Backpropagation

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Fall 2021, Northeastern University

Recap

Batch Gradient Descent

$$L(W) = \frac{1}{N}\sum_{i=1}^{N} L_i(x_i, y_i, W) + \lambda R(W)$$

Problem: Full sum is expensive when N is large!

$$\nabla_W L(W) = \frac{1}{\boldsymbol{B}}\sum_{i=1}^{\boldsymbol{B}} \nabla_W L_i(x_i, y_i, W) + \lambda \nabla_W R(W)$$

Solution: Approximate sum using a **minibatch** of examples, e.g. *B*=32

Slide credit: D Fouhey & J Johnson

Stochastic Gradient Descent (SGD)

$$L(W) = \frac{1}{N}\sum_{i=1}^{N} L_i(x_i, y_i, W) + \lambda R(W)$$

Problem: Full sum is expensive when N is large!

$$\nabla_W L(W) = \frac{1}{\boldsymbol{B}}\sum_{i=1}^{\boldsymbol{B}} \nabla_W L_i(x_i, y_i, W) + \lambda \nabla_W R(W)$$

Solution: Approximate sum using a **minibatch** of examples, e.g. *B*=32

```
# Stochastic gradient descent
w = initialize_weights()
for t in range(num_steps):
  minibatch = sample_data(data, batch_size)
  dw = compute_gradient(loss_fn, minibatch, w)
  w -= learning_rate * dw
```

Hyperparameters:

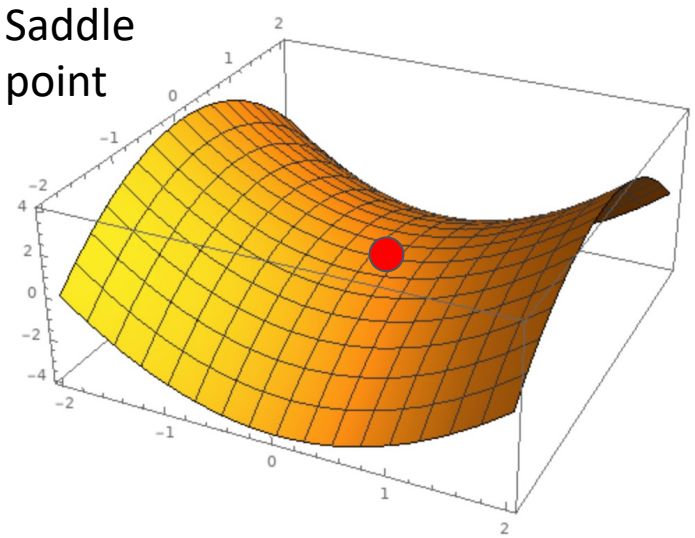
- Weight initialization
- Number of steps
- Learning rate
- Batch size
- Data sampling

Slide credit: D Fouhey & J Johnson

Problems with SGD

What if the loss function has a **local minimum** or **saddle point**?

Gradient is zero,
SGD gets stuck



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Problems with SGD

Our gradients come from minibatches so they can be noisy!

$$L(W) = \frac{1}{N}\sum_{i=1}^{N} L_i(x_i, y_i, W) + \lambda R(W)$$

Slide credit: D Fouhey & J Johnson

SGD

SGD

$$x_{t+1} = x_t - \alpha \nabla f(x_t)$$

```
for t in range(num_steps):
  dw = compute_gradient(w)
  w -= learning_rate * dw
```

Sutskever et al, “On the importance of initialization and momentum in deep learning”, ICML 2013

Slide credit: D Fouhey & J Johnson

SGD + Momentum

SGD

$$x_{t+1} = x_t - \alpha \nabla f(x_t)$$

```
for t in range(num_steps):
  dw = compute_gradient(w)
  w -= learning_rate * dw
```

SGD + Momentum

$$v_{t+1} = \rho v_t + \nabla f(x_t)$$
$$x_{t+1} = x_t - \alpha v_{t+1}$$

```
v = 0
for t in range(num_steps):
  dw = compute_gradient(w)
  v = rho * v + dw
  w -= learning_rate * v
```

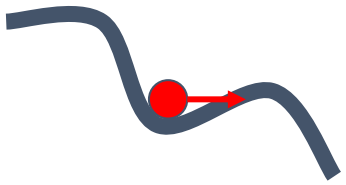
- Build up “velocity” as a running mean of gradients
- Rho gives “friction”; typically $\rho = 0.9$ or 0.99

Sutskever et al, “On the importance of initialization and momentum in deep learning”, ICML 2013

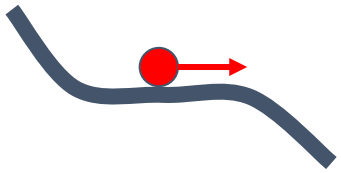
Slide credit: D Fouhey & J Johnson

SGD + Momentum

Local Minima



Saddle points



Gradient Noise

SGD SGD+Momentum

Sutskever et al, “On the importance of initialization and momentum in deep learning”, ICML 2013

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Optimizing Everything

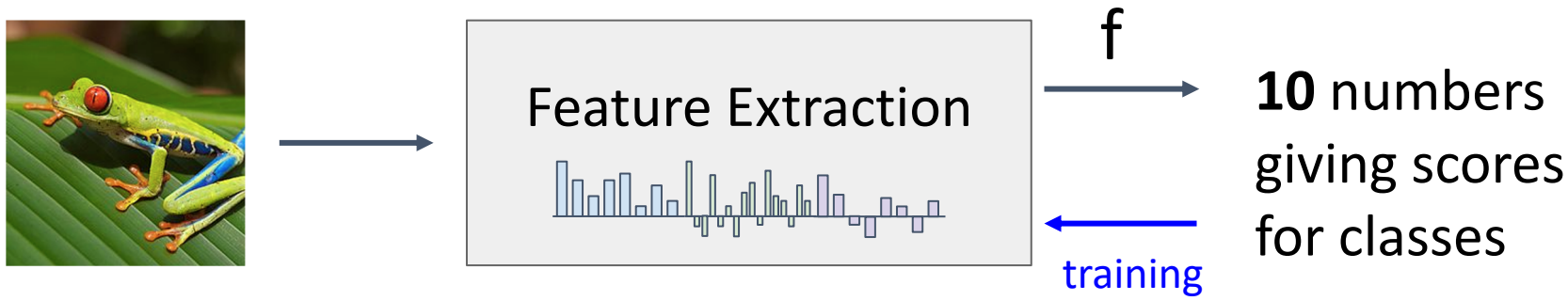
$$L(\boldsymbol{W}) = \boldsymbol{\lambda}\|\boldsymbol{W}\|_{\boldsymbol{2}}^{\boldsymbol{2}} + \sum_{i=1}^{n} -\log\left(\frac{\exp((Wx)_{y_i})}{\sum_k \exp((Wx)_k))}\right)$$

$$L(\boldsymbol{w}) = \lambda\|\boldsymbol{w}\|_2^2 + \sum_{i=1}^{n}\left(y_i - \boldsymbol{w}^{\boldsymbol{T}}\boldsymbol{x}_{\boldsymbol{i}}\right)^2$$

- (Automatically) Optimize **w** on training set with SGD to maximize training accuracy
- (Manually) Optimize λ with random/grid search to maximize validation accuracy

Slide credit: D Fouhey & J Johnson

Image Features vs Neural Networks

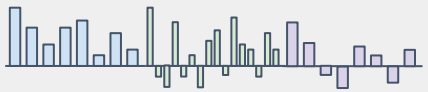


Krizhevsky, Sutskever, and Hinton, "Imagenet classification with deep convolutional neural networks", NIPS 2012

Slide credit: D Fouhey & J Johnson

Image Features vs Neural Networks

Feature Extraction



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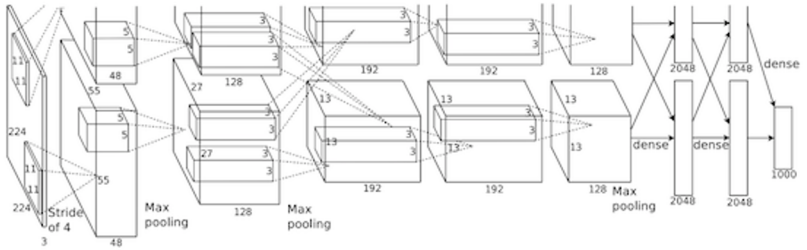
10 numbers giving scores for classes

training

Deep Neural Network



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Neural Networks

Input image: $x \in \mathbb{R}^D$

Category scores: $s \in \mathbb{R}^C$

Linear Classifier:

$$s = Wx$$

$$W \in \mathbb{R}^{C \times D}$$

In practice we add a learnable bias
+b after each matrix multiply

Slide credit: D Fouhey & J Johnson

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Linear Classifier:

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2-layer Neural Net:

$$s = \mathrm{W}_2 \max(0, W_1 x)$$

$$W_1 \in \mathbb{R}^{H \times D}$$

$$W_2 \in \mathbb{R}^{C \times H}$$

In practice we add a learnable bias
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$$W_1 \in \mathbb{R}^{H \times D}$$

$$W_2 \in \mathbb{R}^{C \times H}$$

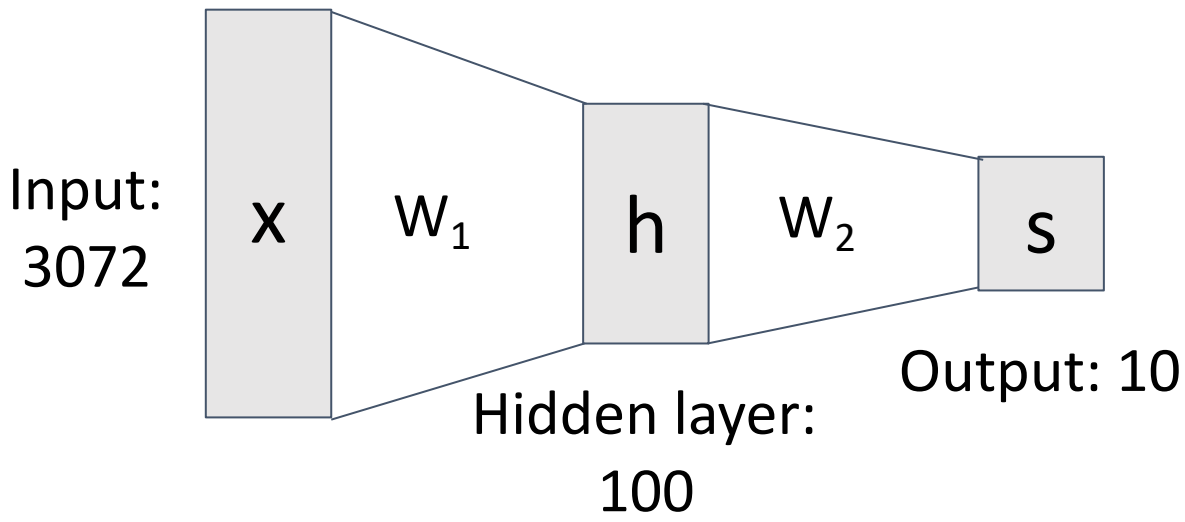
3-layer Neural Net:

$$s = \mathrm{W}_3 \max(0, W_2 \max(0, W_1 x))$$

Slide credit: D Fouhey & J Johnson

Neural Networks

Two-Layer Neural Network: $s = \mathrm{W}_2 \max(0, W_1 x)$



$$x \in \mathbb{R}^D, W_1 \in \mathbb{R}^{H \times D}, W_2 \in \mathbb{R}^{C \times H}$$

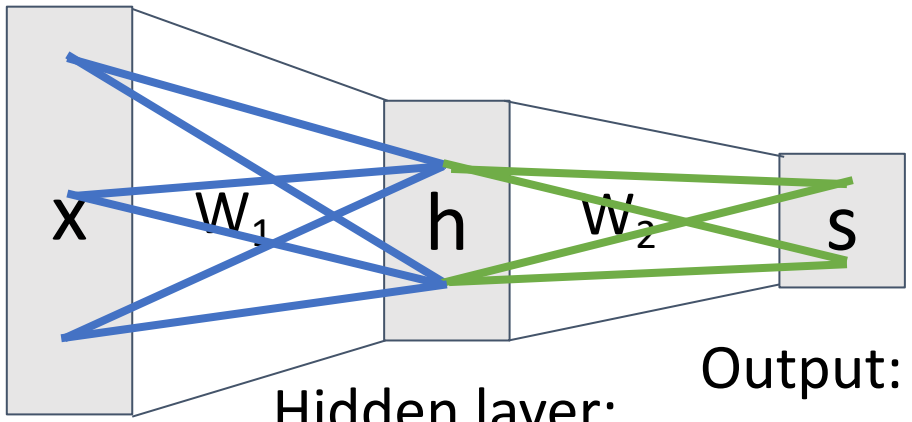
Slide credit: D Fouhey & J Johnson

Neural Networks

Two-Layer Neural Network: $s = W_2 \max(0, W_1 x)$

Element (i, j) of W_1 gives the effect on h_i from x_j

Element (i, j) of W_2 gives the effect on s_i from h_j



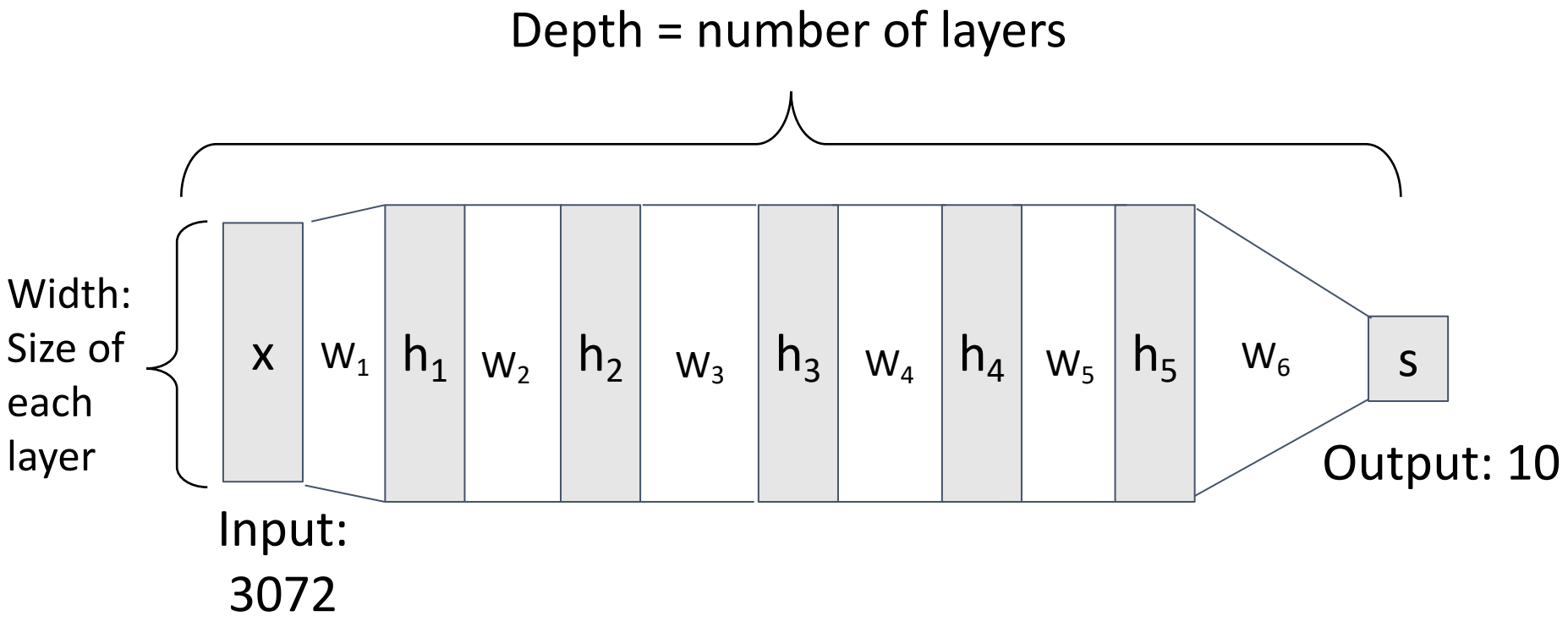
All elements of x affect all elements of h

All elements of h affect all elements of s

"Fully-Connected" neural network
Also "Multi-Layer Perceptron" (MLP)

Slide credit: D Fouhey & J Johnson

Deep Neural Networks



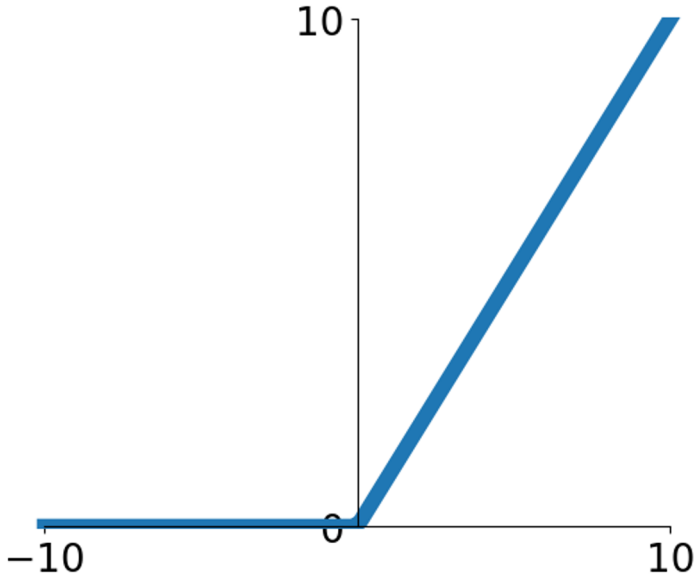
$$s = W_6 \max(0, W_5 \max(0, W_4 \max(0, W_3 \max(0, W_2 \max(0, W_1 x)))))$$

Slide credit: D Fouhey & J Johnson

Activation Functions

2-layer Neural Network

The function $ReLU(z) = \max(0, z)$ is called "Rectified Linear Unit"



$$s = W_2 \max(0, W_1 x)$$

This is called the **activation function** of the neural network

Slide credit: D Fouhey & J Johnson

Activation Functions

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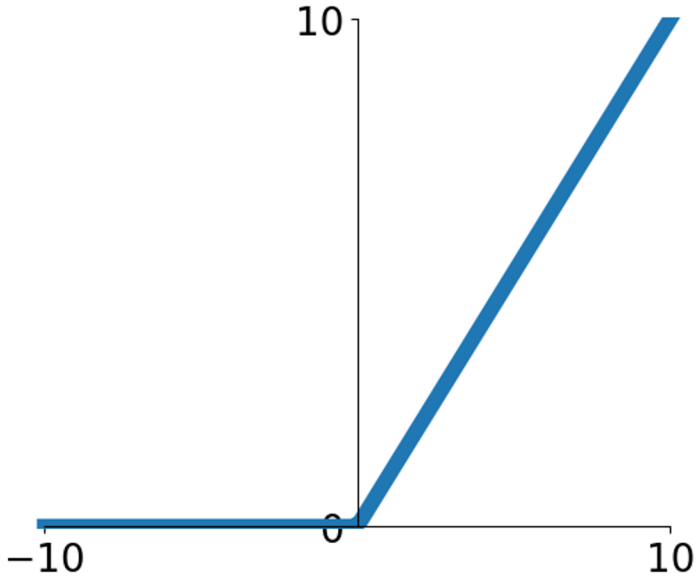

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Q: What happens if we build a neural network with no activation function?

$$s = W_2 W_1 x$$

Slide credit: D Fouhey & J Johnson

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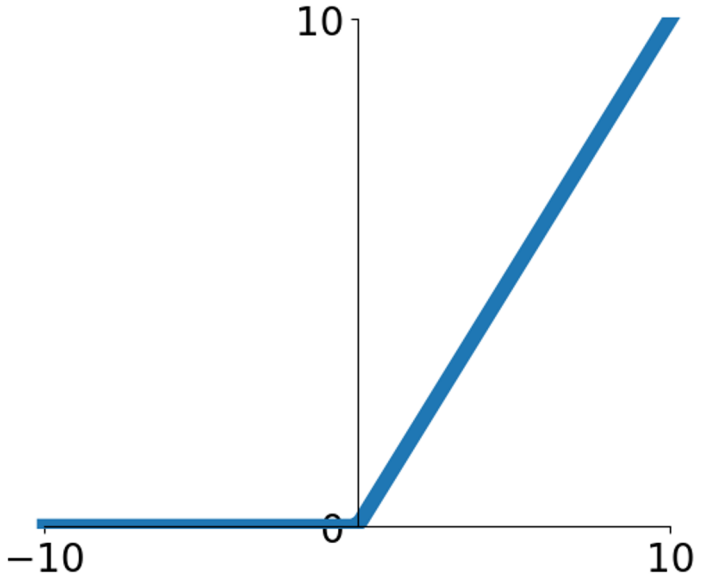


$$s = W_2 \max(0, W_1 x)$$

This is called the **activation function** of the neural network

Q: What happens if we build a neural network with no activation function?

$$s = W_2 W_1 x$$

A: We get a linear classifier!

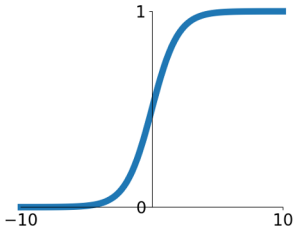
$$W_3 = W_2 W_1 \in \mathbb{R}^{C \times D}$$
$$s = W_3 x$$

Slide credit: D Fouhey & J Johnson

Activation Functions

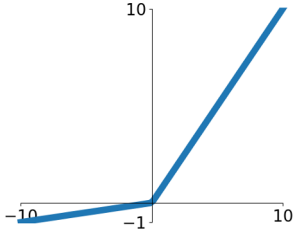
Sigmoid

$$\sigma(x) = \frac{1}{1+e^{-x}}$$



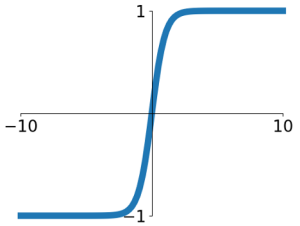
Leaky ReLU

$$\max(0.1x, x)$$



tanh

$$\tanh(x)$$

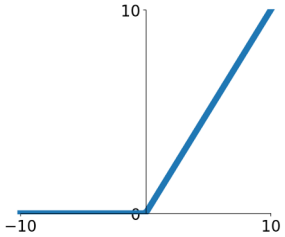


Maxout

$$\max(w_1^T x + b_1, w_2^T x + b_2)$$

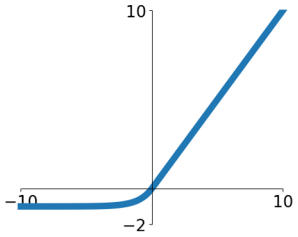
ReLU

$$\max(0, x)$$



ELU

$$\begin{cases} x & x \geq 0 \\ \alpha(e^x - 1) & x < 0 \end{cases}$$



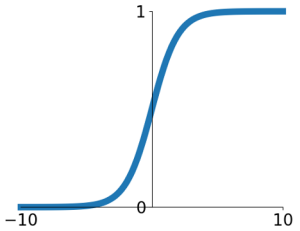
Slide credit: D Fouhey & J Johnson

Activation Functions

ReLU is a good default choice

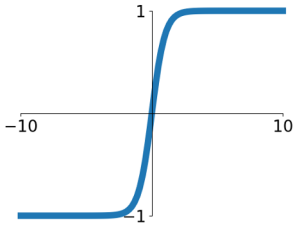
Sigmoid

$$\sigma(x) = \frac{1}{1+e^{-x}}$$



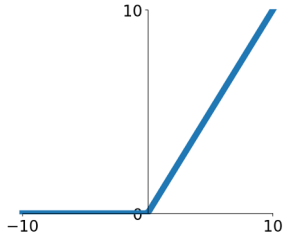
tanh

$$\tanh(x)$$



ReLU

$$\max(0, x)$$



Leaky ReLU

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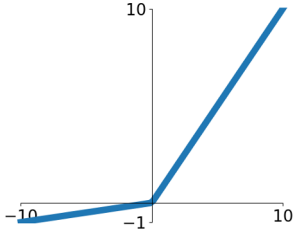
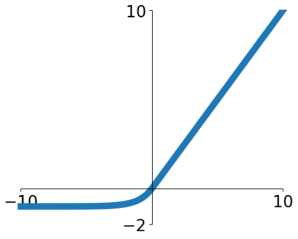


Maxout

$$\max(w_1^T x + b_1, w_2^T x + b_2)$$

ELU

$$\begin{cases} x & x \geq 0 \\ \alpha(e^x - 1) & x < 0 \end{cases}$$



Slide credit: D Fouhey & J Johnson

Today's class

Backpropagation: how to compute gradients and optimize parameters of neural networks

Problem: How to compute gradients?

$$s = W_2 \max(0, W_1 x) + b_2$$ Nonlinear score function

$$L_i = \sum_{j \neq y_i} \max\left(0, s_j - s_{y_i} + 1\right)$$ Per-element data loss

$$R(W) = \sum_k W_k^2$$ L2 Regularization

$$L(W_1, W_2) = \frac{1}{N} \sum_{i=1}^{N} L_i + \lambda R(W_1) + \lambda R(W_2)$$ Total loss

What do we need to optimize with SGD?

