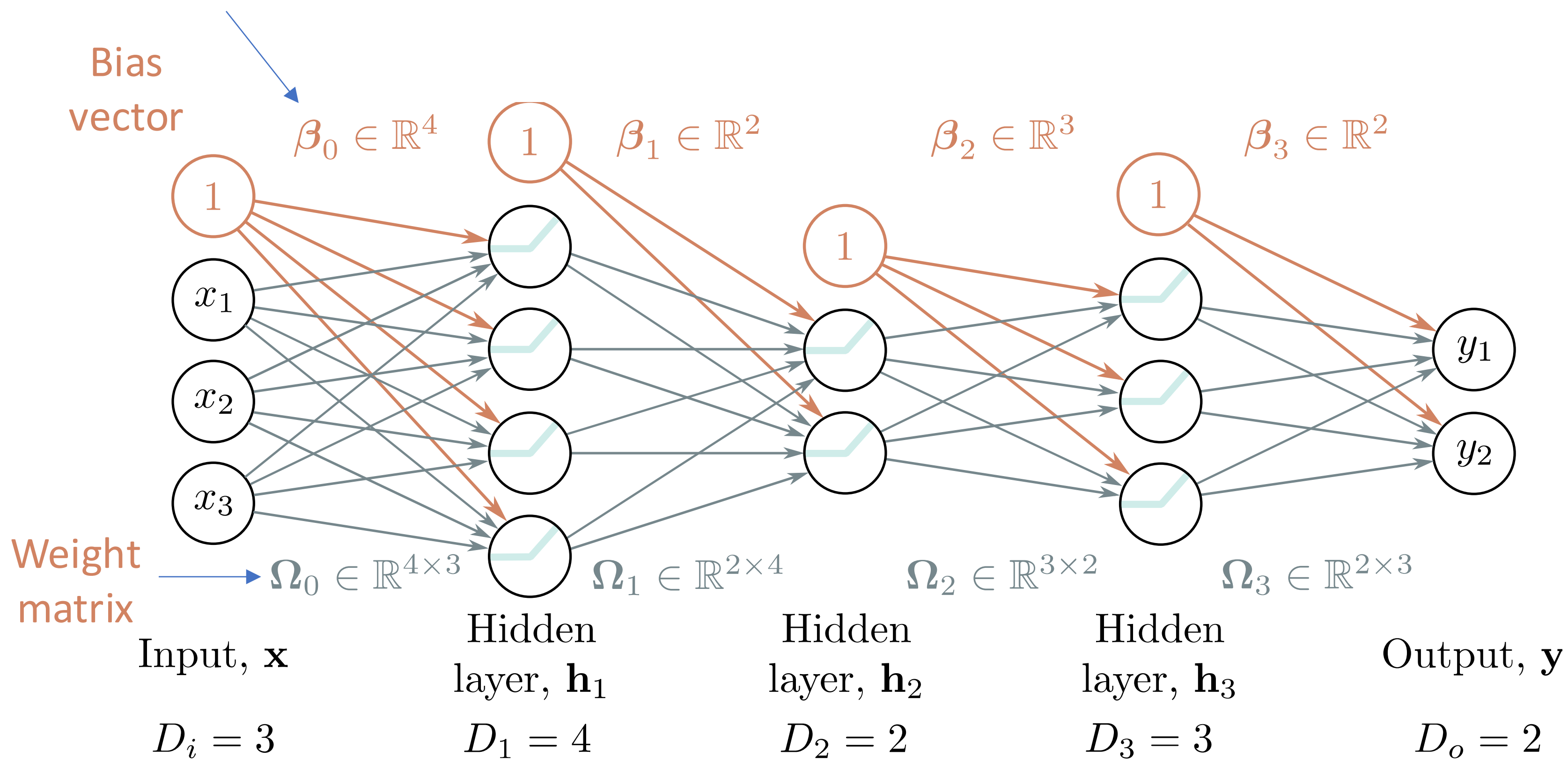
- Monitor learning rate by looking at how fast the objective function decreases



Derivative and Back Propagation

How to take derivatives w.r.t. weights?

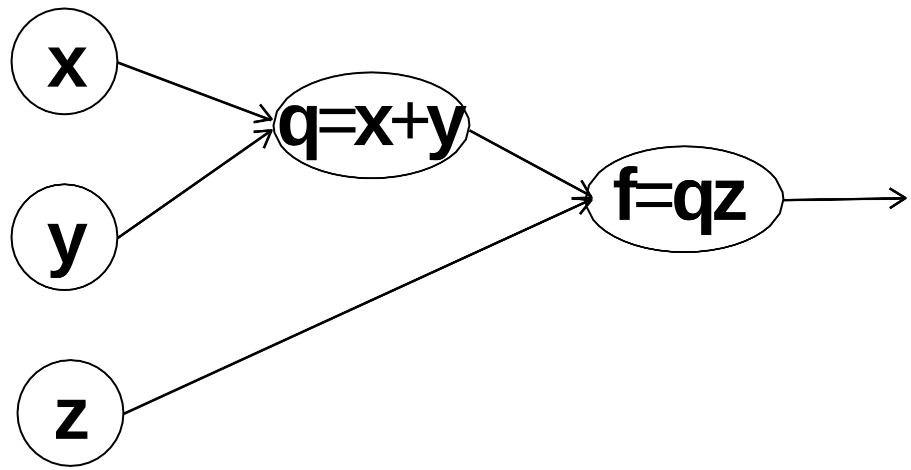
- Training == learning weight and bias



Example of Multi Layer Perceptron (MLP)

