Lecture 4: Neural Networks and Backpropagation

So far: backprop with scalars

What about vector-valued functions?

Recap: Vector derivatives

Scalar to Scalar

$$x \in \mathbb{R}, y \in \mathbb{R}$$

Regular derivative:

$$\frac{\partial y}{\partial x} \in \mathbb{R}$$

If x changes by a small amount, how much will y change?

Recap: Vector derivatives

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Vector to Scalar

$$x \in \mathbb{R}^N, y \in \mathbb{R}$$

Derivative is **Gradient**:

$$\frac{\partial y}{\partial x} \in \mathbb{R}^N \quad \left(\frac{\partial y}{\partial x}\right)_n = \frac{\partial y}{\partial x_n}$$

For each element of x, if it changes by a small amount then how much will y change?

Recap: Vector derivatives

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For each element of x, if it changes by a small amount then how much will y change?

Vector to Vector

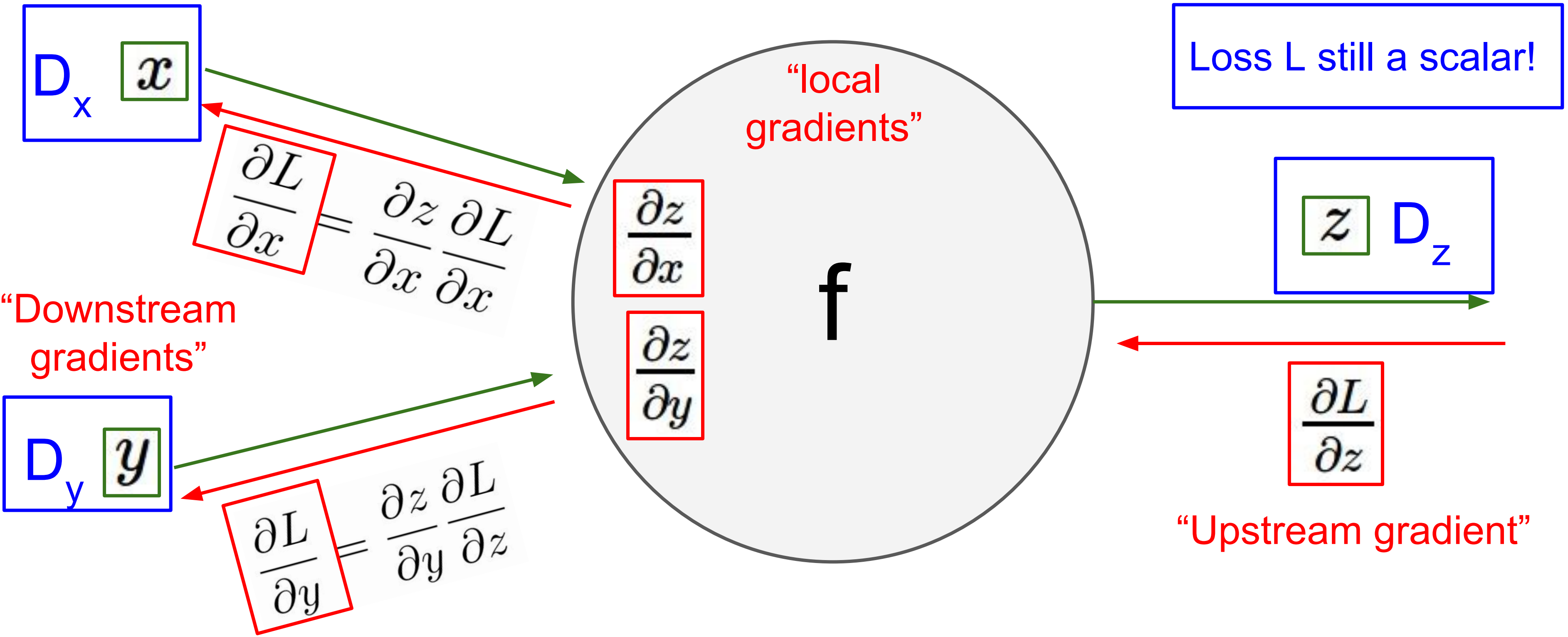
$$x \in \mathbb{R}^N, y \in \mathbb{R}^M$$