Compute $\frac{\partial L}{\partial W_1}, \frac{\partial L}{\partial W_2}$

Slide credit: D Fouhey & J Johnson

(Bad) Idea: Derive $\nabla_W L$ on paper

$$s = f(x; W) = Wx$$

$$L_i = \sum_{j \neq y_i} \max(0, s_j - s_{y_i} + 1)$$

$$= \sum_{j \neq y_i} \max(0, W_{j,:} \cdot x + W_{y_i,:} \cdot x + 1)$$

$$L = \frac{1}{N} \sum_{i=1}^{N} L_i + \lambda \sum_k W_k^2$$

$$= \frac{1}{N} \sum_{i=1}^{N} \sum_{j \neq y_i} \max(0, W_{j,:} \cdot x + W_{y_i,:} \cdot x + 1) + \lambda \sum_k W_k^2$$

$$\nabla_W L = \nabla_W \left(\frac{1}{N} \sum_{i=1}^{N} \sum_{j \neq y_i} \max(0, W_{j,:} \cdot x + W_{y_i,:} \cdot x + 1) + \lambda \sum_k W_k^2 \right)$$

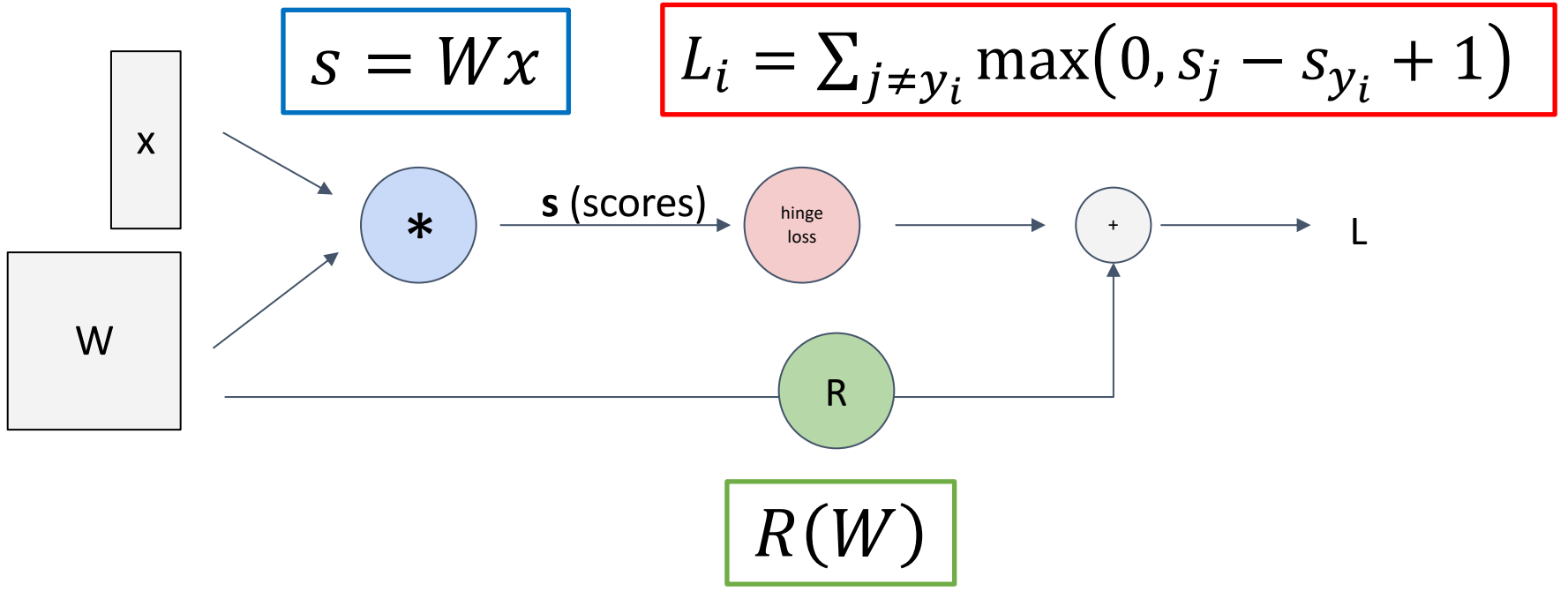
Problem: Very tedious: Lots of matrix calculus, need lots of paper

Problem: What if we want to change loss? E.g. use softmax instead of SVM? Need to re-derive from scratch. Not modular!

Problem: Not feasible for very complex models!

Slide credit: D Fouhey & J Johnson

Better Idea: **Computational Graphs**



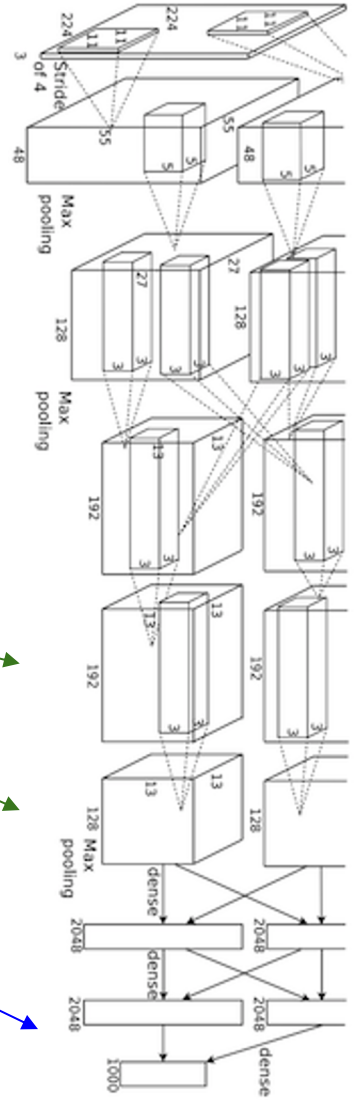
Slide credit: D Fouhey & J Johnson

Deep Network (AlexNet)

input image

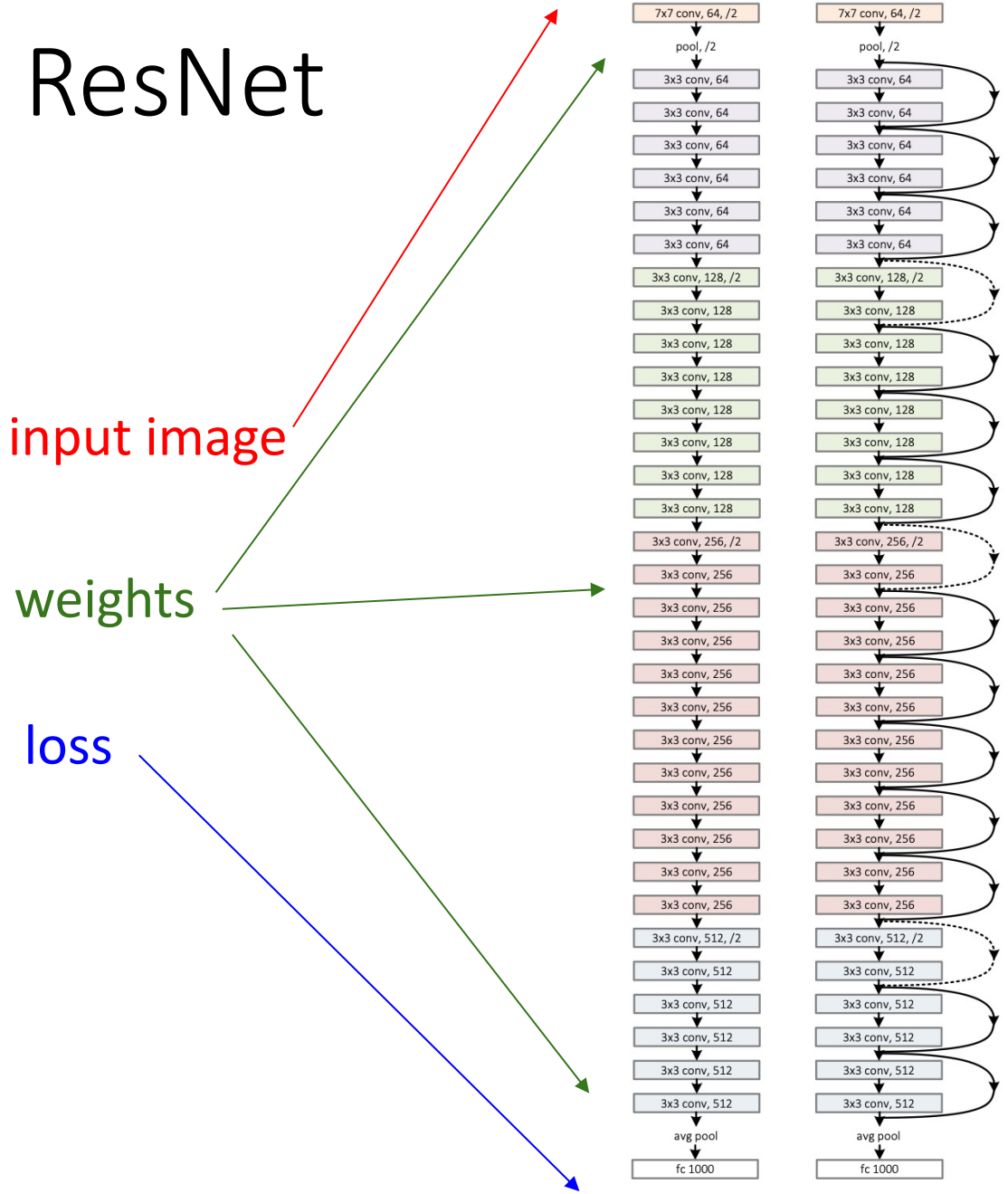
weights

loss



Slide credit: D Fouhey & J Johnson

VGG and ResNet



He et al, CVPR 2016

Overview of where we're going

- We want to **evaluate** the gradient of a Loss function L(x,W,...), with respect to the parameters (weights) of a neural network, at the "point" represented by the arguments to the function (x,W,...).
  - We are **not interested** in an **algebraic expression** for the gradient
  - but rather only in the **evaluation of that gradient at the current value of the function** arguments.

Slide credit: E Learned-Miller

Consider the function

$$z(x, y) = x^2 + y^2,$$

and suppose we are interested in evaluating the gradient of this function at the point

$$(x, y) = (5, 3).$$

Evaluate the gradient:

$$\frac{\partial z}{\partial x} = 2x.$$

$$\frac{\partial z}{\partial y} = 2y.$$

The algebraic expression of the gradient is just the collection of these partials into a "vector":

$$\nabla z = \begin{bmatrix} 2x \\ 2y \end{bmatrix}.$$

Don't care about this

The evaluation of this gradient at the point $(x, y) = (5, 3)$ is simply

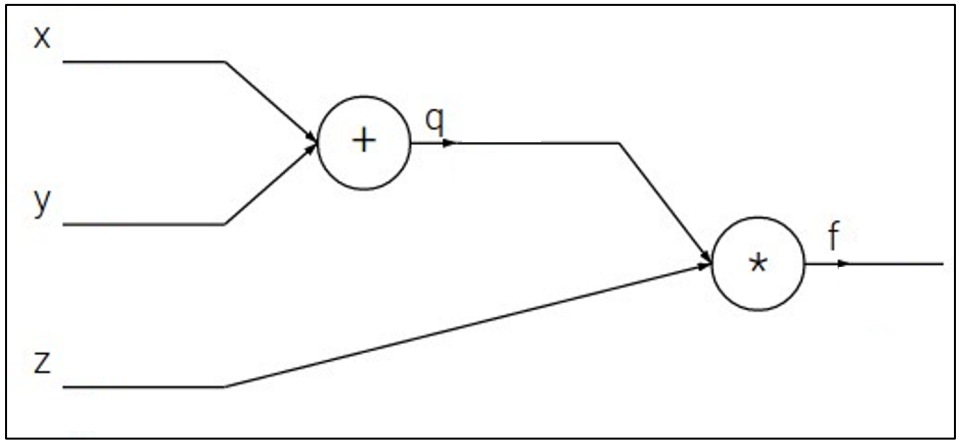
$$\nabla z(5, 3) = \begin{bmatrix} 2 \times 5 \\ 2 \times 3 \end{bmatrix} = \begin{bmatrix} 10 \\ 6 \end{bmatrix}.$$

Do care about this

Slide credit: E Learned-Miller

Backpropagation: Simple Example

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

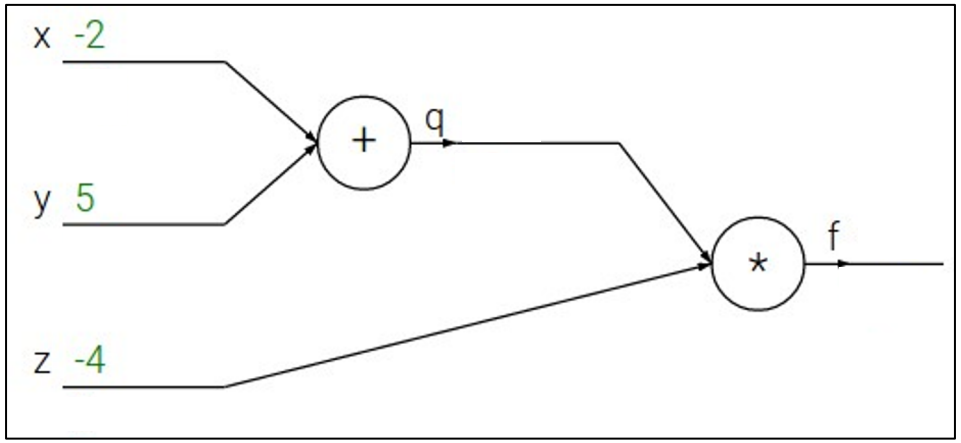


Slide credit: D Fouhey & J Johnson

Backpropagation: Simple Example

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

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



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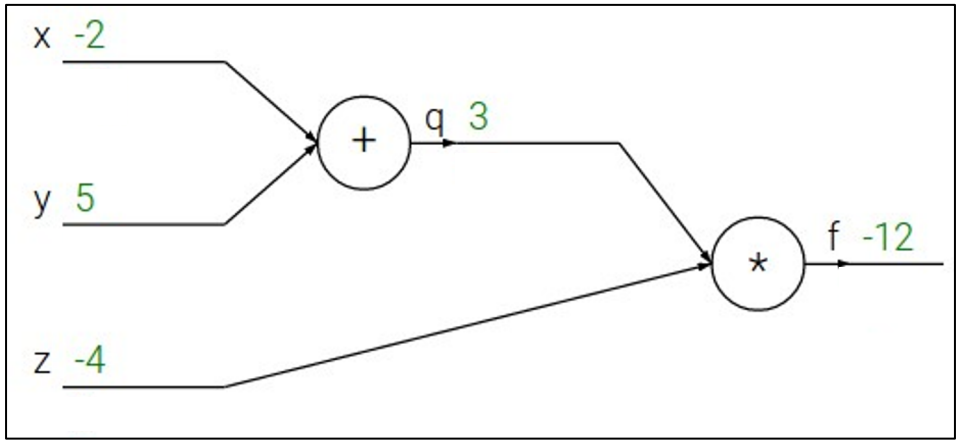


1. Forward pass: Compute outputs

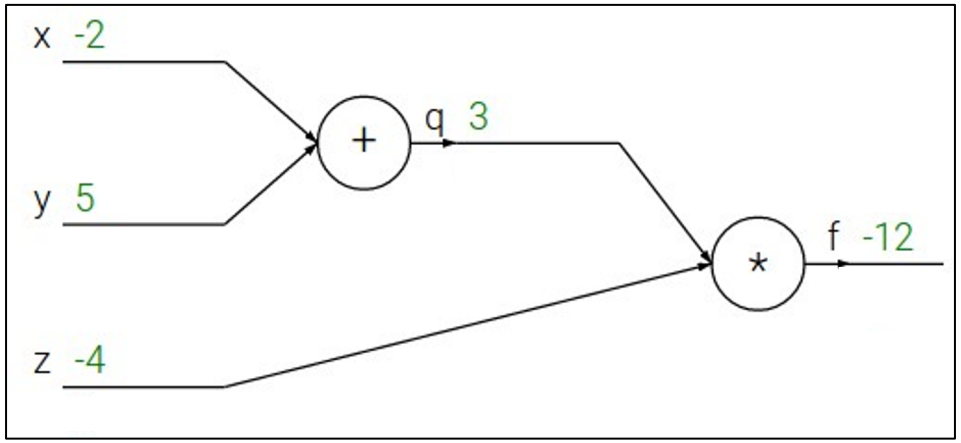
$$q = x + y \quad f = q \cdot z$$

Slide credit: D Fouhey & J Johnson

Backpropagation: Simple Example

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

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



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

Slide credit: D Fouhey & J Johnson

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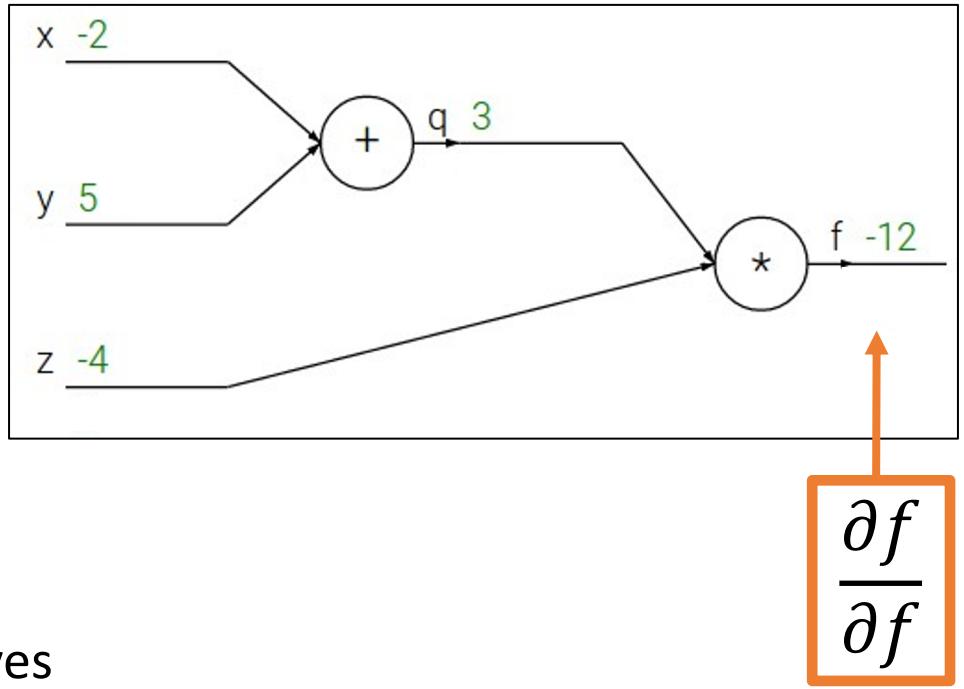

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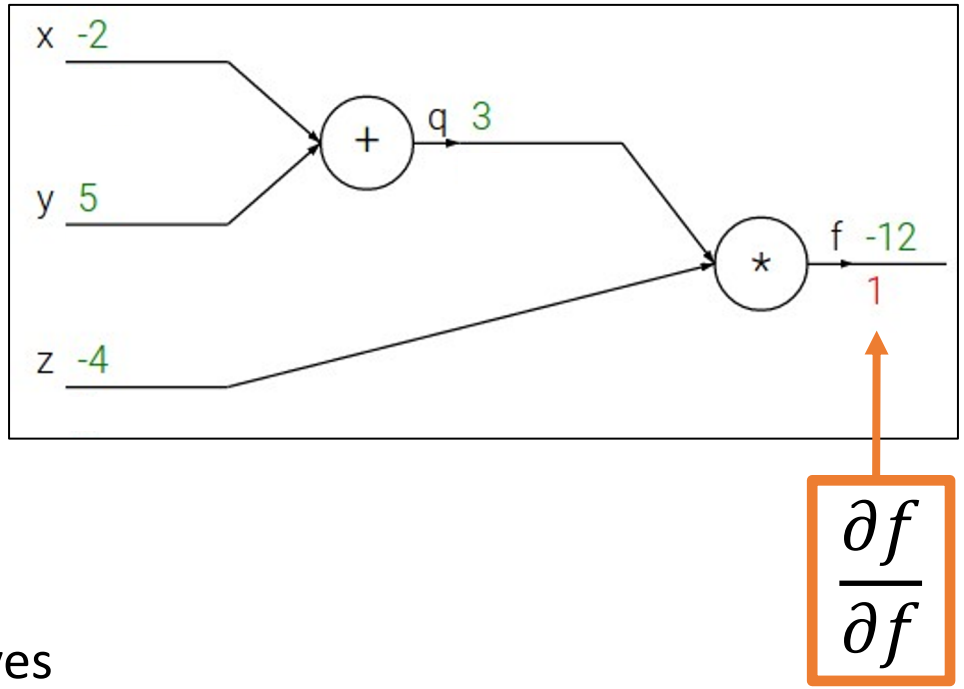

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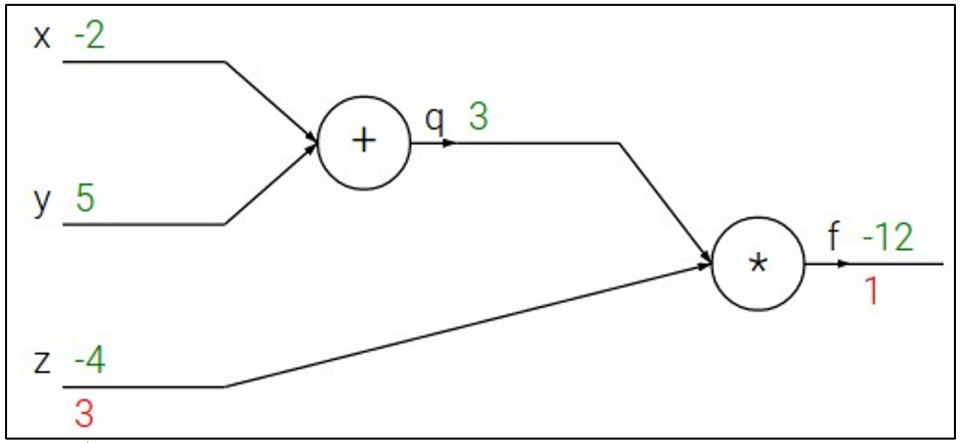

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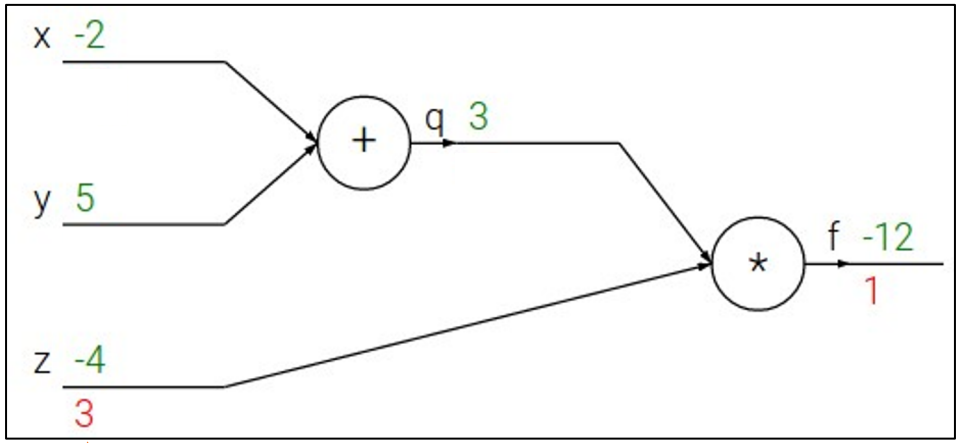

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Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$

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

Slide credit: D Fouhey & J Johnson

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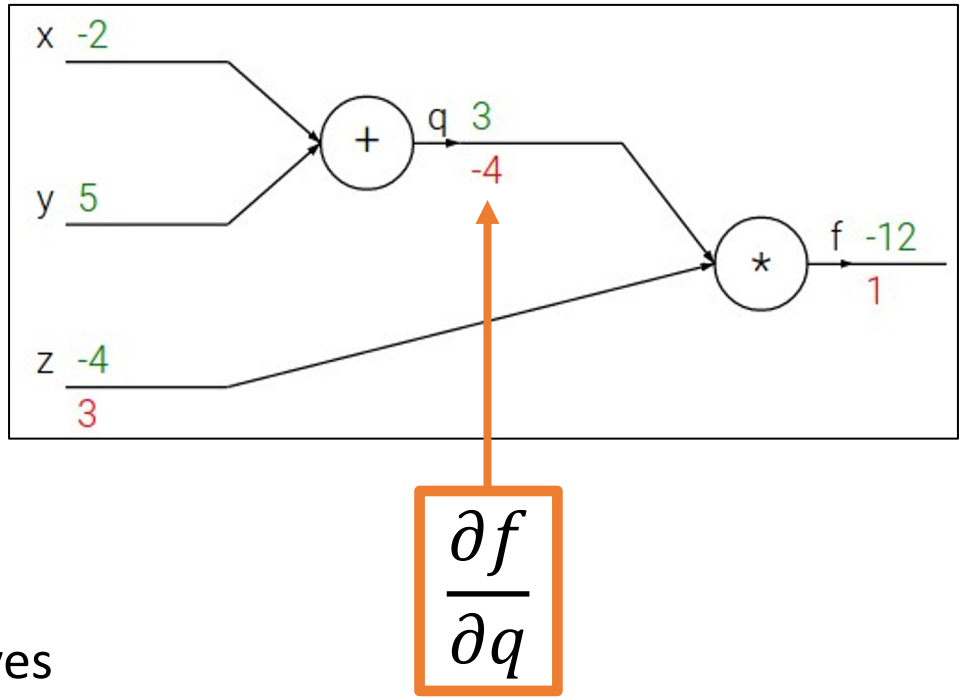

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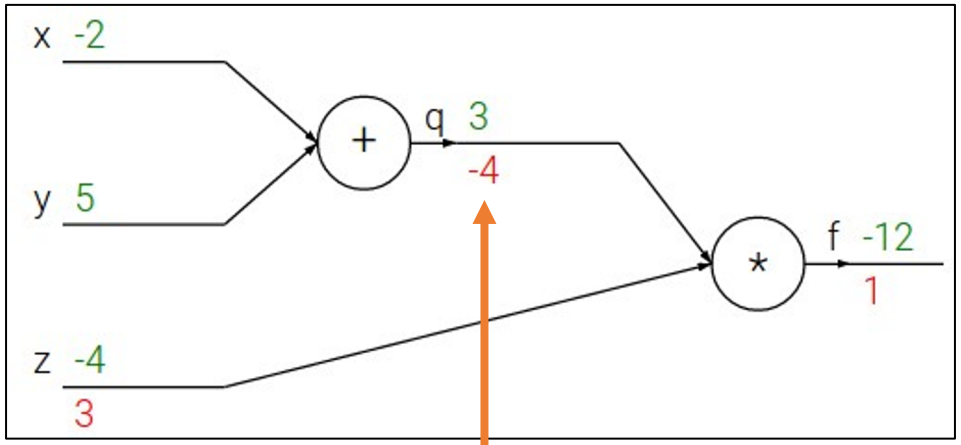

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Slide credit: D Fouhey & J Johnson

