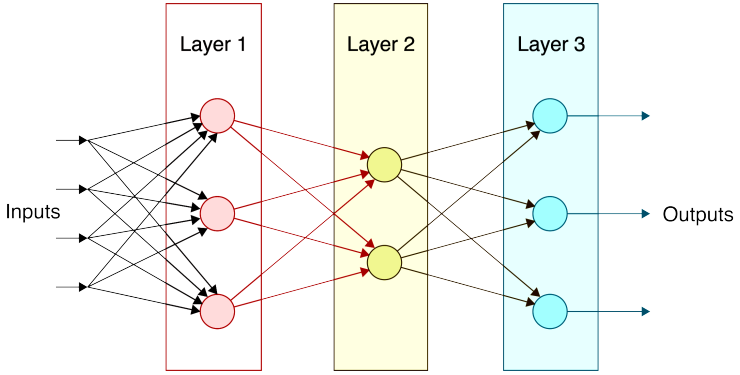
Deep Neural Networks

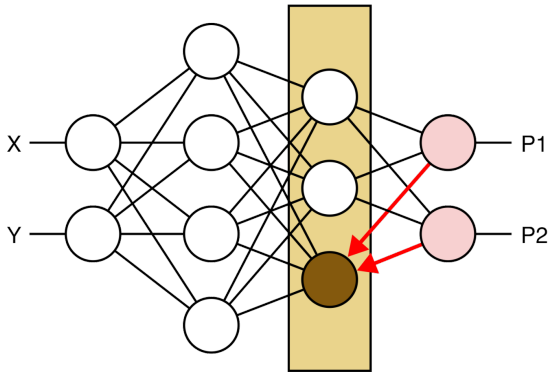
Computer Vision (UW EE/CSE 576)



Richard Szeliski

Facebook & UW

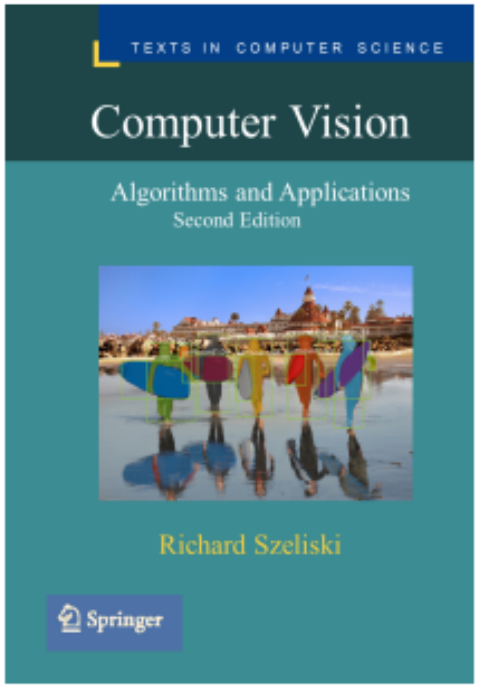
Lecture 7 – Apr 21, 2020



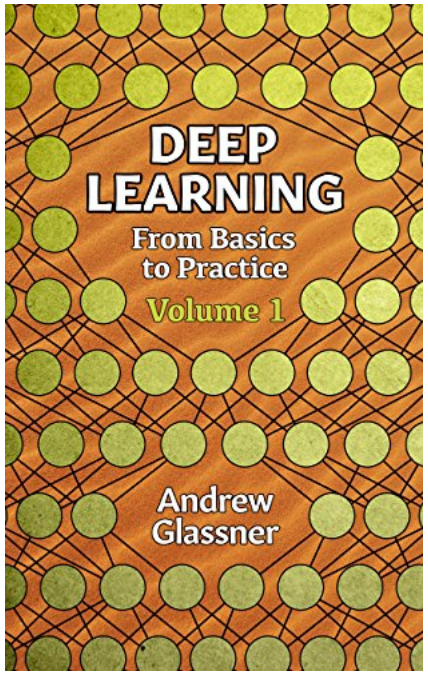
Class calendar

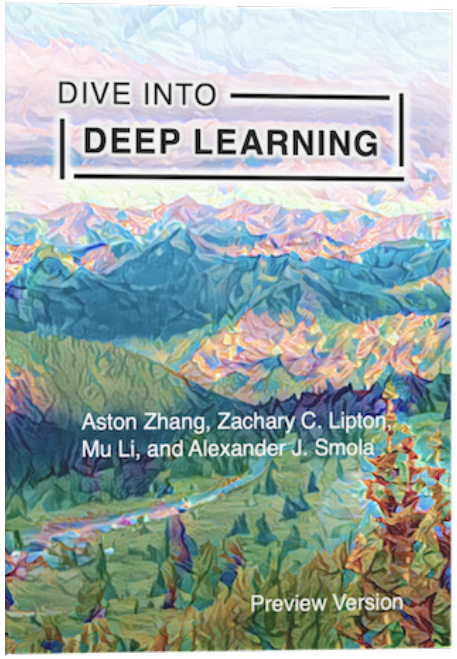
Date	Topic	Slides	Reading	Homework
April 9	Filters and convolutions	Google Slides	Szeliski, Chapter 3	HW1 due, HW2 assigned
April 14	Interpolation and Optimization	pdf, pptx	Szeliski, Chapter 4	
April 16	Machine Learning	pdf, pptx	Szeliski, Chapter 5.1-5.2	
April 21	Deep Neural Networks		Szeliski, Chapter 5.3	
April 23	Convolutional Neural Networks		Szeliski, Chapter 5.4	HW2 due, HW3 assigned
April 28	Network Architectures		Szeliski, Chapter 5.4-5.5	
April 30	Object Detection		Szeliski, Chapter 6.3	
May 5	Detection and Instance Segmentation		Szeliski, Chapter 6.4	
May 7	Edges, features, matching, RANSAC		Szeliski, Chapter 7.1-7.2, 8.1-8.2	HW3 due, HW4 assigned

References



(Thanks, Matt Dietke, for the very helpful comments.)





https://d2l.ai/

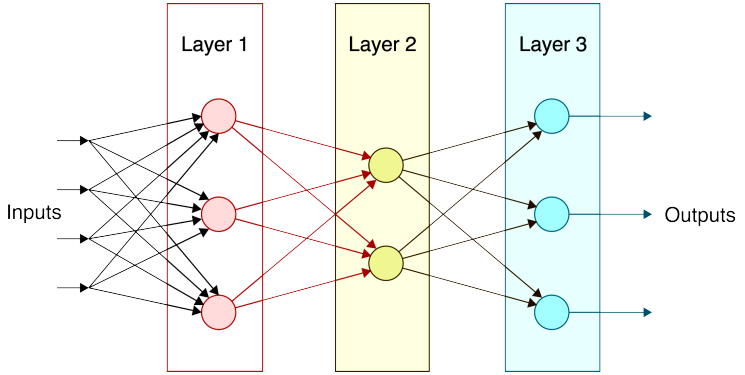
Readings

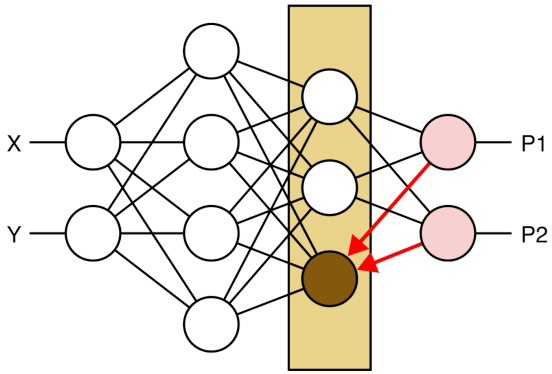
Chapter 5

Deep Learning

Deep neural networks (today's lecture)

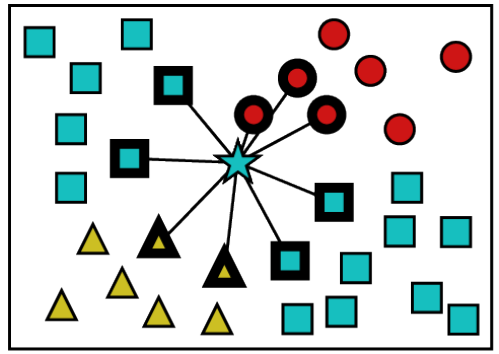
- Loss functions
- Regularization
- Weights and layers
- Activation functions
- Backpropagation
- Training and optimization (?)

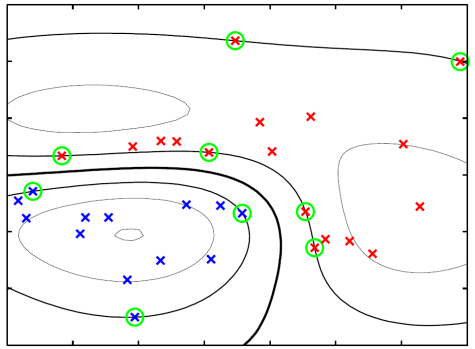




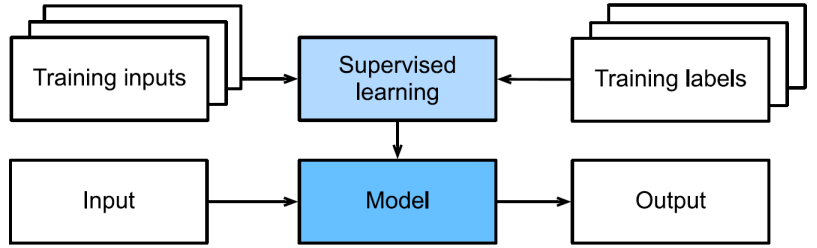
Machine learning (previous lecture)

- Why learning?
- Nearest neighbors
- Bayesian classification
- Logistic regression
- Support vector machines
- Clustering
- Principal component analysis





Supervised learning



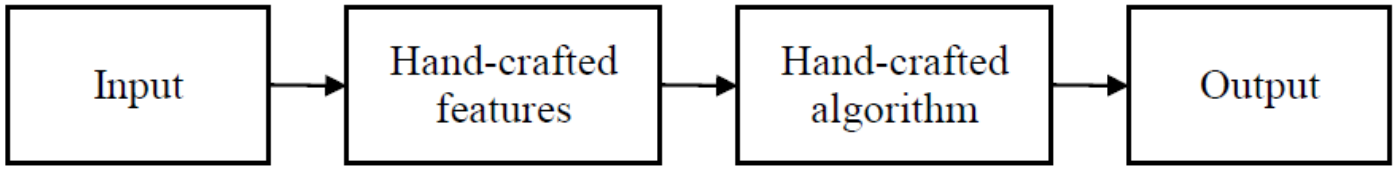
- Goal: provide best output predictions for novel inputs
- How can we predict future performance?
- Placeholder answer: minimize *empirical risk*

$$E_{\text{Risk}}(\mathbf{w}) = \frac{1}{N} \sum L(\mathbf{y}_i, \mathbf{f}(\mathbf{x}_i; \mathbf{w})). \tag{5.1}$$

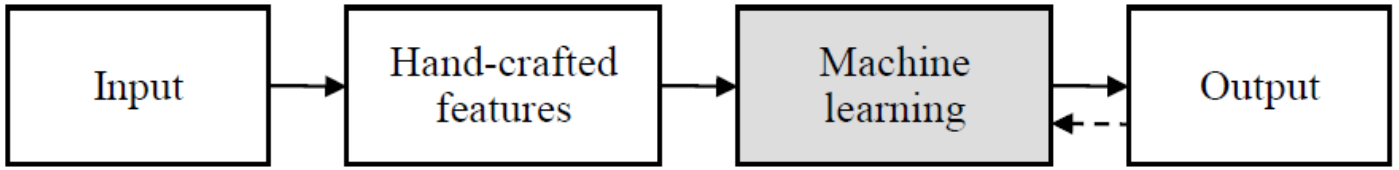
The loss function L measures the "cost" of predicting an output $\mathbf{f}(\mathbf{x}_i; \mathbf{w})$ for input $\mathbf{x}_i$ and model parameters $\mathbf{w}$ when the corresponding target is $\mathbf{y}_i$.

- What are potential *models* and *loss functions*?

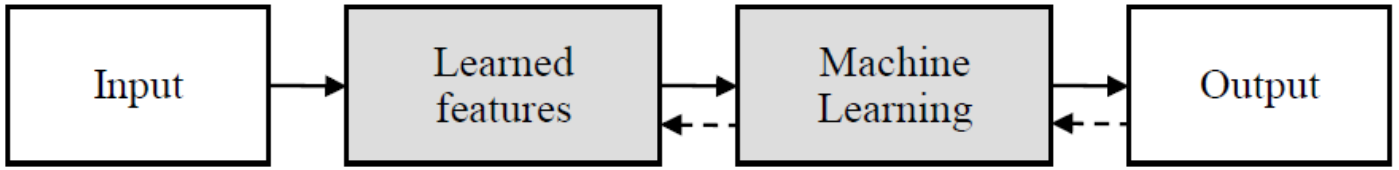
Traditional and deep learning



(a) Traditional vision pipeline

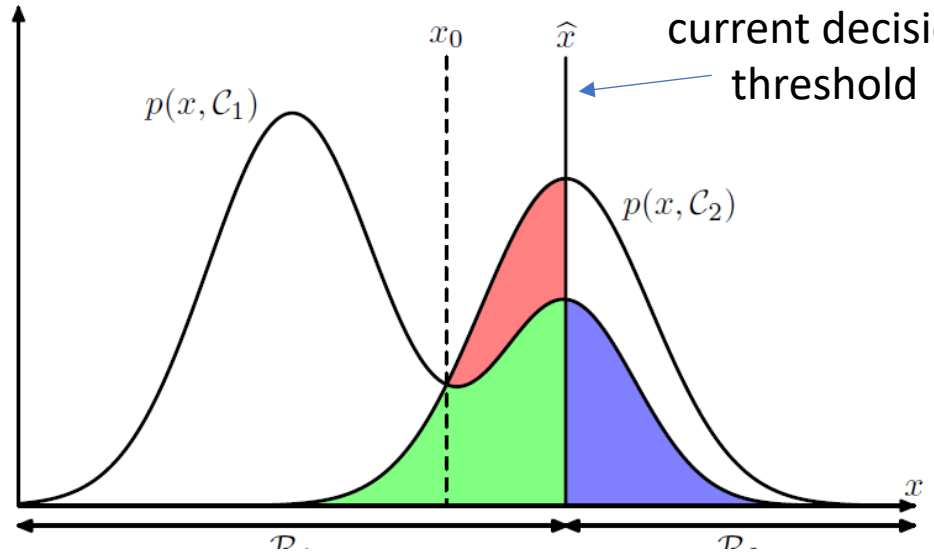


(b) Classic machine learning pipeline



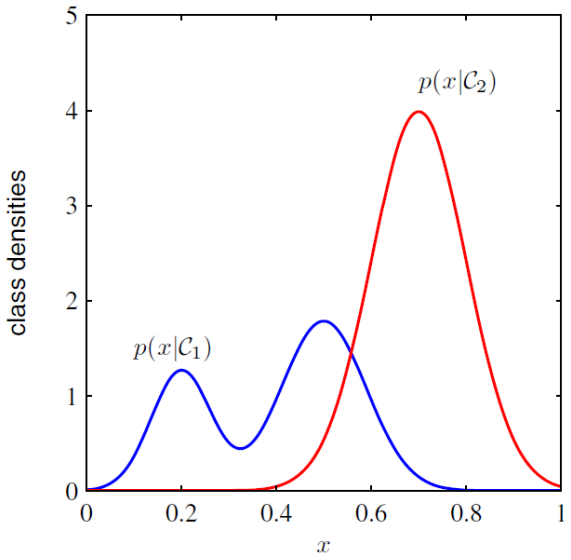
(c) Deep learning pipeline

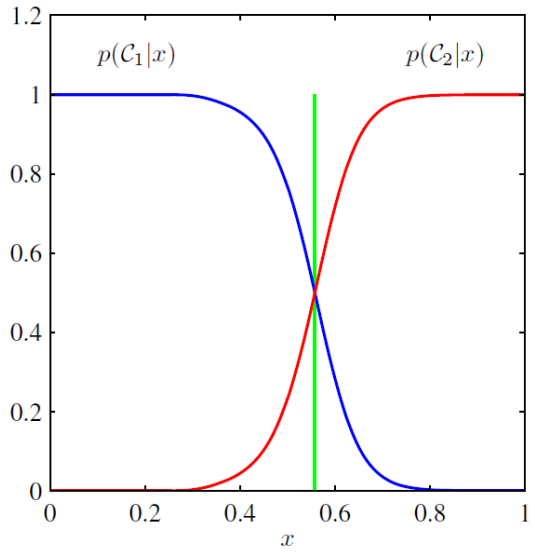
Bayesian classification



Bayes' Rule

$$y_k = p(\mathcal{C}_k|\mathbf{x}) = \frac{p(\mathbf{x}|\mathcal{C}_k)p(\mathcal{C}_k)}{\sum_j p(\mathbf{x}|\mathcal{C}_j)p(\mathcal{C}_j)}$$





Logistic regression

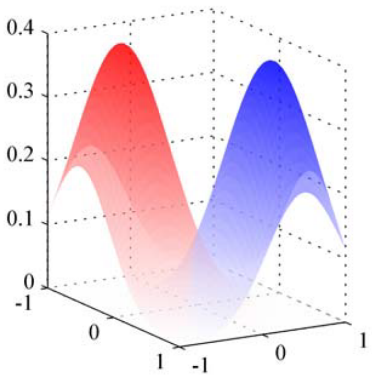
$$p(\mathcal{C}_0|\mathbf{x}) = \sigma(\mathbf{w}^T\mathbf{x} + b), \tag{5.9}$$

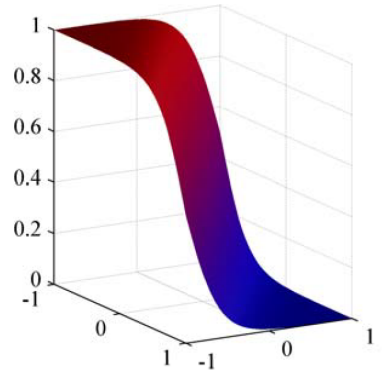
Equation (5.9), which we will revist shortly in the context of non-generative (discriminative) classification (5.18), is called *logistic regression*, since we pass the output of a linear regression formula

$$y(\mathbf{x}) = \mathbf{w}^T\mathbf{x} + b \tag{5.12}$$

through the logistic function to obtain a class probability. Figure 5.7 illustrates this in two dimensions, there the posterior likelihood of the red class $p(\mathcal{C}_0|\mathbf{x})$ is shown on the right side.

In linear regression (5.12), $\mathbf{w}$ plays the role a the *weight* vector along which we project the feature vector $\mathbf{x}$, and b plays the role of the *bias*, which determines where to set the





As before, I'm borrowing slides from

UNIVERSITY OF MICHIGAN

EECS 498-007 / 598-005
Deep Learning for Computer Vision
Fall 2019

Course Description

Computer Vision has become ubiquitous in our society, with applications in search, image understanding, apps, mapping, medicine, drones, and self-driving cars. Core to many of these applications are visual recognition tasks such as image classification and object detection. Recent developments in neural network approaches have greatly advanced the performance of these state-of-the-art visual recognition systems. This course is a deep dive into details of neural-network based deep learning methods for computer vision. During this course, students will learn to implement, train and debug their own neural networks and gain a detailed understanding of cutting-edge research in computer vision. We will cover learning algorithms, neural network architectures, and practical engineering tricks for training and fine-tuning networks for visual recognition tasks.