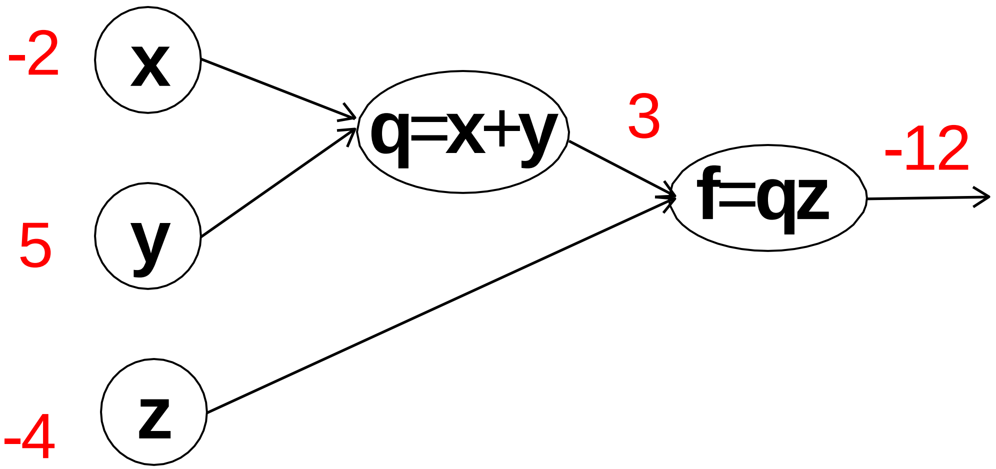
Computing Derivatives: Small Example

- Small network $\mathbf{f}(\mathbf{x},\mathbf{y},\mathbf{z}) = (\mathbf{x}+\mathbf{y})\mathbf{z}$
- Rewrite using
  - $\mathbf{q} = \mathbf{x} + \mathbf{y}$
- $\mathbf{f}(\mathbf{x},\mathbf{y},\mathbf{z}) = \mathbf{qz}$
- each node does one operation



Computing Derivatives: Small Example

- Small network **f(x,y,z)** = (**x**+**y**)**z**
- Rewrite using
  - **q** = **x** + **y**
  - **f**(**x**,**y**,**z**) = **qz**
- Example of computing **f(-2,5,-4)**

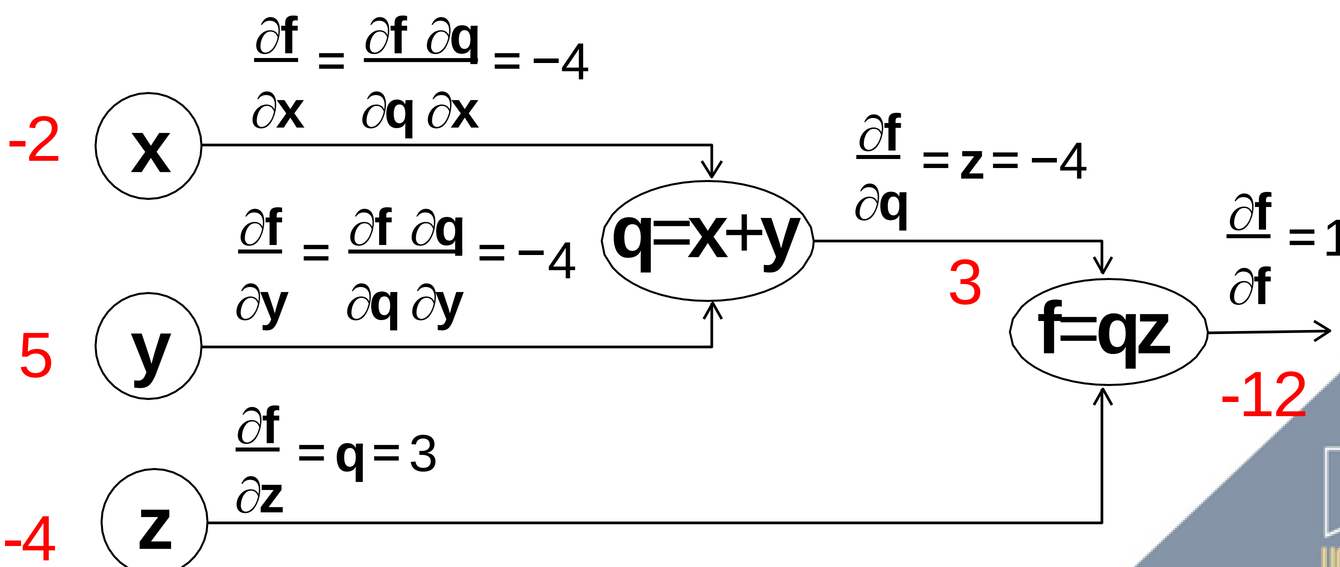


Computing Derivatives: Small Example

- Small network $\mathbf{f(x,y,z)} = (\mathbf{x}+\mathbf{y})\mathbf{z}$
- Rewrite using $\mathbf{q} = \mathbf{x} + \mathbf{y} \;\Rightarrow\; \mathbf{f(x,y,z)} = \mathbf{qz}$
- Want $\frac{\partial \mathbf{f}}{\partial \mathbf{x}}, \frac{\partial \mathbf{f}}{\partial \mathbf{y}}, \frac{\partial \mathbf{f}}{\partial \mathbf{z}}$
- Compute $\frac{\partial \mathbf{f}}{\partial}$ from the end backwards
  - for each edge, with respect to the main variable at edge origin
  - using chain rule with respect to the variable at edge end, if needed

chain rule for $\mathbf{f(y(x))}$

$$\frac{\partial \mathbf{f}}{\partial \mathbf{x}} = \frac{\partial \mathbf{f}}{\partial \mathbf{y}}\frac{\partial \mathbf{y}}{\partial \mathbf{x}}$$