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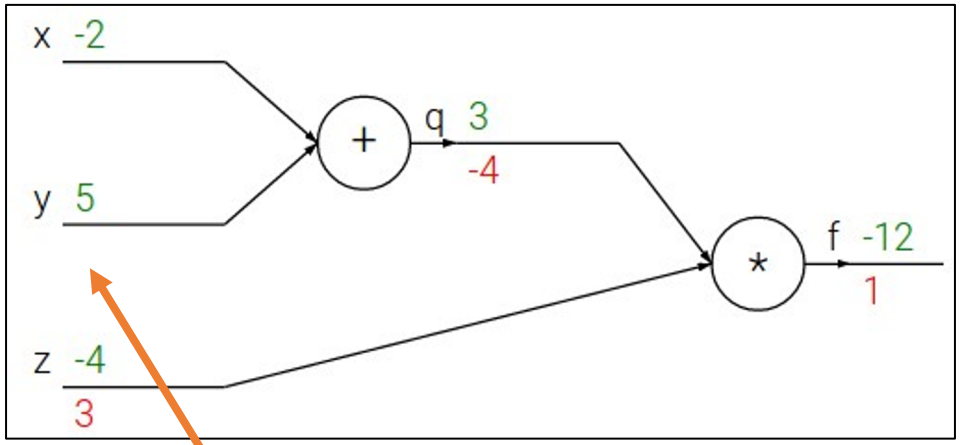

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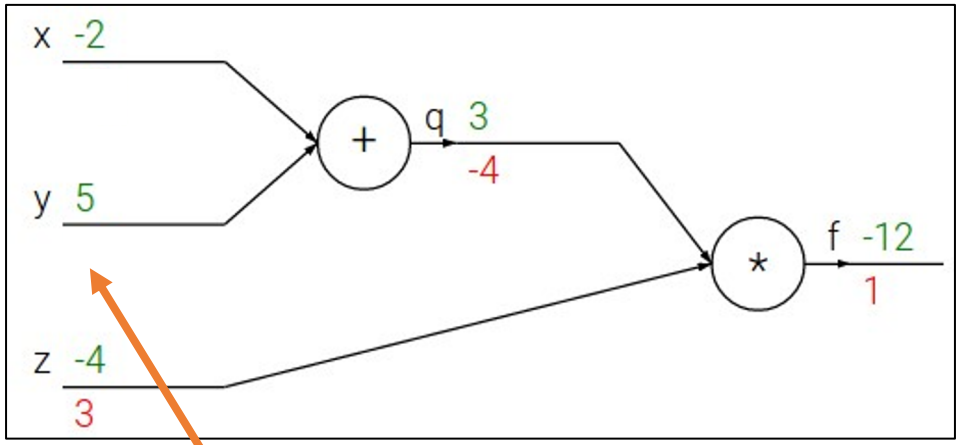

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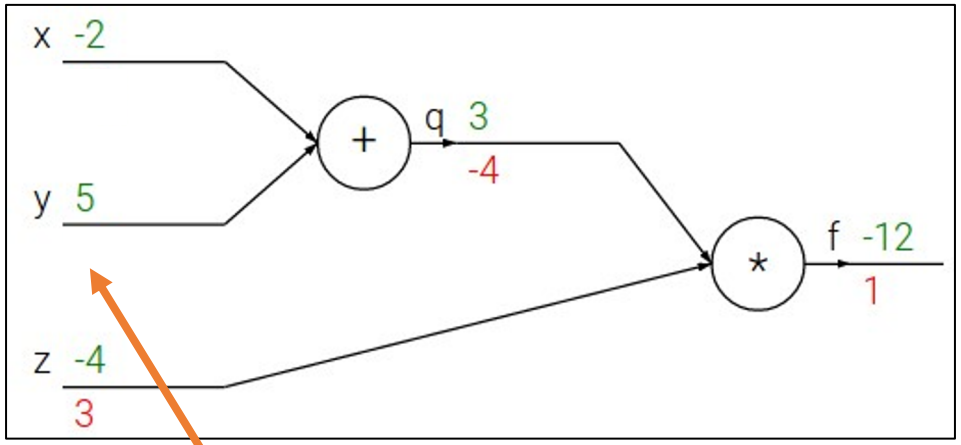

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Chain Rule

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

$$\frac{\partial q}{\partial y} = 1$$

Downstream Gradient **Local Gradient** **Upstream Gradient**

Slide credit: D Fouhey & J Johnson

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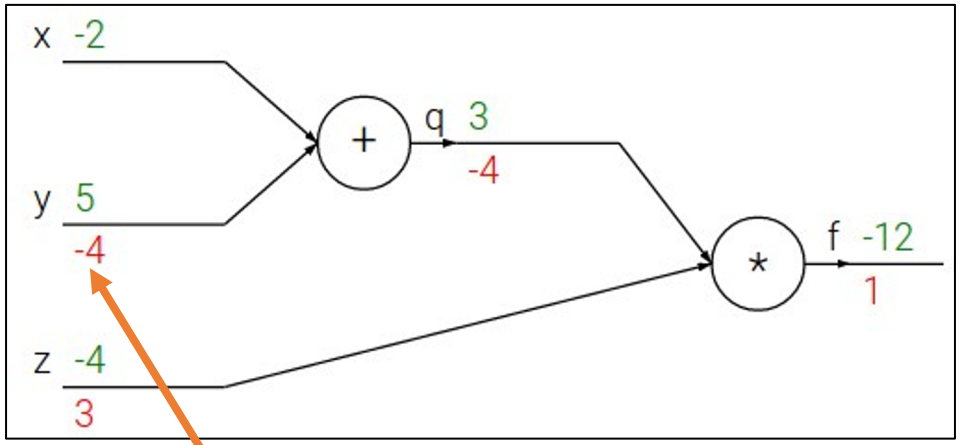

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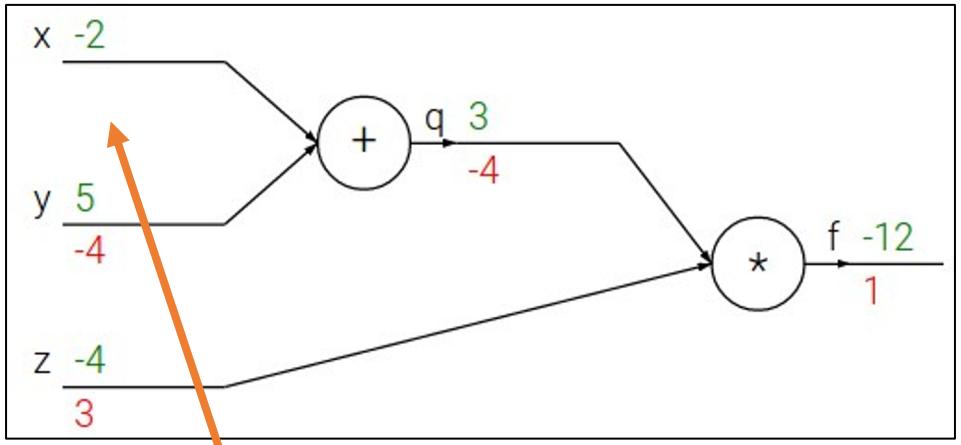

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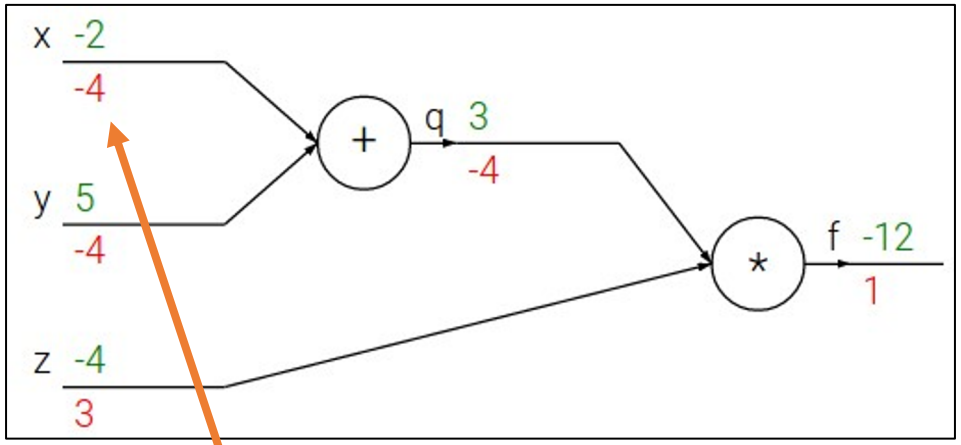

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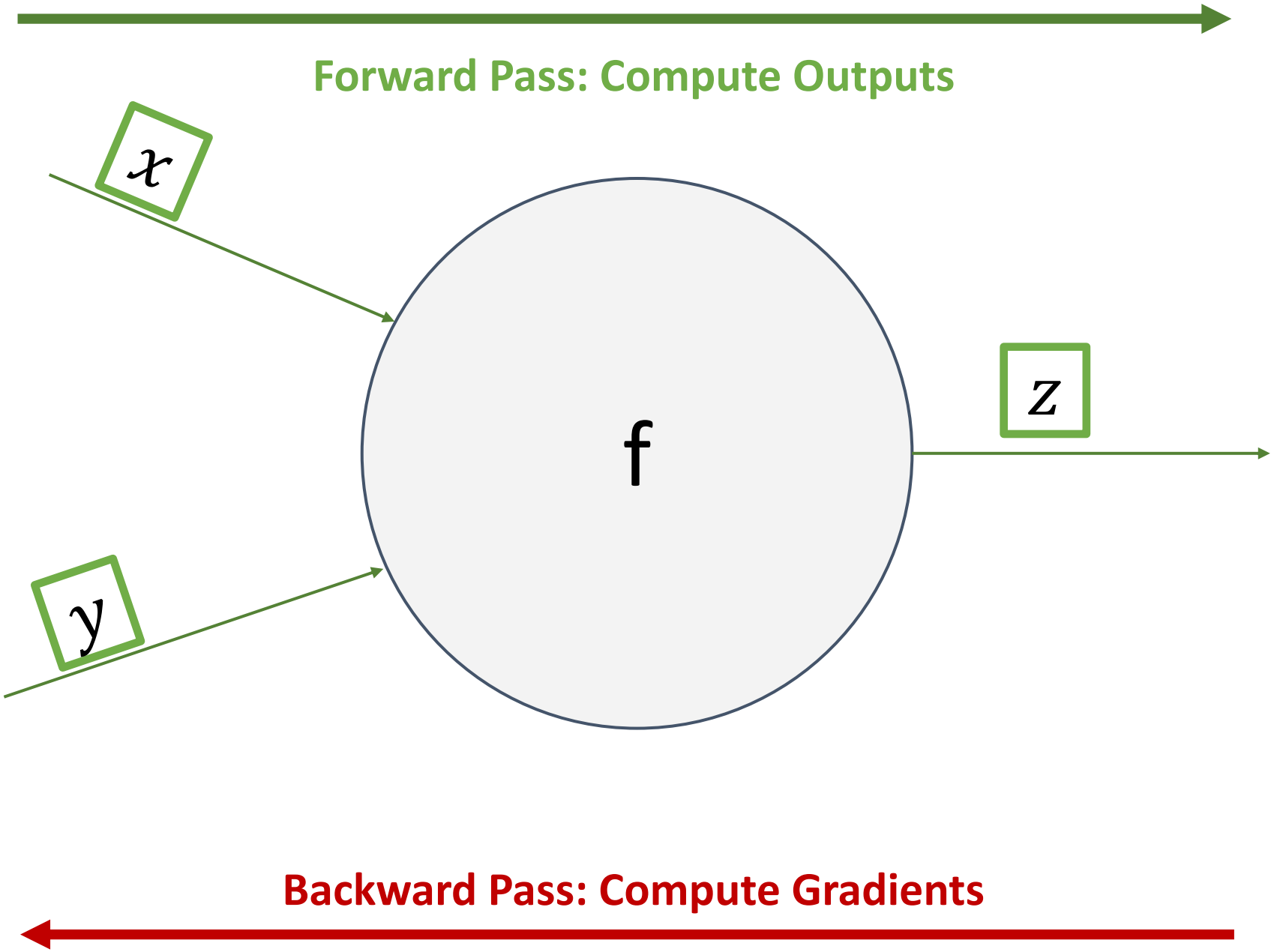

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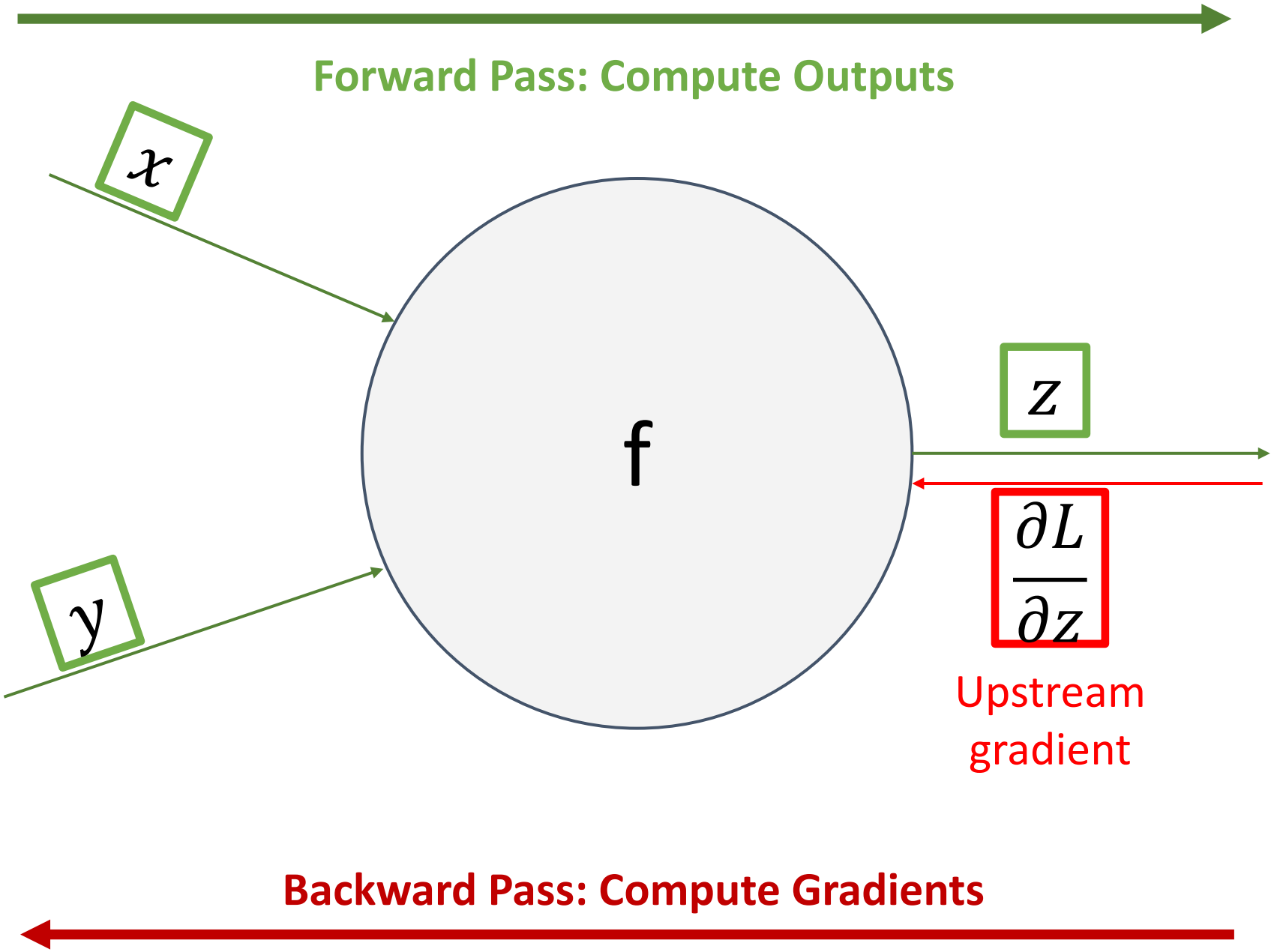

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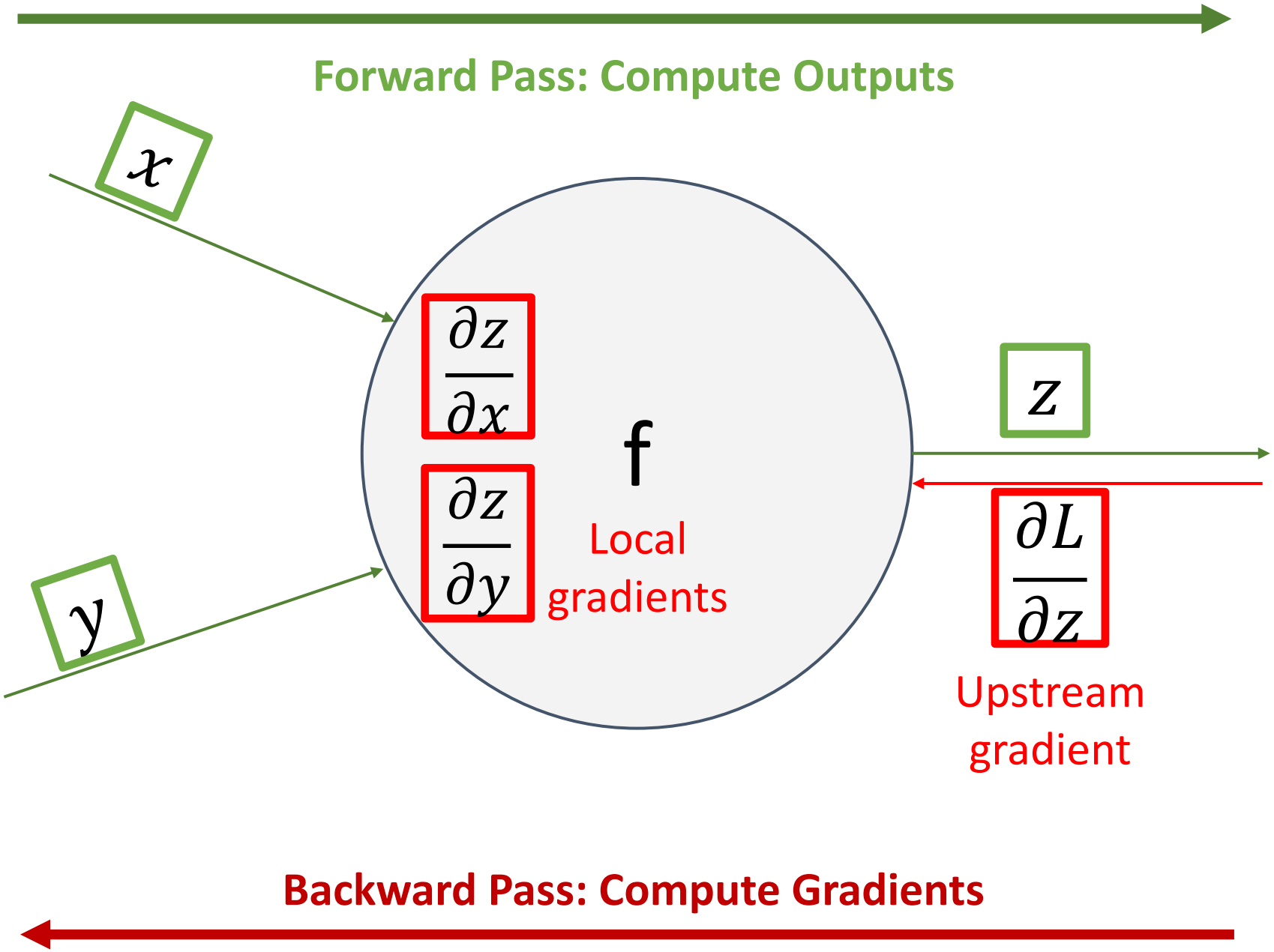

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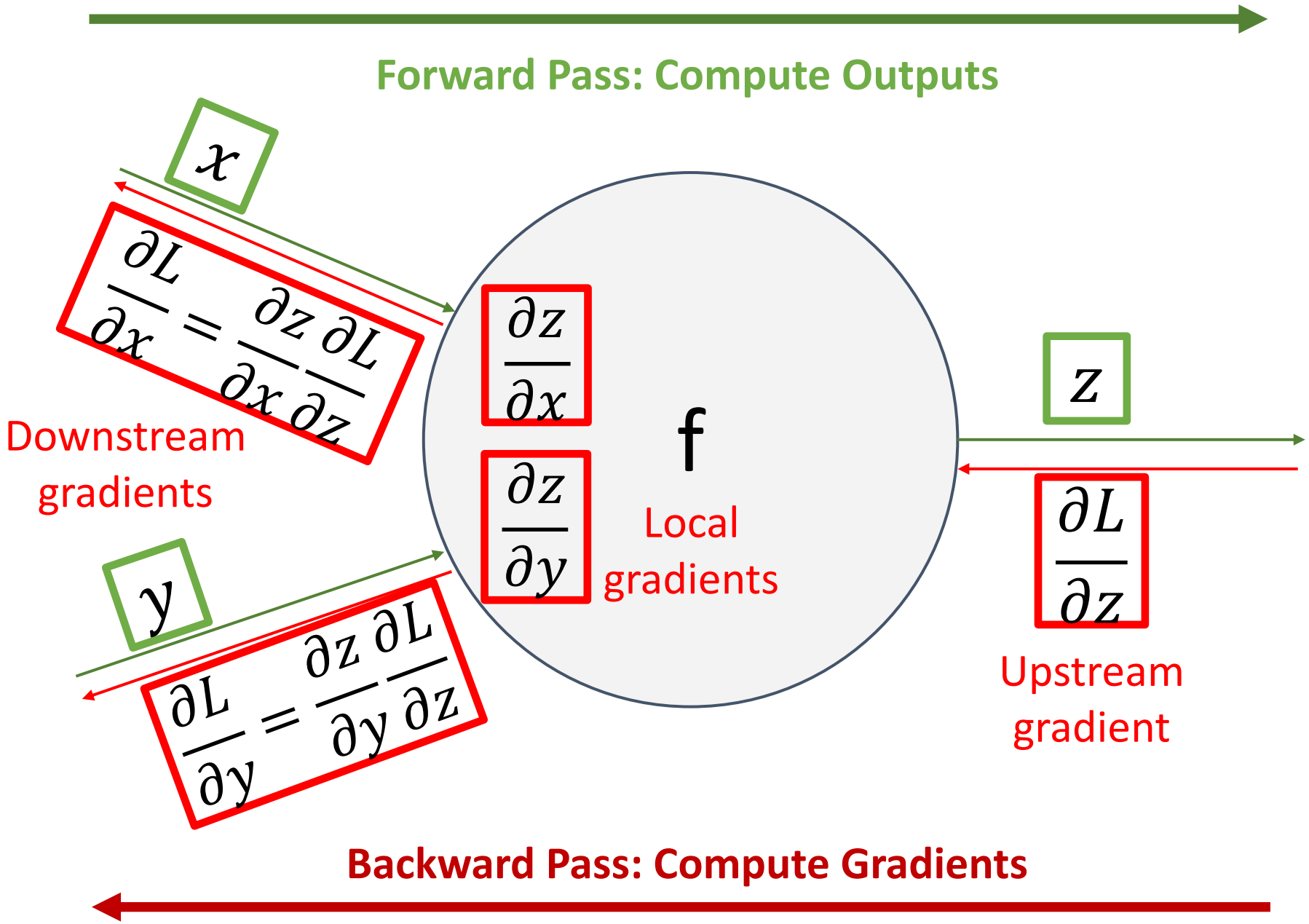

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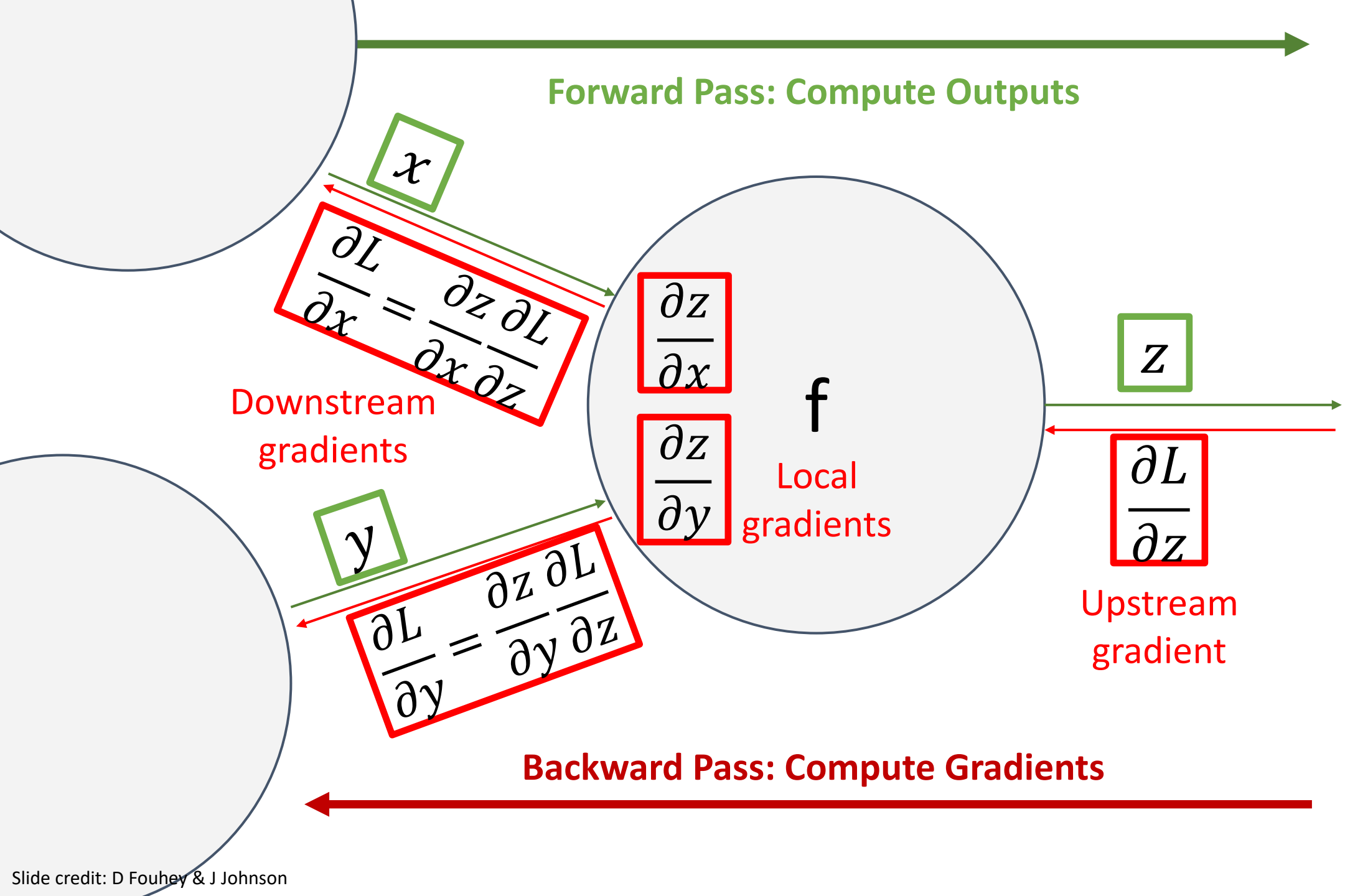
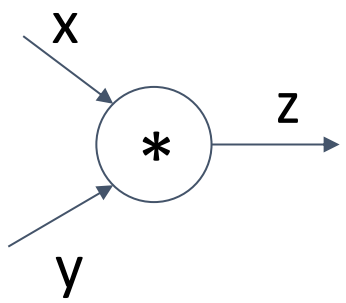