Instructor

Justin Johnson

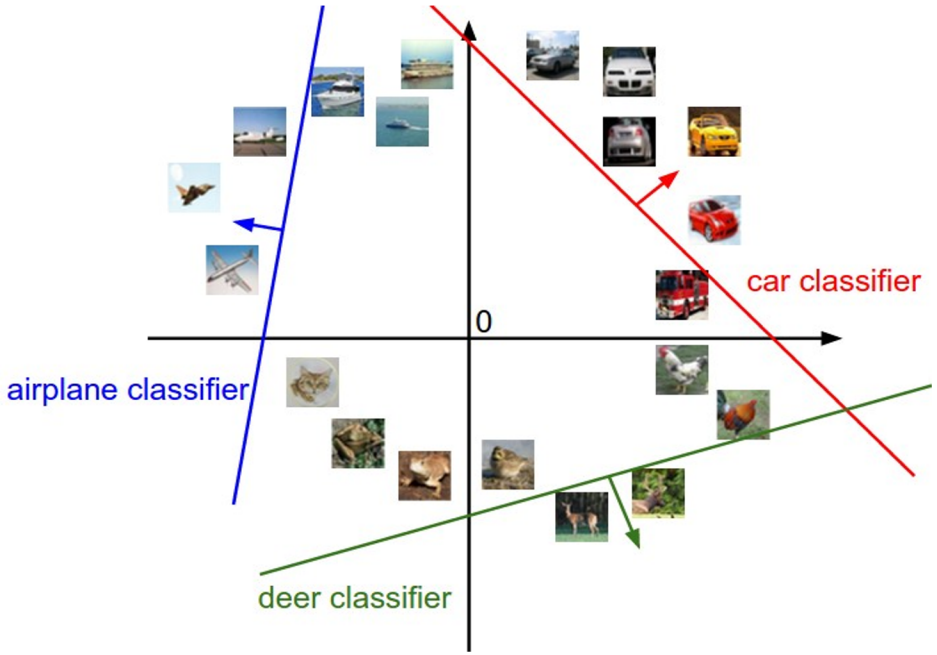
Graduate Student Instructors

Yunseok Jang

Kibok Lee

Luowei Zhou

Lecture 3: Linear Classifiers



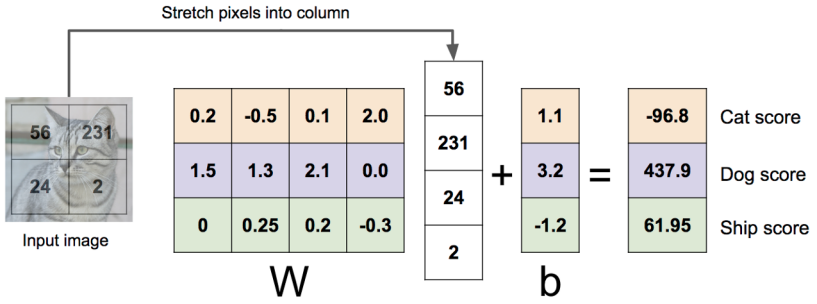
Neural Network

Linear classifiers

Linear Classifier: Three Viewpoints

Algebraic Viewpoint

$$f(x,W) = Wx$$

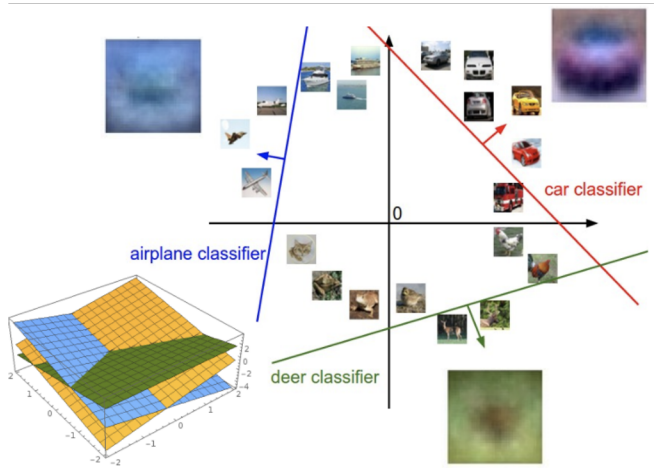


Visual Viewpoint

One template per class

Geometric Viewpoint

Hyperplanes cutting up space



So Far: Defined a linear score function

$$f(x,W) = Wx + b$$

airplane	-3.45	-0.51	3.42
automobile	-8.87	**6.04**	4.64
bird	0.09	5.31	2.65
cat	**2.9**	-4.22	5.1
deer	4.48	-4.19	2.64
dog	8.02	3.58	5.55
frog	3.78	4.49	**-4.34**
horse	1.06	-4.37	-1.5
ship	-0.36	-2.09	-4.79
truck	-0.72	-2.93	6.14

Given a W, we can compute class scores for an image x.

But how can we actually choose a good W?

Choosing a good W

$$f(x,W) = Wx + b$$



airplane	-3.45	-0.51	3.42
automobile	-8.87	**6.04**	4.64
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truck	-0.72	-2.93	6.14

TODO:

1. Use a **loss function** to quantify how good a value of W is

2. Find a W that minimizes the loss function (**optimization**)

Loss Function

A **loss function** tells how good our current classifier is

Low loss = good classifier
High loss = bad classifier

(Also called: **objective function**; **cost function**)

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Negative loss function sometimes called **reward function**, **profit function**, **utility function**, **fitness function**, etc

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Given a dataset of examples

$$\{(x_i, y_i)\}_{i=1}^{N}$$

Where x_i is image and
y_i is (integer) label

Loss Function

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Given a dataset of examples

$$\{(x_i, y_i)\}_{i=1}^{N}$$

Where x_i is image and
y_i is (integer) label

Loss for a single example is

$$L_i(f(x_i, W), y_i)$$

Loss Function

A **loss function** tells how good our current classifier is

Low loss = good classifier
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Given a dataset of examples

$$\{(x_i, y_i)\}_{i=1}^{N}$$

Where x_i is image and
y_i is (integer) label

Loss for a single example is

$$L_i(f(x_i, W), y_i)$$

Loss for the dataset is average of per-example losses:

$$L = \frac{1}{N} \sum_i L_i(f(x_i, W), y_i)$$

Regularization: Beyond Training Error

$$L(W) = \underbrace{\frac{1}{N}\sum_{i=1}^{N} L_i(f(x_i, W), y_i)}$$

Data loss: Model predictions should match training data

Regularization: Beyond Training Error

$$L(W) = \underbrace{\frac{1}{N}\sum_{i=1}^{N} L_i(f(x_i, W), y_i)}_{\text{Data loss}} + \underbrace{\lambda R(W)}_{\text{Regularization}}$$

λ = regularization strength (hyperparameter)

Data loss: Model predictions should match training data

Regularization: Prevent the model from doing *too* well on training data

Simple examples

L2 regularization: $R(W) = \sum_k \sum_l W_{k,l}^2$

L1 regularization: $R(W) = \sum_k \sum_l |W_{k,l}|$

Elastic net (L1 + L2): $R(W) = \sum_k \sum_l \beta W_{k,l}^2 + |W_{k,l}|$

More complex:

Dropout

Batch normalization

Cutout, Mixup, Stochastic depth, etc…

Regularization: Beyond Training Error

$$L(W) = \underbrace{\frac{1}{N}\sum_{i=1}^{N} L_i(f(x_i, W), y_i)}_{\text{Data loss}} + \underbrace{\lambda R(W)}_{\text{Regularization}}$$

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Data loss: Model predictions should match training data

Regularization: Prevent the model from doing *too* well on training data

Purpose of Regularization:

- Express preferences in among models beyond ”minimize training error”
- Avoid **overfitting**: Prefer simple models that generalize better
- Improve optimization by adding curvature

Cross-Entropy Loss (Multinomial Logistic Regression)

Want to interpret raw classifier scores as **probabilities**

$$s = f(x_i; W)$$

$$P(Y = k|X = x_i) = \frac{e^{s_k}}{\sum_j e^{s_j}}$$

Softmax function

$$L_i = -\log P(Y = y_i|X = x_i)$$

	Unnormalized log-probabilities / logits	exp	Probabilities must be >= 0 unnormalized probabilities	normalize	Probabilities must sum to 1 probabilities
cat	**3.2**		**24.5**		**0.13**
car	5.1		164.0		0.87
frog	-1.7		0.18		0.00

$L_i = -\log(0.13)$
$= \mathbf{2.04}$

Maximum Likelihood Estimation
Choose weights to maximize the likelihood of the observed data (next lecture)

Cross-Entropy Loss (Multinomial Logistic Regression)

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car	5.1		164.0		0.87		0.00
frog	-1.7		0.18		0.00		0.00

Kullback–Leibler divergence

$$D_{KL}(P||Q) = \sum_y P(y) \log \frac{P(y)}{Q(y)}$$

Cross-Entropy Loss (Multinomial Logistic Regression)

Want to interpret raw classifier scores as **probabilities**

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frog	-1.7		0.18		0.00		0.00

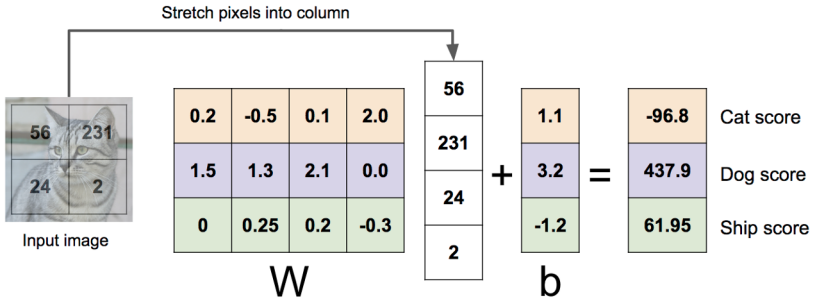
Cross Entropy

$$H(P, Q) = H(p) + D_{KL}(P\|Q)$$

Recap: Three ways to think about linear classifiers

Algebraic Viewpoint

$f(x,W) = Wx$



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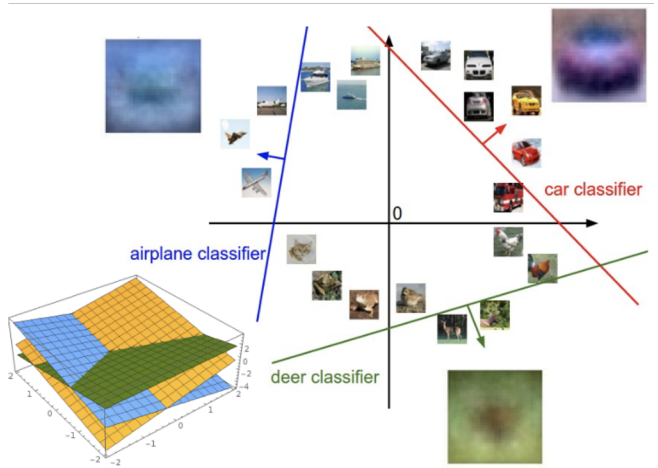


Recap: Loss Functions quantify preferences

- We have some dataset of (x, y)
- We have a **score function:**
- We have a **loss function**:

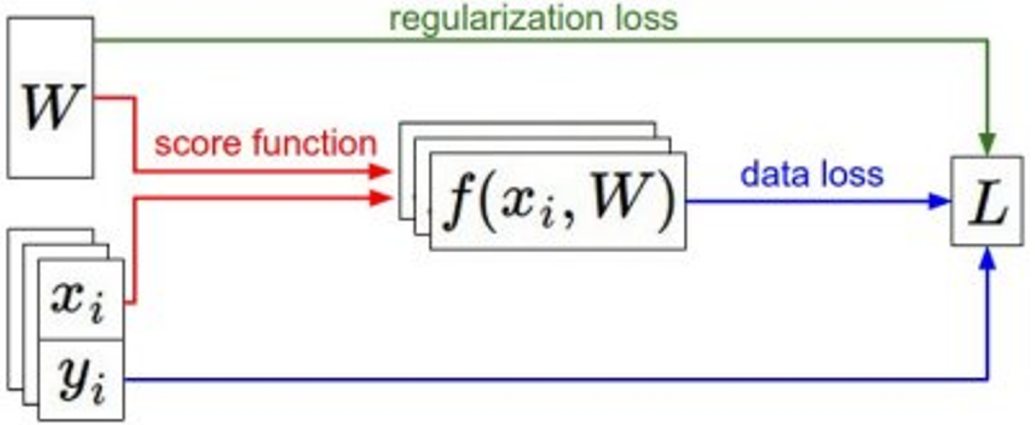
$$s = f(x; W) = Wx$$

Linear classifier

$$L_i = -\log\left(\frac{e^{sy_i}}{\sum_j e^{s_j}}\right)$$ Softmax

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

$$L = \frac{1}{N}\sum_{i=1}^{N} L_i + R(W)$$ Full loss



Recap: Loss Functions quantify preferences

- We have some dataset of (x, y)
- We have a **score function:**
- We have a **loss function**:

Q: How do we find the best W?

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

Linear classifier

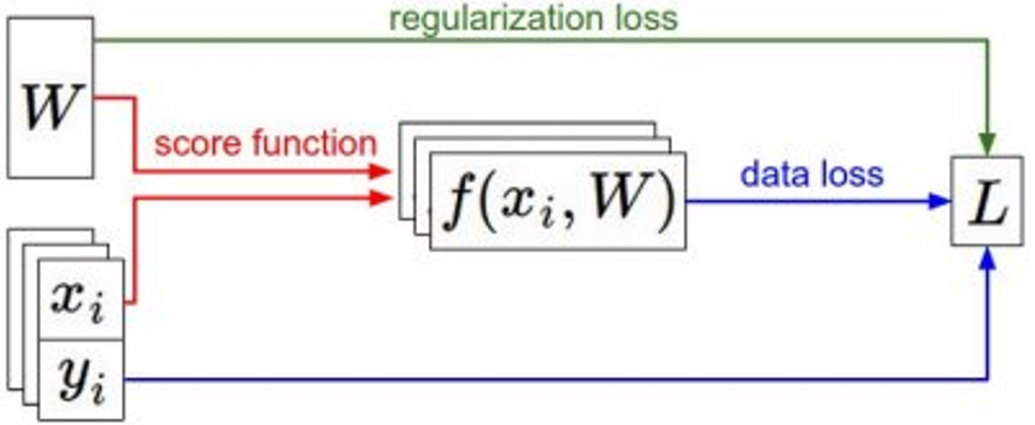
A: Later in this lecture

$$L_i = -\log\left(\frac{e^{sy_i}}{\sum_j e^{s_j}}\right)$$ Softmax

SVM

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

$$L = \frac{1}{N}\sum_{i=1}^{N} L_i + R(W)$$ Full loss

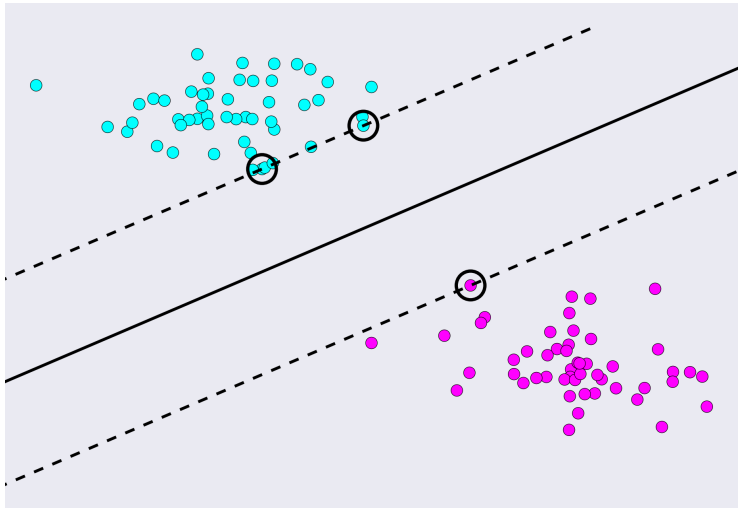


Machine learning

- Why learning?
- Nearest neighbors
- Bayesian classification
- Logistic regression
- Support vector machines
- Clustering
- Principal component analysis

Support vector machines (SVMs)

- Maximize the *margin* between the decision surfaces
- The only points that matter are the circled *support vectors*



n margin classifier, we need to
$l_i = \mathbf{w} \cdot \mathbf{x}_i + b$ (5.17) have an
ıote this more compactly, let

$$\hat{t}_i = 2t_i - 1, \quad \hat{t}_i \in \{-1, 1\}$$

an now re-write the inequality

$$\hat{t}_i(\mathbf{w} \cdot \mathbf{x}_i + b) \geq 1.$$

simply find the smallest norm
ization problem

$$\arg\min_{\mathbf{w},b} \|\mathbf{w}\|^2$$

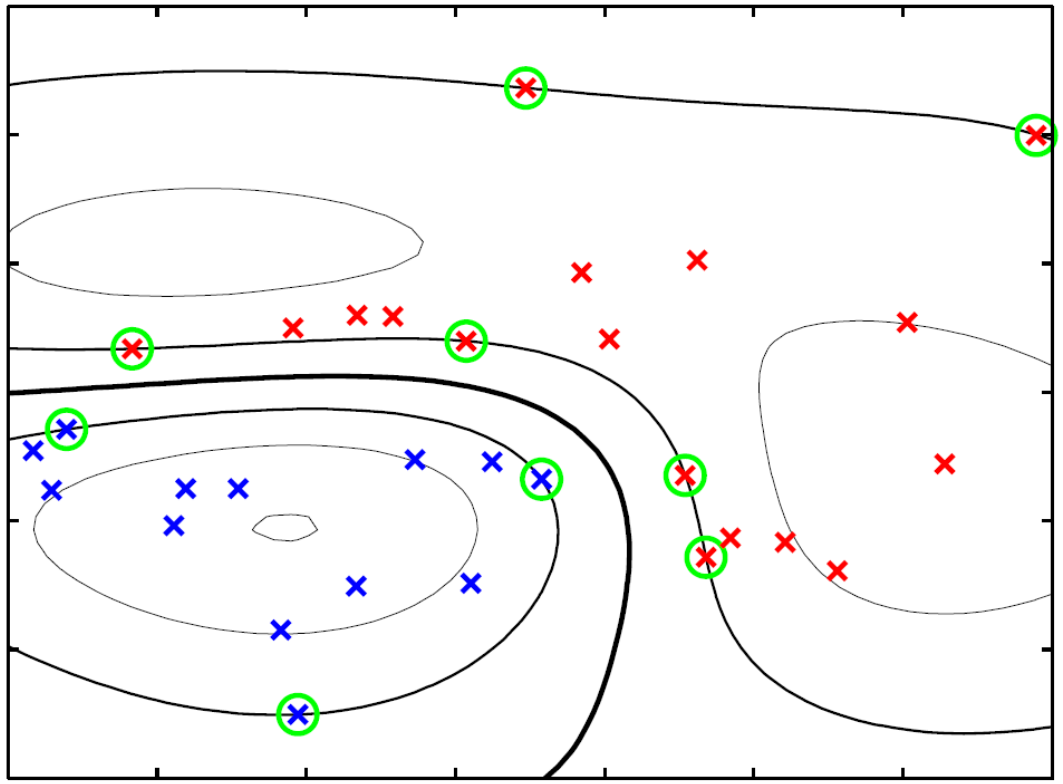
assic *quadratic programming*

Kernelized support vector machines

- Replace linear function with a sum of *kernel functions* (e.g., Gaussian bumps)

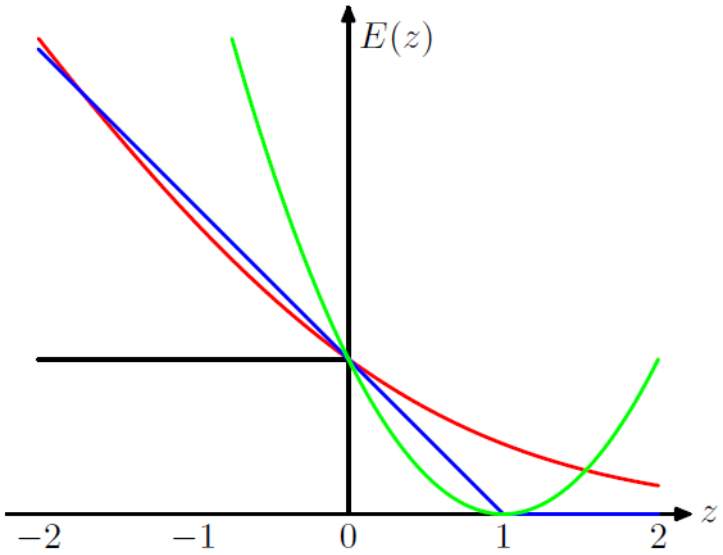
$$l = f(\mathbf{x}) = \sum_k \mathbf{w}_k \phi(\|\mathbf{x} - \mathbf{x}_k\|).$$

- Circled points are *support vectors*, lie on $f = \pm 1$ surfaces ($f = 0$ is the dark curve)



Hinge loss vs. logistic regression

Figure 7.5 Plot of the 'hinge' error function used in support vector machines, shown in blue, along with the error function for logistic regression, rescaled by a factor of $1/\ln(2)$ so that it passes through the point $(0, 1)$, shown in red. Also shown are the misclassification error in black and the squared error in green.



remaining points we have $\xi_n = 1 - y_n t_n$. Thus the objective function (7.21) can be written (up to an overall multiplicative constant) in the form

$$\sum_{n=1}^{N} E_{\mathrm{SV}}(y_n t_n) + \lambda \|\mathbf{w}\|^2 \tag{7.44}$$

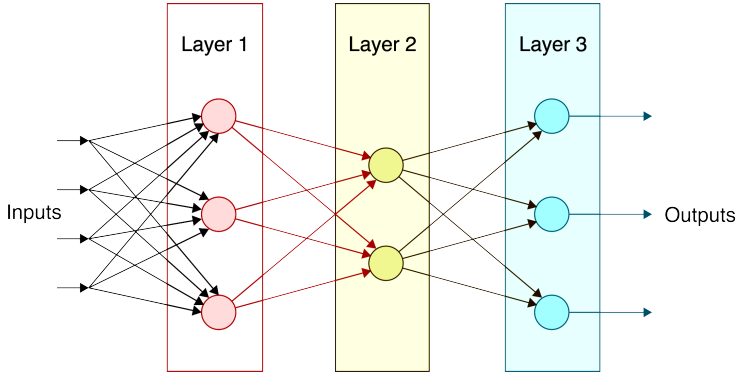
where $\lambda = (2C)^{-1}$, and $E_{\mathrm{SV}}(\cdot)$ is the *hinge* error function defined by

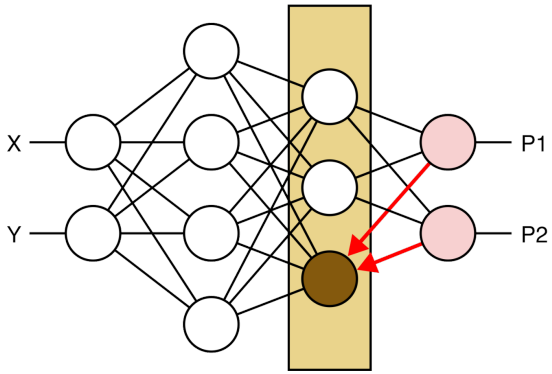
$$E_{\mathrm{SV}}(y_n t_n) = [1 - y_n t_n]_+ \tag{7.45}$$

where $[\cdot]_+$ denotes the positive part. The hinge error function, so-called because of its shape, is plotted in Figure 7.5. It can be viewed as an approximation to the misclassification error, i.e., the error function that ideally we would like to minimize, which is also shown in Figure 7.5.