Computing Derivatives: Chain of Chain Rule

- Compute $\frac{\partial \mathbf{d}}{\partial}$ from the end backwards
  - for each edge, with respect to the main variable at edge origin
  - using chain rule with respect to the variable at edge end, if needed

direction of computation

$$\xrightarrow{\mathbf{a}} \left(\mathbf{b}=\mathbf{h}(\mathbf{a})\right) \longrightarrow \left(\mathbf{c}=\mathbf{h}(\mathbf{b})\right) \longrightarrow \left(\mathbf{d}=\mathbf{h}(\mathbf{c})\right) \xrightarrow{\mathbf{d}}$$

$$\frac{\partial \mathbf{d}}{\partial \mathbf{a}} = \underbrace{\frac{\partial \mathbf{d}}{\partial \mathbf{b}}}_{\text{prev}} \underbrace{\frac{\partial \mathbf{b}}{\partial \mathbf{a}}}_{\text{local}} \qquad \frac{\partial \mathbf{d}}{\partial \mathbf{b}} = \underbrace{\frac{\partial \mathbf{d}}{\partial \mathbf{c}}}_{\text{prev}} \underbrace{\frac{\partial \mathbf{c}}{\partial \mathbf{b}}}_{\text{local}} \qquad \underbrace{\frac{\partial \mathbf{d}}{\partial \mathbf{c}}}_{\text{local}}$$

$$\boxed{\textbf{example}: \textbf{ if } \mathbf{h}(\mathbf{c}) = \mathbf{c}^2, \textbf{ then } \frac{\partial \mathbf{d}}{\partial \mathbf{c}} = \frac{\partial \mathbf{h}}{\partial \mathbf{c}} = 2\mathbf{c}}$$

Computing Derivatives Backwards

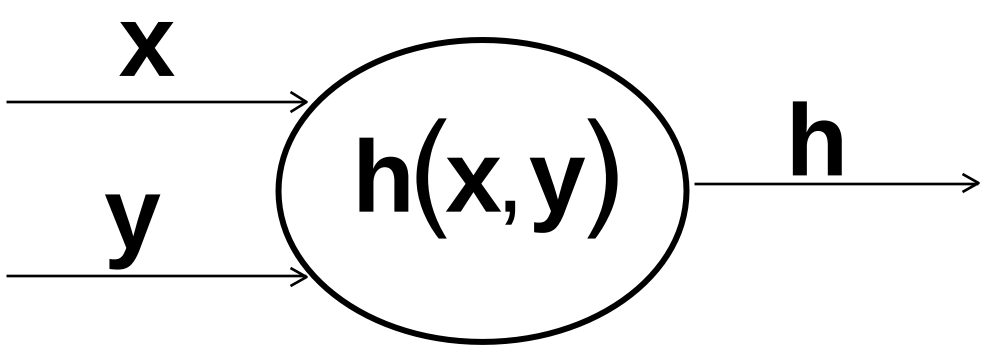
$$\xrightarrow{\mathbf{x}} \boxed{h(W^1\mathbf{x}+b^1)} \xrightarrow{\mathbf{h}^1} \boxed{h(W^2\mathbf{h}^1+b^2)} \xrightarrow{\mathbf{h}^2} \boxed{h(W^3\mathbf{h}^2+b^3)} \xrightarrow{\mathbf{o}} \boxed{\mathbf{L}(\mathbf{o})}$$

direction of computation

- Have loss function $\mathbf{L}(\mathbf{o})$
- Need derivatives for all $\frac{\partial \mathbf{L}}{\partial \mathbf{w}}, \frac{\partial \mathbf{L}}{\partial \mathbf{b}}$
- Will compute derivatives from end to front, backwards
- On the way will also compute intermediate derivatives $\frac{\partial \mathbf{L}}{\partial \mathbf{h}}$