Slide credit: D Fouhey & J Johnson

Example: PyTorch Autograd Functions with Modular API



(x,y,z are scalars)

```
class Multiply(torch.autograd.Function):
  @staticmethod
  def forward(ctx, x, y):
    ctx.save_for_backward(x, y)
    z = x * y
    return z
  @staticmethod
  def backward(ctx, grad_z):
    x, y = ctx.saved_tensors
    grad_x = y * grad_z   # dz/dx * dL/dz
    grad_y = x * grad_z   # dz/dy * dL/dz
    return grad_x, grad_y
```

Need to stash some values for use in backward

Upstream gradient

Multiply upstream and local gradients

Slide credit: D Fouhey & J Johnson

Example: PyTorch operators

pytorch / pytorch

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Tree: 517c7c9861 ▾ pytorch / aten / src / THNN / generic / | Create new file | Upload files | Find file | History

ezyang and facebook-github-bot Canonicalize all includes in PyTorch. (#14849) ··· Latest commit 517c7c9 on Dec 8, 2018

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AbsCriterion.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
BCECriterion.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
ClassNLLCriterion.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
Col2Im.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
ELU.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
FeatureLPPooling.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
GatedLinearUnit.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
HardTanh.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
Im2Col.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
IndexLinear.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
LeakyReLU.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
LogSigmoid.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
MSECriterion.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
MultiLabelMarginCriterion.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
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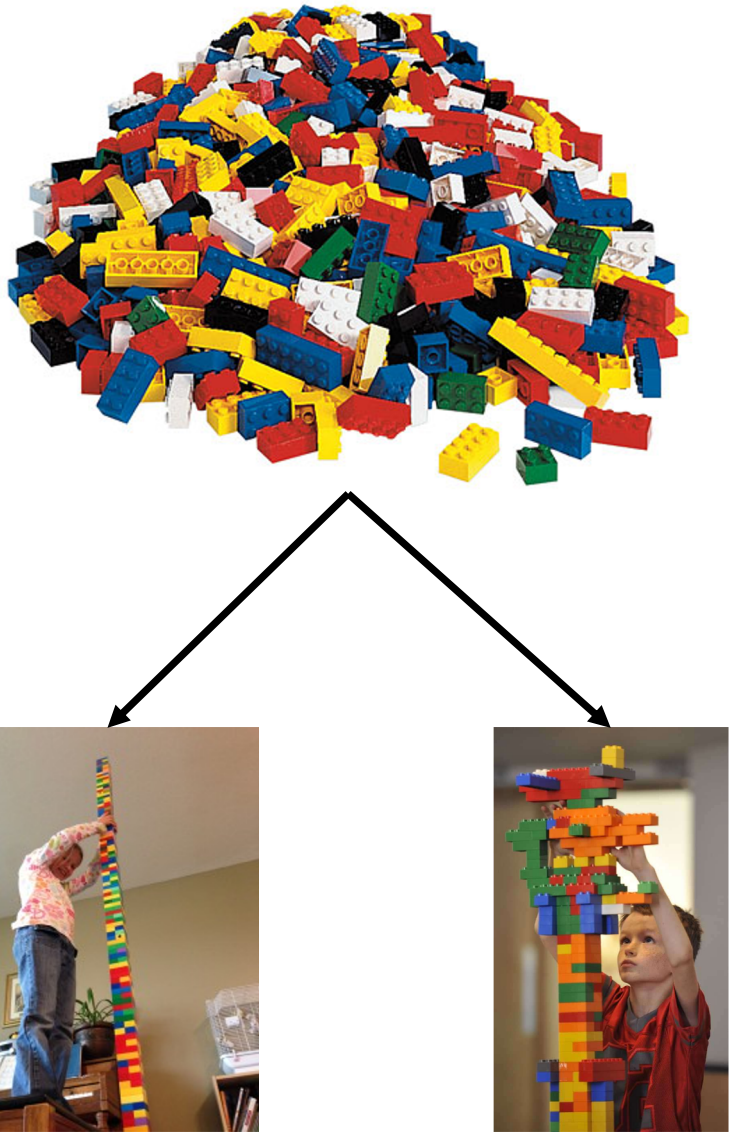
RReLU.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago



Slide credit: D Fouhey & J Johnson, E Learned-Miller

Building NNs using PyTorch with AutoGrad

```python
import torch.nn as nn

class MLP(nn.Module):
    def __init__(self, input_dim, output_dim, hidden_dim):
        super(MLP, self).__init__()

        # hidden layer
        self.h_mult = nn.Linear(input_dim, hidden_dim)
        self.h_relu = nn.ReLU()

        # output layer
        self.out = nn.Linear(hidden_dim, output_dim)

    def forward(self, x):
        h = self.h_mult(x)
        h = self.h_relu(h)
        y = self.out(h)
        return y
```

So far: Backprop with scalars

What about vector-valued functions?

Slide credit: D Fouhey & J Johnson

Vector Derivatives

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

Regular derivative:

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

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

Slide credit: D Fouhey & J Johnson

Vector Derivatives

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

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

Derivative is **Gradient**:

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

$$\left(\frac{\partial y}{\partial x}\right)_i = \frac{\partial y}{\partial x_i}$$

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

Slide credit: D Fouhey & J Johnson

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

Derivative is **Jacobian**:

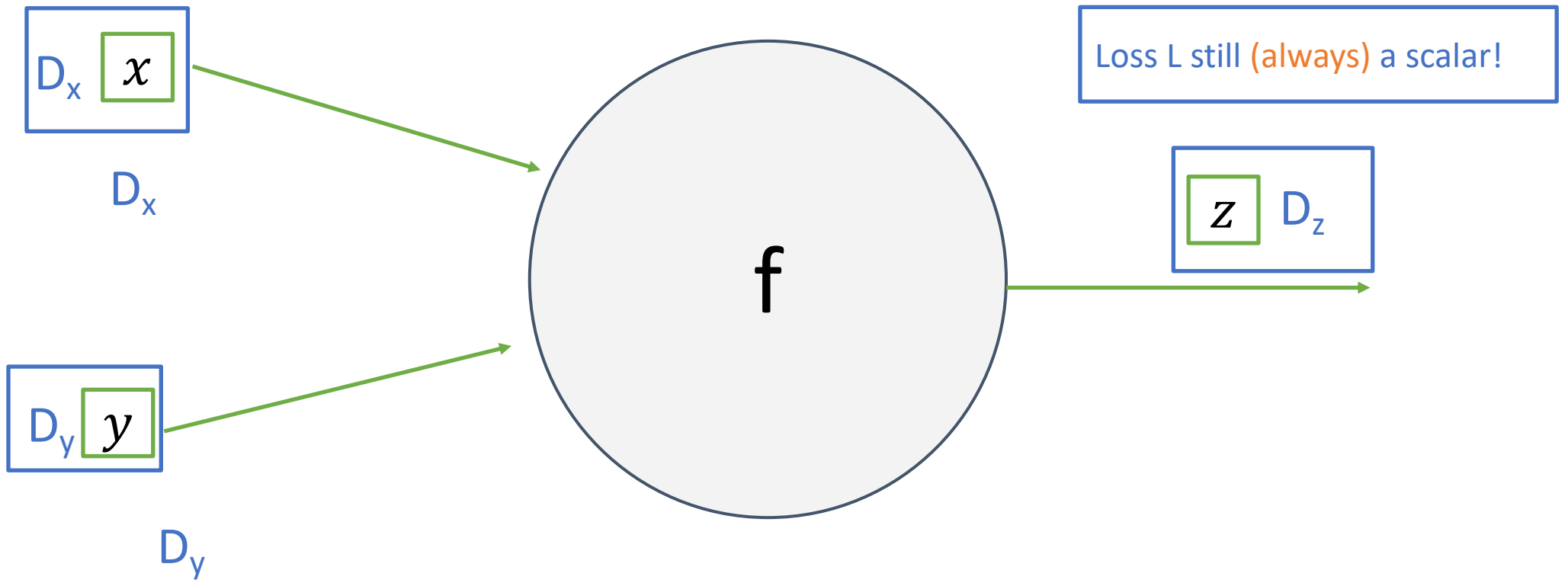
$$\frac{\partial y}{\partial x} \in \mathbb{R}^{N \times M}$$

$$\left(\frac{\partial y}{\partial x}\right)_{i,j} = \frac{\partial y_j}{\partial x_i}$$

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

Slide credit: D Fouhey & J Johnson

Backprop with Vectors



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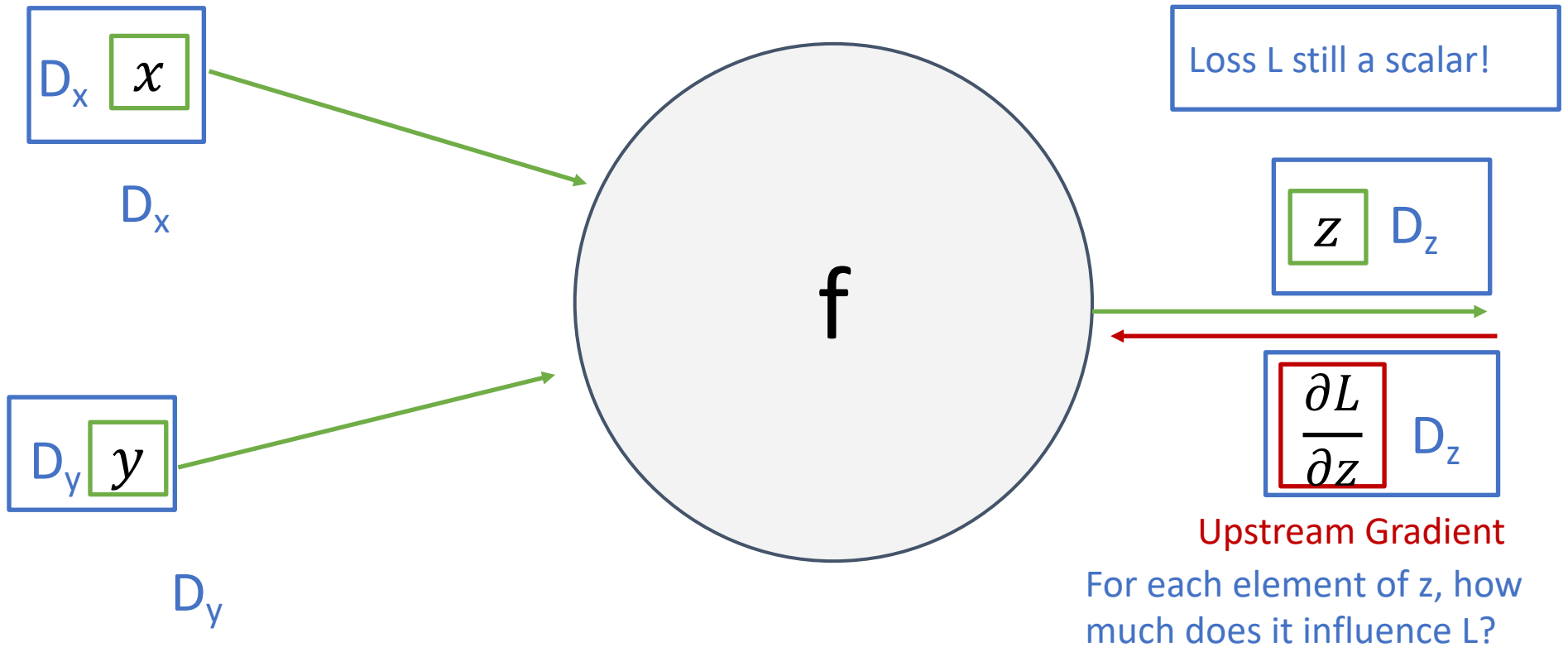

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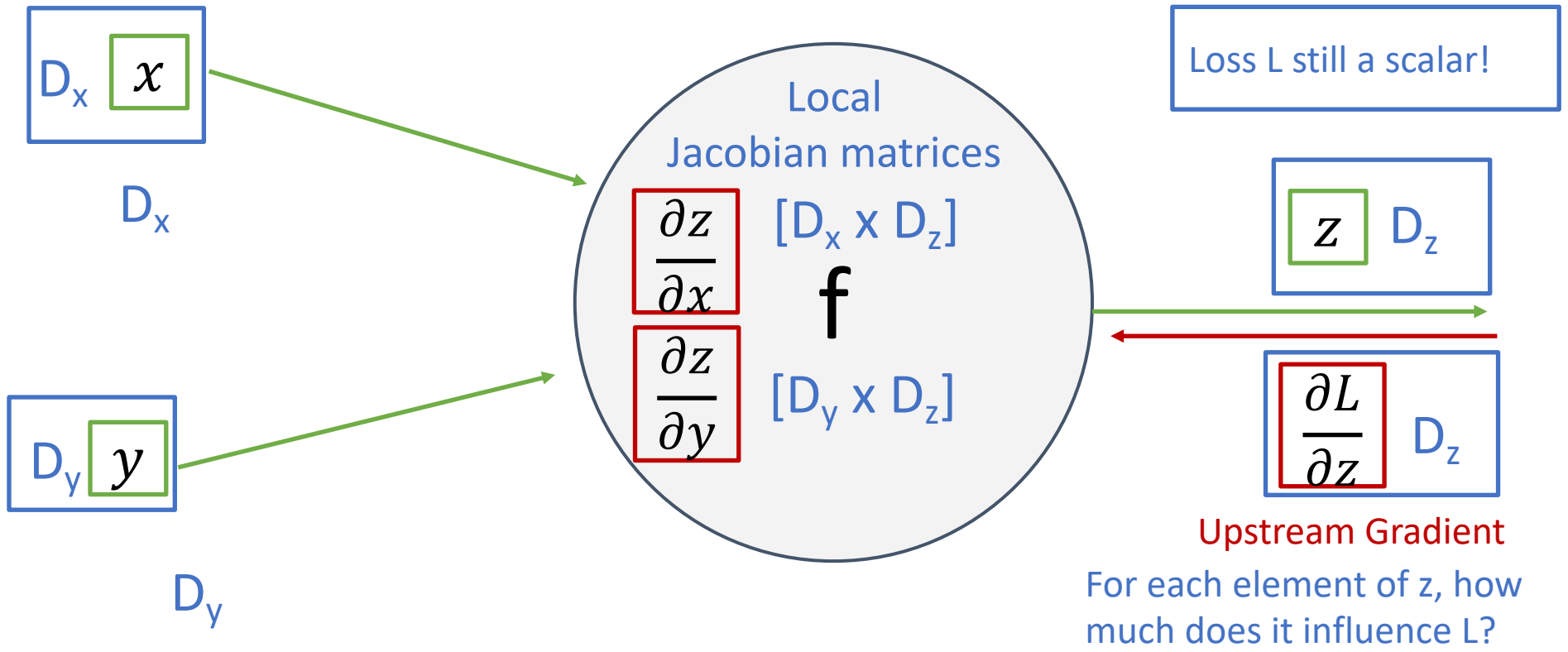

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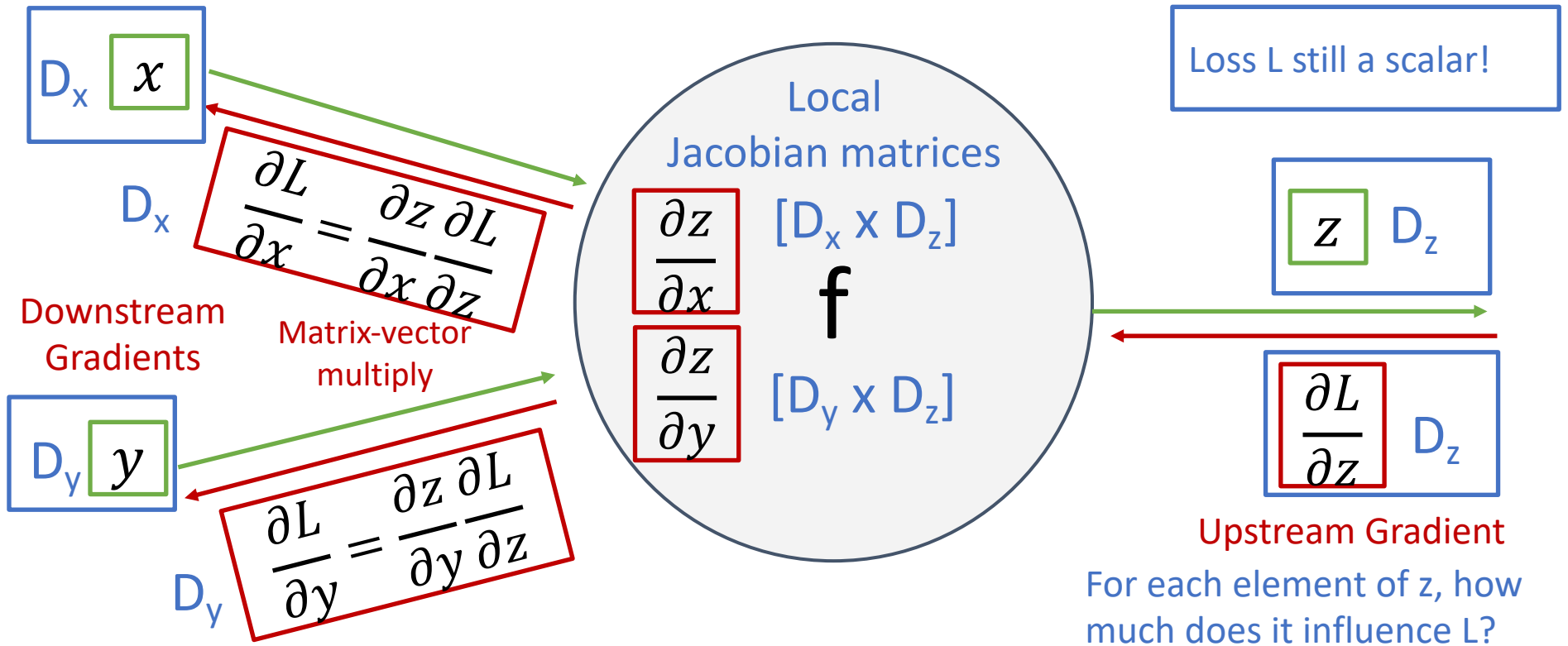

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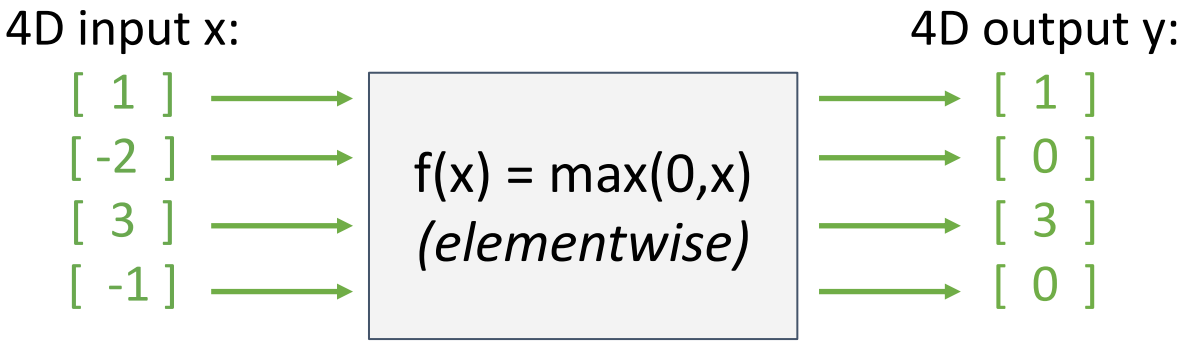

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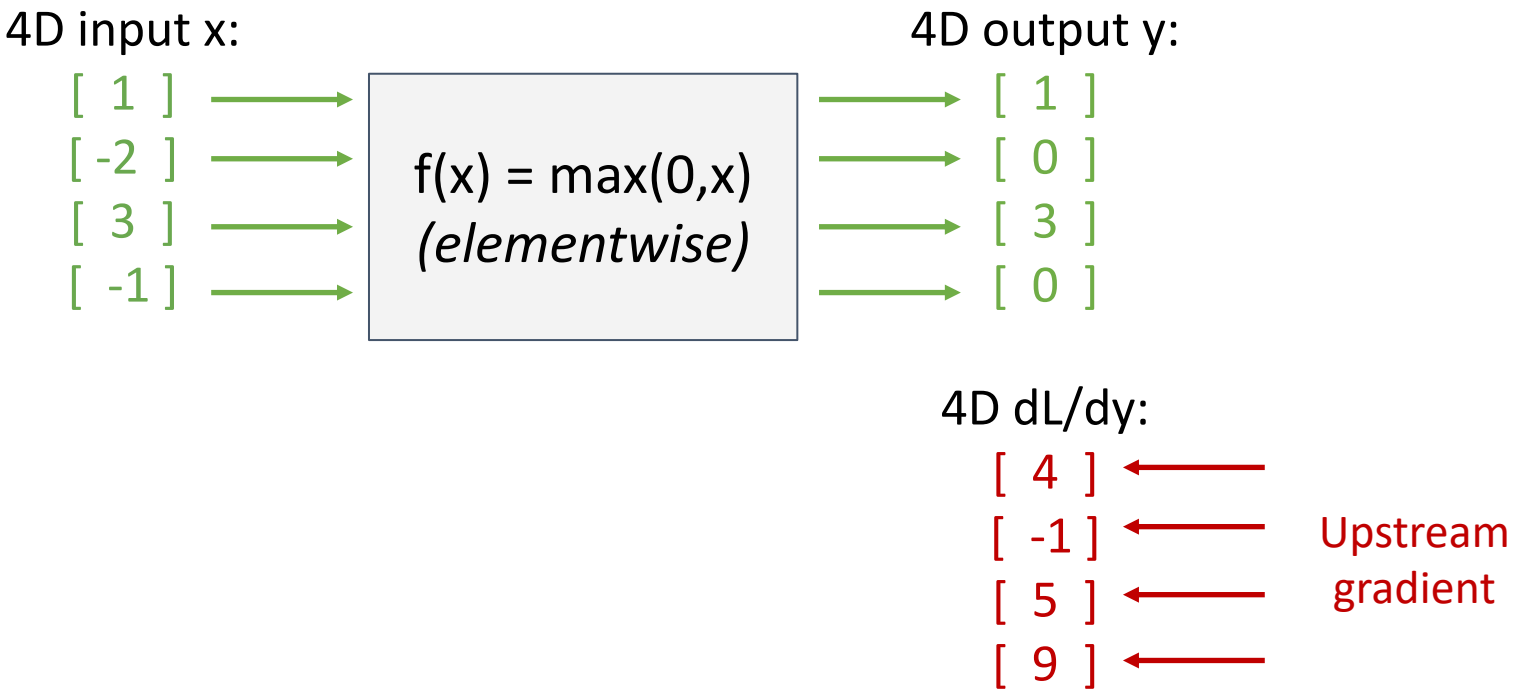

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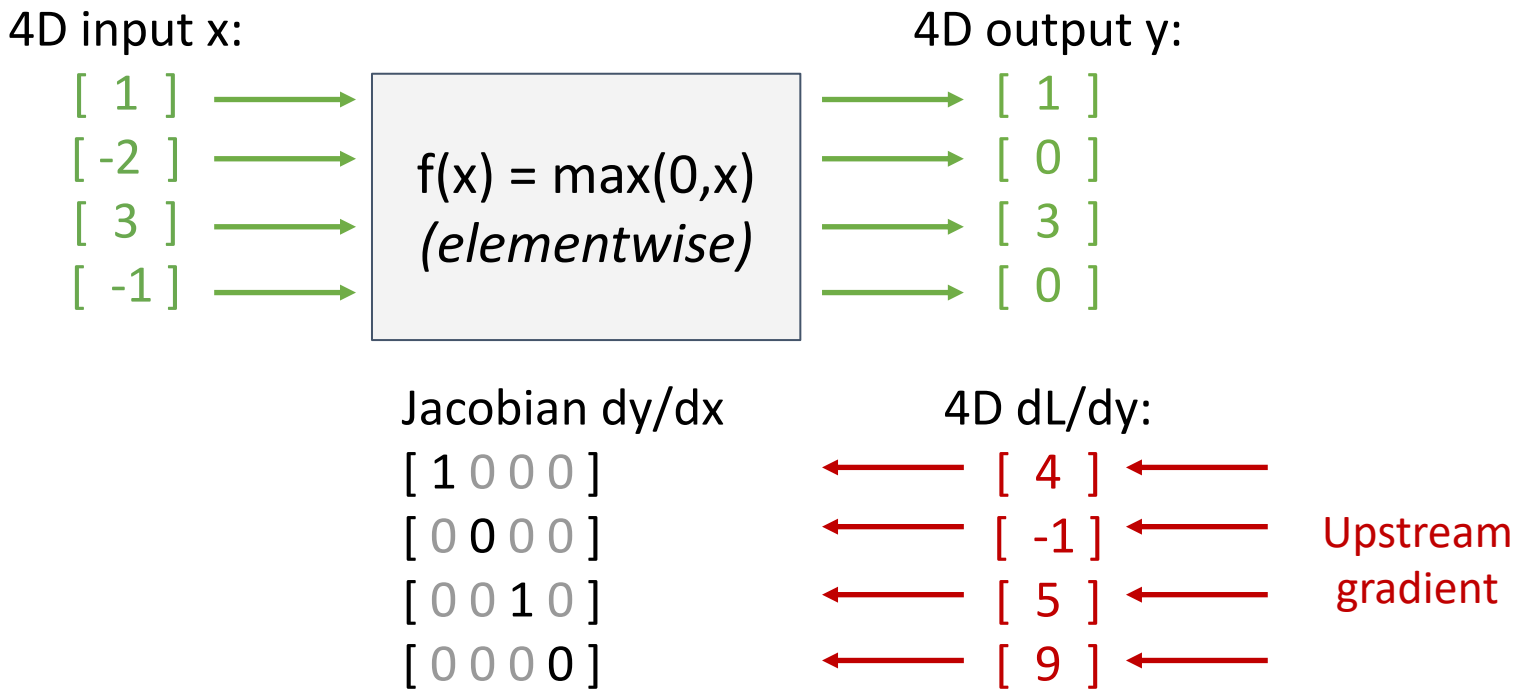