Deep neural networks (today's lecture)

- Loss functions
- Regularization
- Weights and layers
- Activation functions
- Backpropagation
- Training and optimization

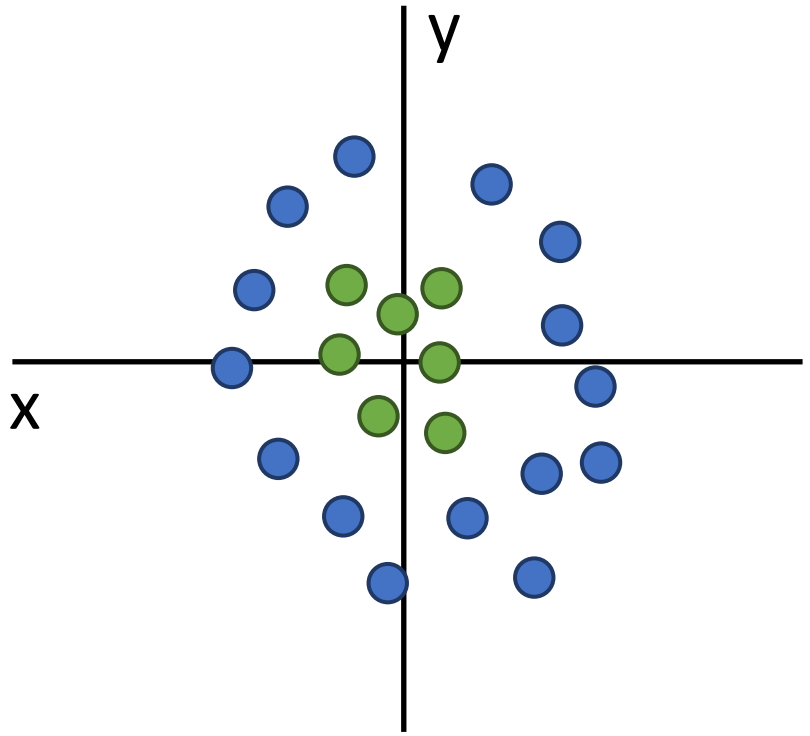




Lecture 5:
Neural Networks

Problem: Linear Classifiers aren't that powerful

Geometric Viewpoint

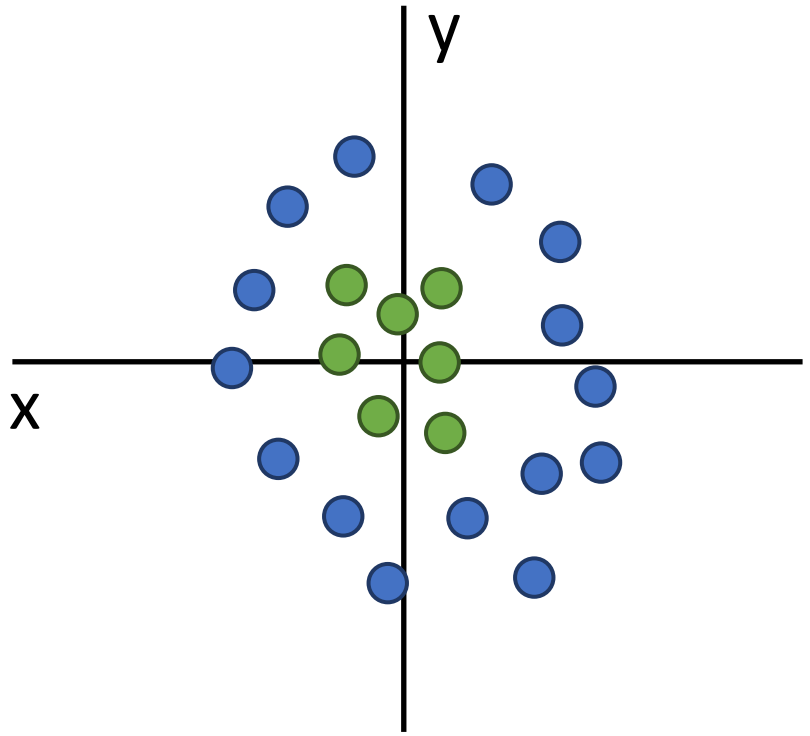


Visual Viewpoint

One template per class:
Can't recognize different
modes of a class

One solution: **Feature Transforms**

Original space

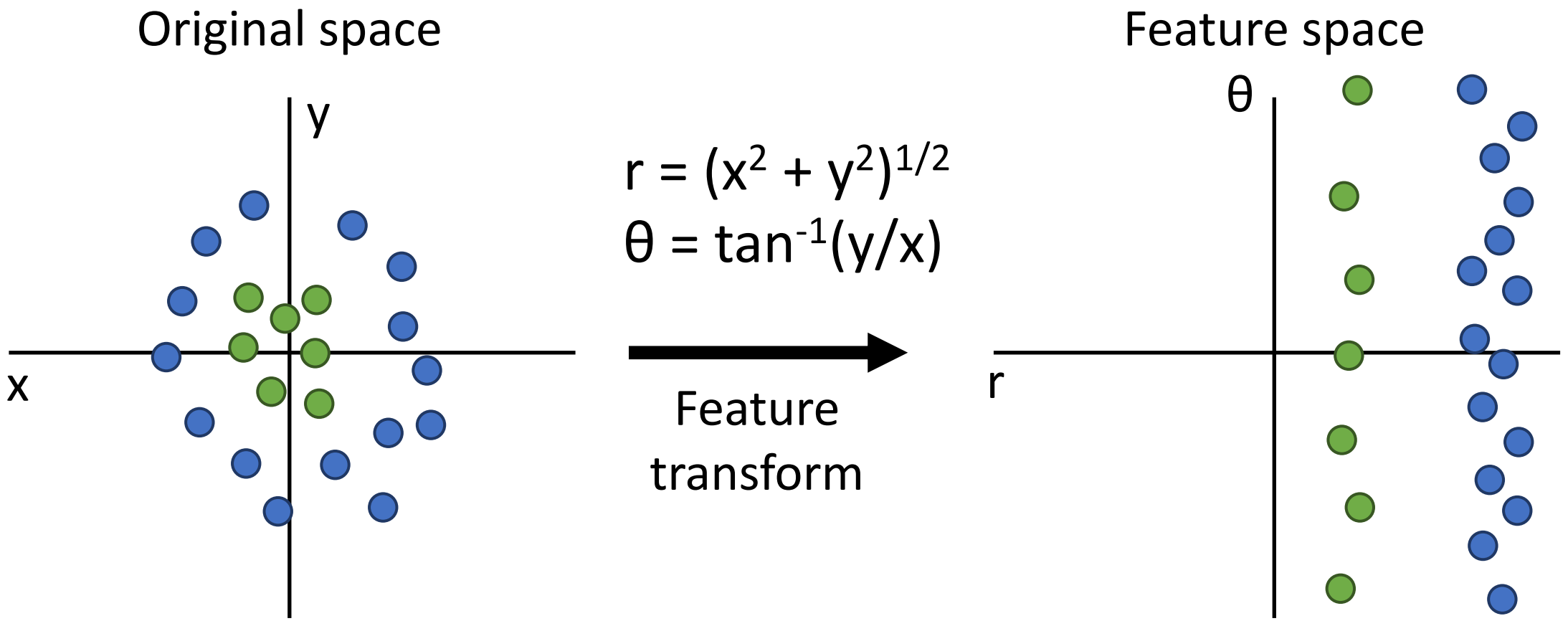


$r = (x^2 + y^2)^{1/2}$

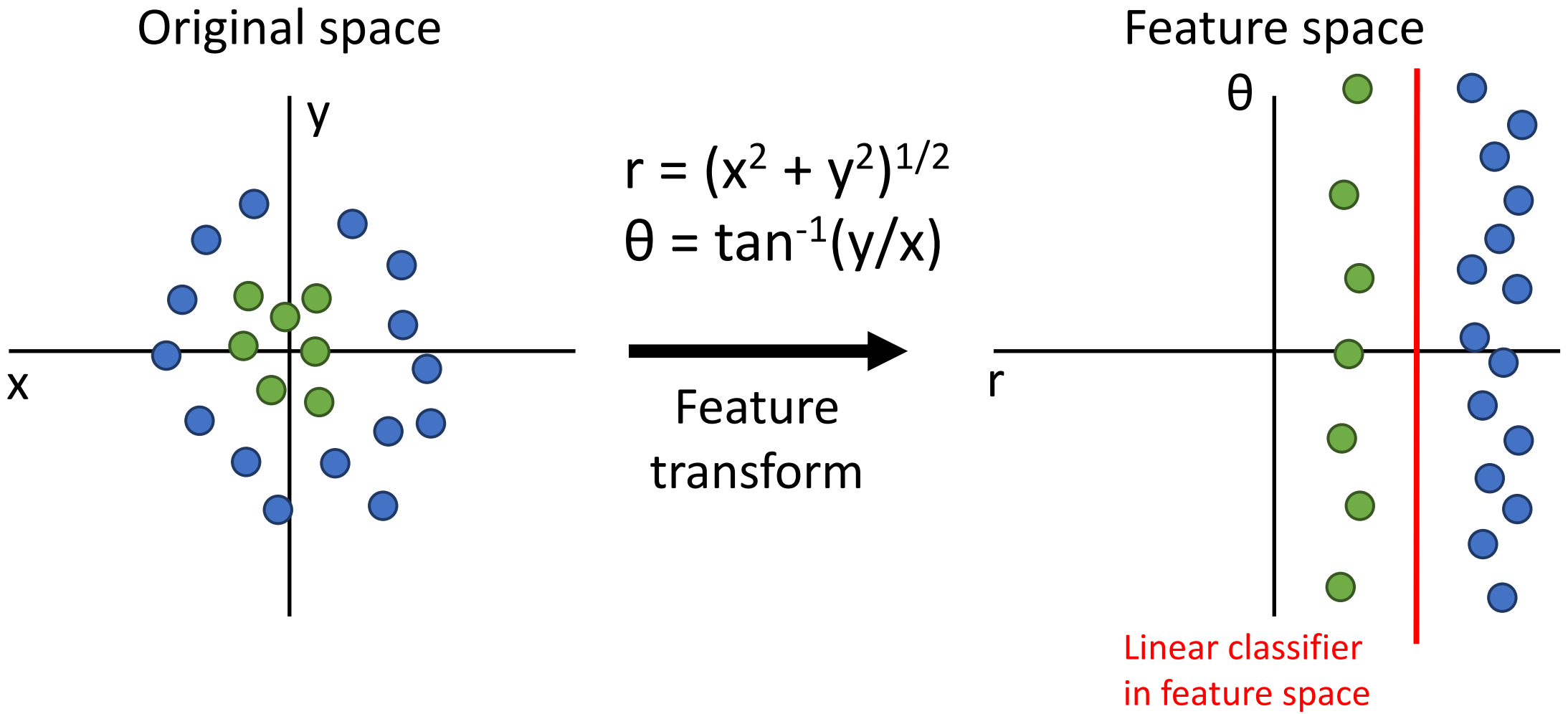
$\theta = \tan^{-1}(y/x)$

Feature transform

One solution: **Feature Transforms**



One solution: **Feature Transforms**



One solution: **Feature Transforms**

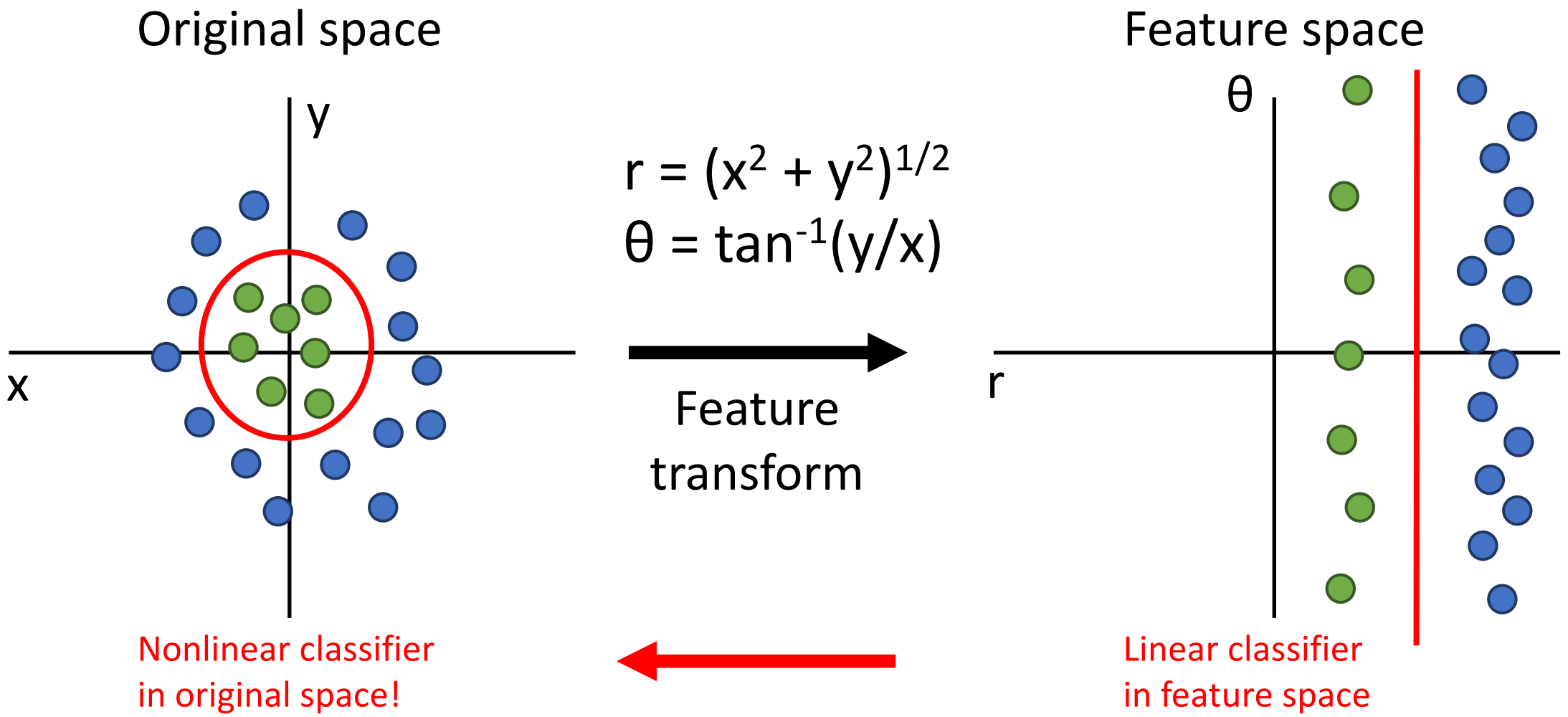
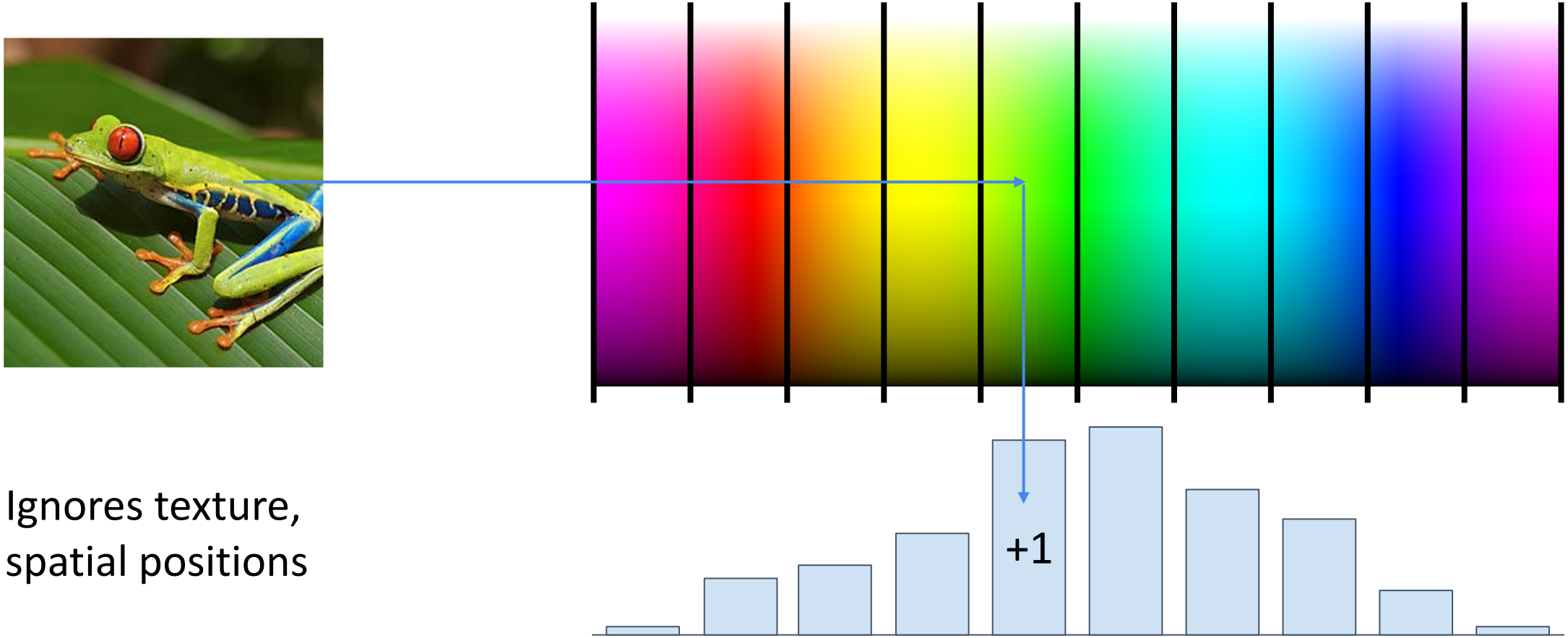


Image Features: Color Histogram



Ignores texture,
spatial positions

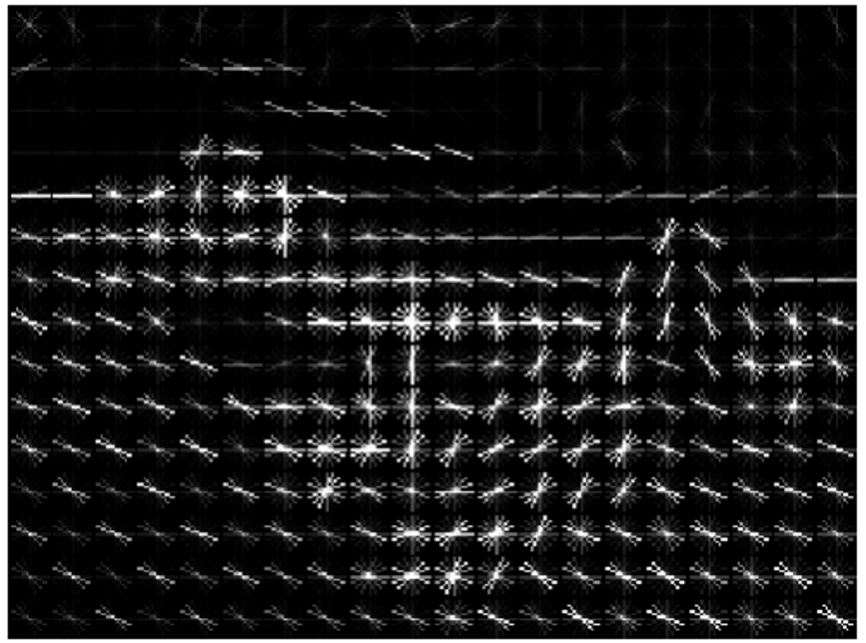
Frog image is in the public domain

Image Features: Histogram of Oriented Gradients (HoG)

1. Compute edge direction / strength at each pixel
2. Divide image into 8x8 regions
3. Within each region compute a histogram of edge directions weighted by edge strength

Lowe, “Object recognition from local scale-invariant features”, ICCV 1999
Dalal and Triggs, "Histograms of oriented gradients for human detection," CVPR 2005

Image Features: Histogram of Oriented Gradients (HoG)

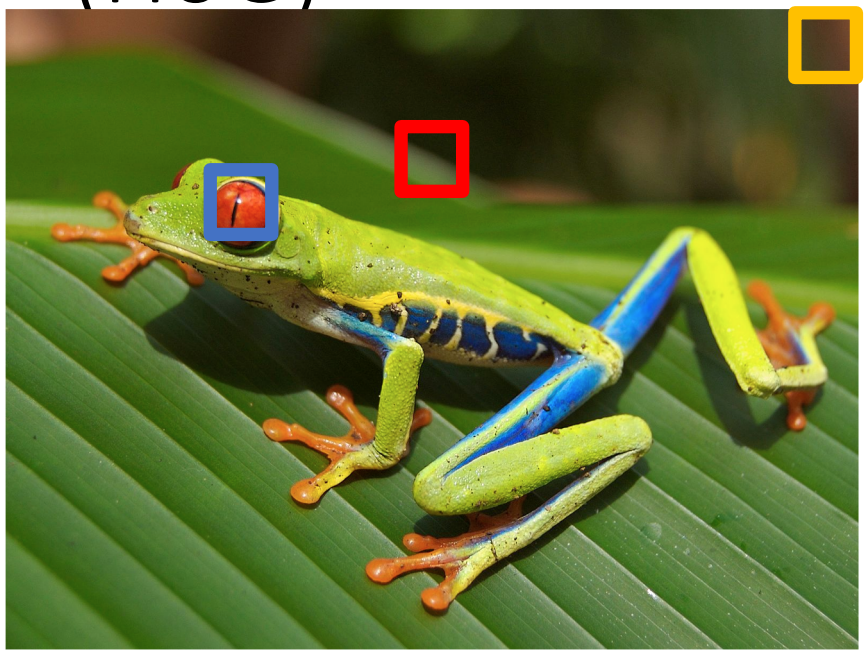


1. Compute edge direction / strength at each pixel
2. Divide image into 8x8 regions
3. Within each region compute a histogram of edge directions weighted by edge strength