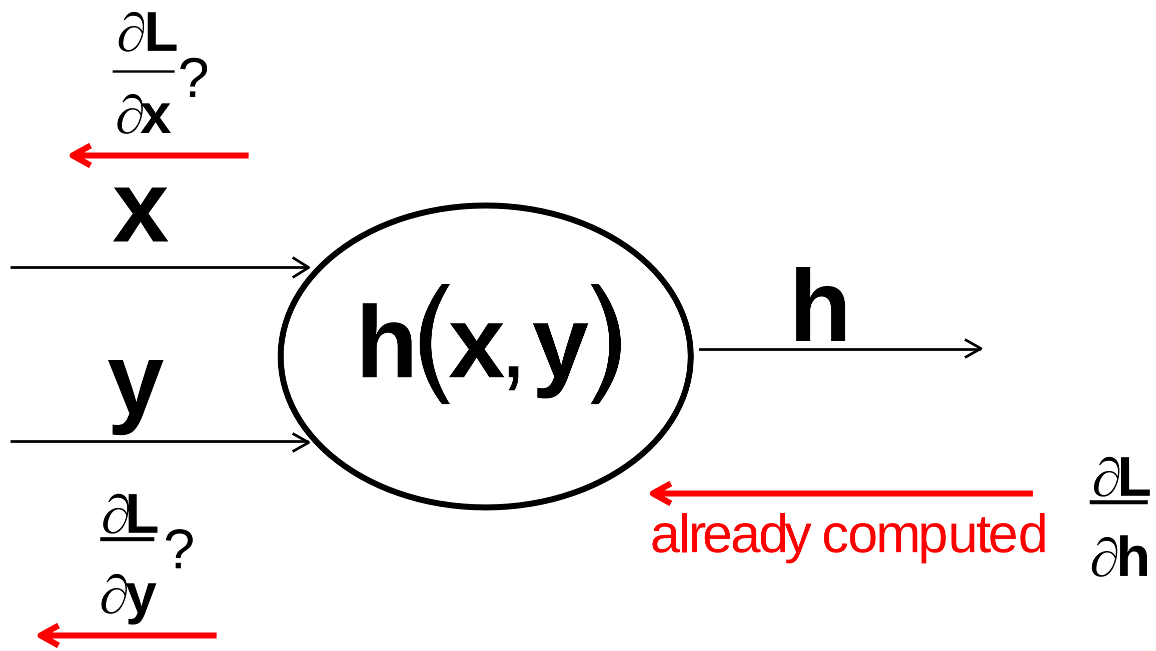
Computing Derivatives: Look at One Node

- Simplified view at a network node
  - inputs **x**,**y** come in
  - node computes some function **h**(**x**,**y**)



Computing Derivatives: Look at One Node

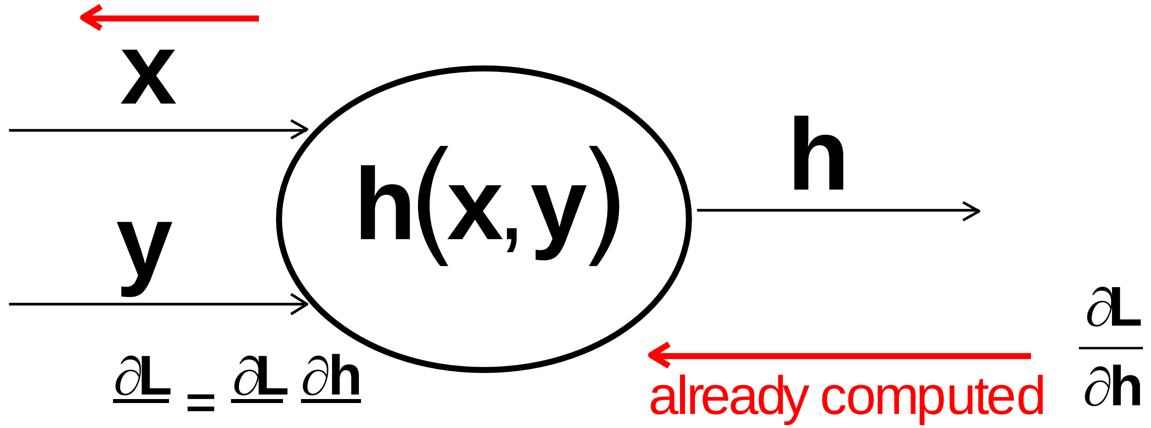
- At each network node
  - inputs **x**,**y** come in
  - nodes computes activation function **h**(**x**,**y**)
- Have loss function **L**(·)



Computing Derivatives: Look at One Node

- Need $\frac{\partial L}{\partial x}, \frac{\partial L}{\partial y}$
- Easy to compute local node derivatives $\frac{\partial h}{\partial x}, \frac{\partial h}{\partial y}$

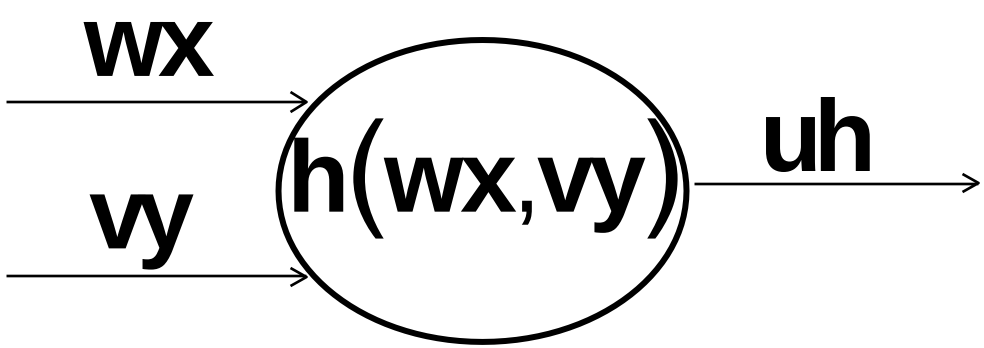
$$\frac{\partial L}{\partial x} = \frac{\partial L}{\partial h}\frac{\partial h}{\partial x}$$



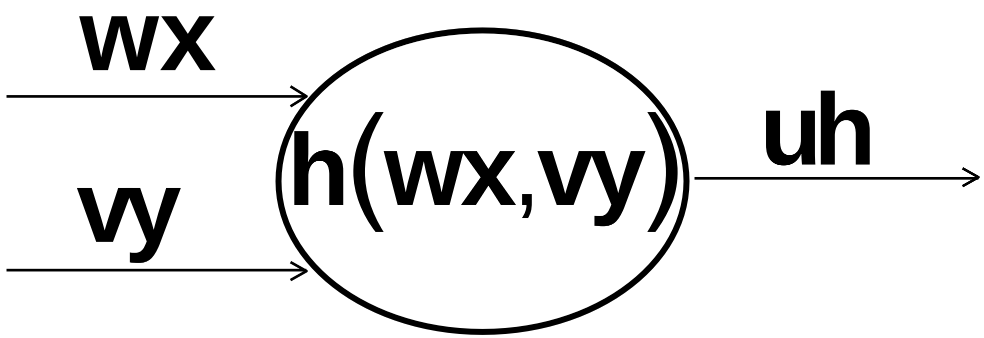
$$\frac{\partial L}{\partial y} = \frac{\partial L}{\partial h}\frac{\partial h}{\partial y}$$