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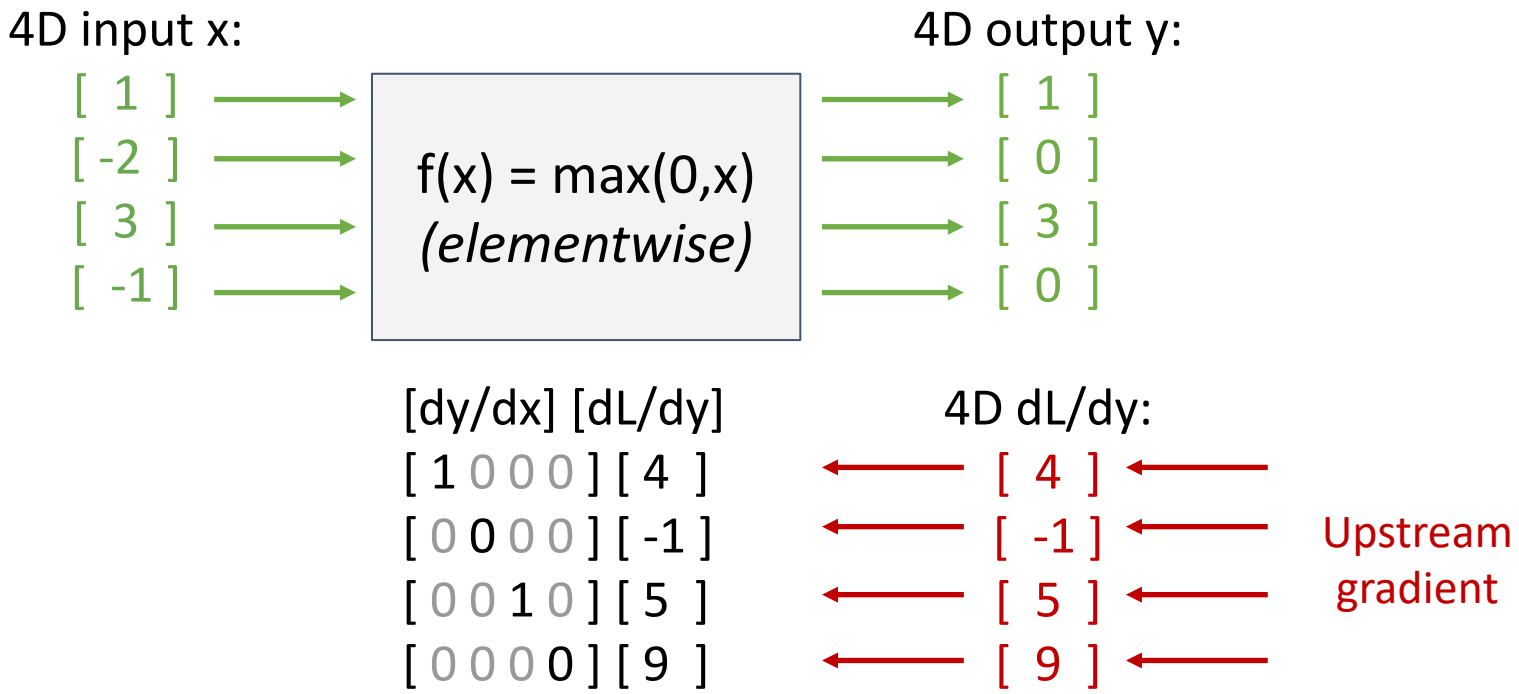

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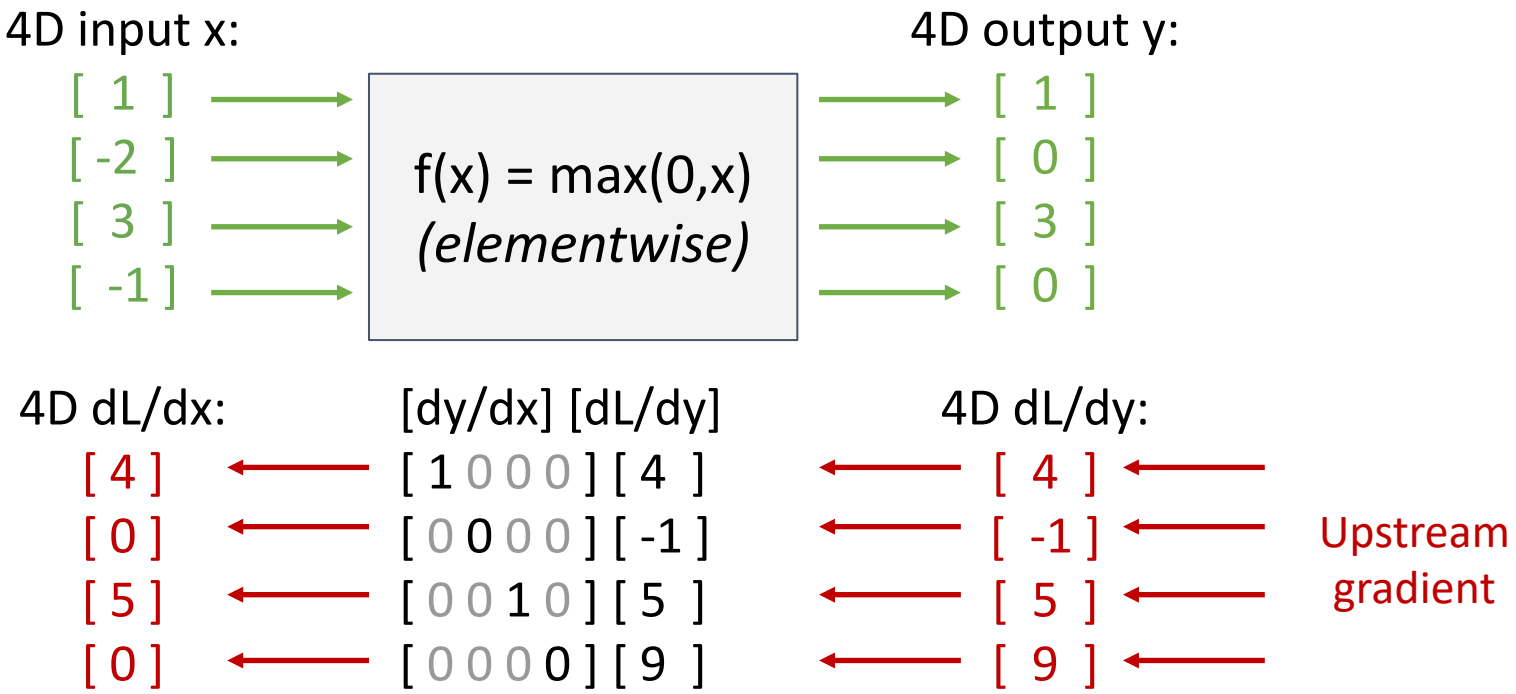
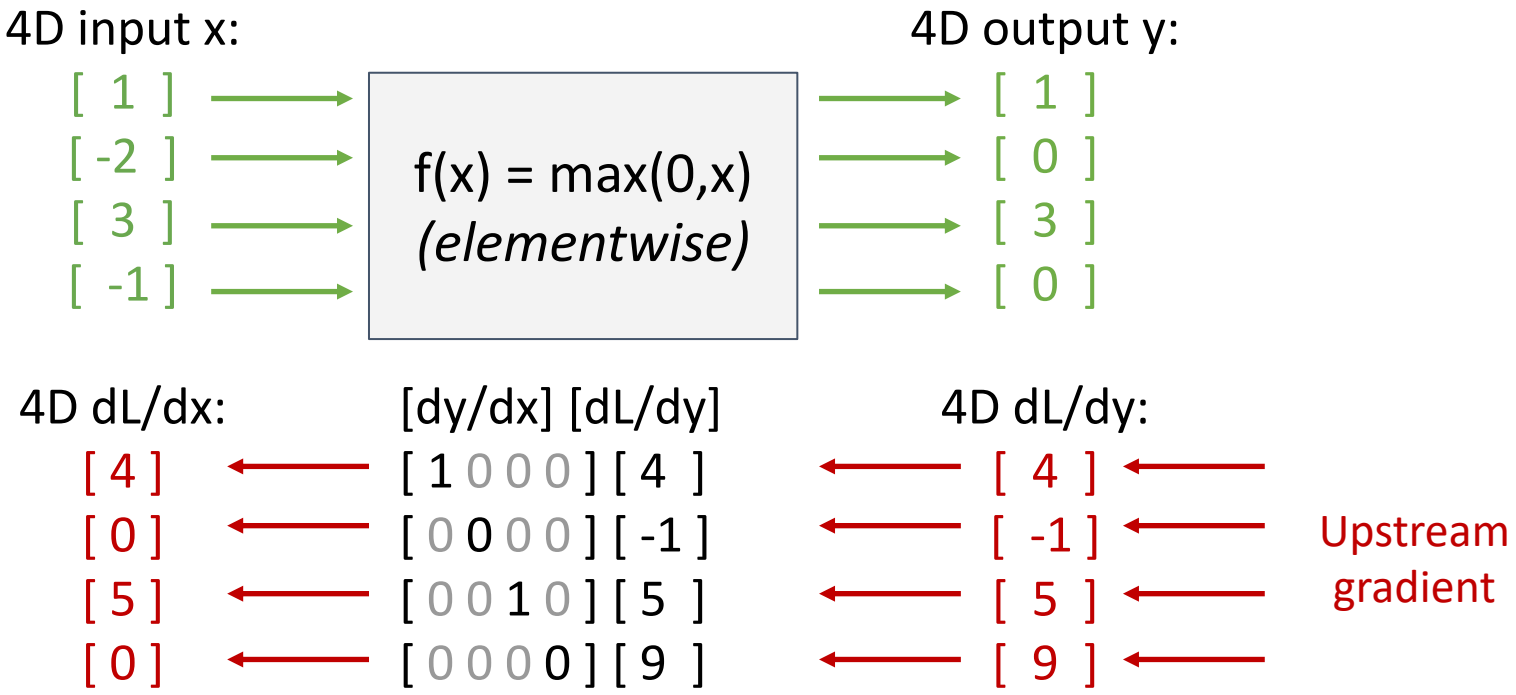
Backprop with Vectors



Slide credit: D Fouhey & J Johnson

Backprop with Vectors

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



Slide credit: D Fouhey & J Johnson

Backprop with Vectors

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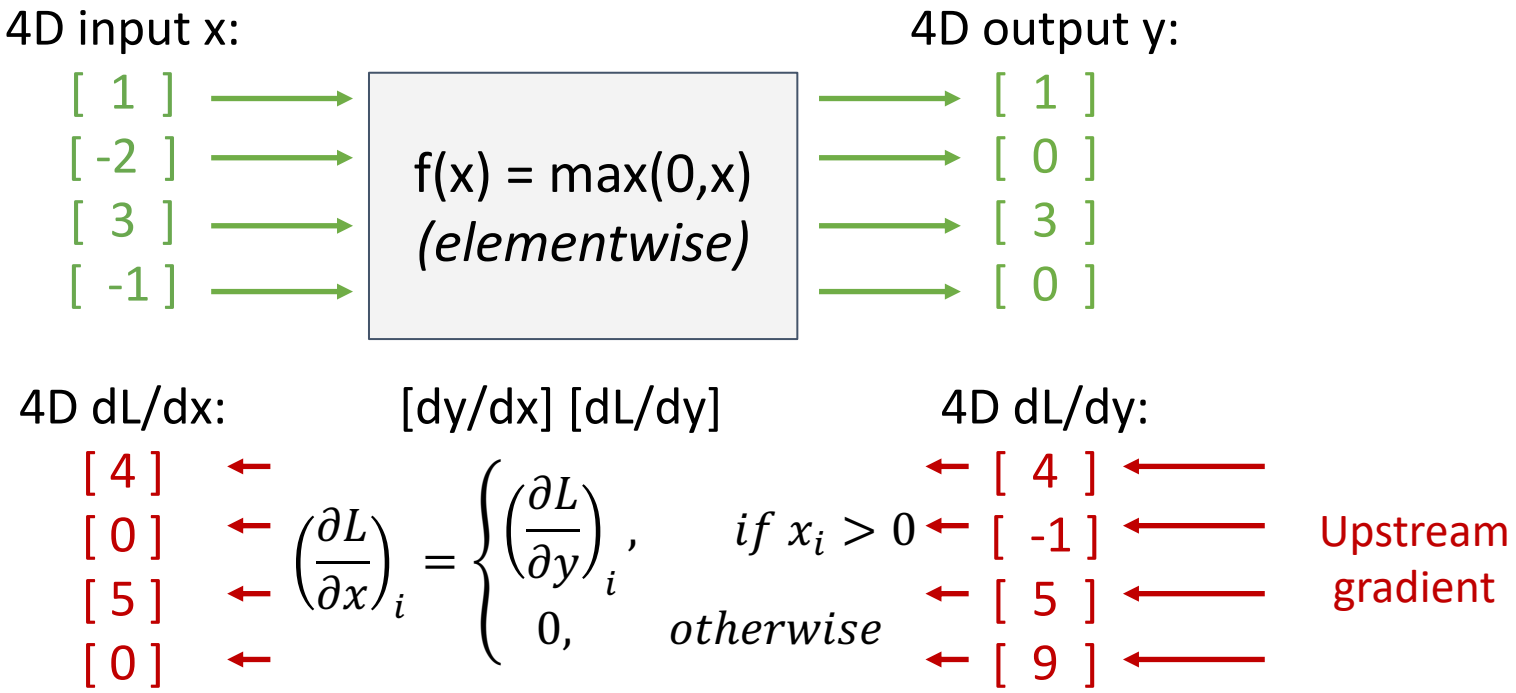
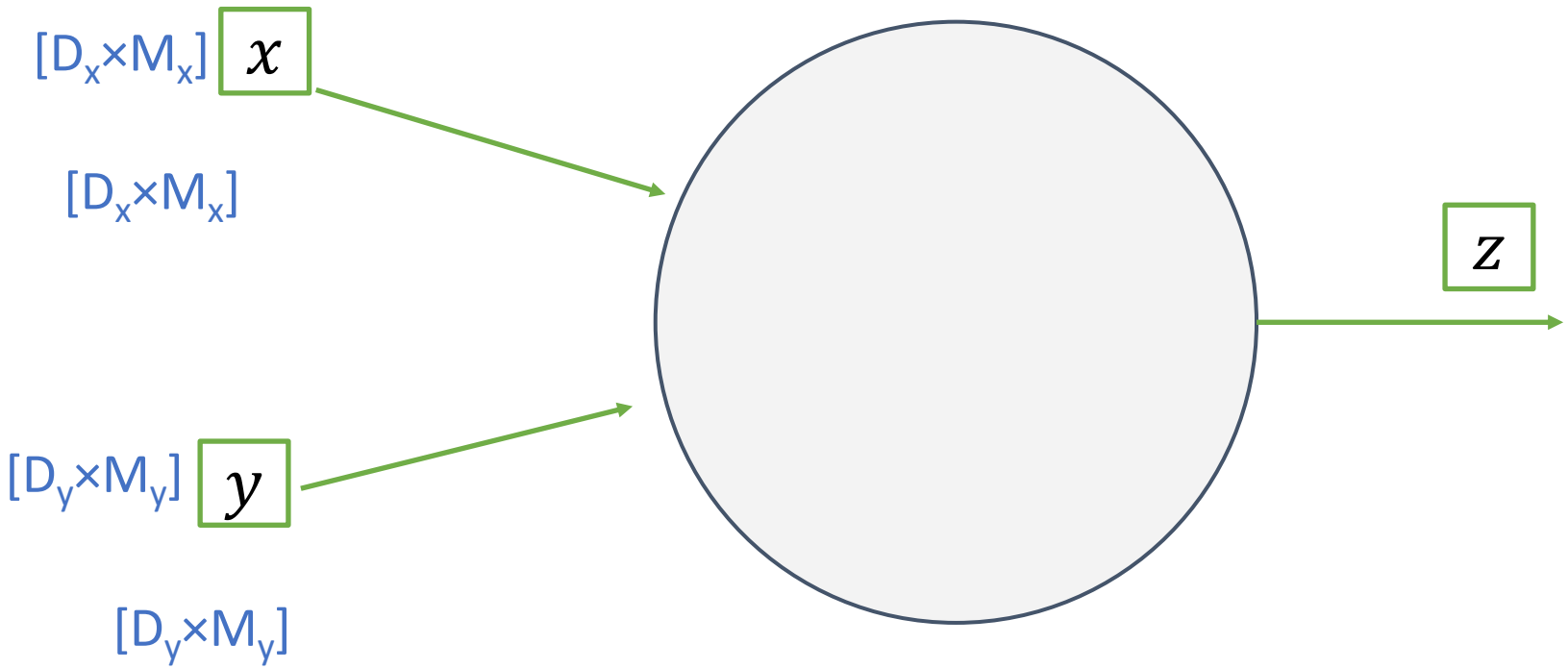


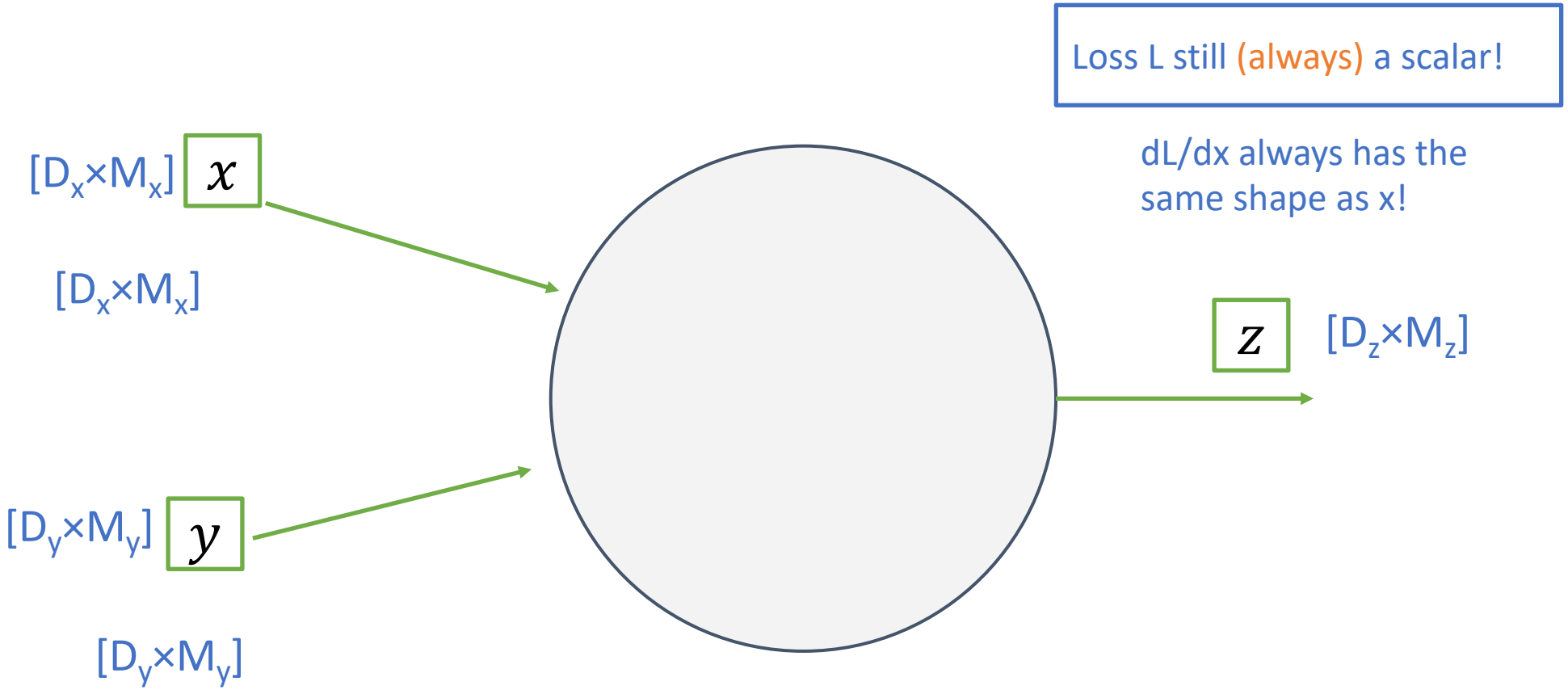
Slide credit: D Fouhey & J Johnson

Backprop with Matrices (or Tensors):



Slide credit: D Fouhey & J Johnson

Backprop with Matrices (or Tensors):



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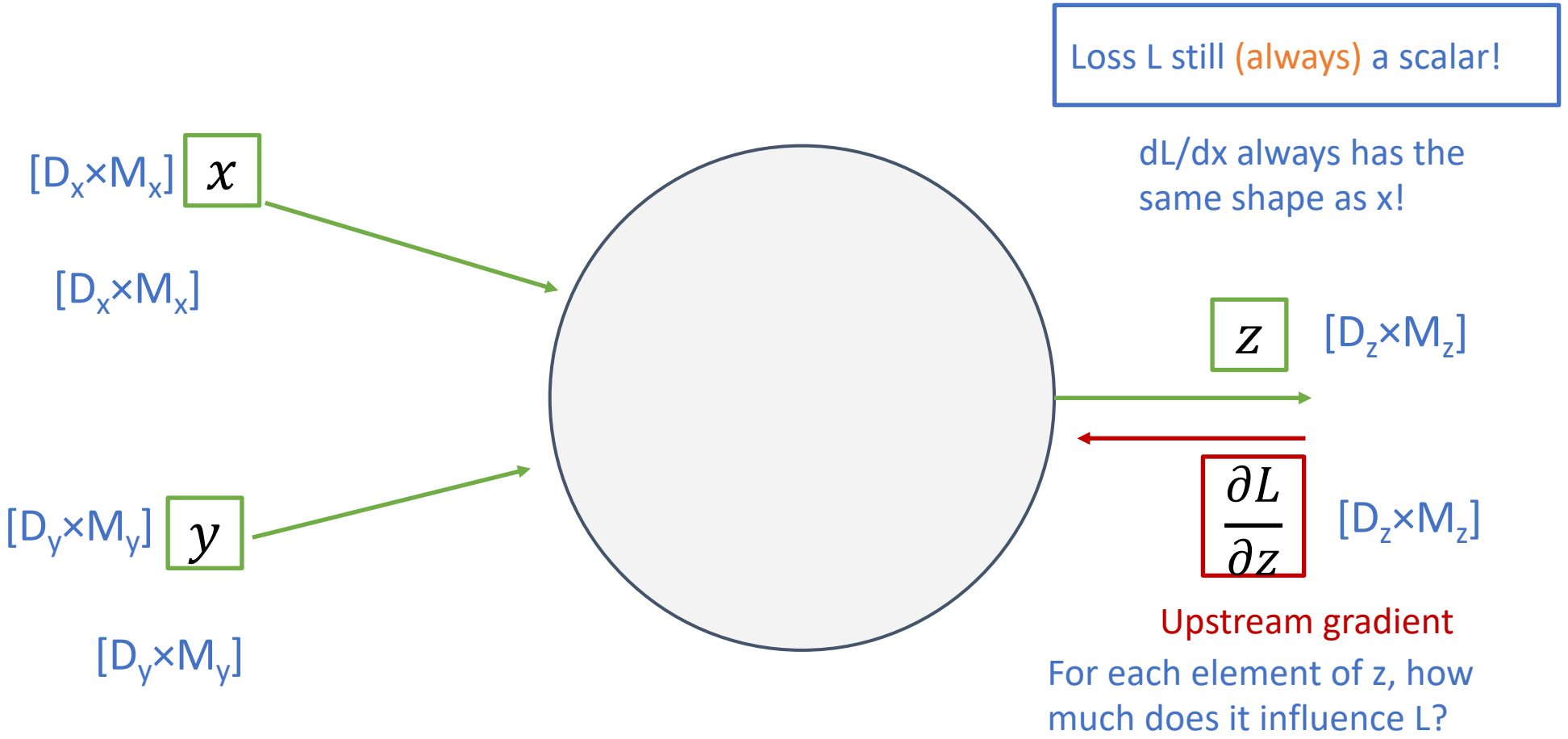
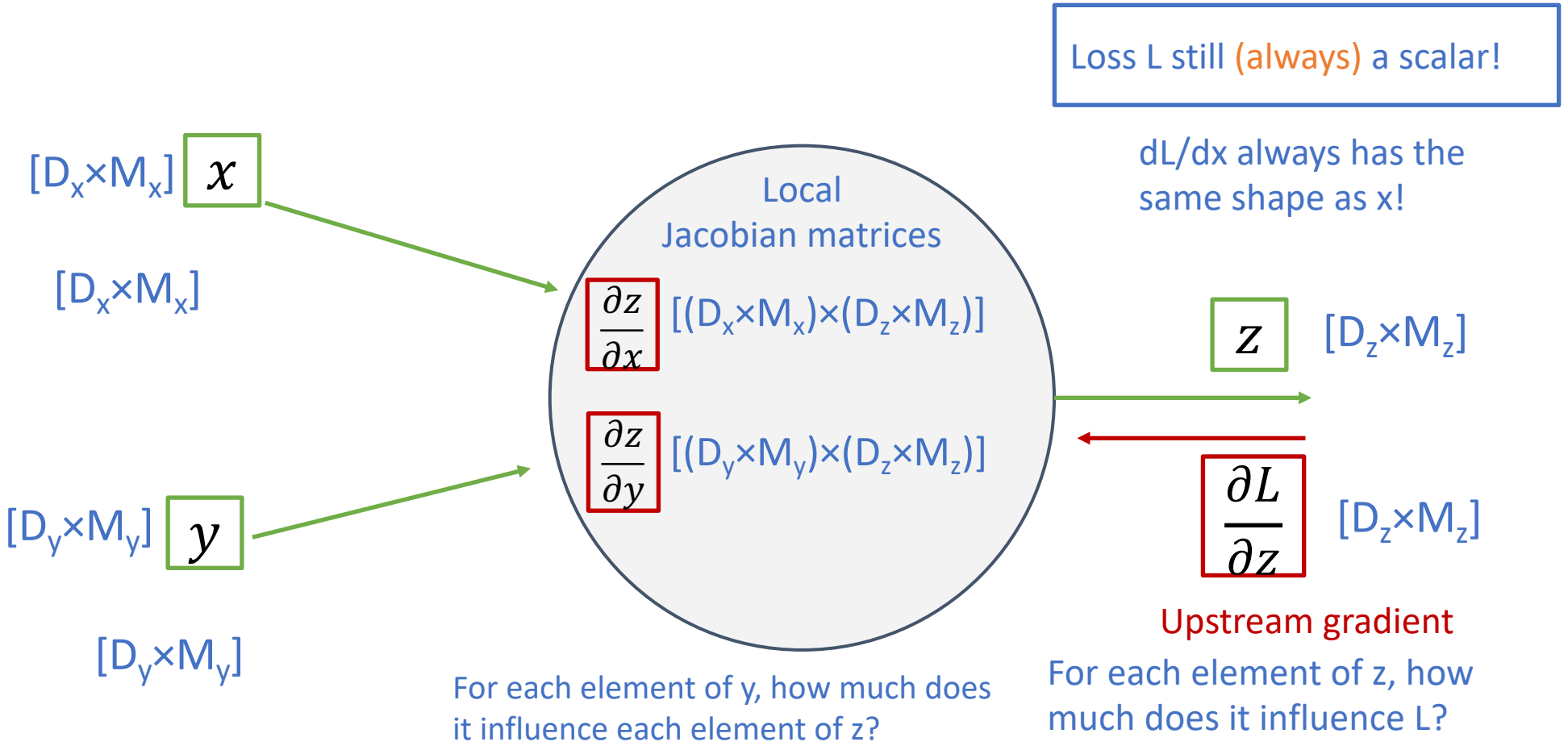