Example: 320x240 image gets divided into 40x30 bins; 8 directions per bin; feature vector has 30*40*9 = 10,800 numbers

Lowe, “Object recognition from local scale-invariant features”, ICCV 1999
Dalal and Triggs, "Histograms of oriented gradients for human detection," CVPR 2005

Image Features: Histogram of Oriented Gradients (HoG)



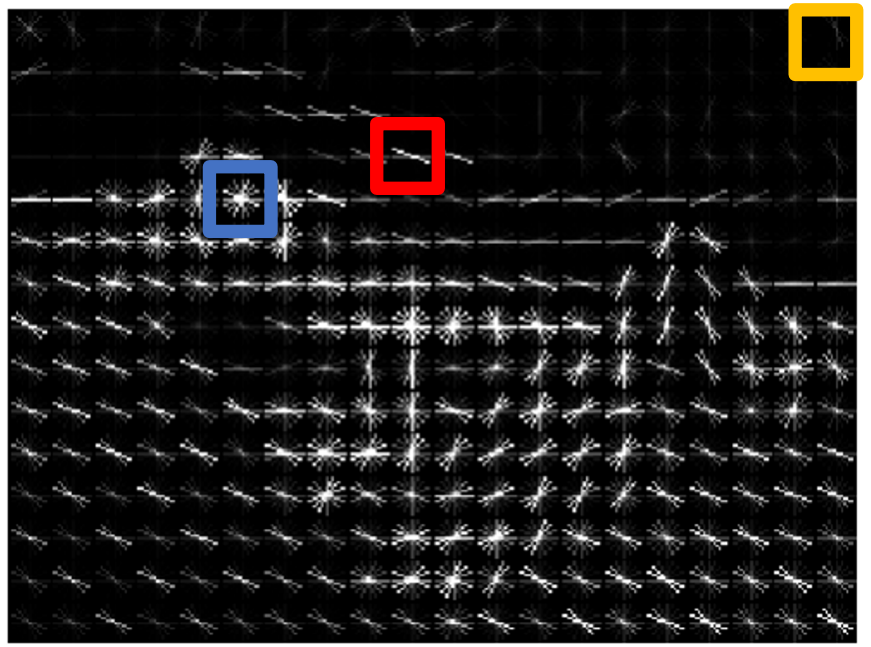
1. Compute edge direction / strength at each pixel
2. Divide image into 8x8 regions
3. Within each region compute a histogram of edge directions weighted by edge strength

Weak edges

Strong diagonal edges

Edges in all directions

Captures texture and position, robust to small image changes



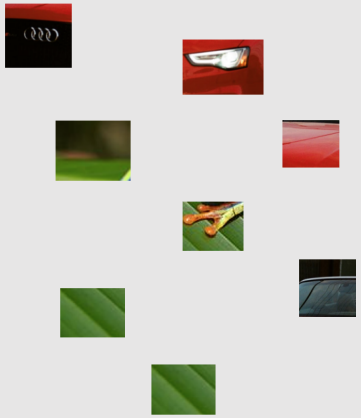
Example: 320x240 image gets divided into 40x30 bins; 8 directions per bin; feature vector has 30*40*9 = 10,800 numbers

Lowe, “Object recognition from local scale-invariant features”, ICCV 1999
Dalal and Triggs, "Histograms of oriented gradients for human detection," CVPR 2005

Image Features: Bag of Words (Data-Driven!)

Step 1: Build codebook

Extract random patches



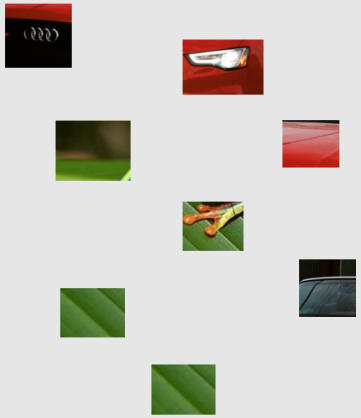
Cluster patches to form “codebook” of “visual words”

Fei-Fei and Perona, “A bayesian hierarchical model for learning natural scene categories”, CVPR 2005

Image Features: Bag of Words (Data-Driven!)

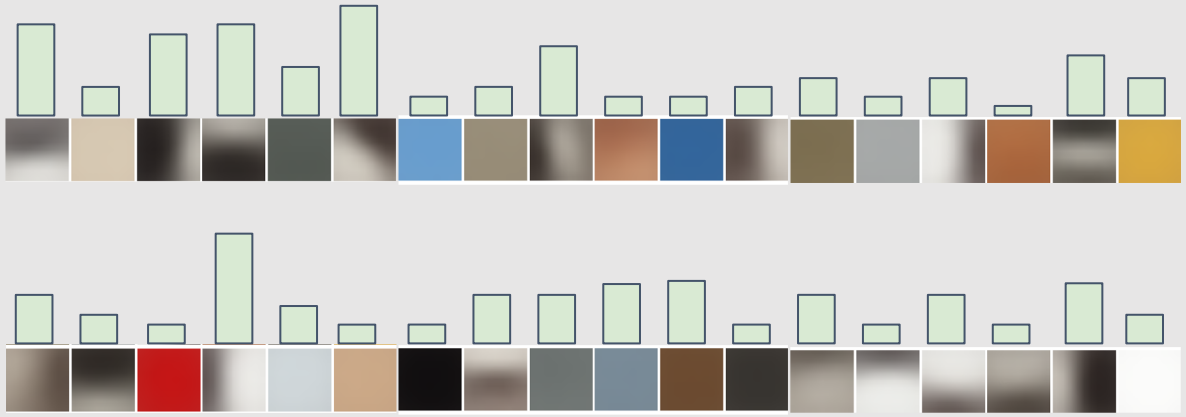
Step 1: Build codebook

Extract random patches



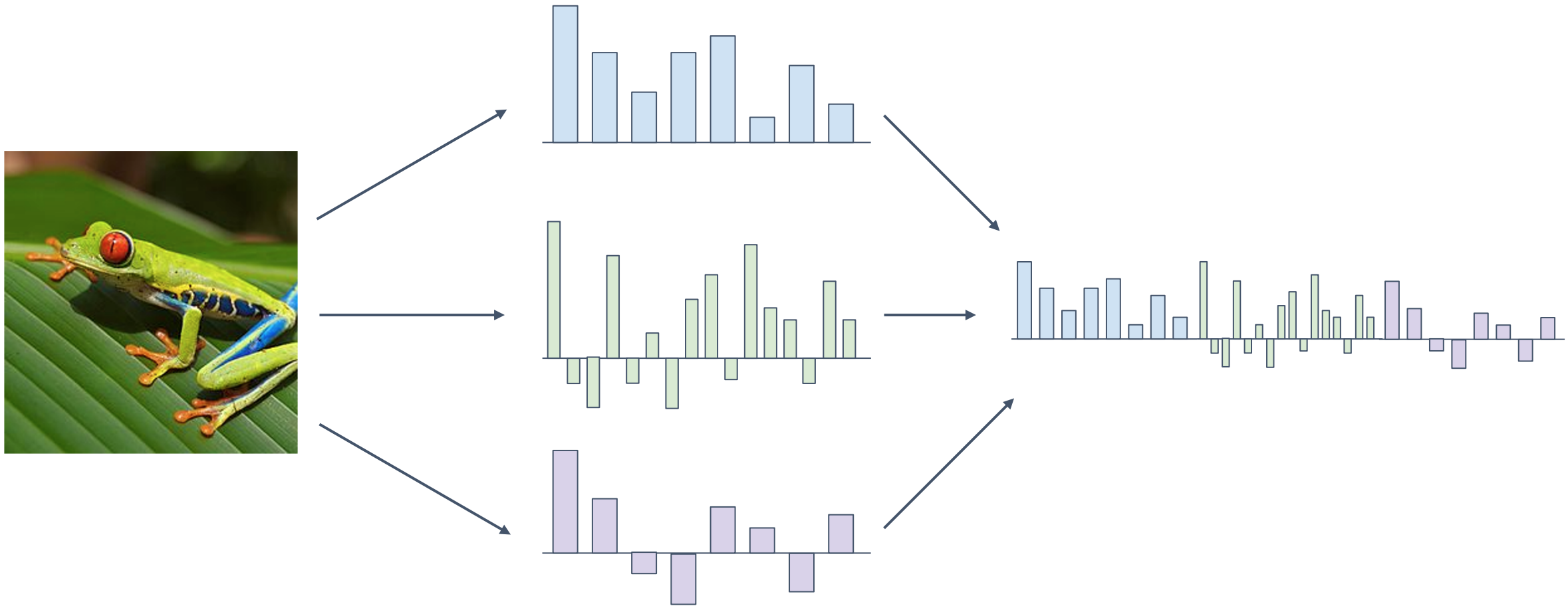
Cluster patches to form “codebook” of “visual words”

Step 2: Encode images



Fei-Fei and Perona, “A bayesian hierarchical model for learning natural scene categories”, CVPR 2005

Image Features



Example: Winner of 2011 ImageNet challenge

Low-level feature extraction ≈ 10k patches per image

- SIFT: 128-dim
- color: 96-dim

} reduced to 64-dim with PCA

FV extraction and compression:

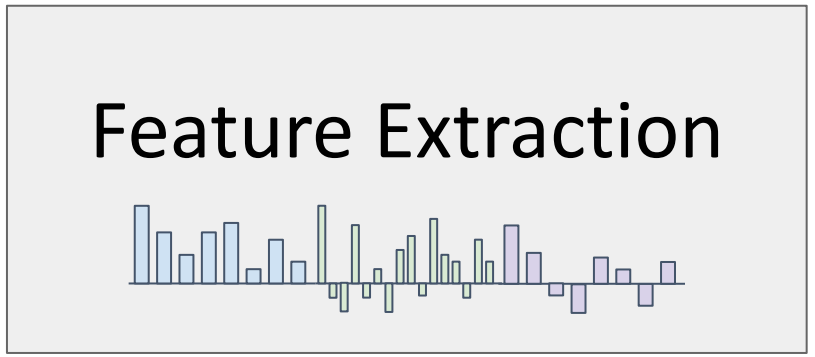
- N=1,024 Gaussians, R=4 regions ⇨ 520K dim x 2
- compression: G=8, b=1 bit per dimension

One-vs-all SVM learning with SGD

Late fusion of SIFT and color systems

F. Perronnin, J. Sánchez, "Compressed Fisher vectors for LSVRC", PASCAL VOC / ImageNet workshop, ICCV, 2011.

Image Features



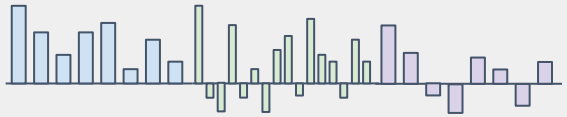
f

10 numbers giving scores for classes

training

Image Features vs Neural Networks

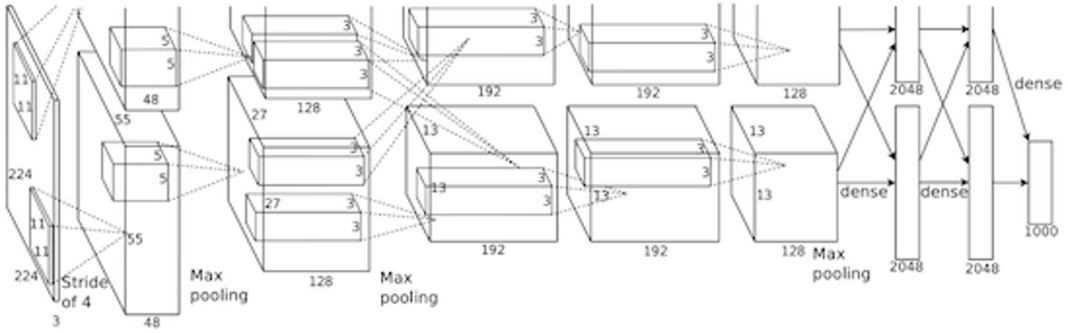
Feature Extraction



f

10 numbers giving scores for classes

training



Krizhevsky, Sutskever, and Hinton, "Imagenet classification with deep convolutional neural networks", NIPS 2012. Figure copyright Krizhevsky, Sutskever, and Hinton, 2012. Reproduced with permission.

10 numbers giving scores for classes

training

Neural Networks

(**Before**) Linear score function: $f = Wx$

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

Neural Networks

(**Before**) Linear score function: $f = Wx$

(**Now**) 2-layer Neural Network $f = W_2 \max(0, W_1 x)$

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

(In practice we will usually add a learnable bias at each layer as well)

Neural Networks

(**Before**) Linear score function: $f = Wx$

(**Now**) 2-layer Neural Network $f = W_2 \max(0, W_1 x)$

or 3-layer Neural Network

$$f = W_3 \max(0, W_2 \max(0, W_1 x))$$

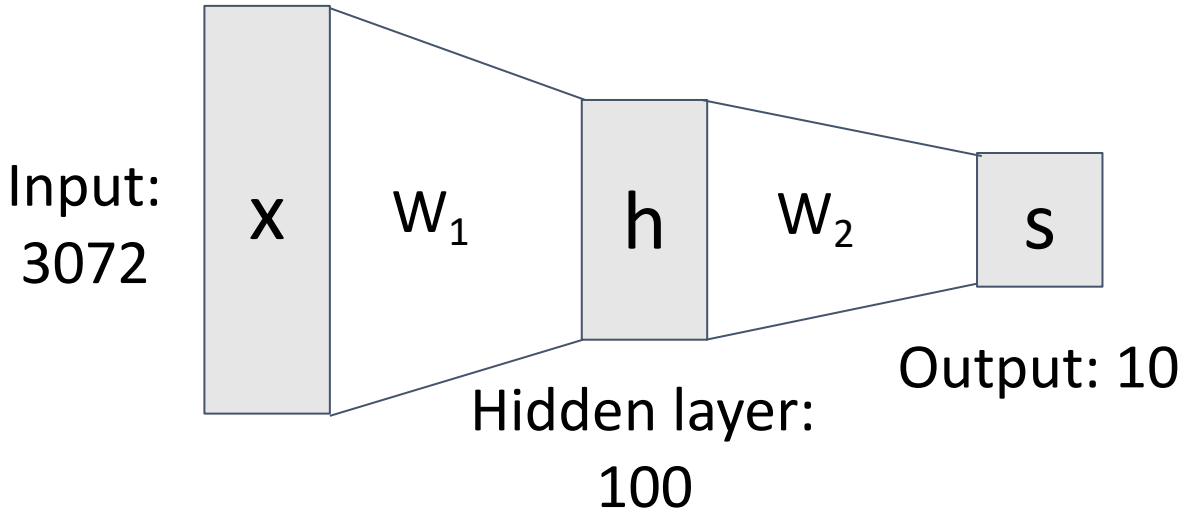
$W_3 \in \mathbb{R}^{C \times H_2}$ $W_2 \in \mathbb{R}^{H_2 \times H_1}$ $W_1 \in \mathbb{R}^{H_1 \times D}$ $x \in \mathbb{R}^D$

(In practice we will usually add a learnable bias at each layer as well)

Neural Networks

(**Before**) Linear score function: $f = Wx$

(**Now**) 2-layer Neural Network $f = W_2 \max(0, W_1 x)$



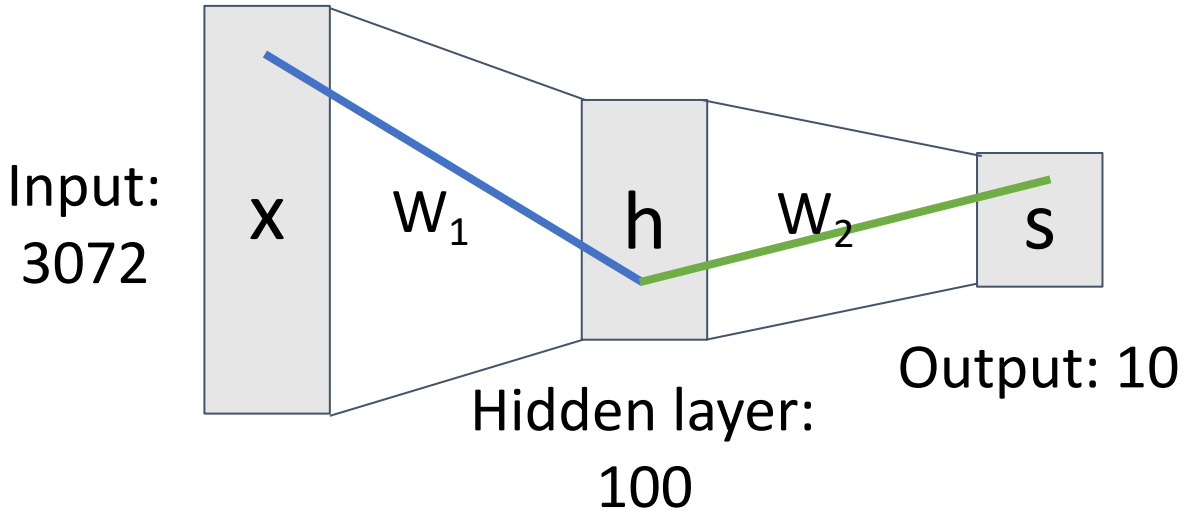
$$x \in \mathbb{R}^D, W_1 \in \mathbb{R}^{H \times D}, W_2 \in \mathbb{R}^{C \times H}$$

Neural Networks

(**Before**) Linear score function: $f = Wx$

(**Now**) 2-layer Neural Network $f = W_2 \max(0, W_1 x)$

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

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

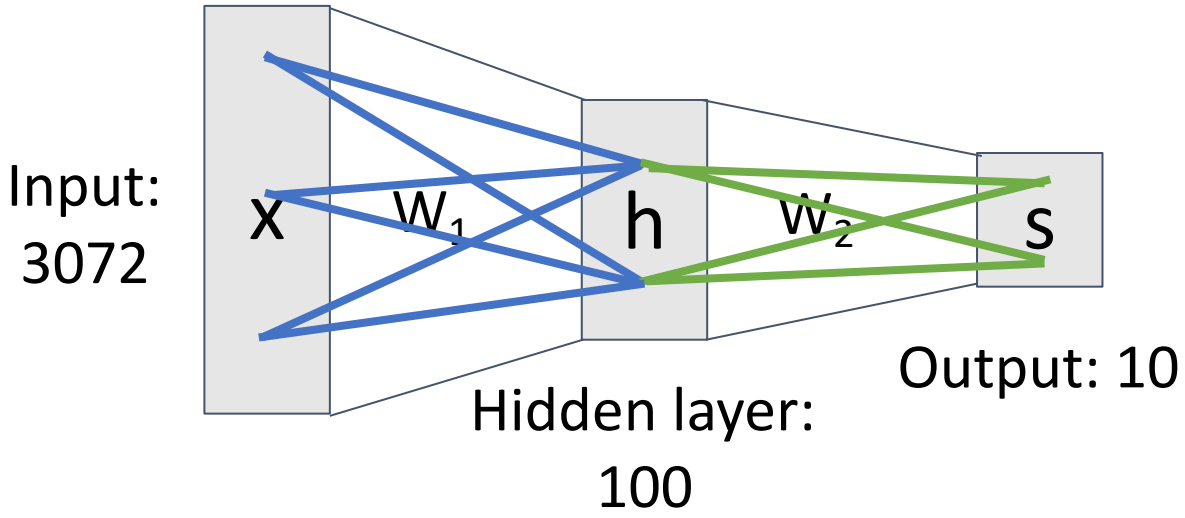
Neural Networks

(**Before**) Linear score function: $f = Wx$

(**Now**) 2-layer Neural Network $f = W_2 \max(0, W_1 x)$

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

All elements of x affect all elements of h



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

All elements of h affect all elements of s

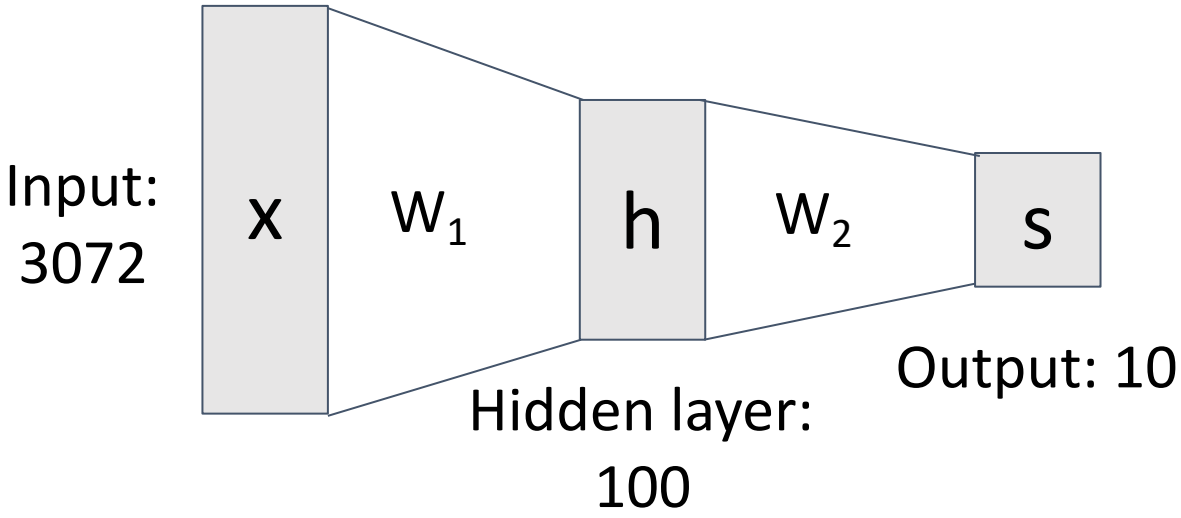
Fully-connected neural network
Also "Multi-Layer Perceptron" (MLP)