Computing Derivatives: Look at One Node

- More complete view at a network node
  - inputs **x**,**y** come in, get multiplied by weight **w** and **v**
  - node computes function **h**(**wx**,**vy**)
  - node output **h** gets multiplied by **u**

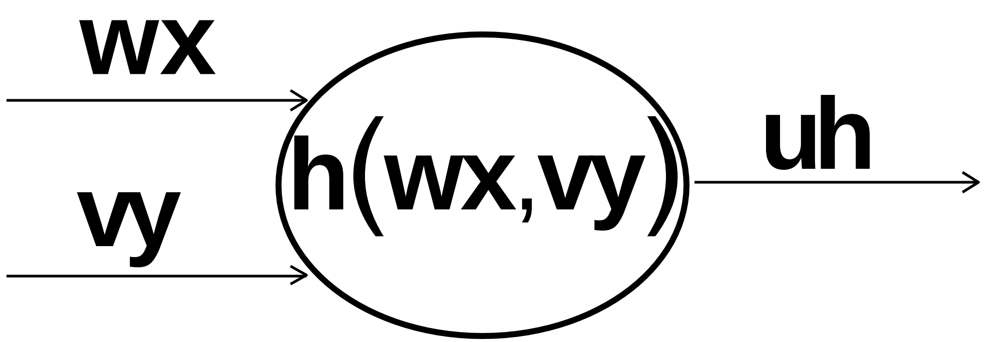


Computing Derivatives: Look at One Node



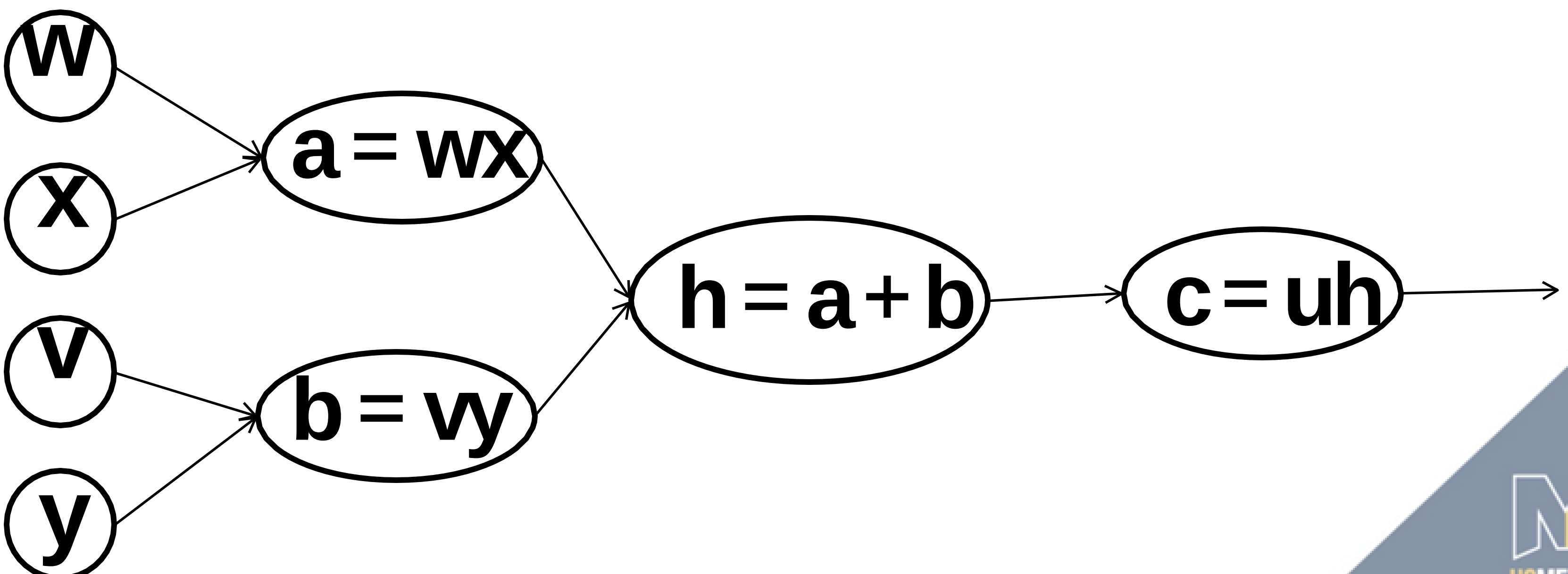
- To be concrete, let **h**(**i**,**j**) = **i** + **j**