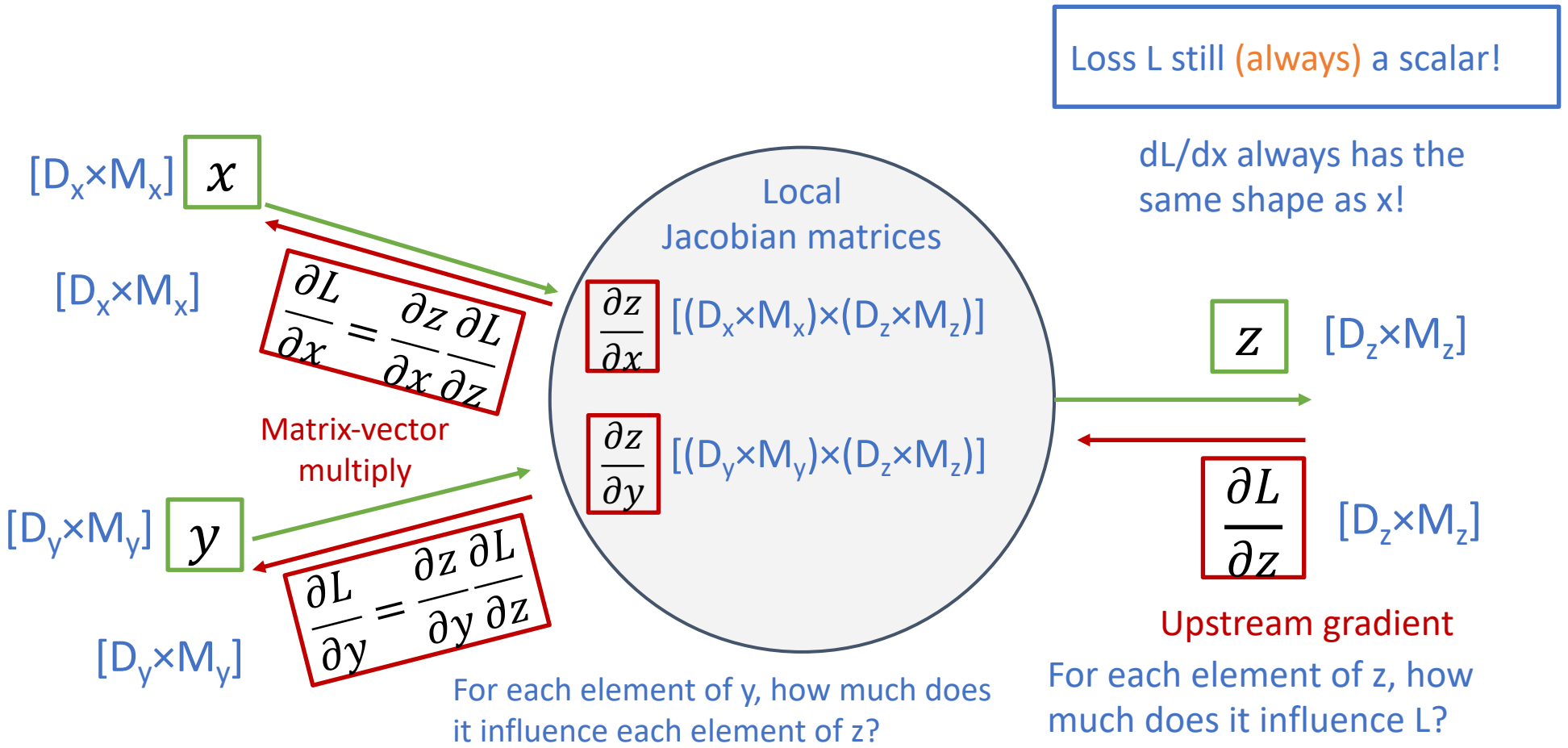
Slide credit: D Fouhey & J Johnson

Backprop with Matrices (or Tensors):



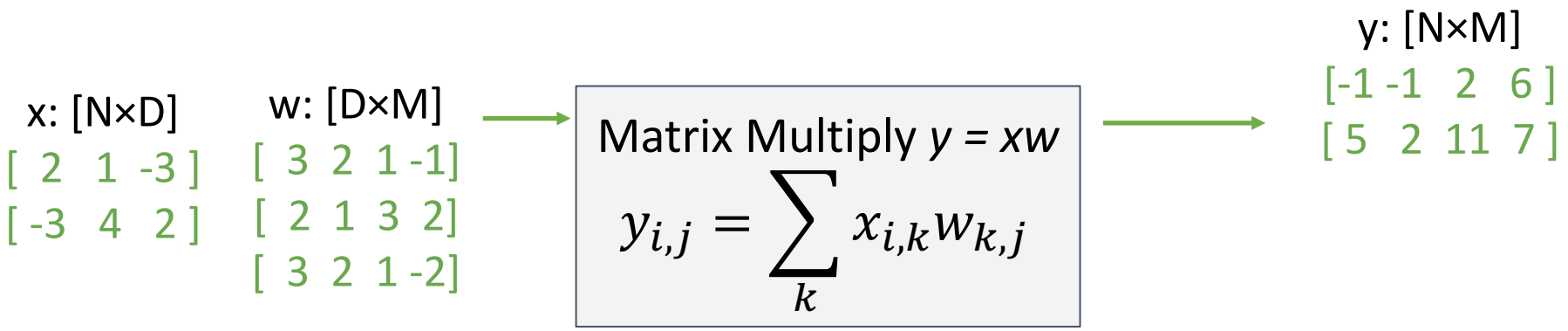
Slide credit: D Fouhey & J Johnson

Backprop with Matrices (or Tensors):



Slide credit: D Fouhey & J Johnson

Example: Matrix Multiplication Operator



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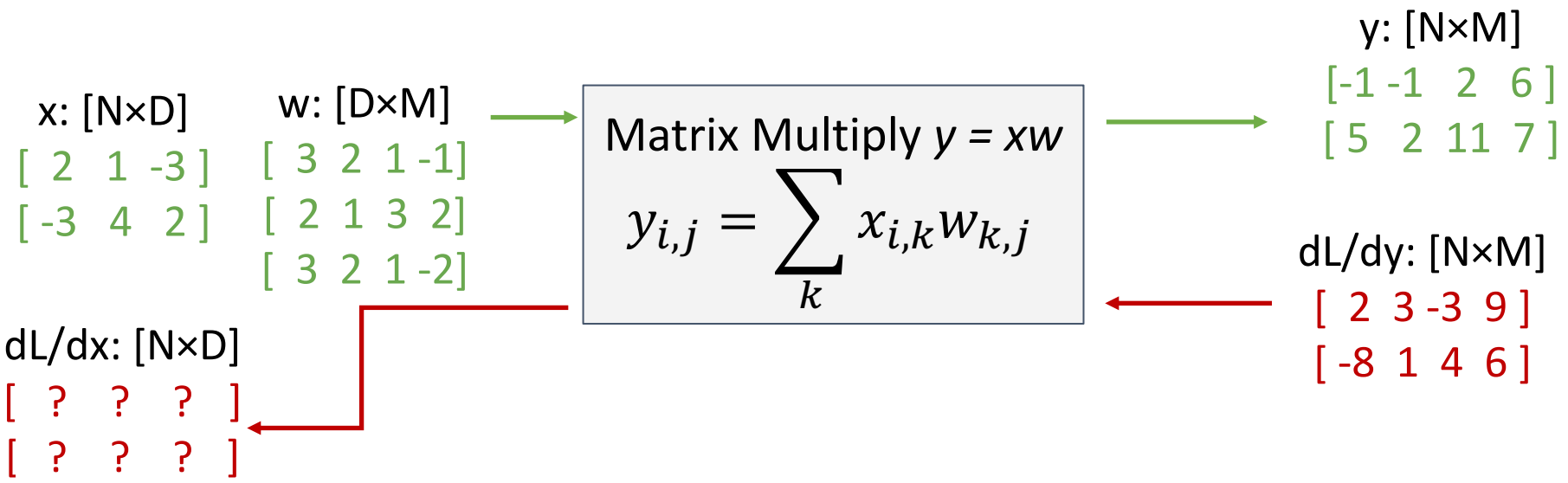

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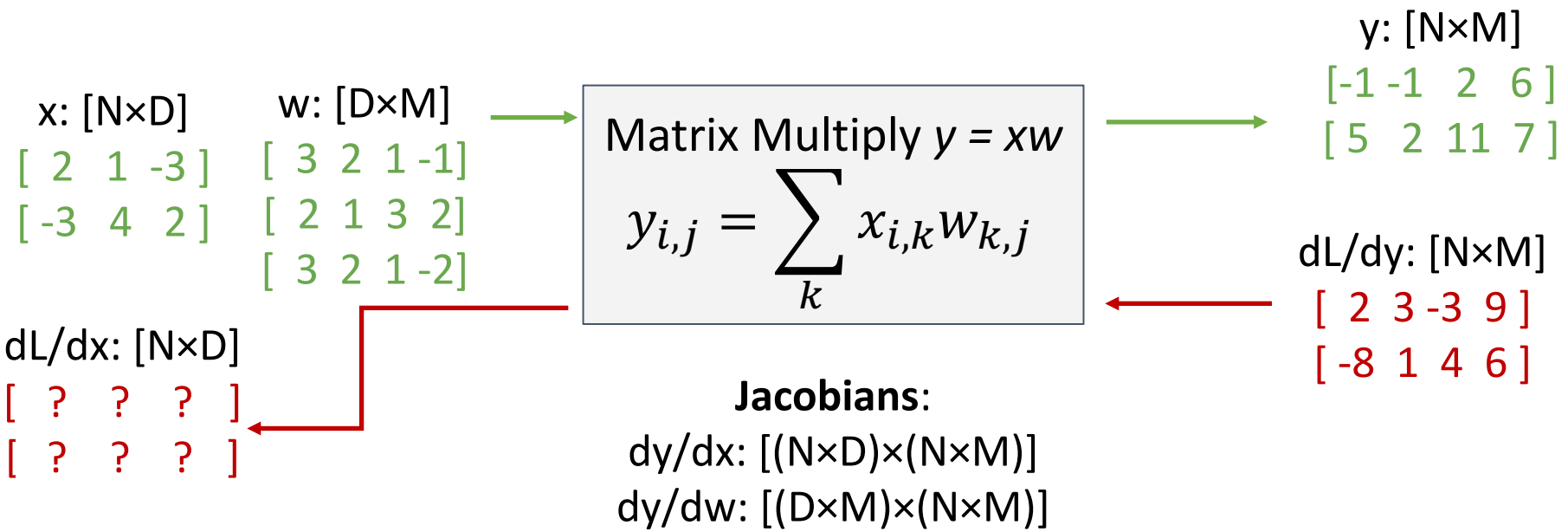
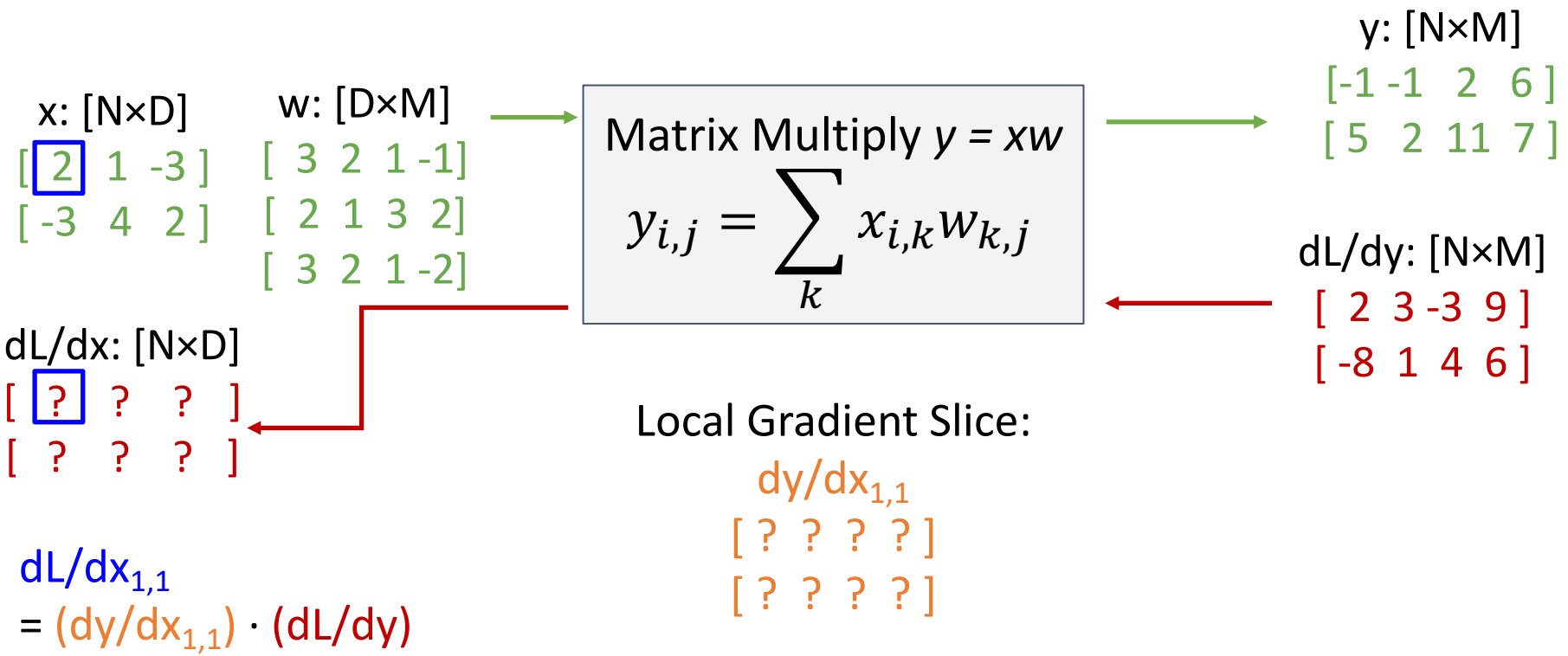


For a neural net we may have
N=64, D=M=4096
Each Jacobian takes 256 GB of memory!
Must work with them implicitly!

Slide credit: D Fouhey & J Johnson

Example: Matrix Multiplication Operator



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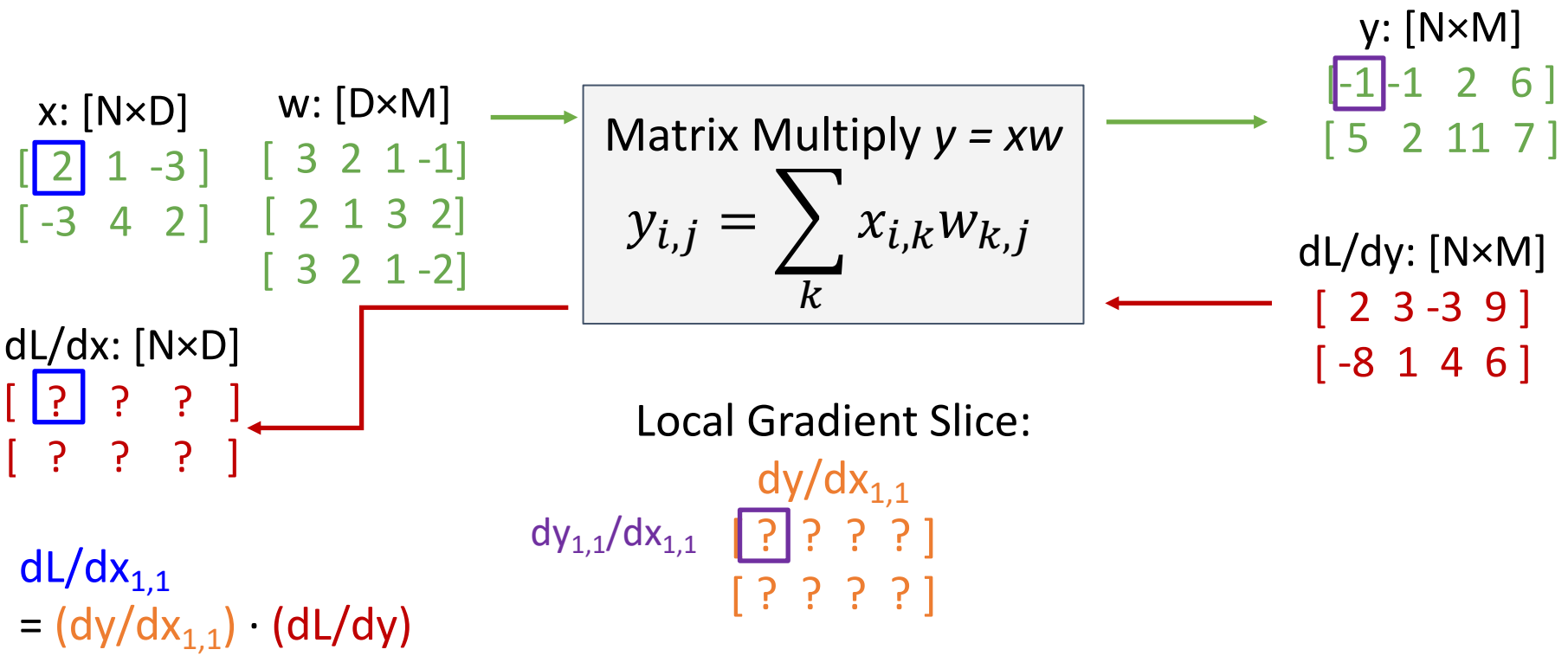

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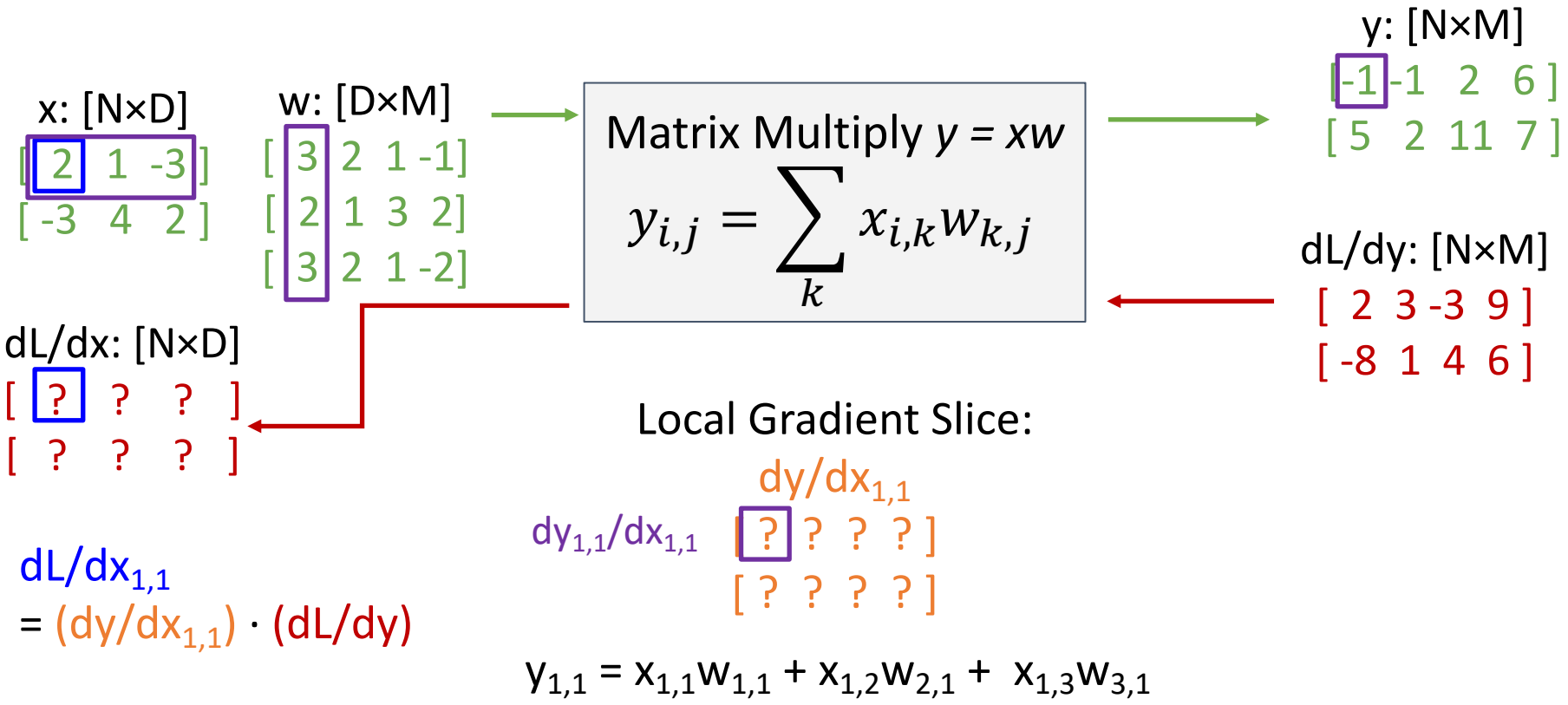

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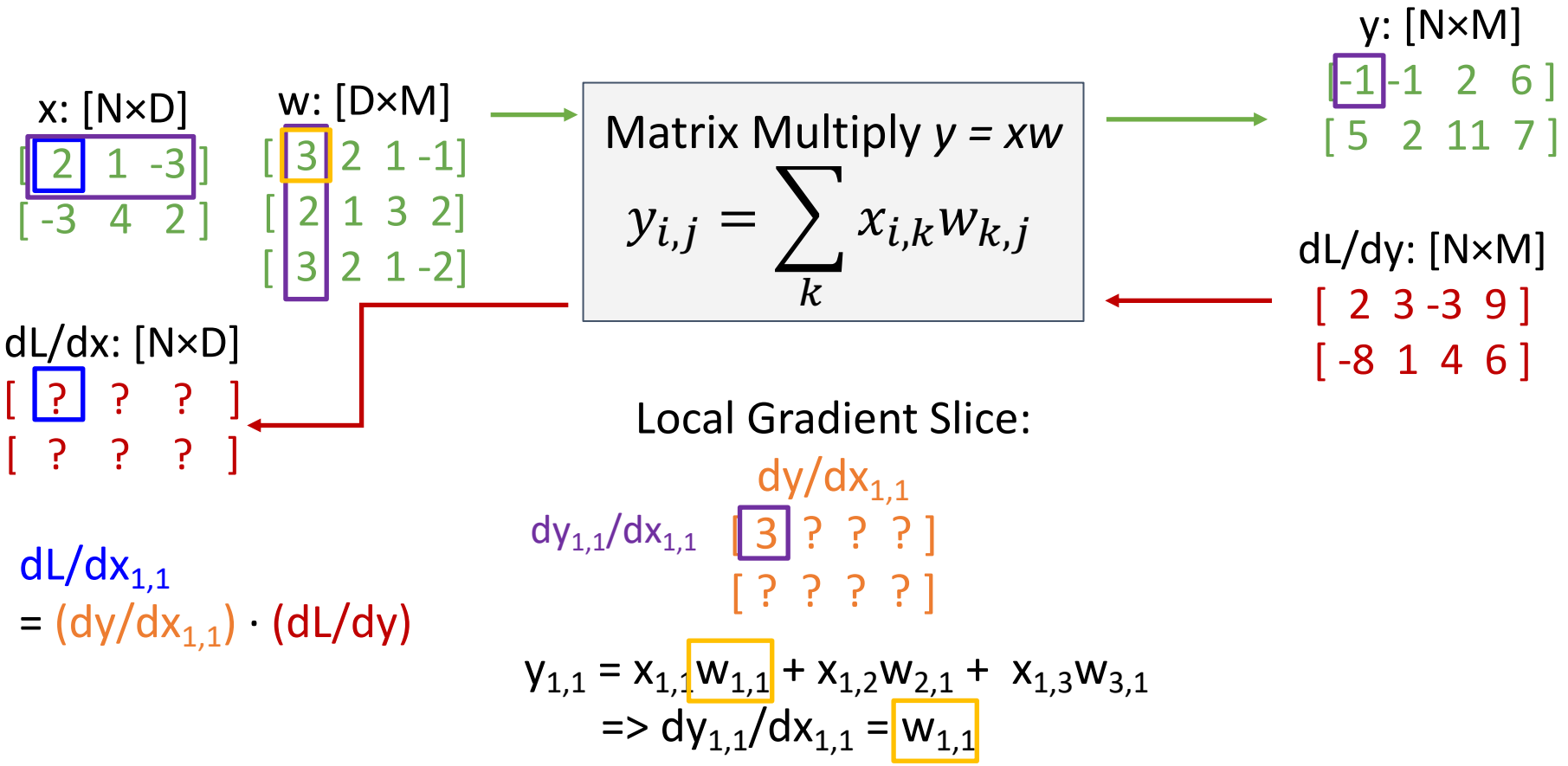
Example: Matrix Multiplication Operator