Neural Networks

Linear classifier: One template per class

(**Before**) Linear score function:

(**Now**) 2-layer Neural Network



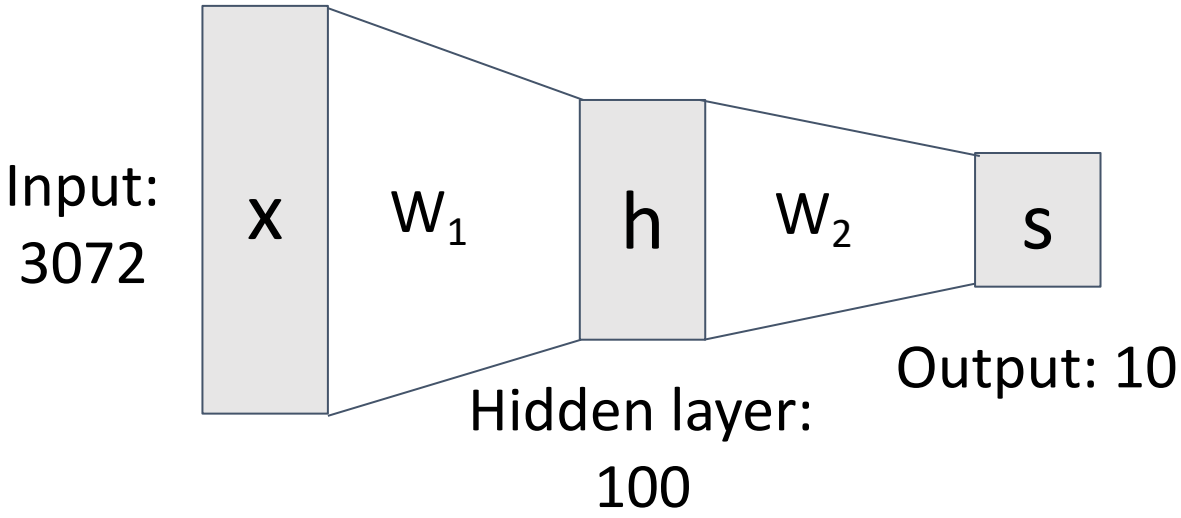
$$x \in \mathbb{R}^D, W_1 \in \mathbb{R}^{H \times D}, W_2 \in \mathbb{R}^{C \times H}$$

Neural Networks

Neural net: first layer is bank of templates;
Second layer recombines templates

(**Before**) Linear score function:

(**Now**) 2-layer Neural Network



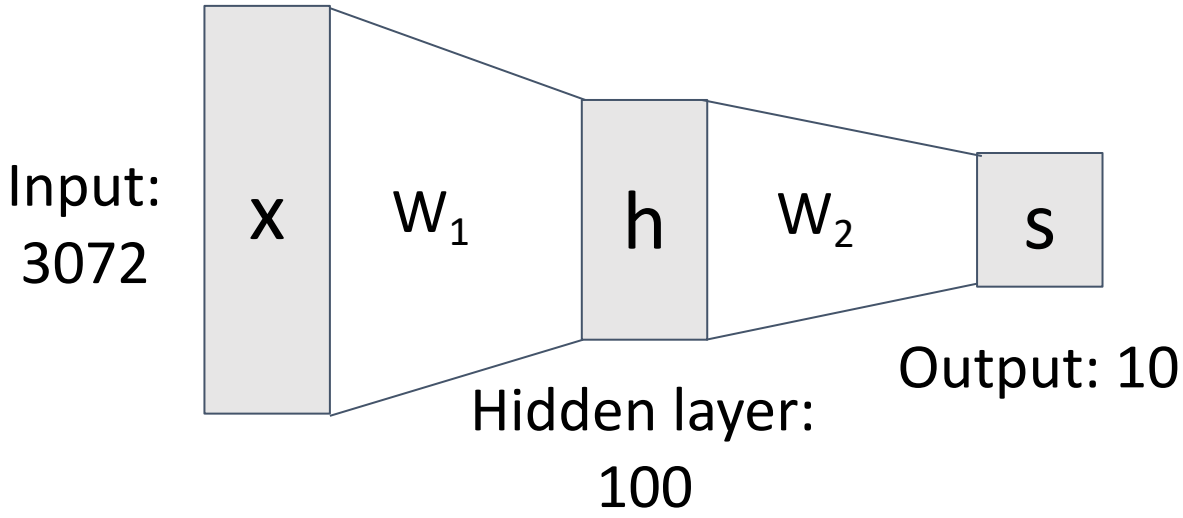
$$x \in \mathbb{R}^D, W_1 \in \mathbb{R}^{H \times D}, W_2 \in \mathbb{R}^{C \times H}$$

Neural Networks

Can use different templates to cover multiple modes of a class!

(**Before**) Linear score function:

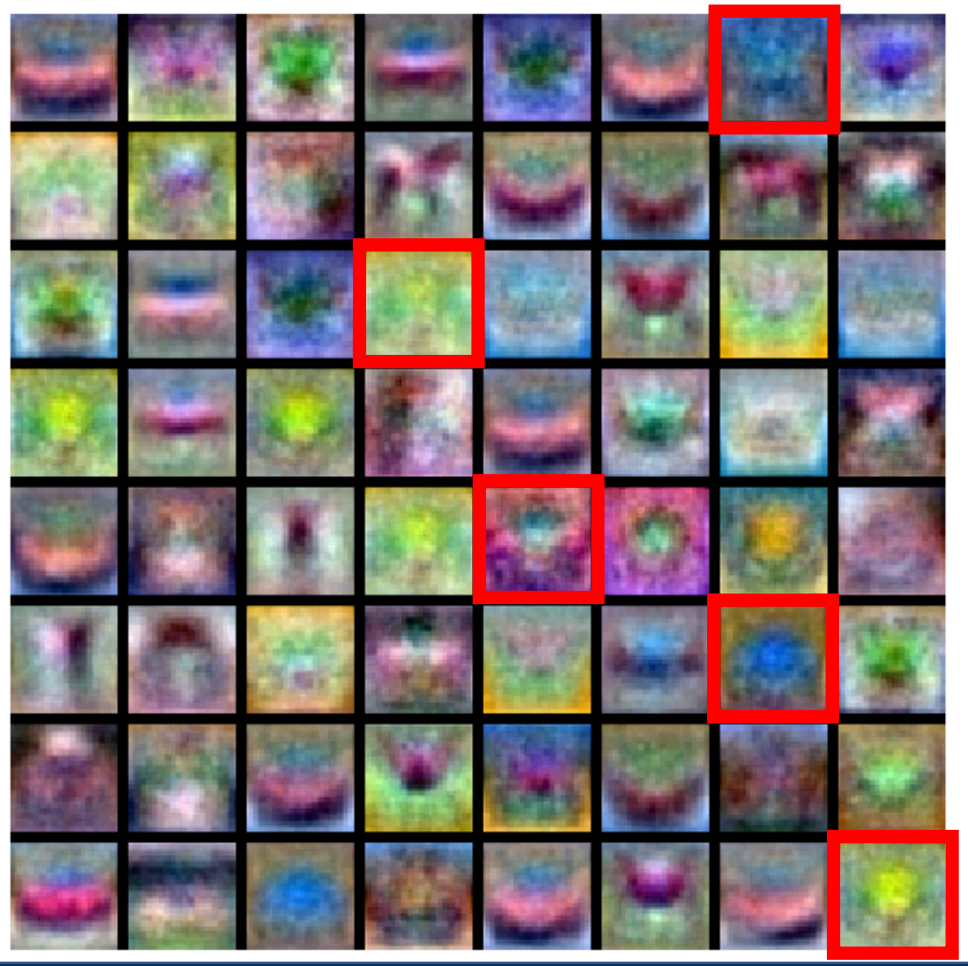
(**Now**) 2-layer Neural Network



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

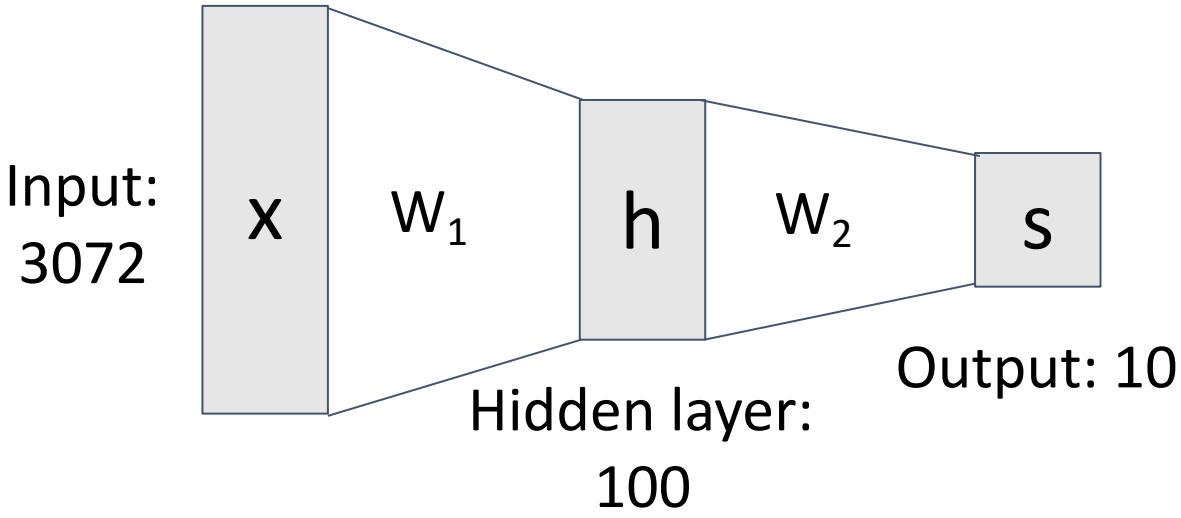
Neural Networks

"Distributed representation":
Most templates not interpretable!



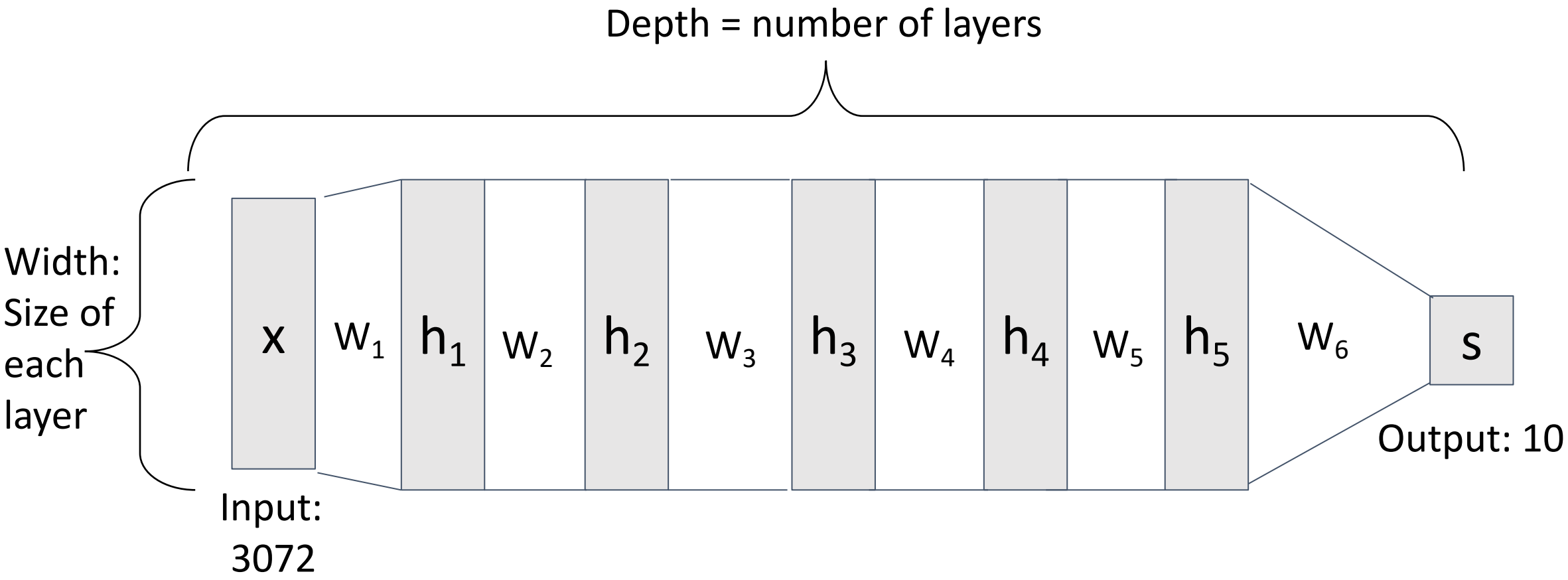
(**Before**) Linear score function:

(**Now**) 2-layer Neural Network



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

Deep Neural Networks



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

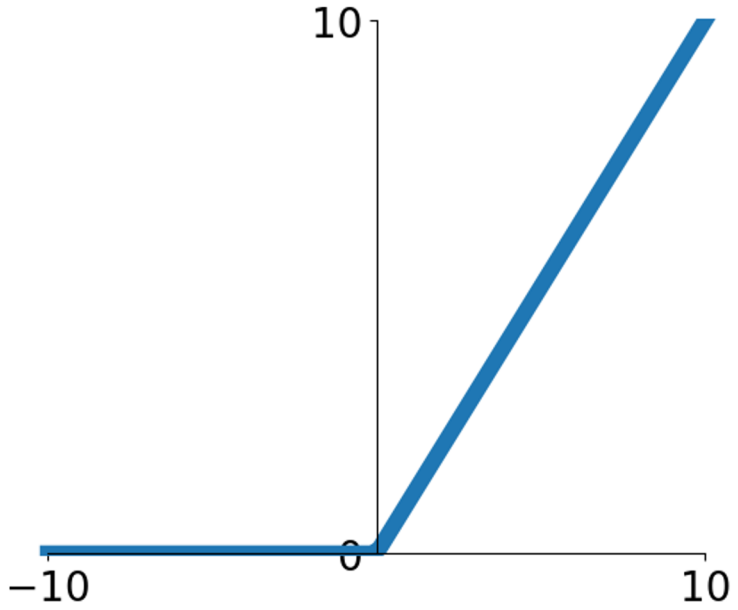
Activation Functions

2-layer Neural Network

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

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

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



Activation Functions

2-layer Neural Network

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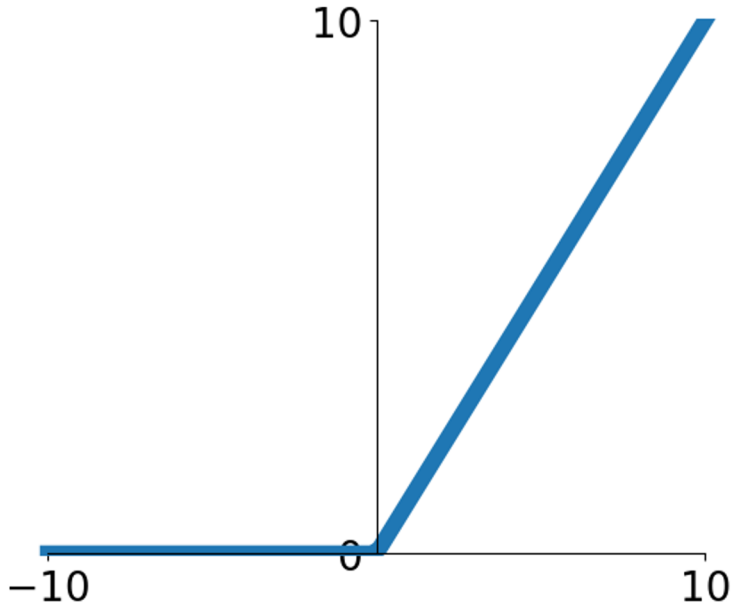


$$f = W_2 \max(0, W_1 x)$$

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

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

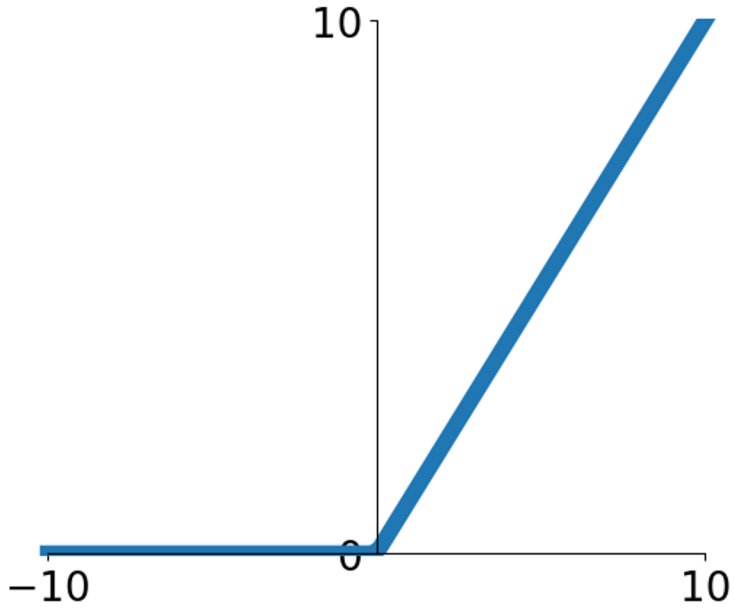
$$s = W_2 W_1 x$$

Activation Functions

2-layer Neural Network

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

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



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

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

$$s = W_2 W_1 x$$

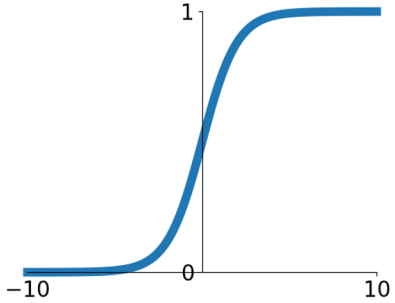
$$W_3 = W_2 W_1 \in \mathbb{R}^{C \times H} \qquad s = W_3 x$$

A: We end up with a linear classifier!

Activation Functions

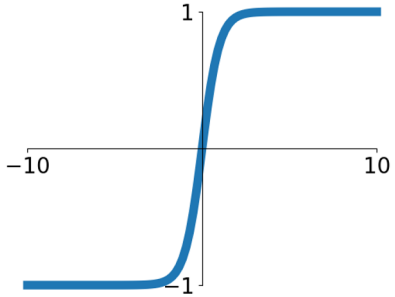
Sigmoid

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



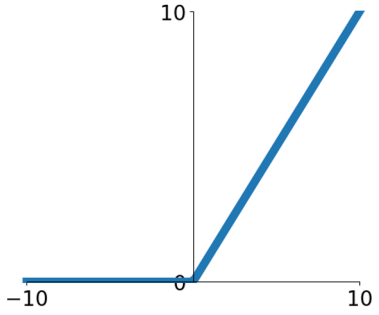
tanh

$$\tanh(x)$$



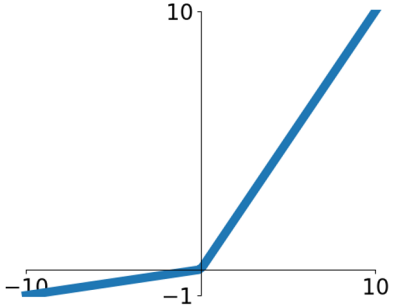
ReLU

$$\max(0, x)$$



Leaky ReLU

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

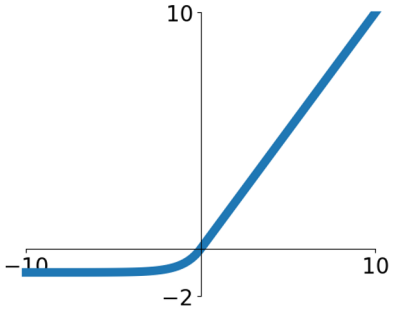


Maxout

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

ELU

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

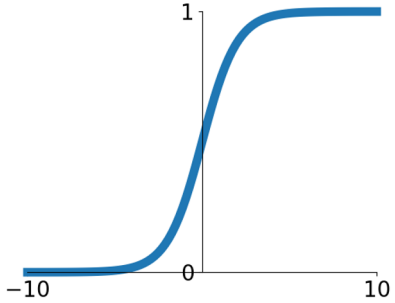


Activation Functions

ReLU is a good default choice for most problems

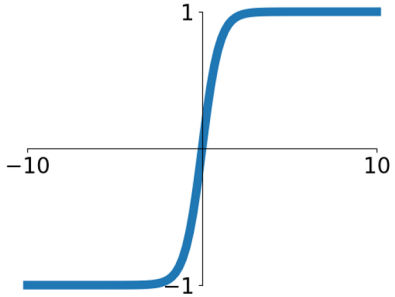
Sigmoid

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



tanh

$$\tanh(x)$$



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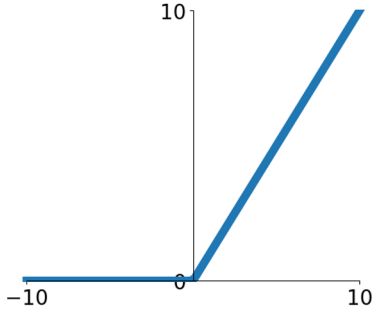
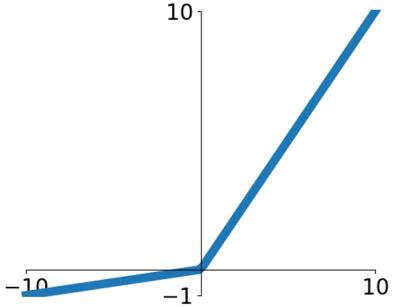
$$\max(0, x)$$



Leaky ReLU

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

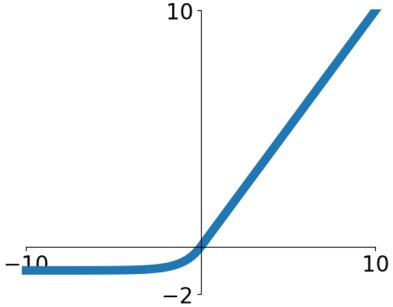


Maxout

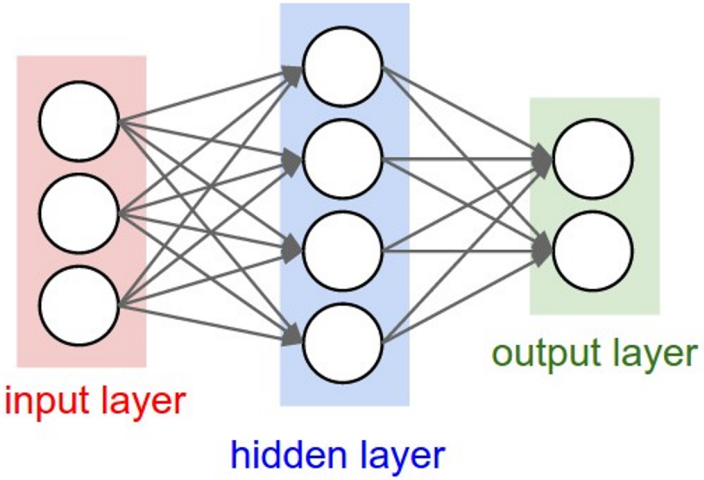
$$\max(w_1^T x + b_1, w_2^T x + b_2)$$

ELU

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



Neural Net in <20 lines!