Computing Derivatives: Look at One Node

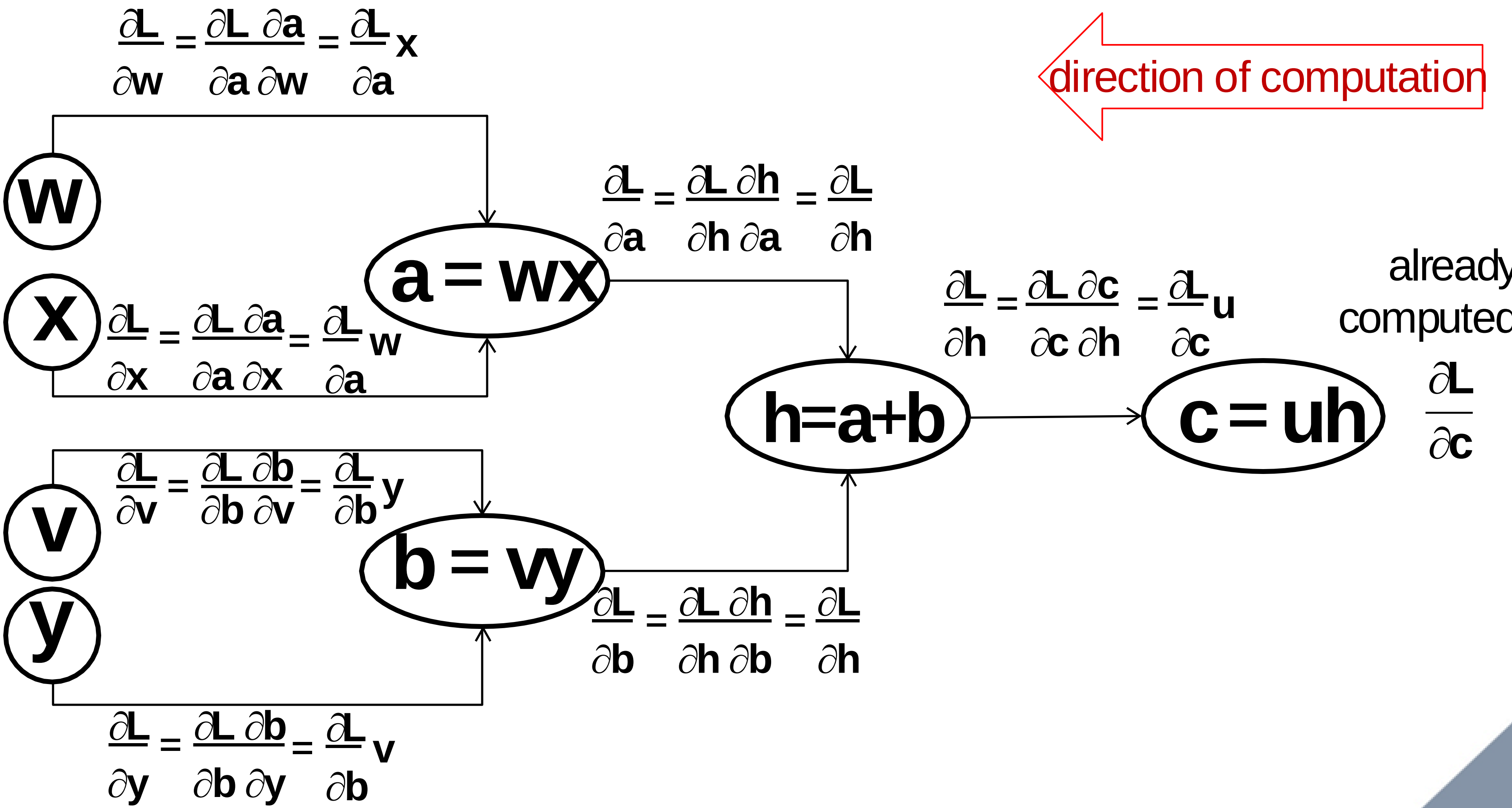


- **h(i,j) = i + j**

- Break into more computational nodes
  - all computation happens inside nodes, not on edges