Derivative is **Jacobian**:

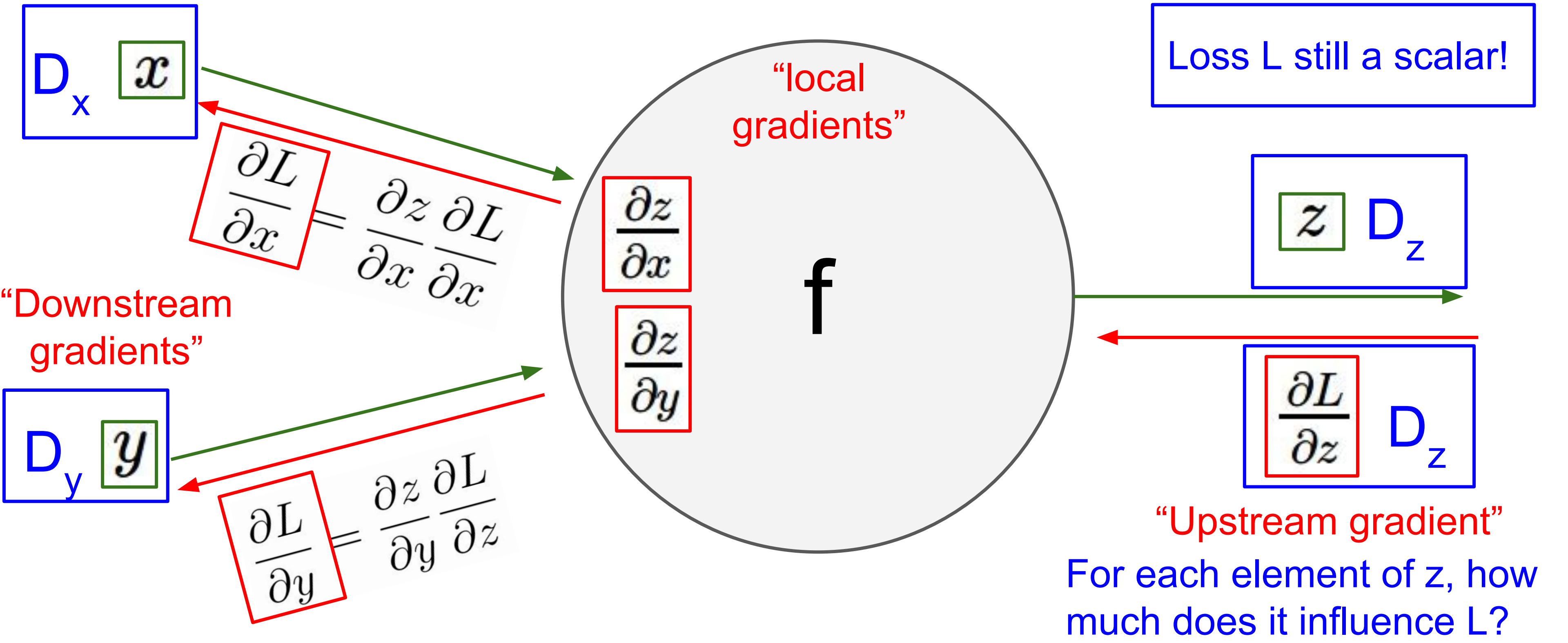
$$\frac{\partial y}{\partial x} \in \mathbb{R}^{N \times M} \quad \left(\frac{\partial y}{\partial x}\right)_{n,m} = \frac{\partial y_m}{\partial x_n}$$

For each element of x, if it changes by a small amount then how much will each element of y change?