Initialize weights and data

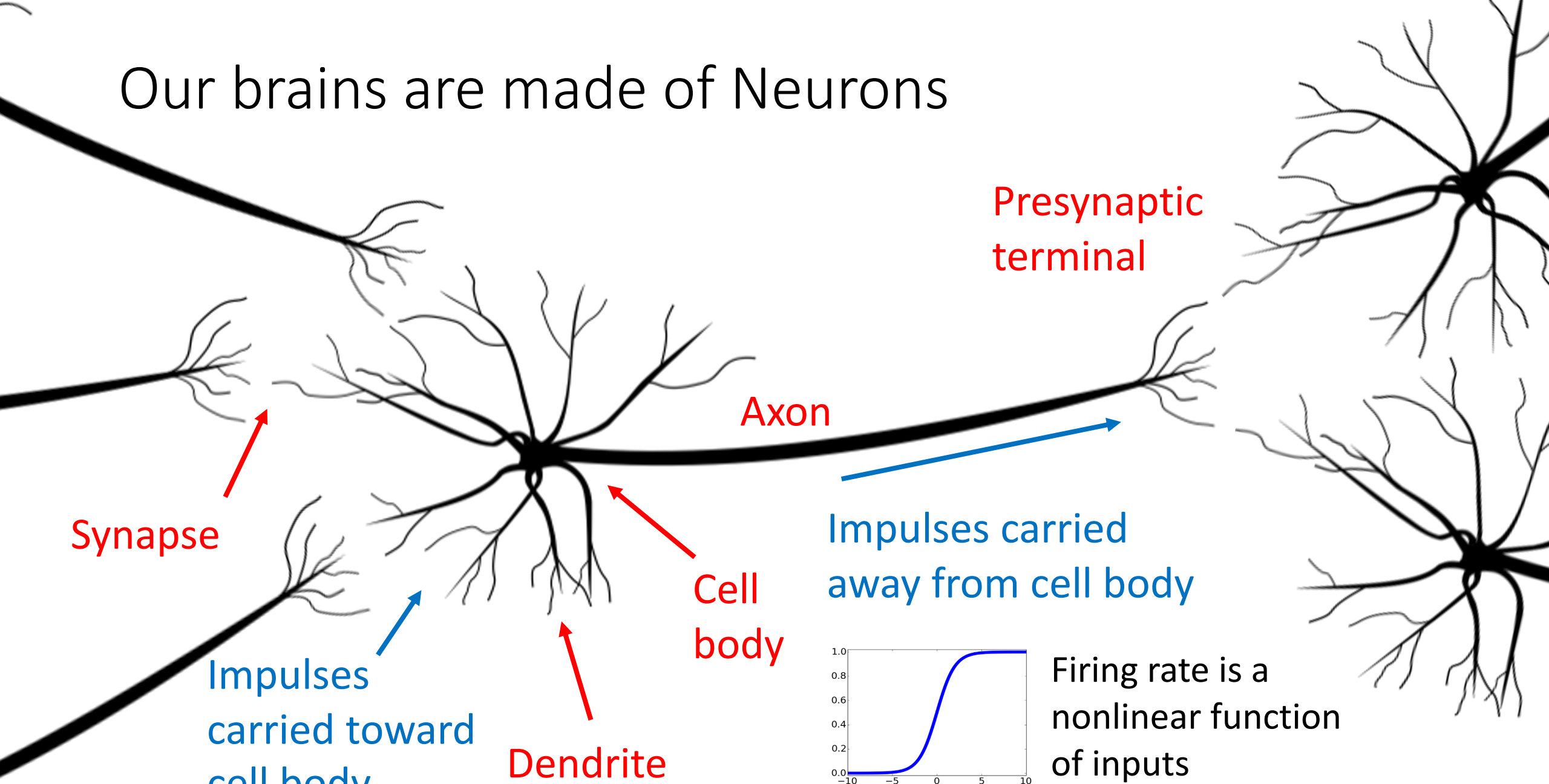
Compute loss (sigmoid activation, L2 loss)

Compute gradients

Stochastic Gradient Descent (SGD) step

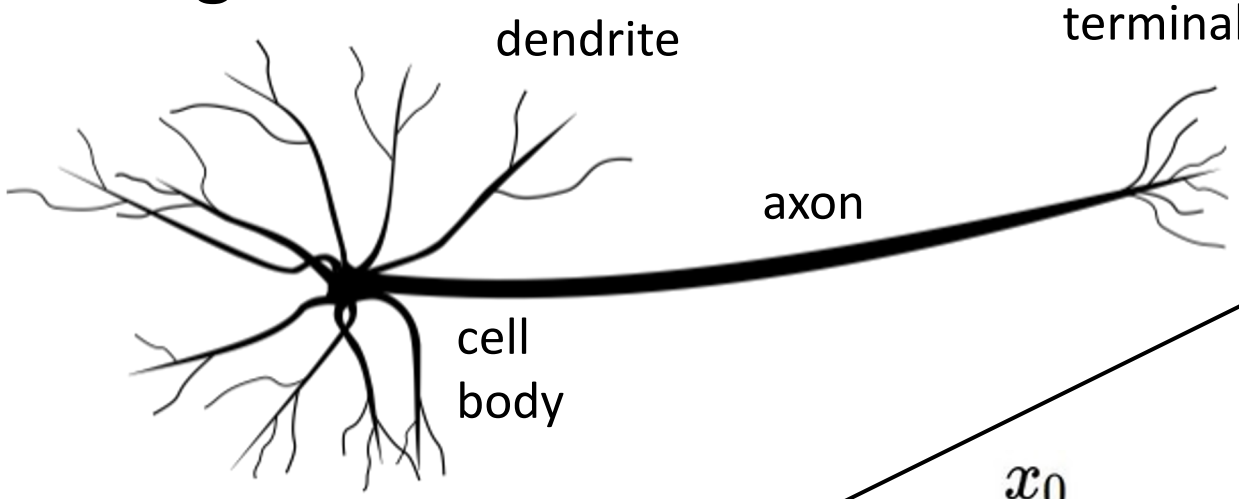
```
1   import numpy as np
2   from numpy.random import randn
3
4   N, Din, H, Dout = 64, 1000, 100, 10
5   x, y = randn(N, Din), randn(N, Dout)
6   w1, w2 = randn(Din, H), randn(H, Dout)
7   for t in range(10000):
8     h = 1.0 / (1.0 + np.exp(-x.dot(w1)))
9     y_pred = h.dot(w2)
10    loss = np.square(y_pred - y).sum()
11    dy_pred = 2.0 * (y_pred - y)
12    dw2 = h.T.dot(dy_pred)
13    dh = dy_pred.dot(w2.T)
14    dw1 = x.T.dot(dh * h * (1 - h))
15    w1 -= 1e-4 * dw1
16    w2 -= 1e-4 * dw2
```

Our brains are made of Neurons

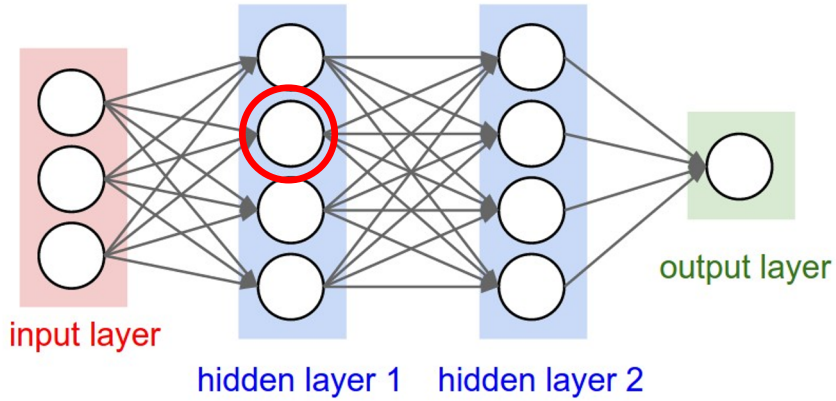


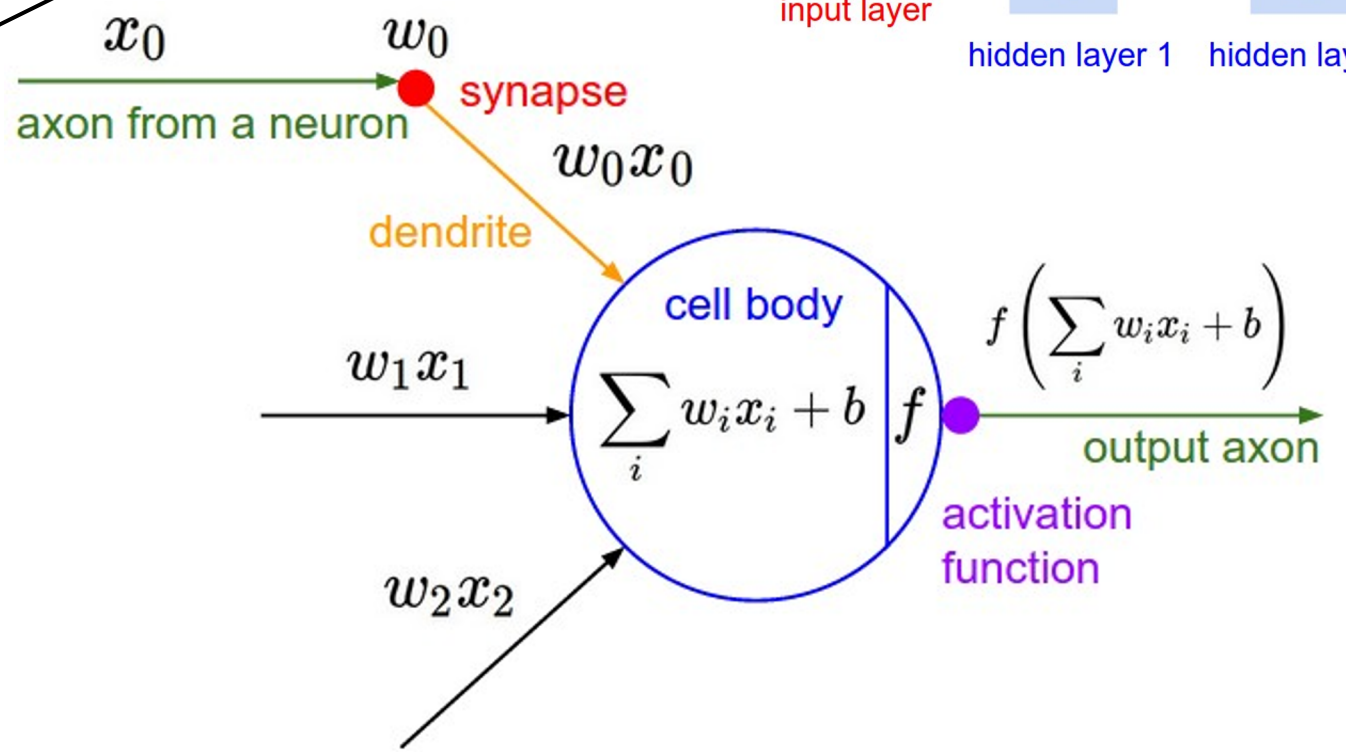
Firing rate is a nonlinear function of inputs

Biological Neuron



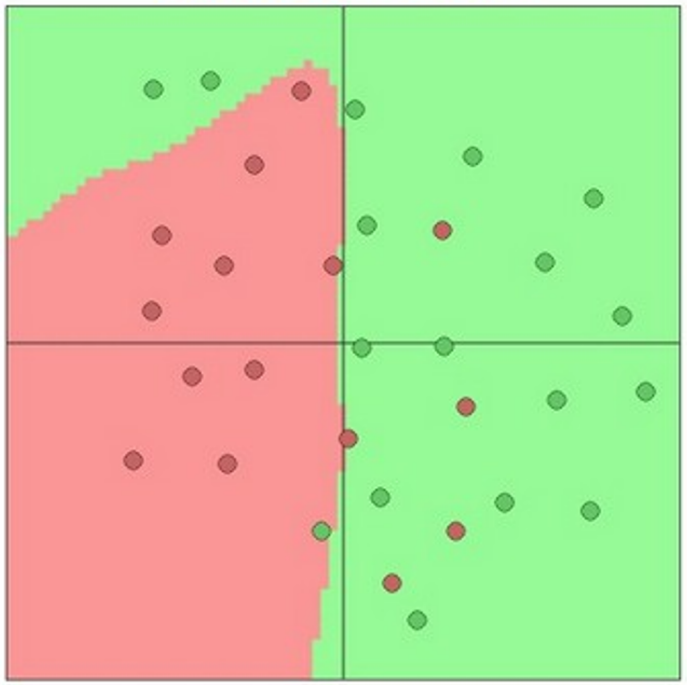
Artificial Neuron



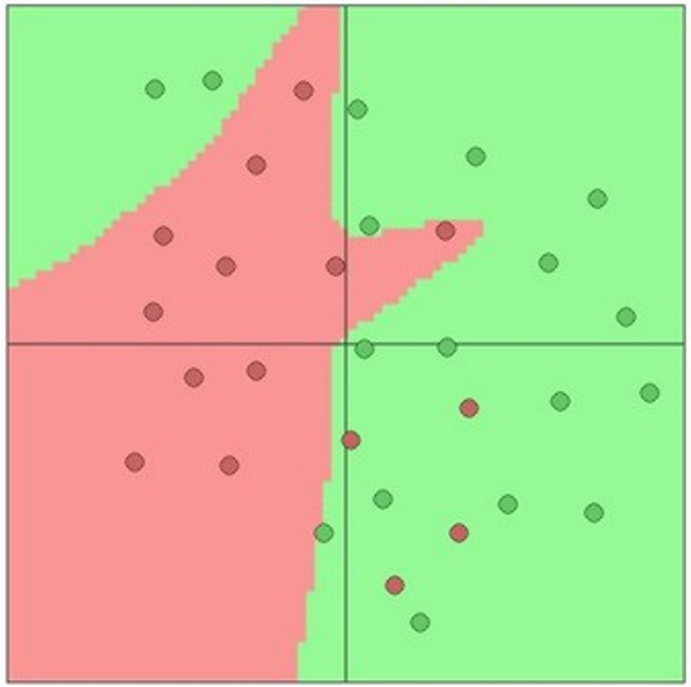


Setting the number of layers and their sizes

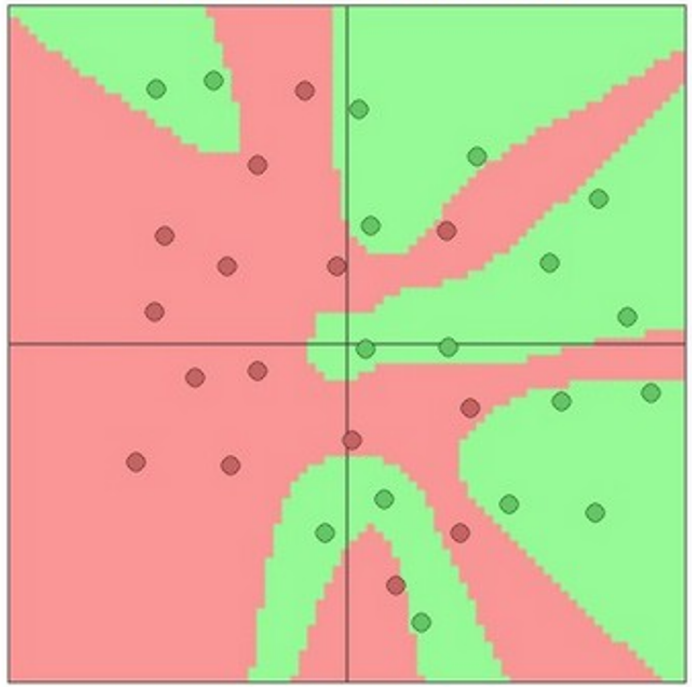
3 hidden units



6 hidden units

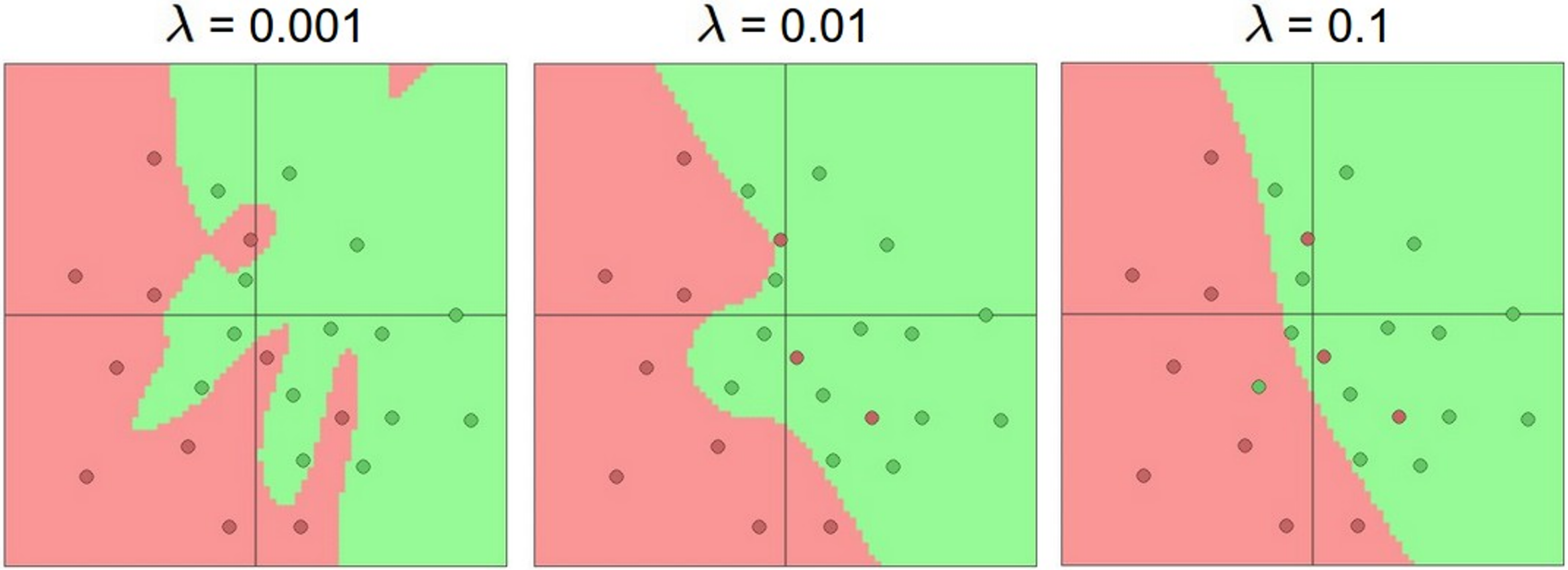


20 hidden units



More hidden units = more capacity

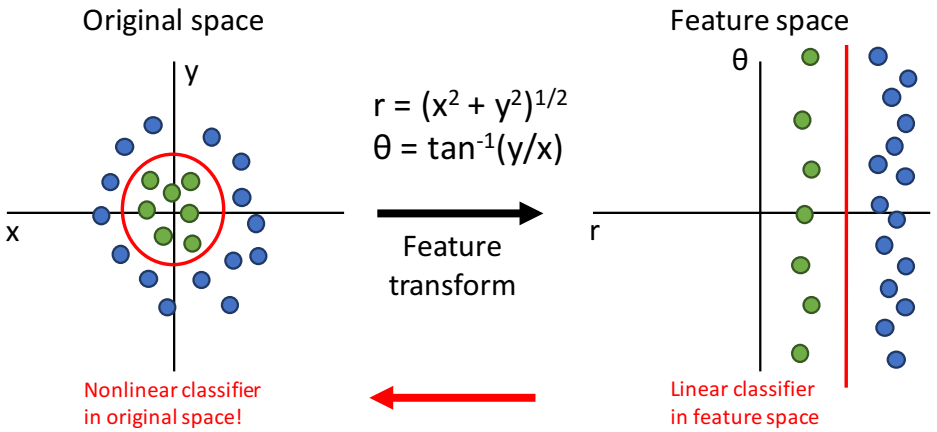
Don’t regularize with size; instead use stronger L2