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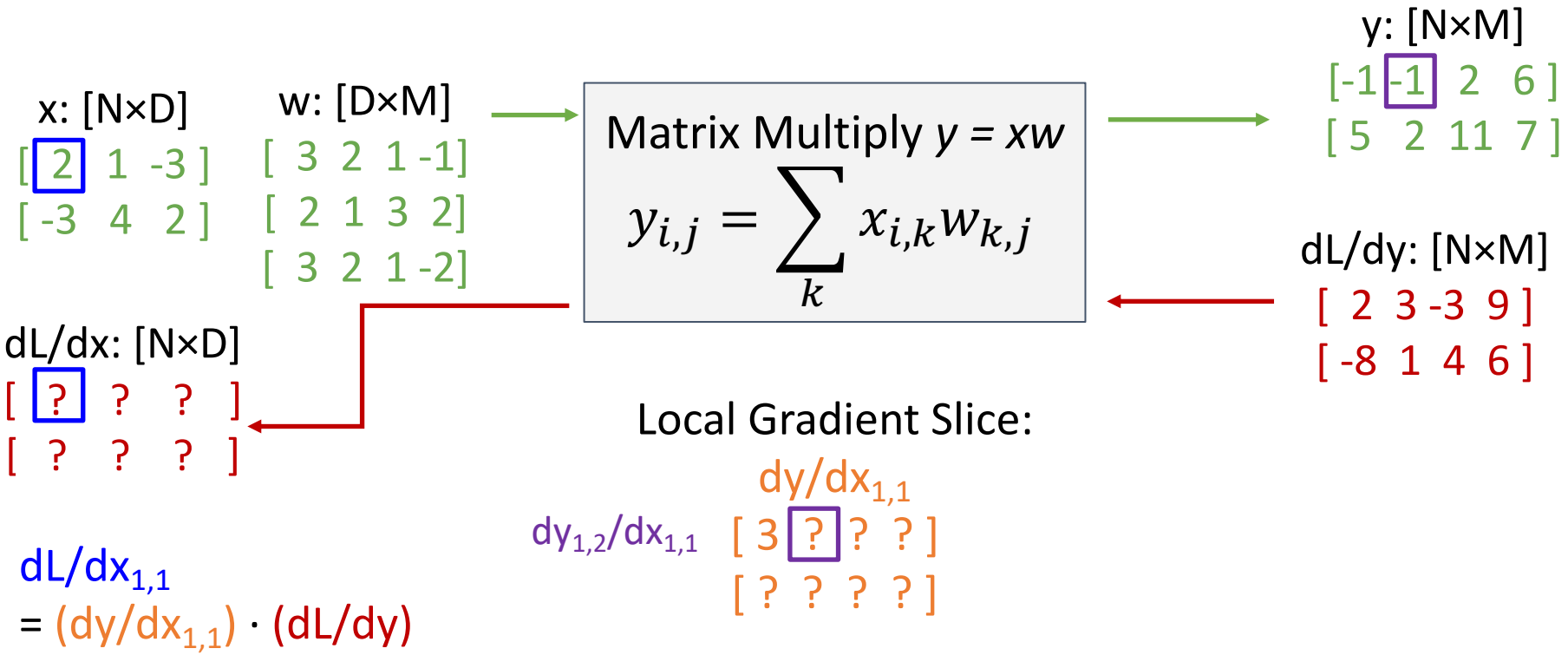

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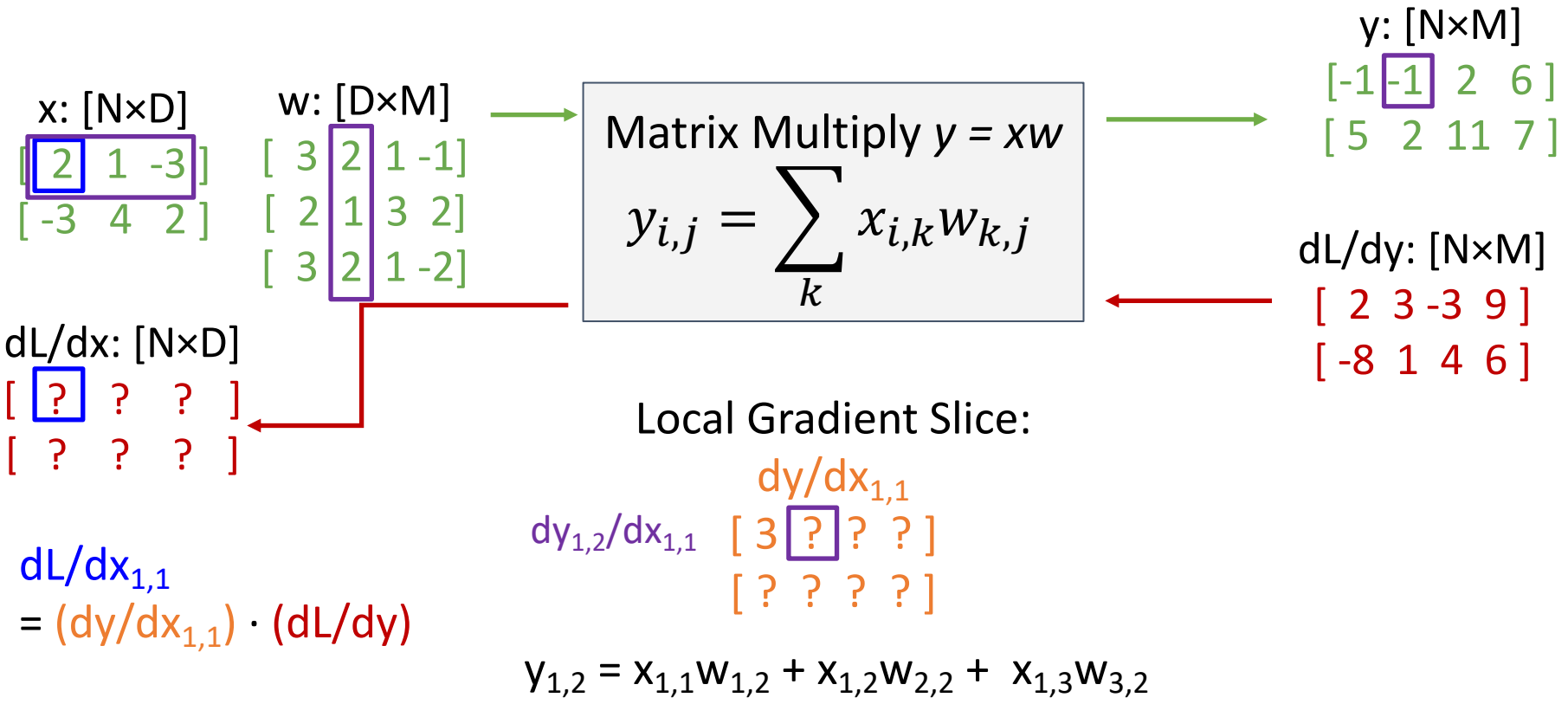

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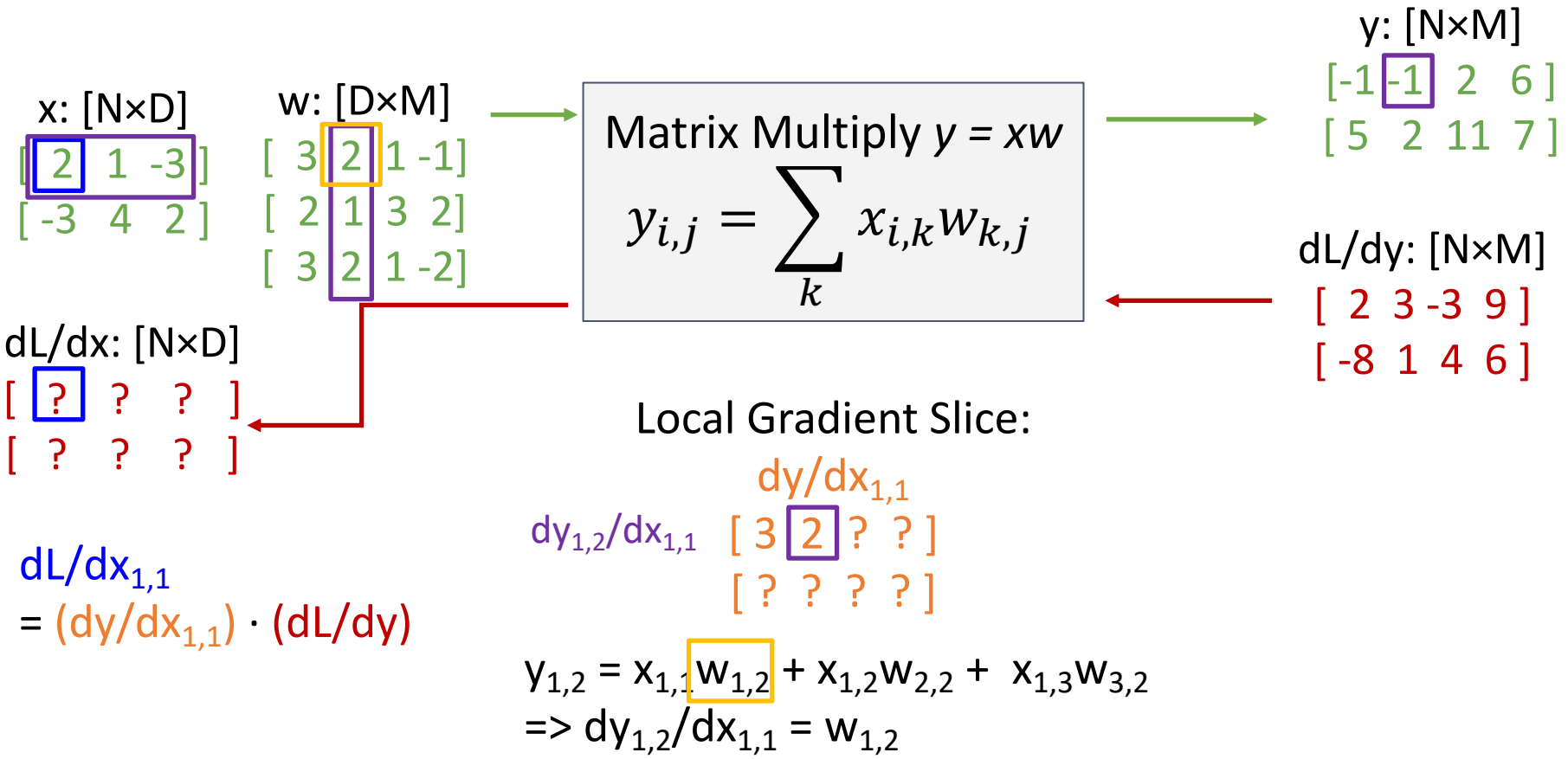
Example: Matrix Multiplication Operator



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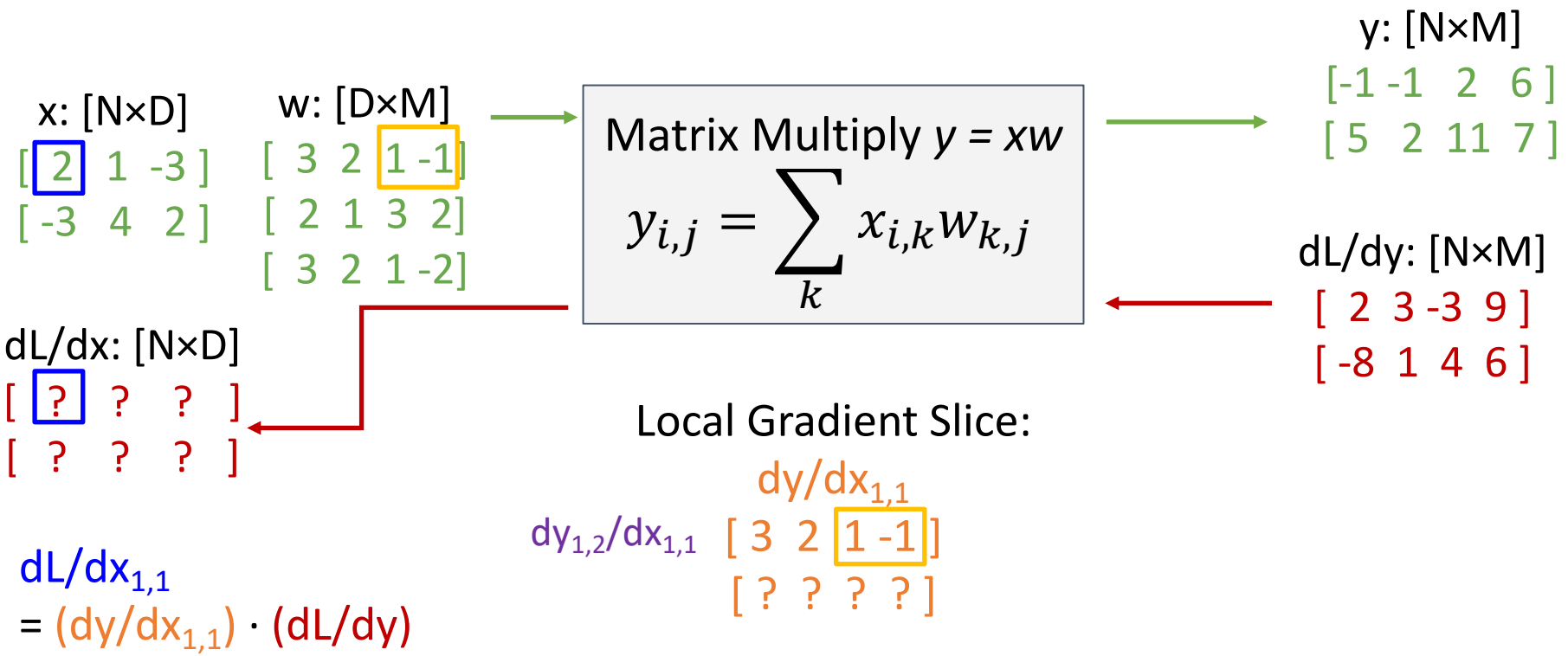

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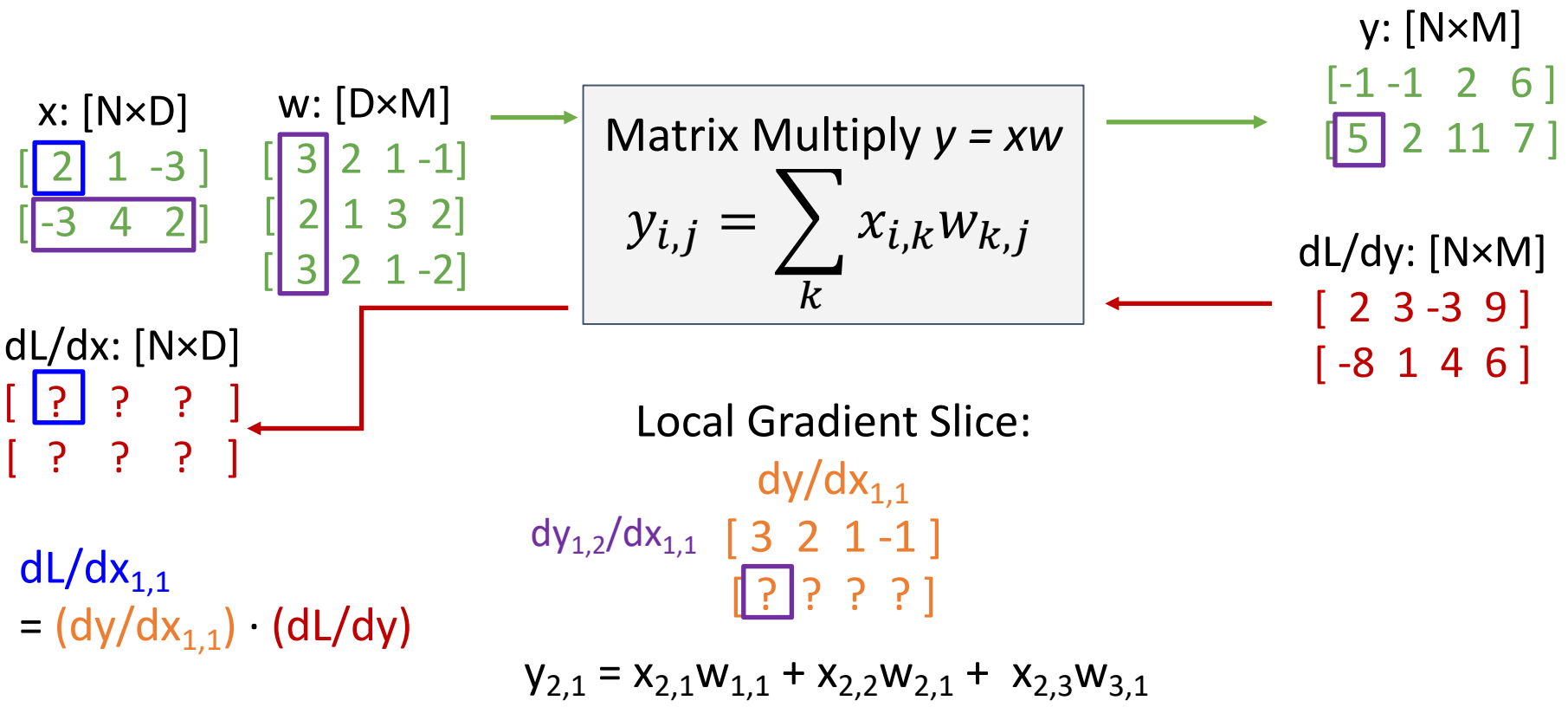

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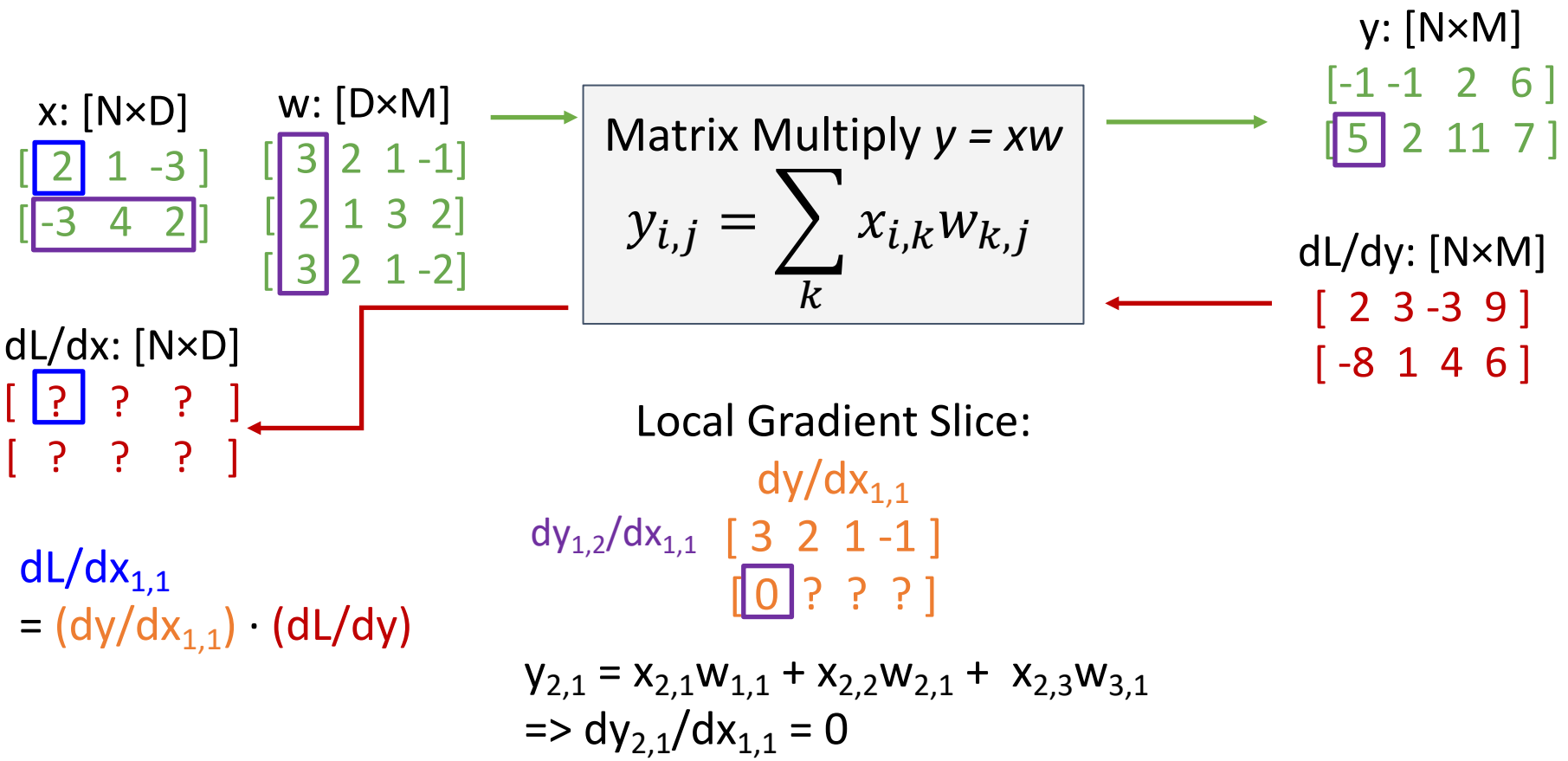

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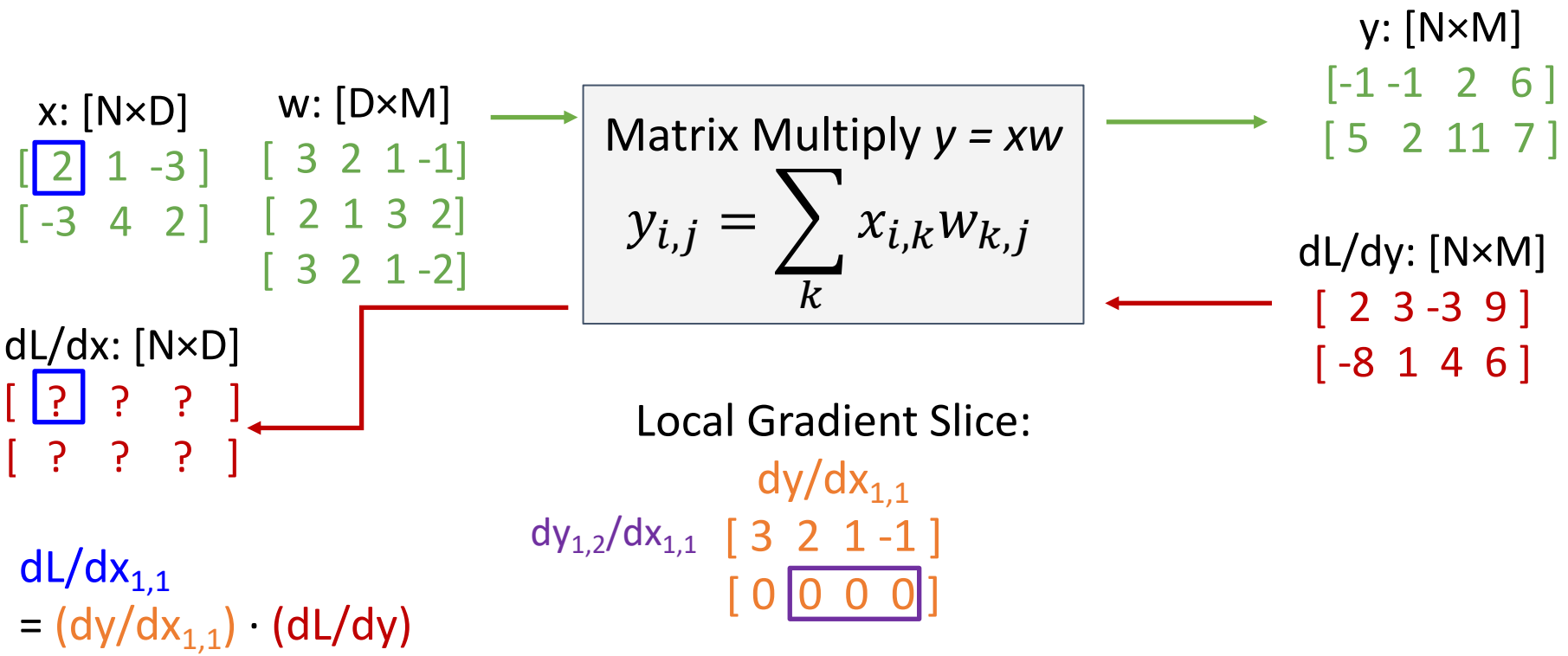