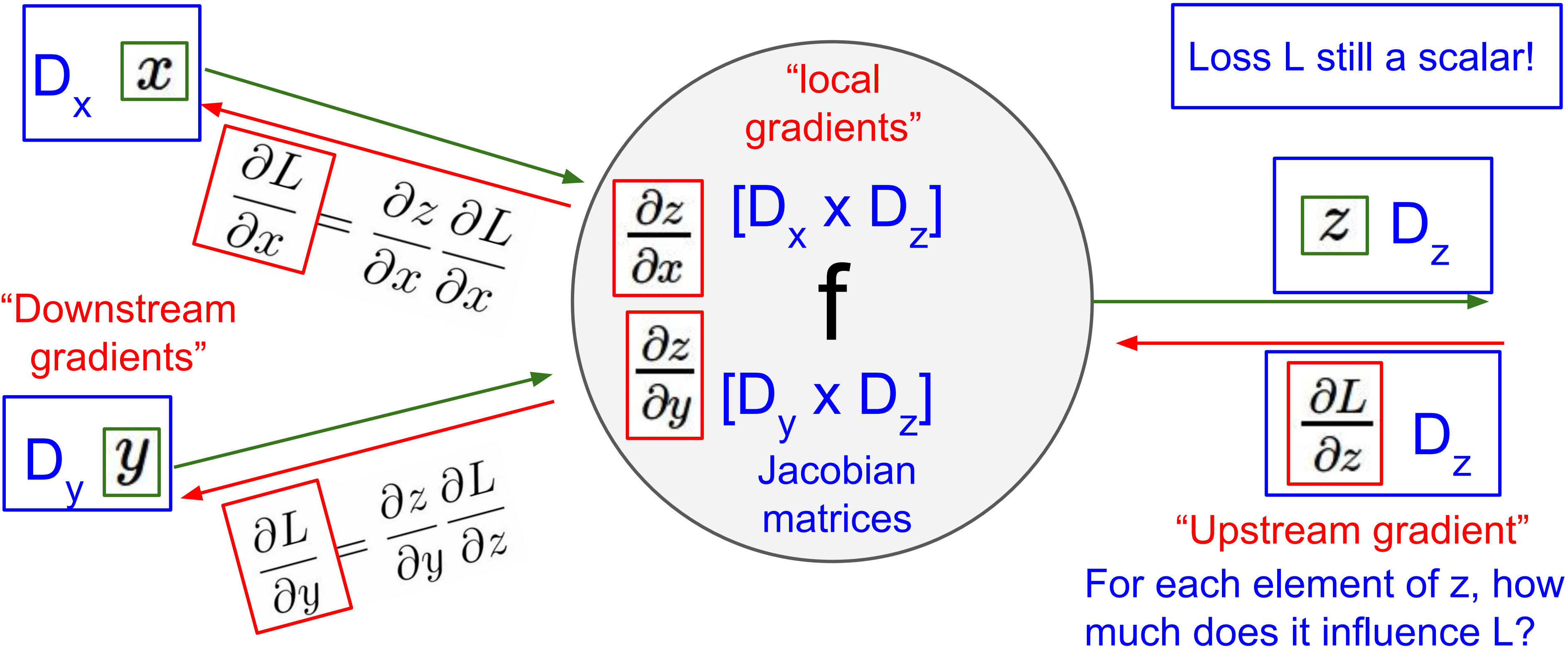
Backprop with Vectors



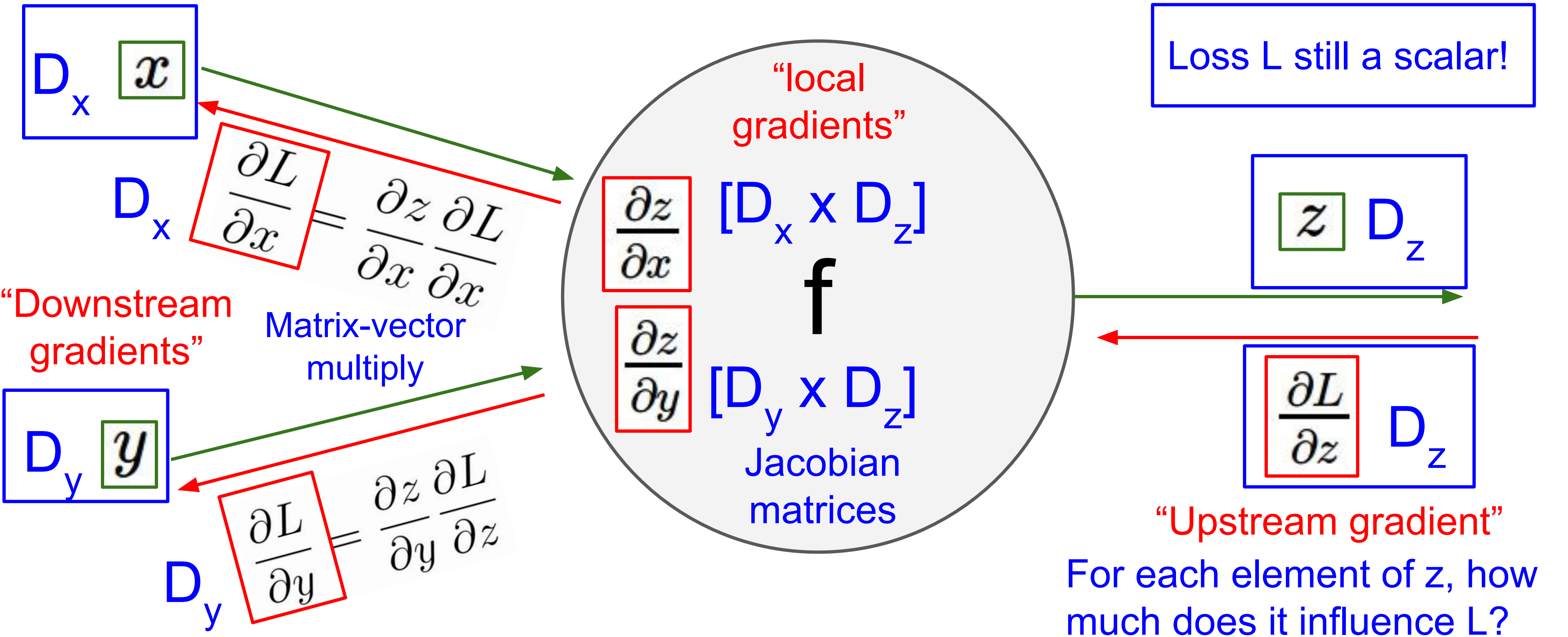
Backprop with Vectors



Backprop with Vectors



Backprop with Vectors



Backprop with Vectors

4D input x:

$$\begin{bmatrix} 1 \\ -2 \\ 3 \\ -1 \end{bmatrix} \longrightarrow \boxed{\begin{matrix} f(x) = \max(0,x) \\ \textit{(elementwise)} \end{matrix}} \longrightarrow \begin{bmatrix} 1 \\ 0 \\ 3 \\ 0 \end{bmatrix}$$

4D output y:

Backprop with Vectors

4D input x:

[1]
[-2]
[3]
[-1]

f(x) = max(0,x)
(elementwise)

4D output y:

[1]
[0]
[3]
[0]

4D dL/dy:

[4]
[-1]
[5]
[9]

Upstream gradient

Backprop with Vectors

4D input x:

$$\begin{bmatrix} 1 \\ -2 \\ 3 \\ -1 \end{bmatrix}$$

f(x) = max(0,x)
(elementwise)

4D output y:

$$\begin{bmatrix} 1 \\ 0 \\ 3 \\ 0 \end{bmatrix}$$

Jacobian dy/dx

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

4D dL/dy:

$$\begin{bmatrix} 4 \\ -1 \\ 5 \\ 9 \end{bmatrix}$$

Upstream gradient

Backprop with Vectors

4D input x:

$$\begin{bmatrix} 1 \\ -2 \\ 3 \\ -1 \end{bmatrix}$$

$f(x) = \max(0,x)$
(elementwise)

4D output y:

$$\begin{bmatrix} 1 \\ 0 \\ 3 \\ 0 \end{bmatrix}$$

[dy/dx] [dL/dy]

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} 4 \\ -1 \\ 5 \\ 9 \end{bmatrix}$$