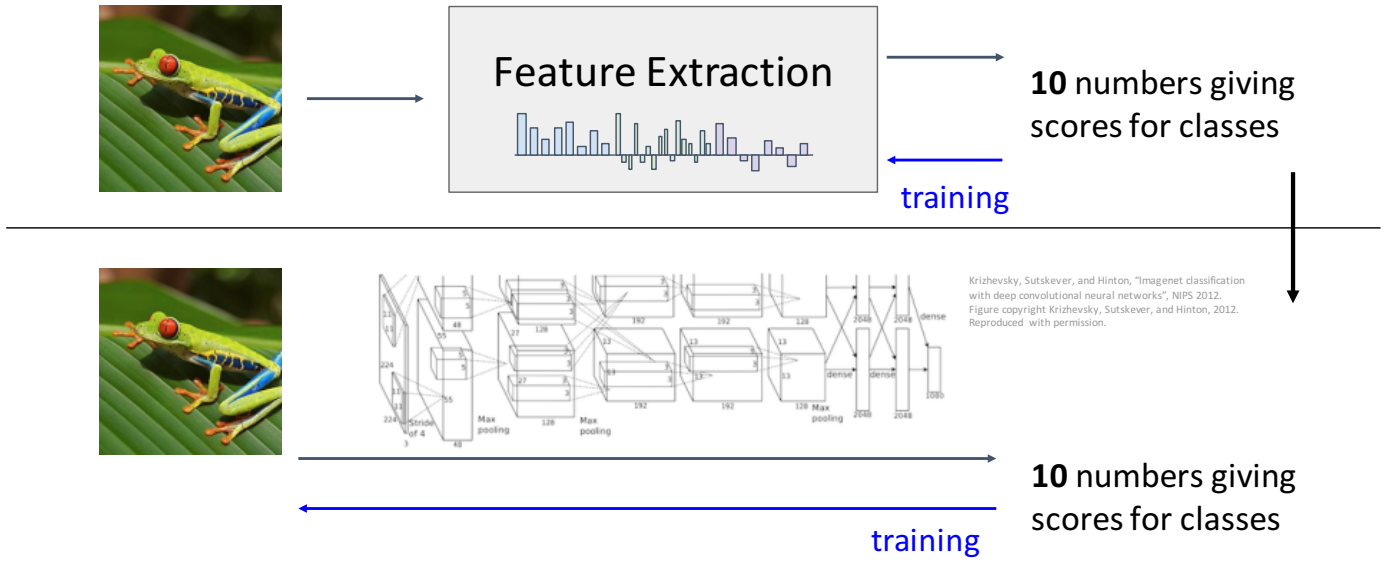
(Web demo with ConvNetJS:
http://cs.stanford.edu/people/karpathy/convnetjs/demo/classify2d.html)

Summary

Feature transform + Linear classifier allows nonlinear decision boundaries



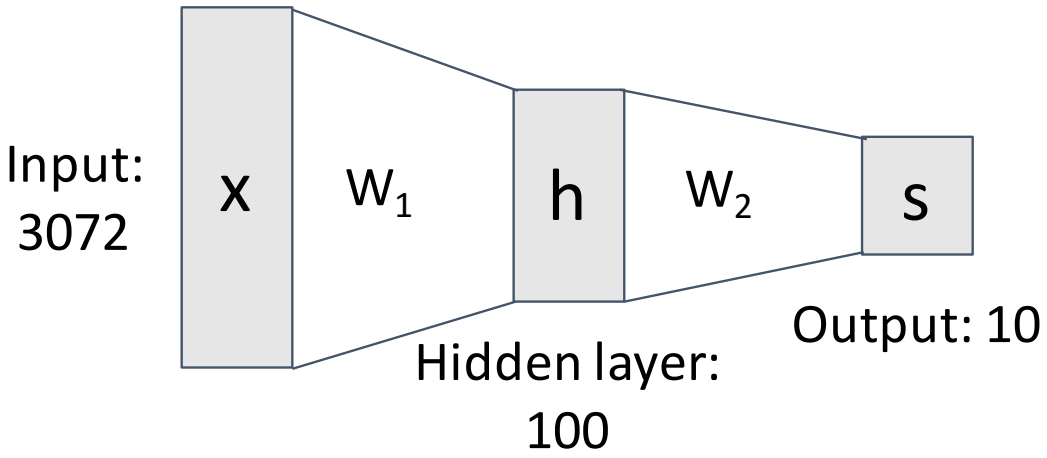
Neural Networks as learnable feature transforms



Summary

From linear classifiers to fully-connected networks

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

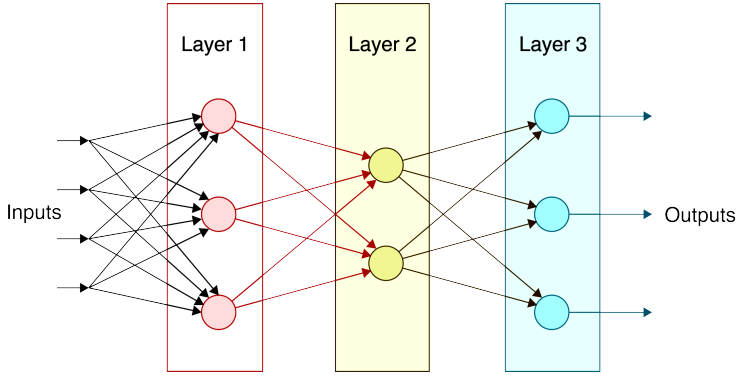


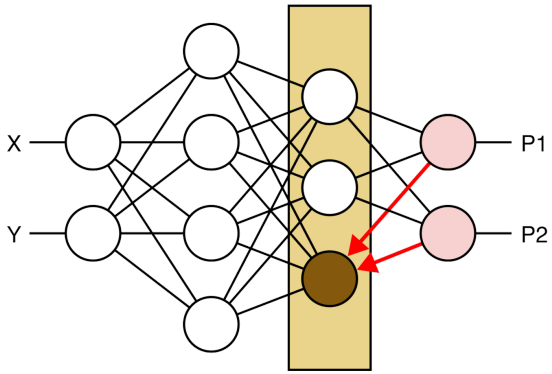
Linear classifier: One template per class

Neural networks: Many reusable templates

Deep neural networks

- Loss functions
- Regularization
- Weights and layers
- Activation functions
- Backpropagation
- Training and optimization





Lecture 6: Backpropagation

Problem: How to compute gradients?

$$s = f(x; W_1, W_2) = W_2 \max(0, W_1 x)$$ Nonlinear score function

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

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

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

If we can compute $\frac{\partial L}{\partial W_1}, \frac{\partial L}{\partial W_2}$ then we can learn W_1 and W_2

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

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

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

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

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

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

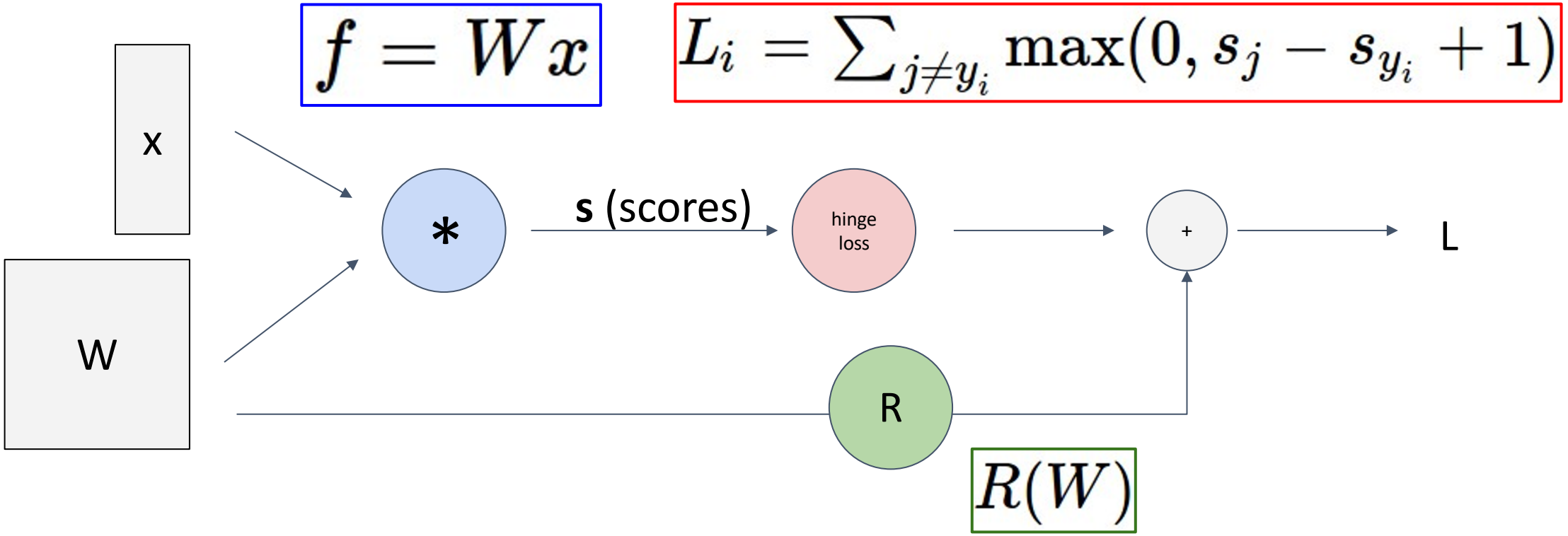
$$\nabla_W L = \nabla_W \left(\frac{1}{N} \sum_{i=1}^{N} \sum_{j \neq y_i} \max(0, W_{j,:} \cdot x + W_{y_i,:} \cdot x + 1) + \lambda \sum_k W_k^2 \right)$$

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!

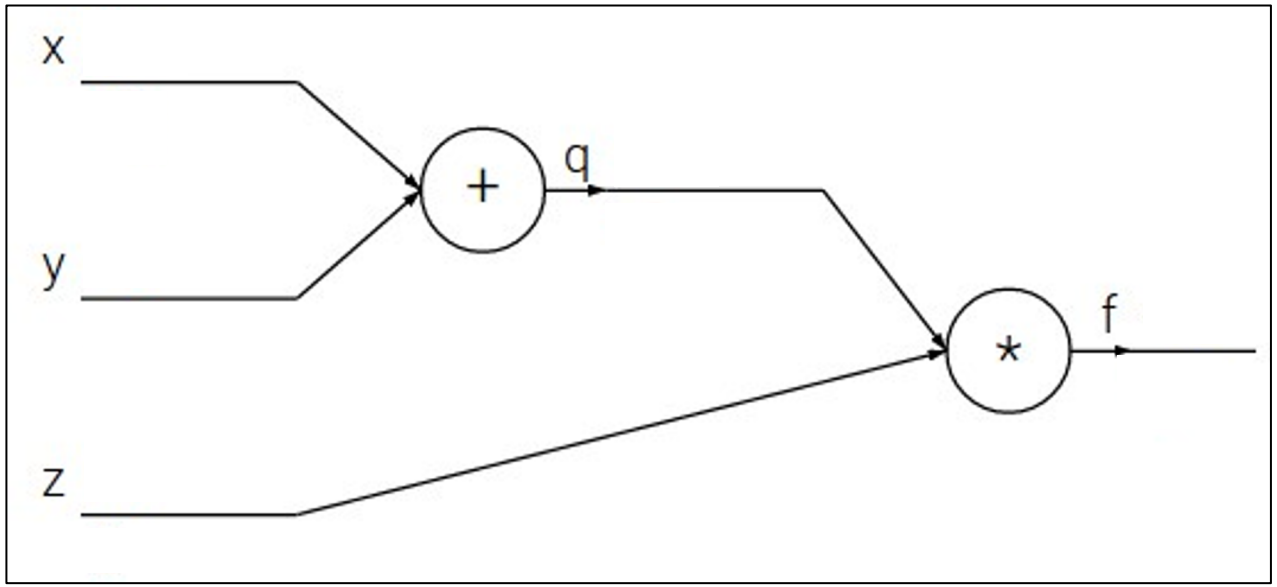
Problem: Not feasible for very complex models!

Better Idea: Computational Graphs



Backpropagation: Simple Example

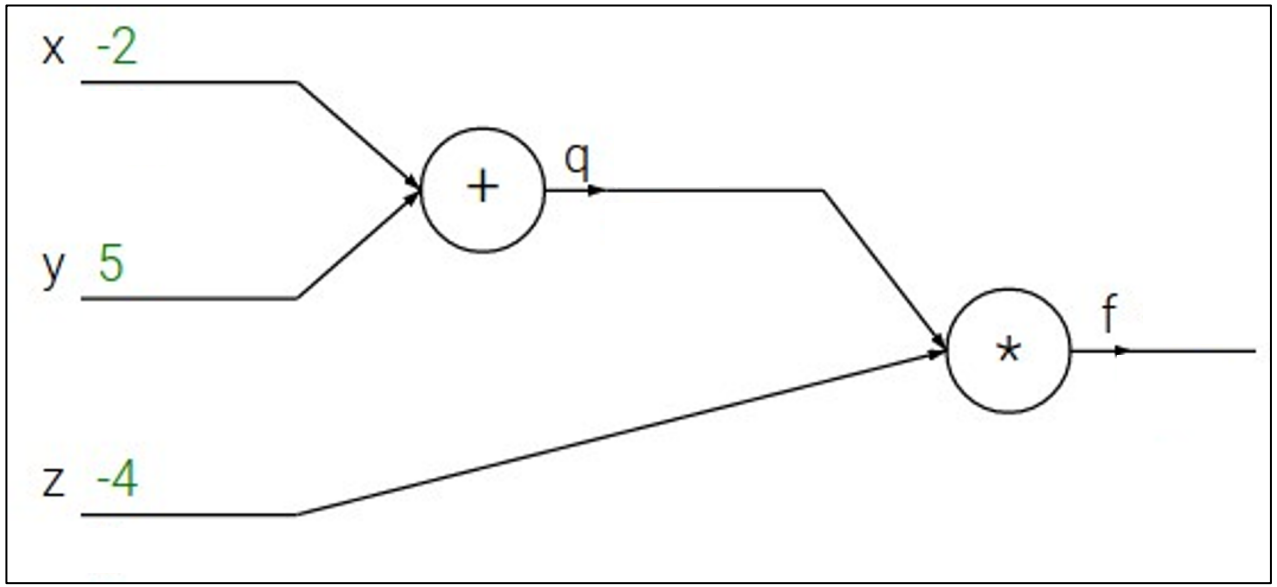
$$f(x, y, z) = (x + y)z$$



Backpropagation: Simple Example

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

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



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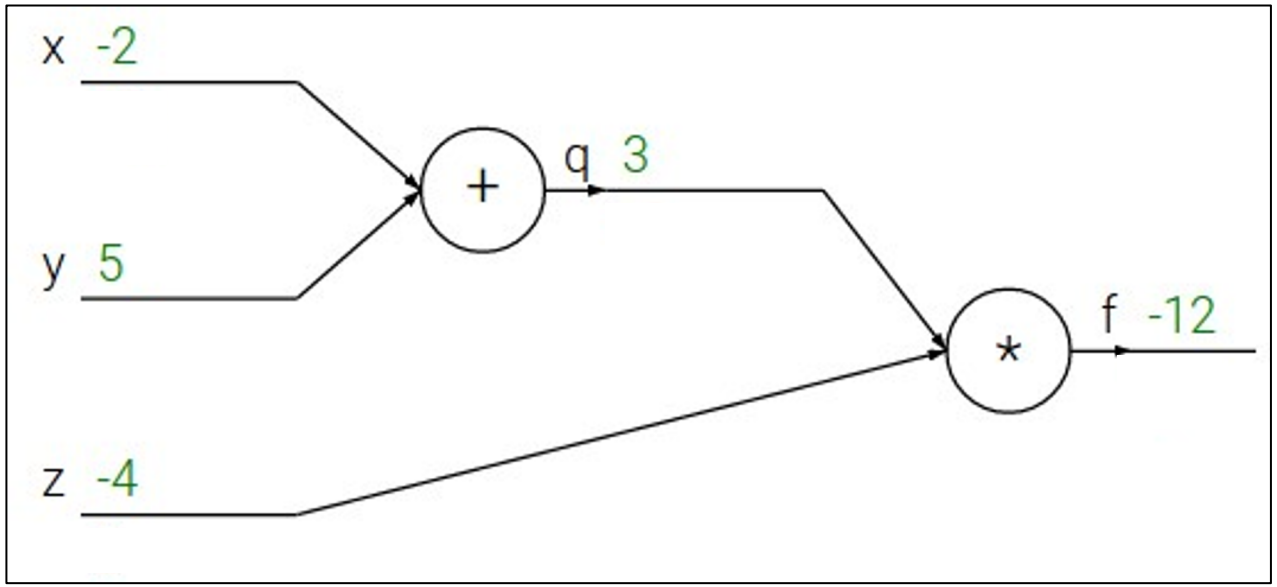


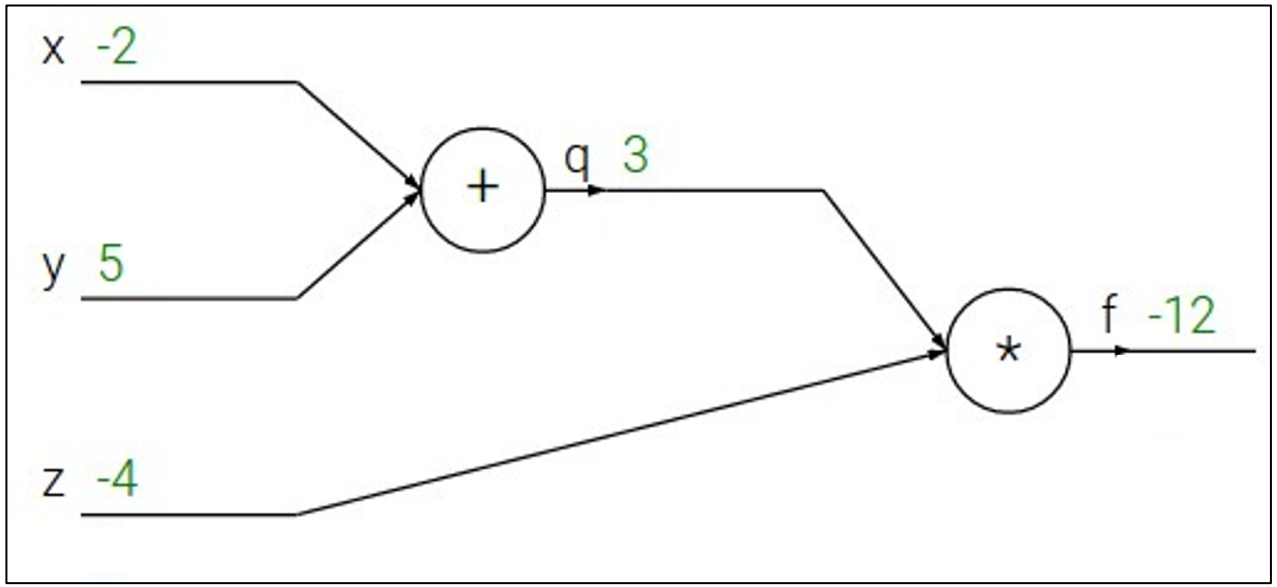
1. Forward pass: Compute outputs

$$q = x + y \qquad f = qz$$

Backpropagation: Simple Example

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

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



1. Forward pass: Compute outputs

$$q = x + y \qquad f = qz$$

2. Backward pass: Compute derivatives

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

Backpropagation: Simple Example

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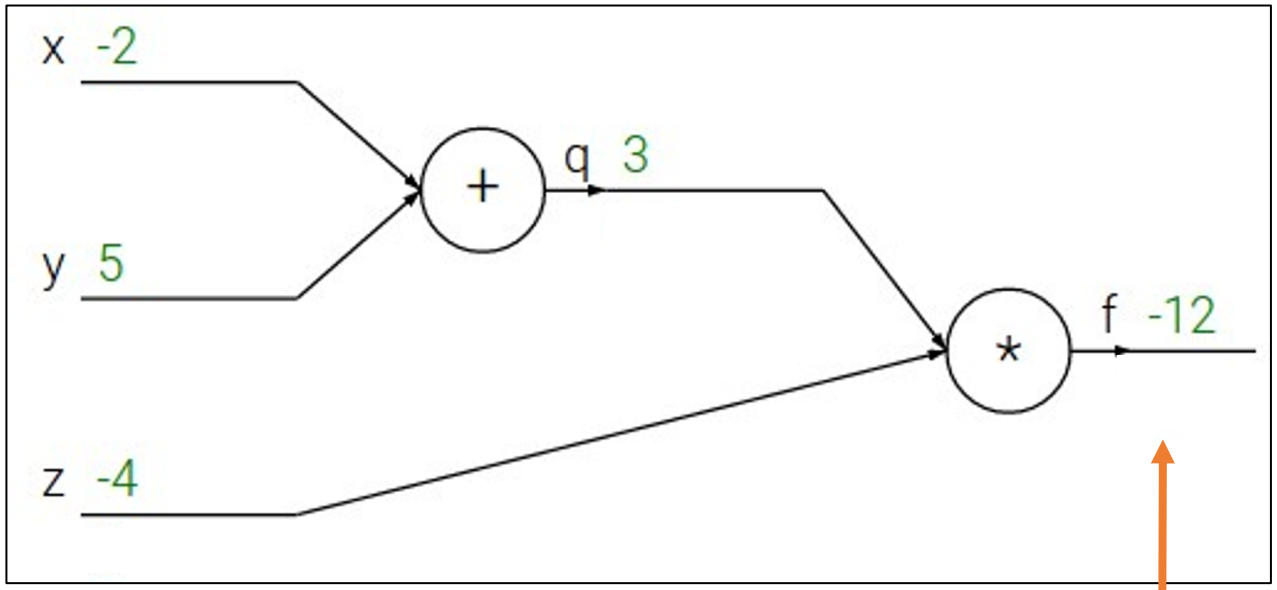