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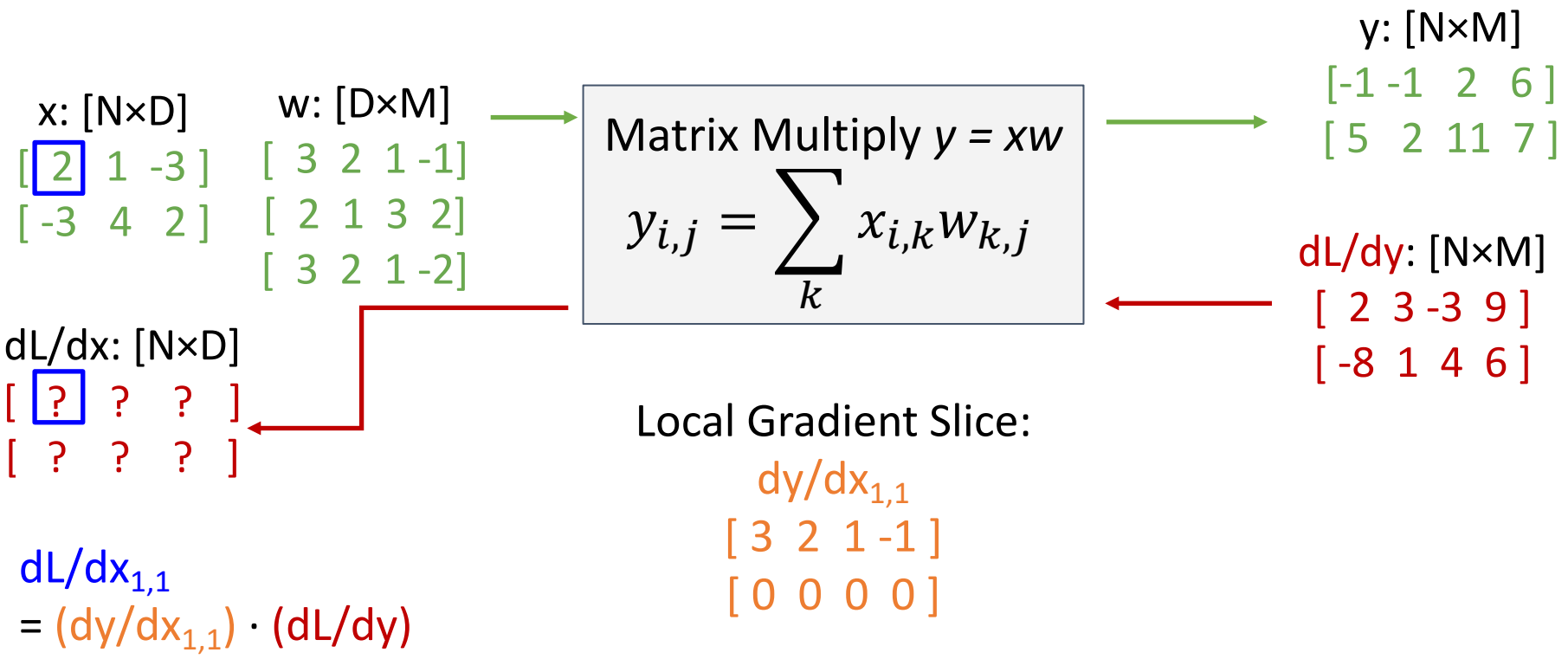

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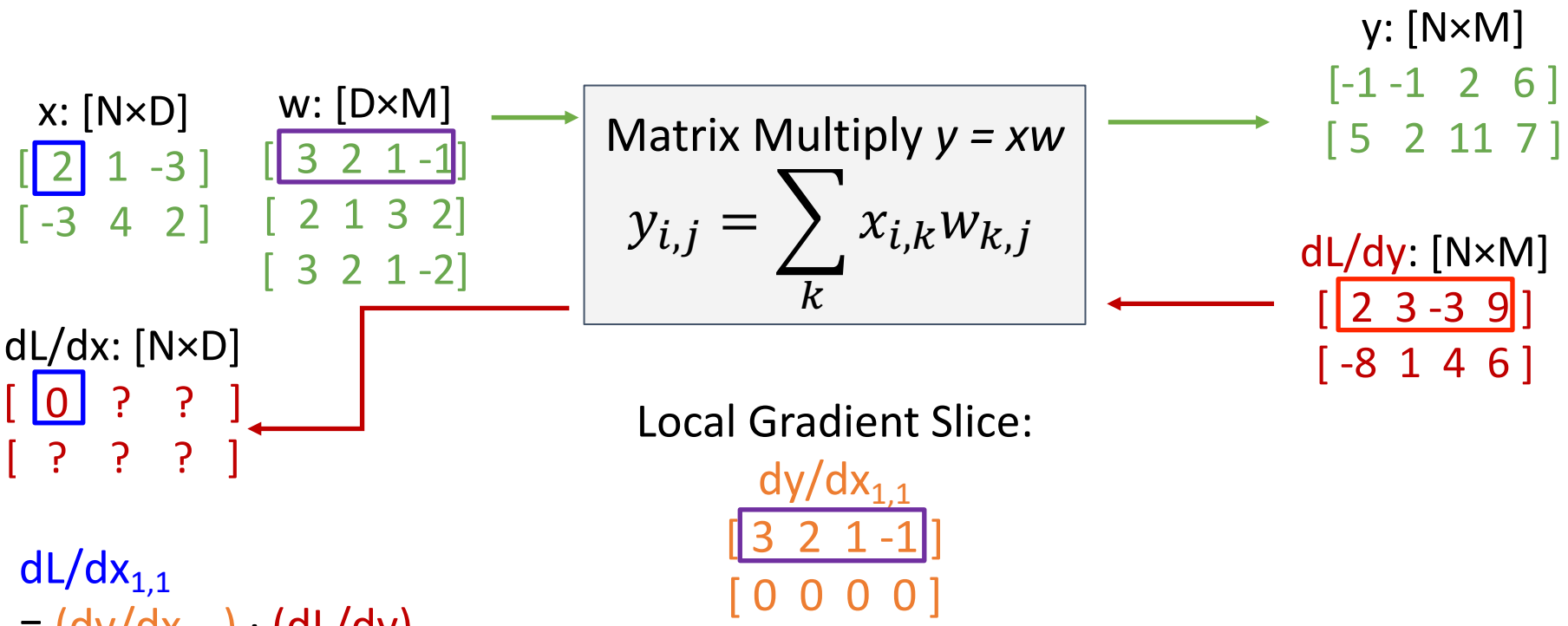
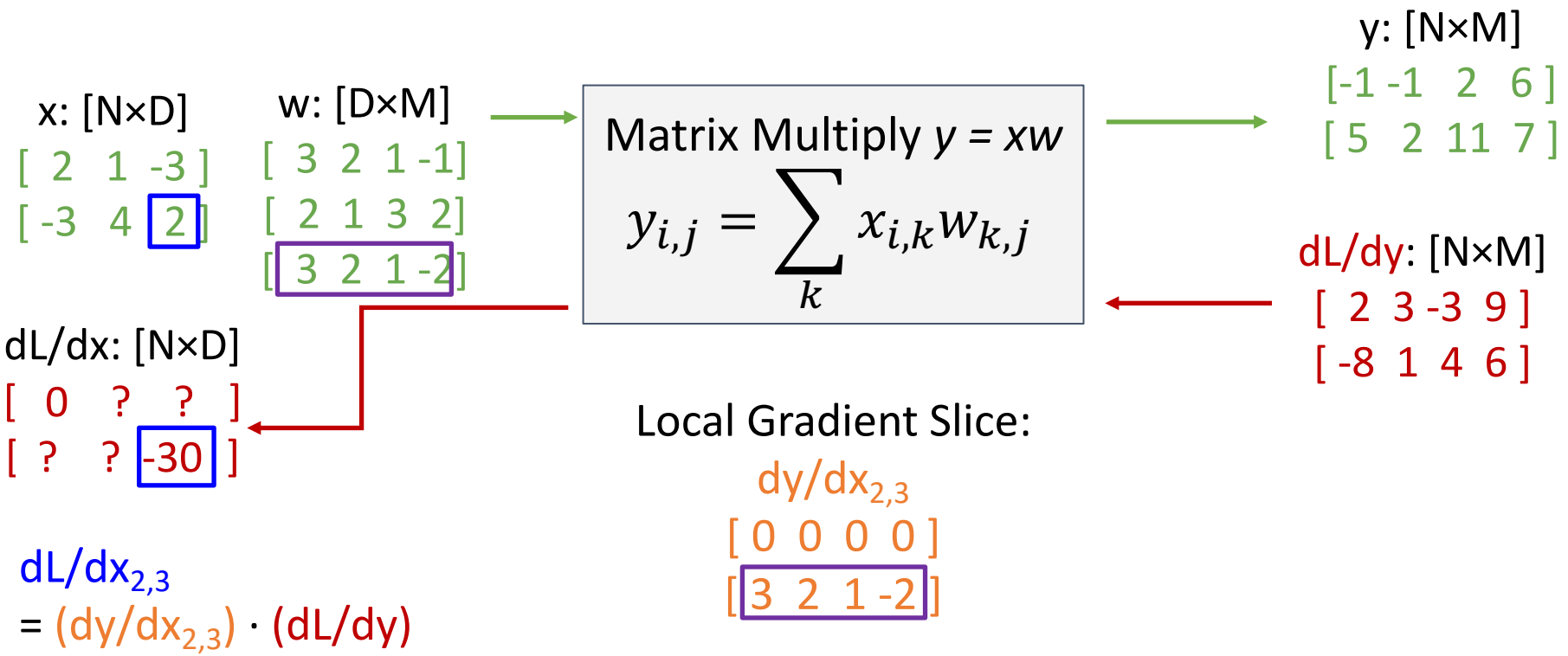


$dL/dx_{1,1}$
$= (dy/dx_{1,1}) \cdot (dL/dy)$
$= (w_{1,:}) \cdot (dL/dy_{1,:})$
$= 3*2 + 2*3 + 1*(-3) + (-1)*9 = 0$

Slide credit: D Fouhey & J Johnson

Example: Matrix Multiplication Operator



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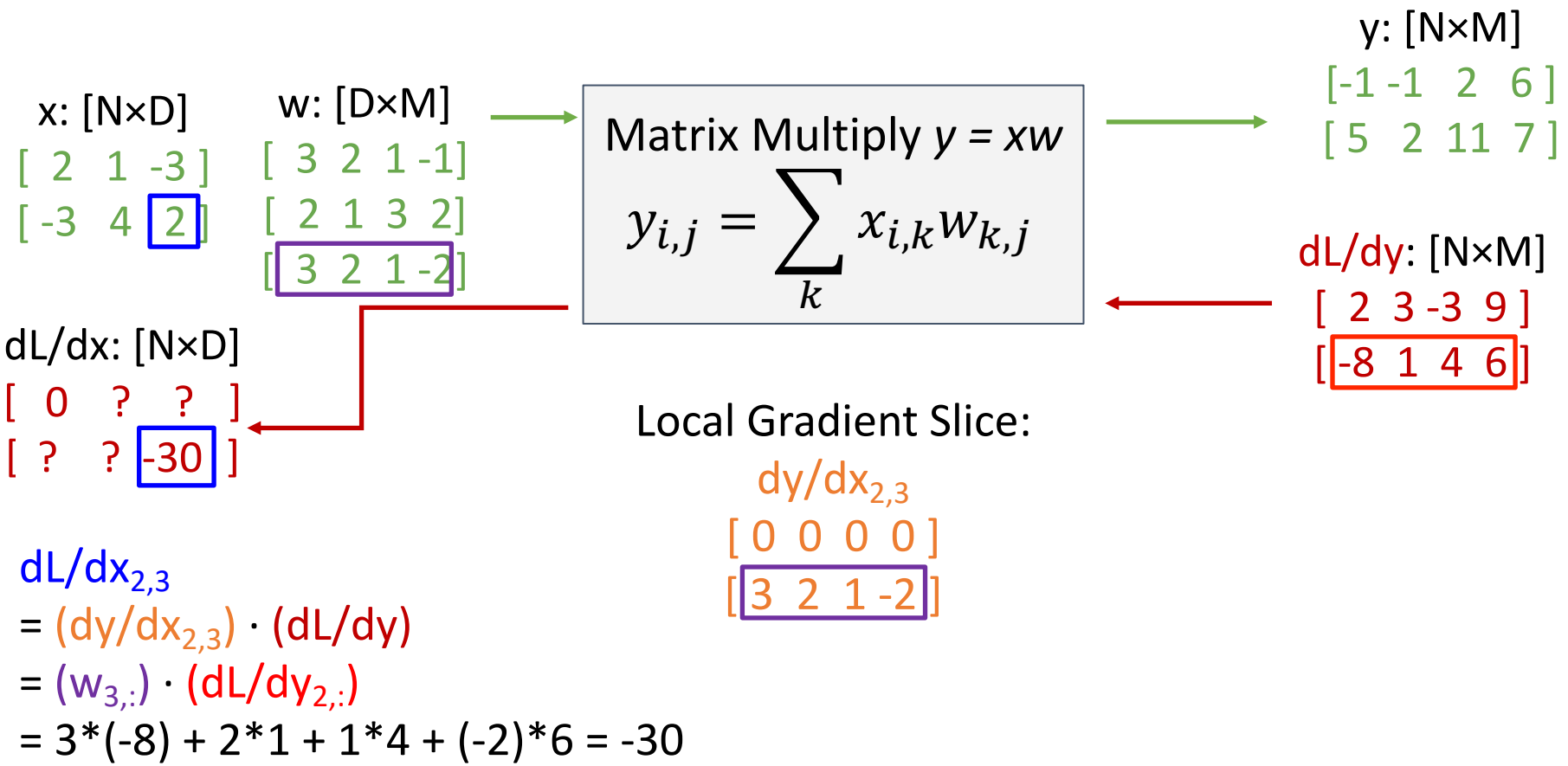
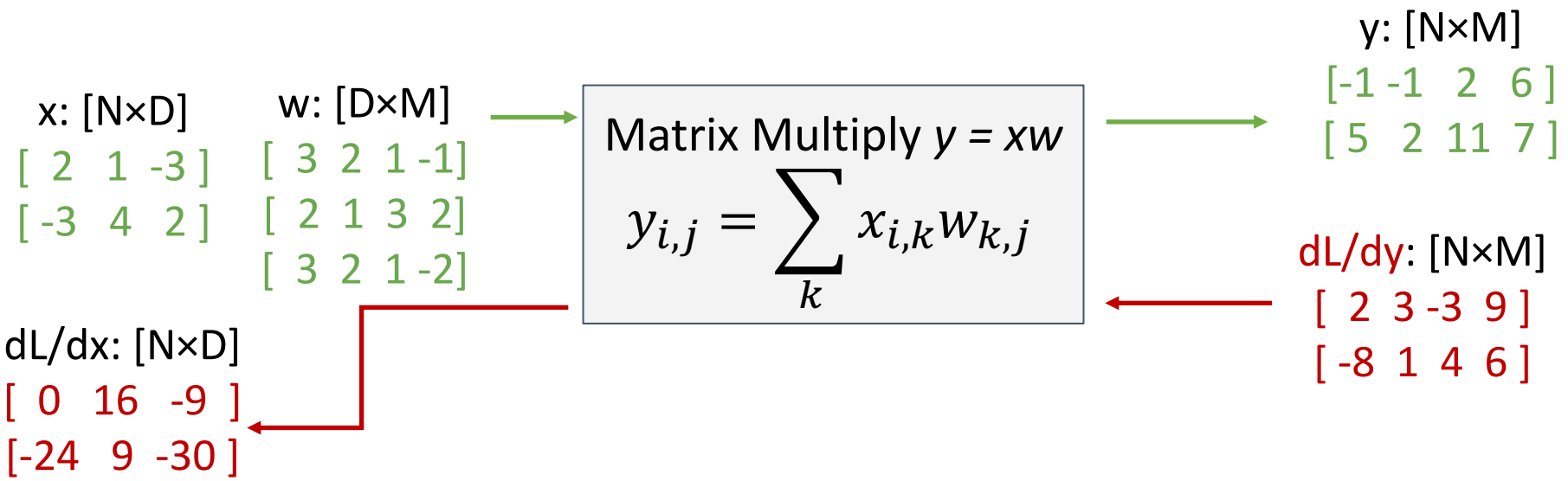


$dL/dx_{2,3}$
$= (dy/dx_{2,3}) \cdot (dL/dy)$
$= (w_{3,:}) \cdot (dL/dy_{2,:})$
$= 3*(-8) + 2*1 + 1*4 + (-2)*6 = -30$

Slide credit: D Fouhey & J Johnson

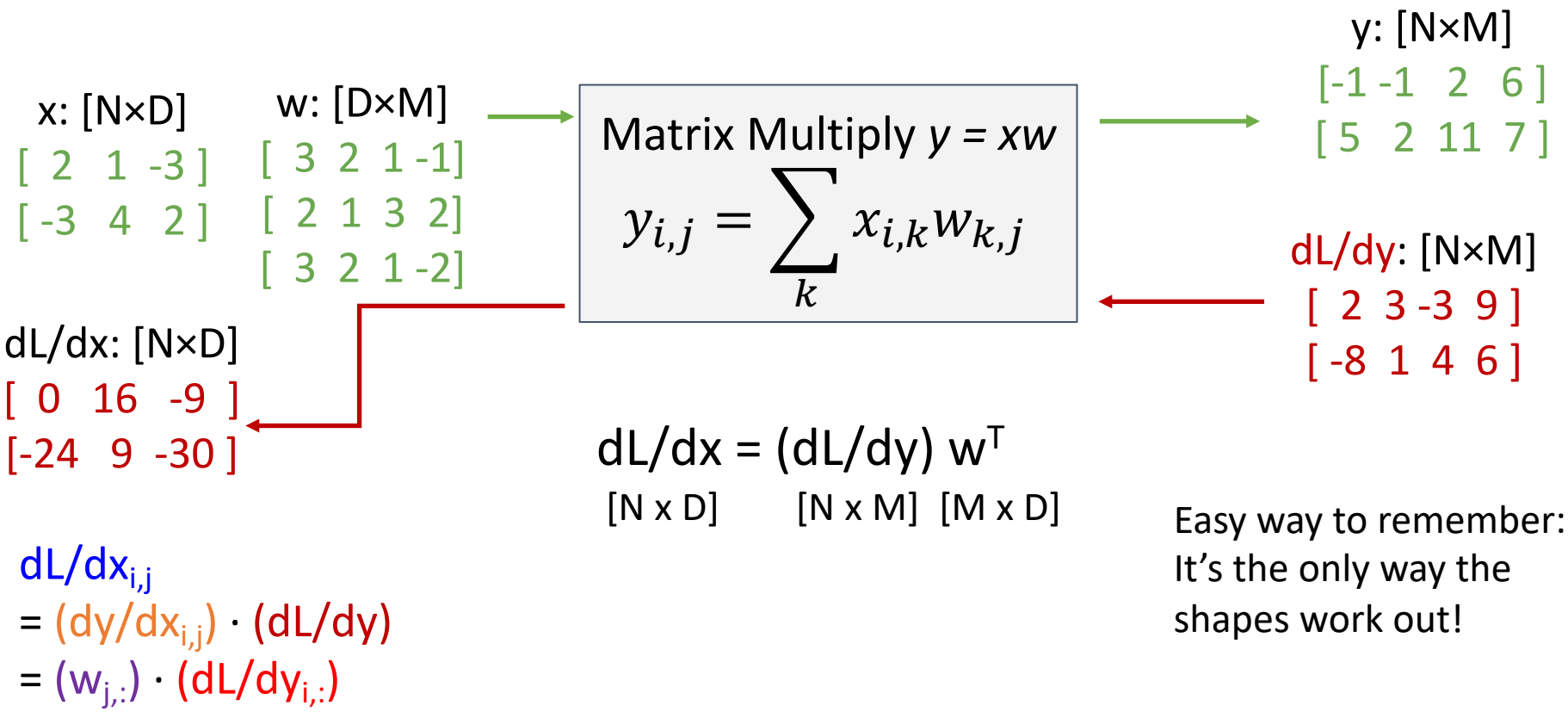
Example: Matrix Multiplication Operator



$dL/dx_{i,j}$
$= (dy/dx_{i,j}) \cdot (dL/dy)$
$= (w_{j,:}) \cdot (dL/dy_{i,:})$

Slide credit: D Fouhey & J Johnson

Example: Matrix Multiplication Operator



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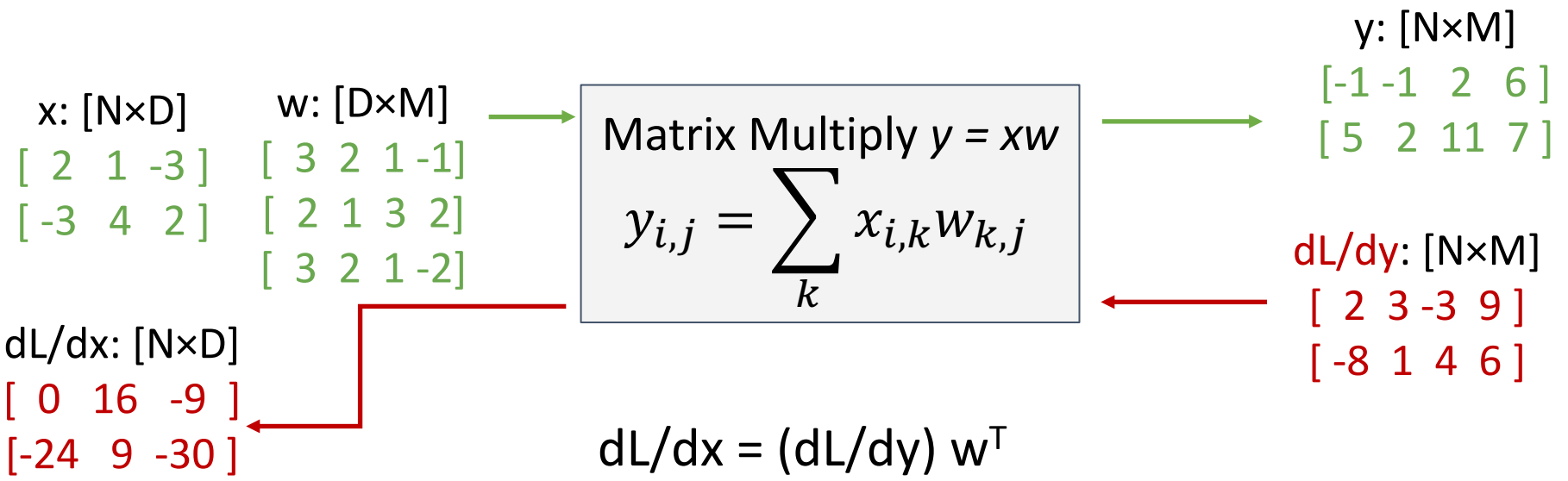


$dL/dx = (dL/dy)\, w^T$

[N x D] [N x M] [M x D]

$dL/dw = x^T\, (dL/dy)$

[D x M] [D x N] [N x M]

Easy way to remember:
It's the only way the shapes work out!

Slide credit: D Fouhey & J Johnson

Extra Resources

- Prof. Erik Learned-Miller's notes on vector, matrix, and tensor derivatives

  https://compsci682-fa21.github.io/docs/vecDerivs.pdf

- Prof. Justin Johnson's notes for a derivation of backprop for matrix multiplication

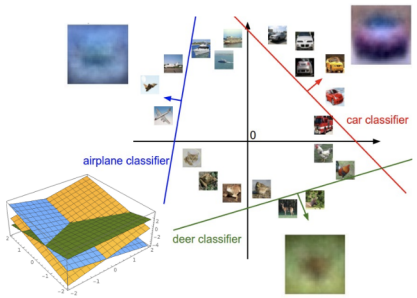
  https://web.eecs.umich.edu/~justincj/teaching/eecs442/notes/linear-backprop.html

Summary

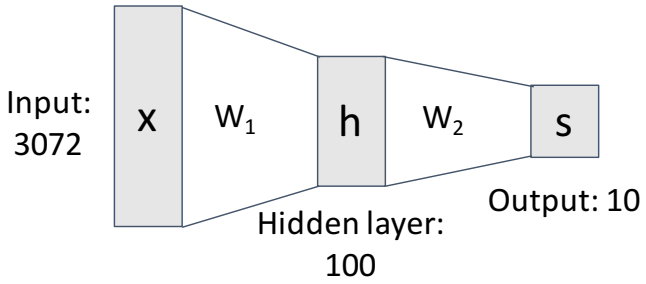
- **Computational graphs** are a useful data structure for organizing computation
- **Backpropagation** lets us compute compute gradients in a computational graph
- **Modular backprop** code composes pairs of forward and backward functions
- Backprop extends to vector and tensor-valued functions

Slide adapted from: D Fouhey & J Johnson

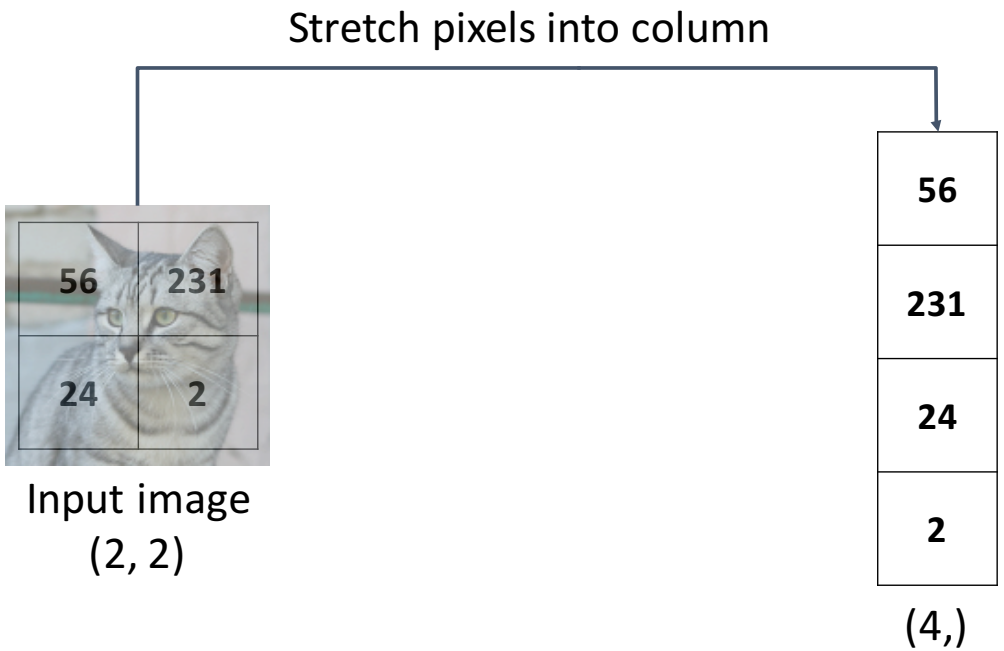
f(x,W) = Wx



$$f = W_2 \max(0, W_1 x)$$



Problem: So far our classifiers don't respect the spatial structure of images!



Slide credit: D Fouhey & J Johnson

Next Class

Convolutional Neural Networks!