4D dL/dy:

$$\begin{bmatrix} 4 \\ -1 \\ 5 \\ 9 \end{bmatrix}$$

Upstream gradient

Backprop with Vectors

4D input x:

$$\begin{bmatrix} 1 \\ -2 \\ 3 \\ -1 \end{bmatrix} \rightarrow \boxed{\begin{array}{c} f(x) = \max(0,x) \\ \textit{(elementwise)} \end{array}} \rightarrow \begin{bmatrix} 1 \\ 0 \\ 3 \\ 0 \end{bmatrix}$$

4D output y:

4D dL/dx: [dy/dx] [dL/dy] 4D dL/dy:

$$\begin{bmatrix} 4 \\ 0 \\ 5 \\ 0 \end{bmatrix} \leftarrow \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} 4 \\ -1 \\ 5 \\ 9 \end{bmatrix} \leftarrow \begin{bmatrix} 4 \\ -1 \\ 5 \\ 9 \end{bmatrix} \leftarrow$$

Upstream gradient

Backprop with Vectors

Jacobian is **sparse**: off-diagonal entries always zero! Never **explicitly** form Jacobian -- instead use **implicit** multiplication

4D input x:

$$\begin{bmatrix} 1 \\ -2 \\ 3 \\ -1 \end{bmatrix} \longrightarrow \boxed{\begin{matrix} f(x) = \max(0,x) \\ \textit{(elementwise)} \end{matrix}} \longrightarrow \begin{bmatrix} 1 \\ 0 \\ 3 \\ 0 \end{bmatrix}$$

4D output y:

4D dL/dx:

[dy/dx] [dL/dy]

4D dL/dy:

$$\begin{bmatrix} 4 \\ 0 \\ 5 \\ 0 \end{bmatrix} \longleftarrow \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} 4 \\ -1 \\ 5 \\ 9 \end{bmatrix} \longleftarrow \begin{bmatrix} 4 \\ -1 \\ 5 \\ 9 \end{bmatrix} \longleftarrow$$

Upstream gradient

Backprop with Vectors

Jacobian is **sparse**: off-diagonal entries always zero! Never **explicitly** form Jacobian -- instead use **implicit** multiplication

4D input x:

[1]
[-2]
[3]
[-1]

$f(x) = \max(0,x)$ *(elementwise)*

4D output y:

[1]
[0]
[3]
[0]

4D dL/dx:

[4]
[0]
[5]
[0]

[dy/dx] [dL/dy]

$$\left(\frac{\partial L}{\partial x}\right)_i = \begin{cases} \left(\frac{\partial L}{\partial y}\right)_i & \text{if } x_i > 0 \\ 0 & \text{otherwise} \end{cases}$$

4D dL/dy:

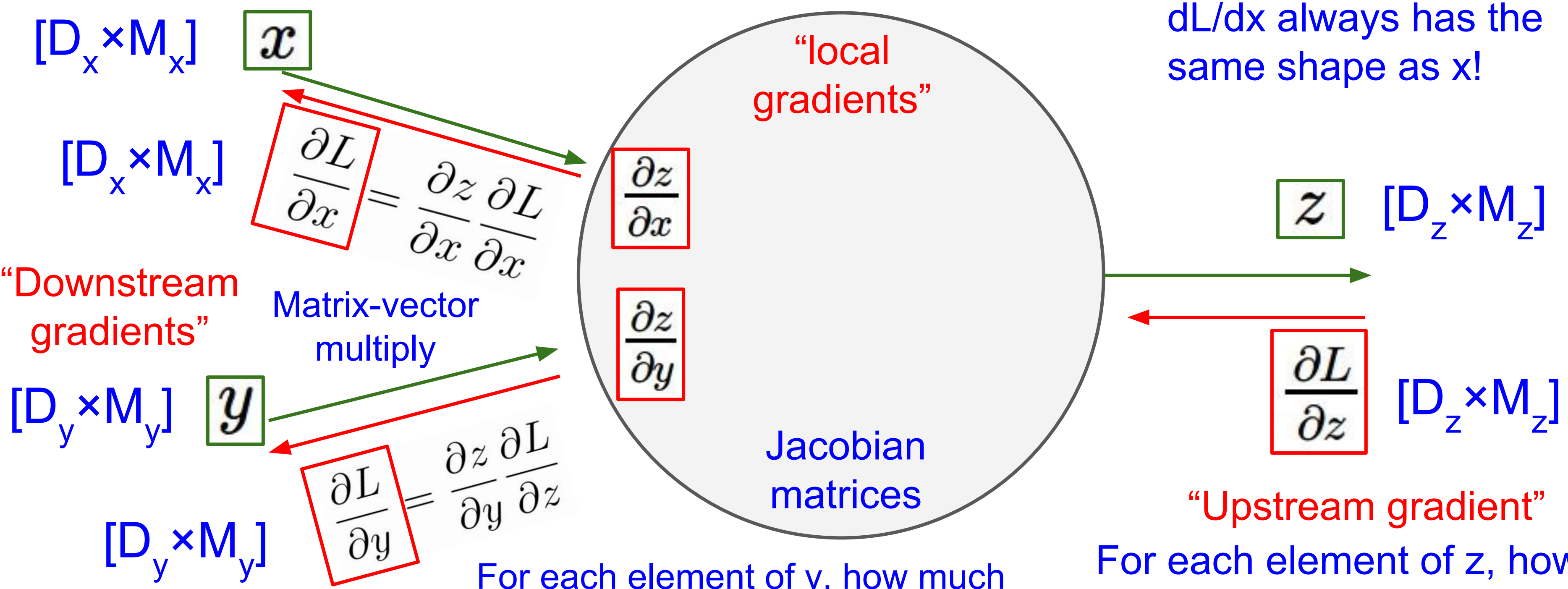
[4]
[-1]
[5]
[9]

Upstream gradient

Backprop with Matrices (or Tensors)

Loss L still a scalar!

dL/dx always has the same shape as x!