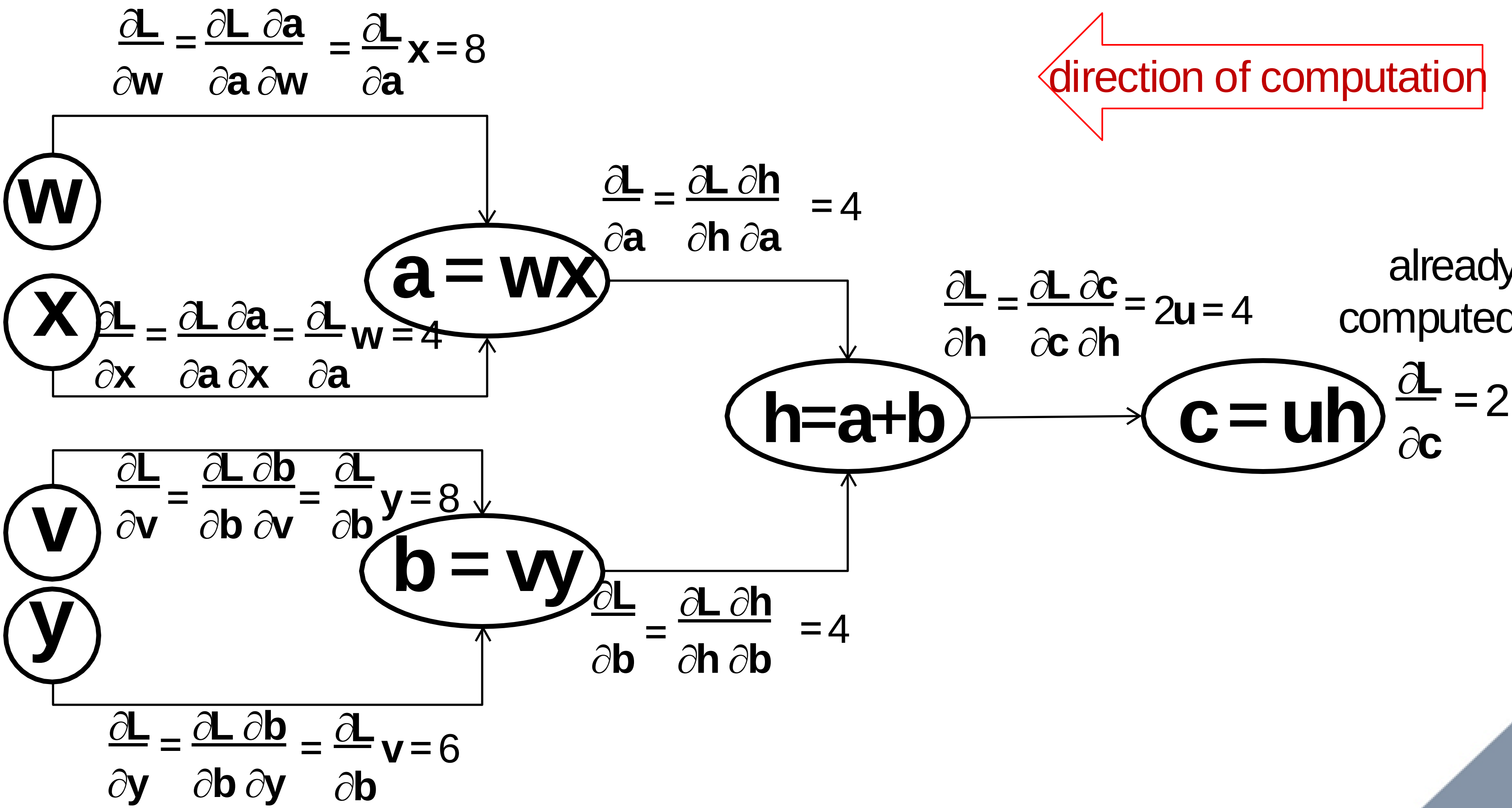


Computing Derivatives: Look at One Node



- Some of these partial derivatives are intermediate
  - their values will not be used for gradient descent

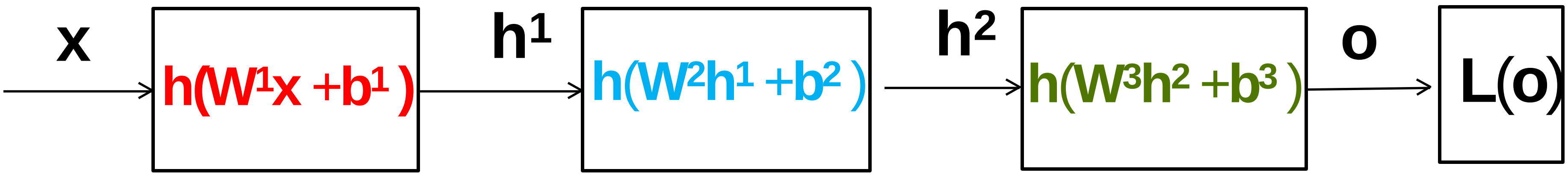
Computing Derivatives: Look at One Node



- Example when **w** = 1, **x** = 2, **v** = 3, **y** = 4, u = 2, $\frac{\partial L}{\partial c} = 2$

Computing Derivatives: Vector Notation

- Inputs outputs are often vectors



- **h**(a) is a function from $\mathbf{R}^n$ to $\mathbf{R}^m$
- Chain rule generalizes to vector functions

Computing Derivatives: Vector Notation

- Let $\mathbf{f}(\mathbf{x})$: $\mathbf{R}^{\mathbf{n}} \to \mathbf{R}^{\mathbf{m}}$,
  - $\mathbf{x}$ is $\mathbf{n}$-dimensional vector and output $\mathbf{f}(\mathbf{x})$ is $\mathbf{m}$-dimensional vector
- Jacobian matrix
  - has $\mathbf{m}$ rows and $\mathbf{n}$ columns
  - has $\frac{\partial \mathbf{f_i}}{\partial \mathbf{x_j}}$ in row $\mathbf{i}$, column $\mathbf{j}$

Computing Derivatives: Vector Notation

- $\mathbf{f}(\mathbf{x})$: $\mathbf{R}^n \rightarrow \mathbf{R}^m$ and $\mathbf{g}(\mathbf{x})$: $\mathbf{R}^k \rightarrow \mathbf{R}^n$
- $\mathbf{f}(\mathbf{g}(\mathbf{x}))$: $\mathbf{R}^k \rightarrow \mathbf{R}^m$
- Chain rule for vector functions

$$\frac{\partial \mathbf{f}}{\partial \mathbf{x}} = \frac{\partial \mathbf{f}}{\partial \mathbf{g}} \frac{\partial \mathbf{g}}{\partial \mathbf{x}}$$

Jacobian matrices

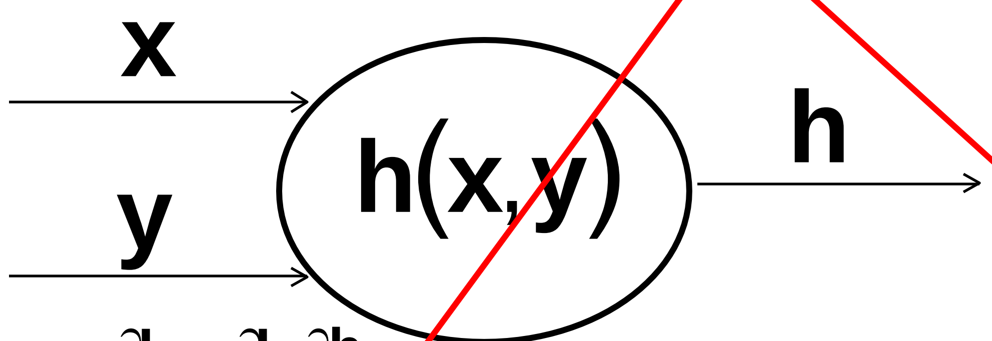
Vector Notation: Look at One Node

- **h**, **x**, **y** are vectors
- already computed Jacobian $\frac{\partial \mathbf{L}}{\partial \mathbf{h}}$
- Need Jacobians $\frac{\partial \mathbf{L}}{\partial \mathbf{x}}, \frac{\partial \mathbf{L}}{\partial \mathbf{y}}$