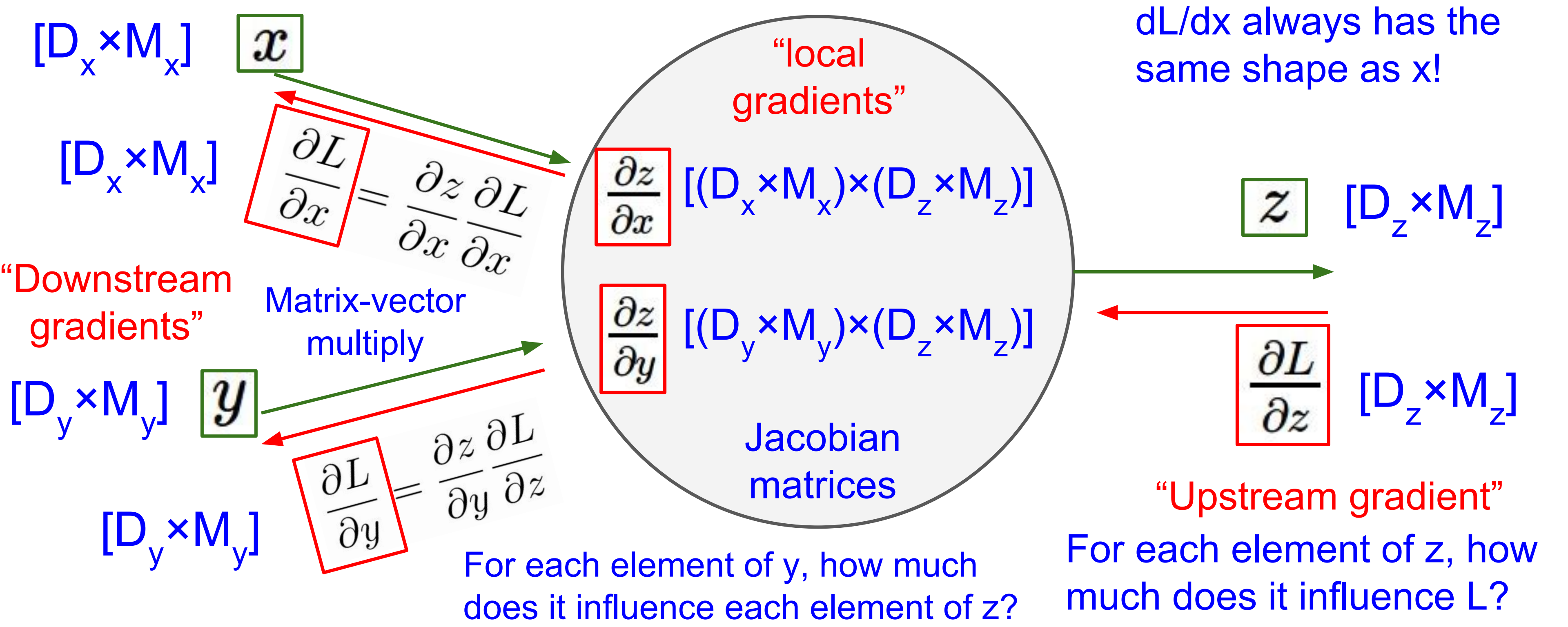


For each element of y, how much does it influence each element of z?

For each element of z, how much does it influence L?

Backprop with Matrices (or Tensors)

Loss L still a scalar!



Backprop with Matrices

x: [N×D]

$$\begin{bmatrix} 2 & 1 & -3 \\ -3 & 4 & 2 \end{bmatrix}$$

w: [D×M]

$$\begin{bmatrix} 3 & 2 & 1 & -1 \\ 2 & 1 & 3 & 2 \\ 3 & 2 & 1 & -2 \end{bmatrix}$$

Matrix Multiply

$$y_{n,m} = \sum_d x_{n,d} w_{d,m}$$

y: [N×M]

$$\begin{bmatrix} 13 & 9 & -2 & -6 \\ 5 & 2 & 17 & 1 \end{bmatrix}$$

dL/dy: [N×M]

$$\begin{bmatrix} 2 & 3 & -3 & 9 \\ -8 & 1 & 4 & 6 \end{bmatrix}$$

Also see derivation in the course notes:
http://cs231n.stanford.edu/handouts/linear-backprop.pdf

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Jacobians:
dy/dx: [(N×D)×(N×M)]
dy/dw: [(D×M)×(N×M)]

For a neural net we may have
N=64, D=M=4096
Each Jacobian takes 256 GB of memory!
Must work with them implicitly!

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Q: What parts of y are affected by one element of x?

Backprop with Matrices

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[2 1 3 2]
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[$\boxed{13 \ 9 \ -2 \ -6}$]
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dL/dy: [N×M]

[$\boxed{2 \ 3 \ -3 \ 9}$]
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Q: What parts of y are affected by one element of x?

A: $\boxed{x_{n,d}}$ affects the whole row $y_{n,\cdot}$

$$\frac{\partial L}{\partial x_{n,d}} = \sum_m \frac{\partial L}{\partial y_{n,m}} \frac{\partial y_{n,m}}{\partial x_{n,d}}$$

Backprop with Matrices

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$$y_{n,m} = \sum_d x_{n,d} w_{d,m}$$

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dL/dy: [N×M]

[2 3 -3 9]
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Q: How much does $\boxed{x_{n,d}}$ affect $\boxed{y_{n,m}}$?

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[N×D] [N×M] [M×D]

$$\boxed{\frac{\partial L}{\partial x} = \left(\frac{\partial L}{\partial y}\right) w^T}$$

$$\frac{\partial L}{\partial x_{n,d}} = \sum_m \frac{\partial L}{\partial y_{n,m}} \frac{\partial y_{n,m}}{\partial x_{n,d}} = \sum_m \frac{\partial L}{\partial y_{n,m}} w_{d,m}$$

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dL/dy: [N×M]

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By similar logic:

[N×D] [N×M] [M×D]

$$\frac{\partial L}{\partial x} = \left(\frac{\partial L}{\partial y}\right) w^T$$

[D×M] [D×N] [N×M]

$$\frac{\partial L}{\partial w} = x^T \left(\frac{\partial L}{\partial y}\right)$$

These formulas are easy to remember: they are the only way to make shapes match up!