- Easy to compute local node Jacobians $\frac{\partial \mathbf{h}}{\partial \mathbf{x}}, \frac{\partial \mathbf{h}}{\partial \mathbf{y}}$

$$\frac{\partial \mathbf{L}}{\partial \mathbf{x}} = \frac{\partial \mathbf{L}}{\partial \mathbf{h}} \frac{\partial \mathbf{h}}{\partial \mathbf{x}}$$

Jacobian matrices



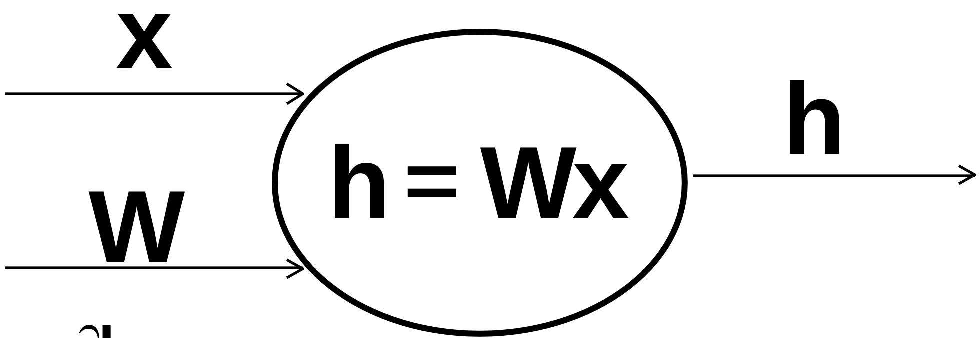
already computed $\frac{\partial \mathbf{L}}{\partial \mathbf{h}}$

$$\frac{\partial \mathbf{L}}{\partial \mathbf{y}} = \frac{\partial \mathbf{L}}{\partial \mathbf{h}} \frac{\partial \mathbf{h}}{\partial \mathbf{y}}$$

Vector Notation: Look at One Node

- Can apply to matrices (and tensors) as well
- But first vectorize matrix (or tensor)
- Say $\mathbf{W}$ is 10 x 5, stretch into 50x1 vector
- Still denote Jacobian by $\frac{\partial \mathbf{h}}{\partial \mathbf{W}}$

$$\frac{\partial \mathbf{L}}{\partial \mathbf{x}} = \frac{\partial \mathbf{L}}{\partial \mathbf{h}} \frac{\partial \mathbf{h}}{\partial \mathbf{x}}$$



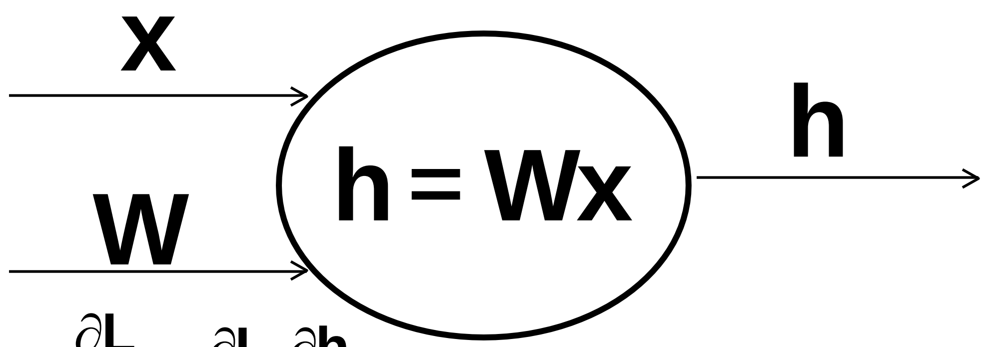
already computed $\frac{\partial \mathbf{L}}{\partial \mathbf{h}}$

$$\frac{\partial \mathbf{L}}{\partial \mathbf{W}} = \frac{\partial \mathbf{L}}{\partial \mathbf{h}} \frac{\partial \mathbf{h}}{\partial \mathbf{W}}$$

Vector Notation: Look at One Node

- Easy to compute local node Jacobians $\frac{\partial \mathbf{h}}{\partial \mathbf{x}}, \frac{\partial \mathbf{h}}{\partial \mathbf{W}}$
- But they can get very large (although sparse)
- Say $\mathbf{h}$ is 1000 x 1, $\mathbf{W}$ is 1000 x 500, then $\frac{\partial \mathbf{h}}{\partial \mathbf{W}}$ is 1000 x 500,000

$$\frac{\partial \mathbf{L}}{\partial \mathbf{x}} = \frac{\partial \mathbf{L}}{\partial \mathbf{h}} \frac{\partial \mathbf{h}}{\partial \mathbf{x}}$$



already computed

$$\frac{\partial \mathbf{L}}{\partial \mathbf{h}}$$

$$\frac{\partial \mathbf{L}}{\partial \mathbf{W}} = \frac{\partial \mathbf{L}}{\partial \mathbf{h}} \frac{\partial \mathbf{h}}{\partial \mathbf{W}}$$

Summary

- ❑Gradient Descent Optimization
- ❑Chain rule of derivatives
- ❑Back propagation