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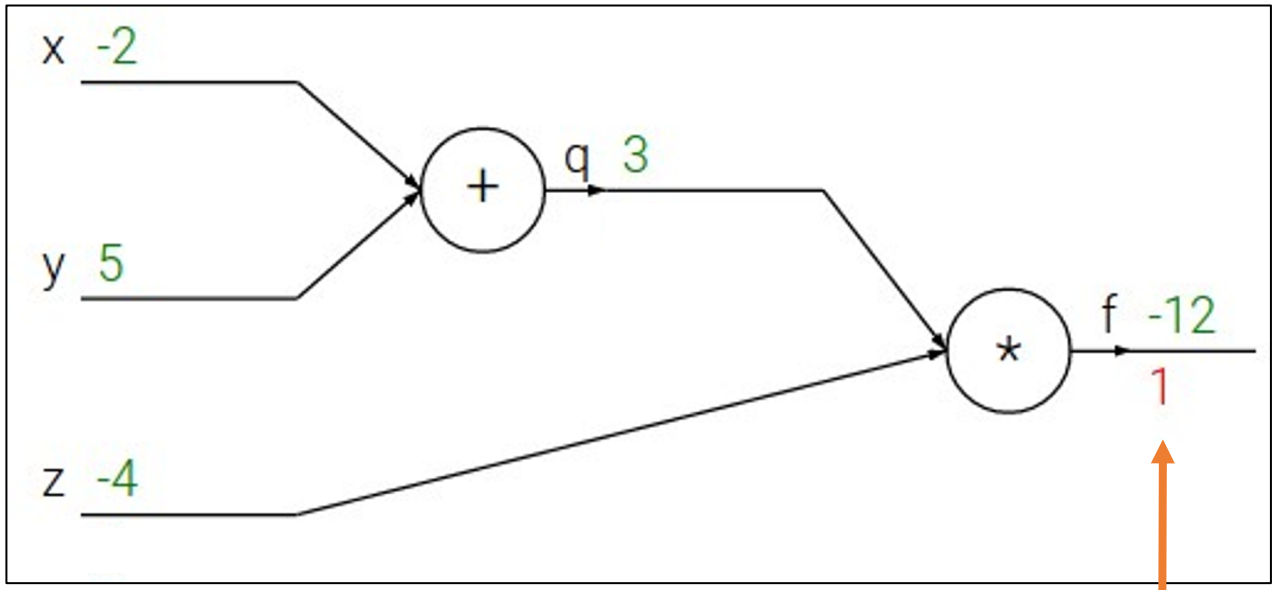

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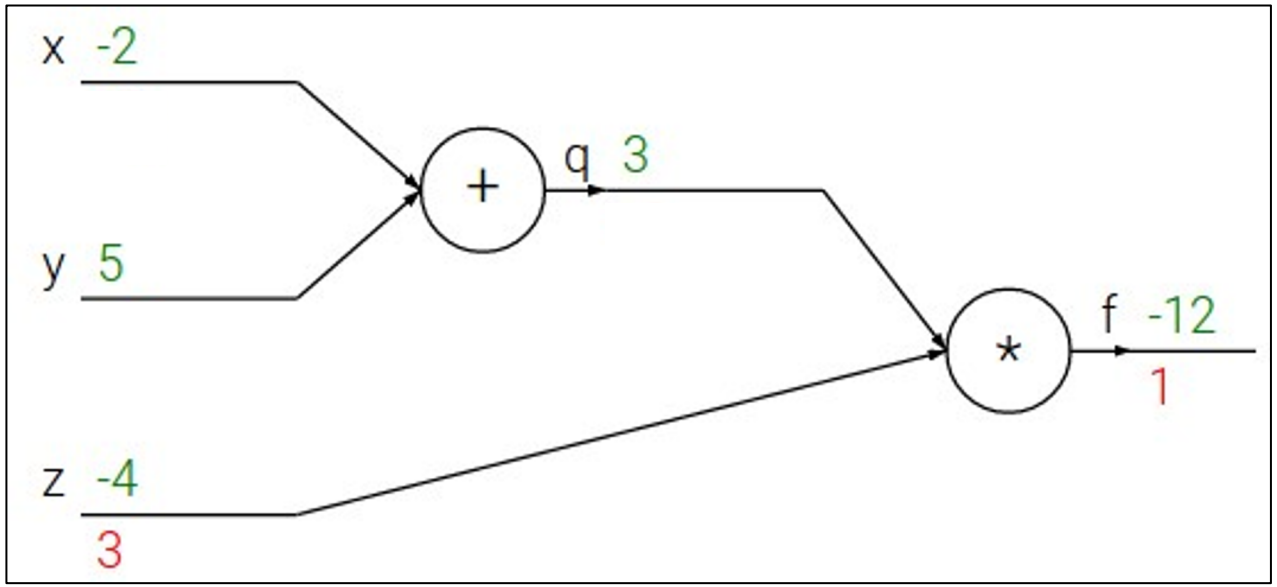

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Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$

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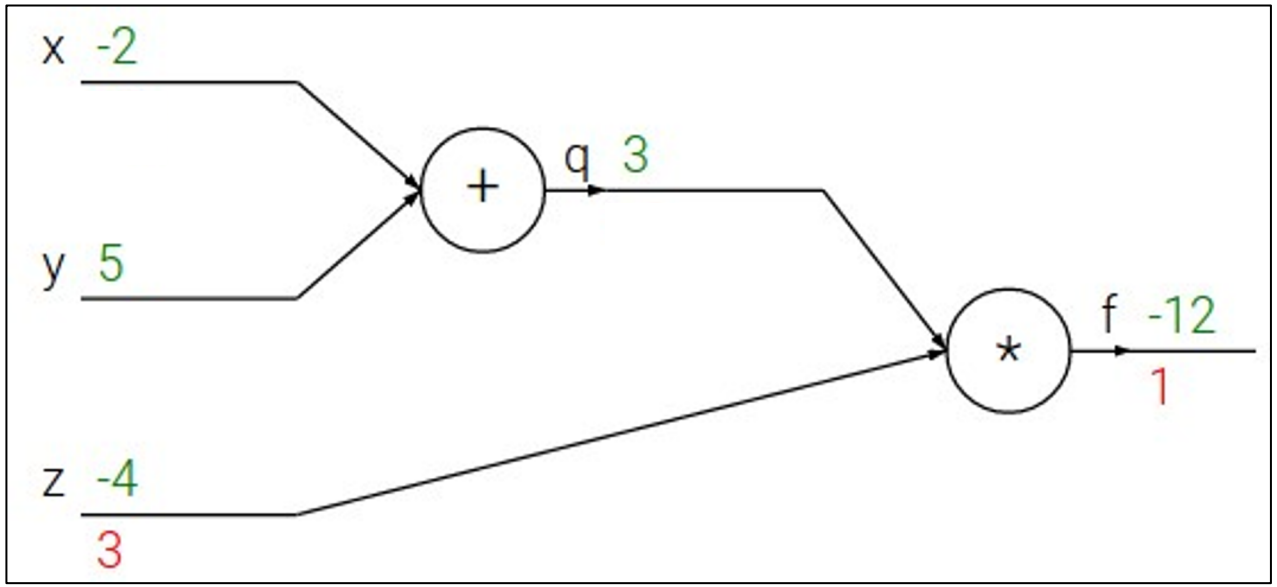

1. Forward pass: Compute outputs

$$q = x + y \qquad f = qz$$

2. Backward pass: Compute derivatives

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

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

Backpropagation: Simple Example

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

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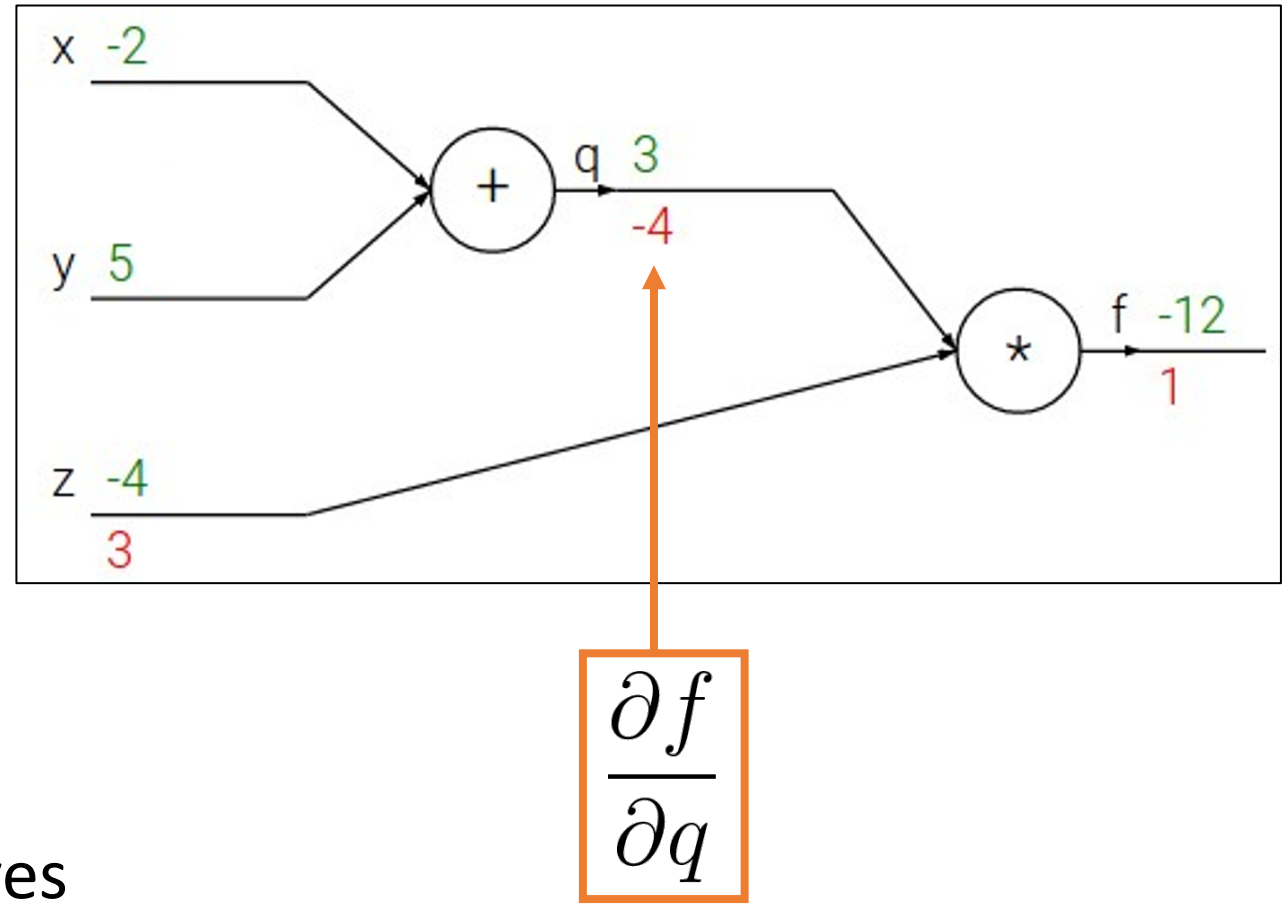

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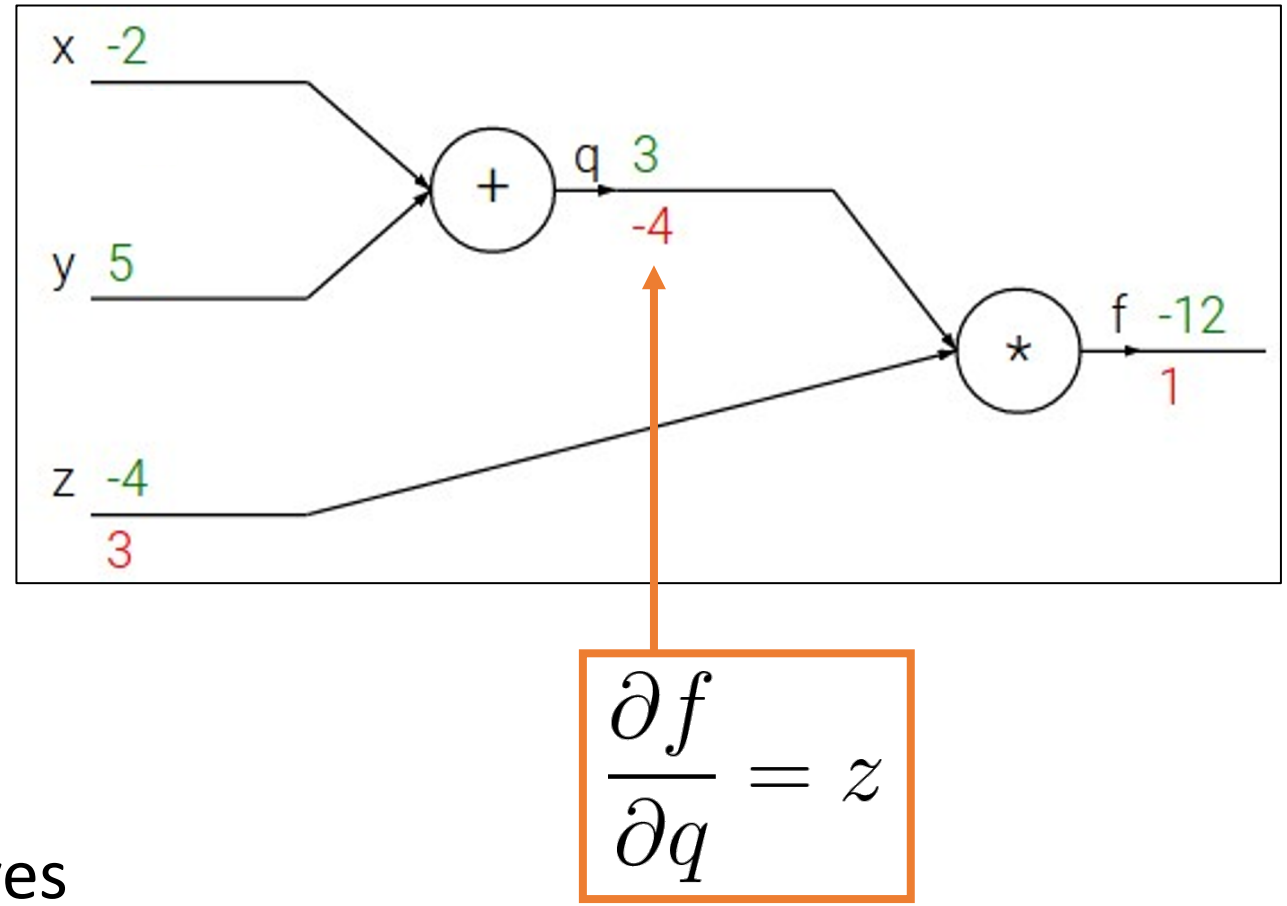

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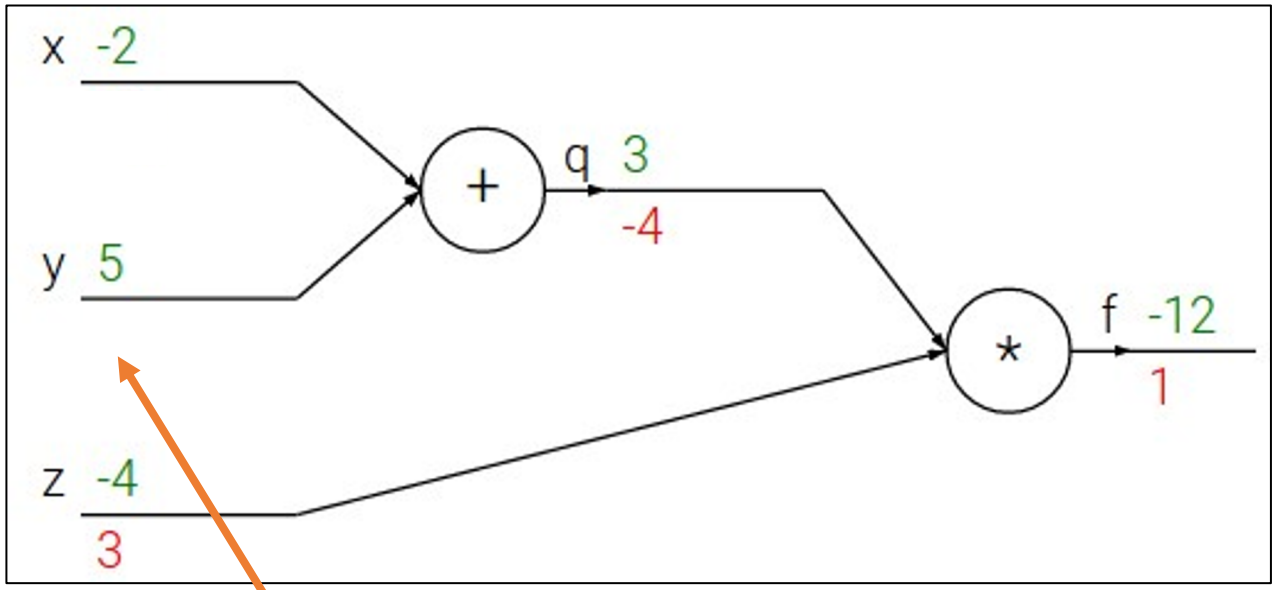

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$\frac{\partial f}{\partial y}$

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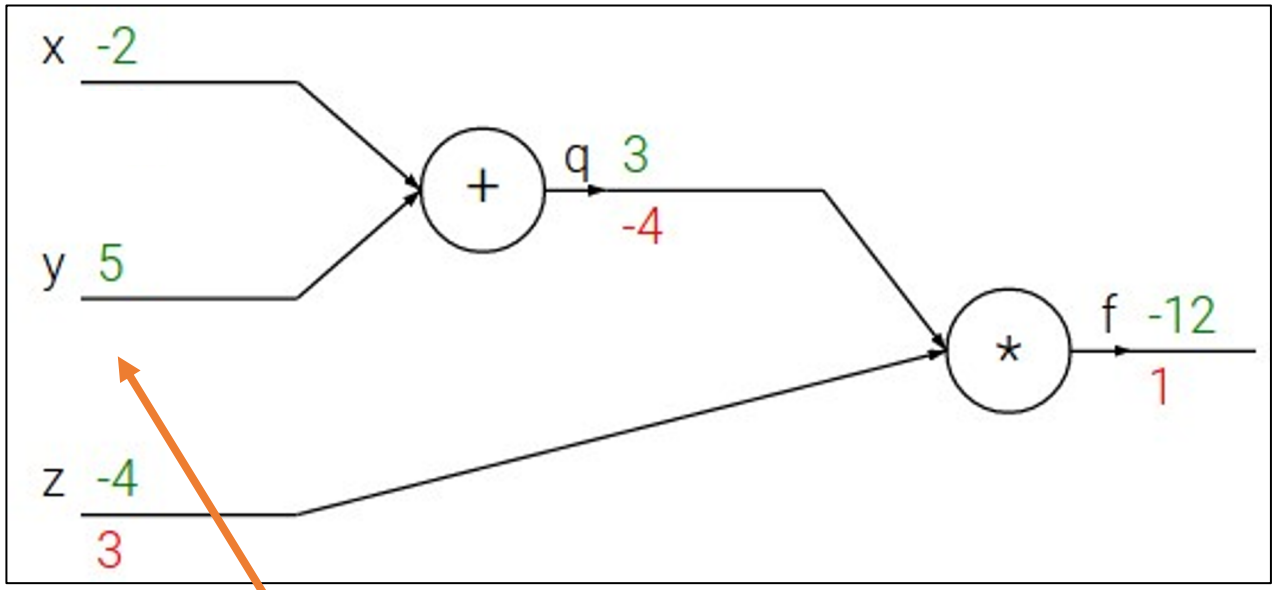


1. Forward pass: Compute outputs

$$q = x + y \qquad f = qz$$

2. Backward pass: Compute derivatives

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

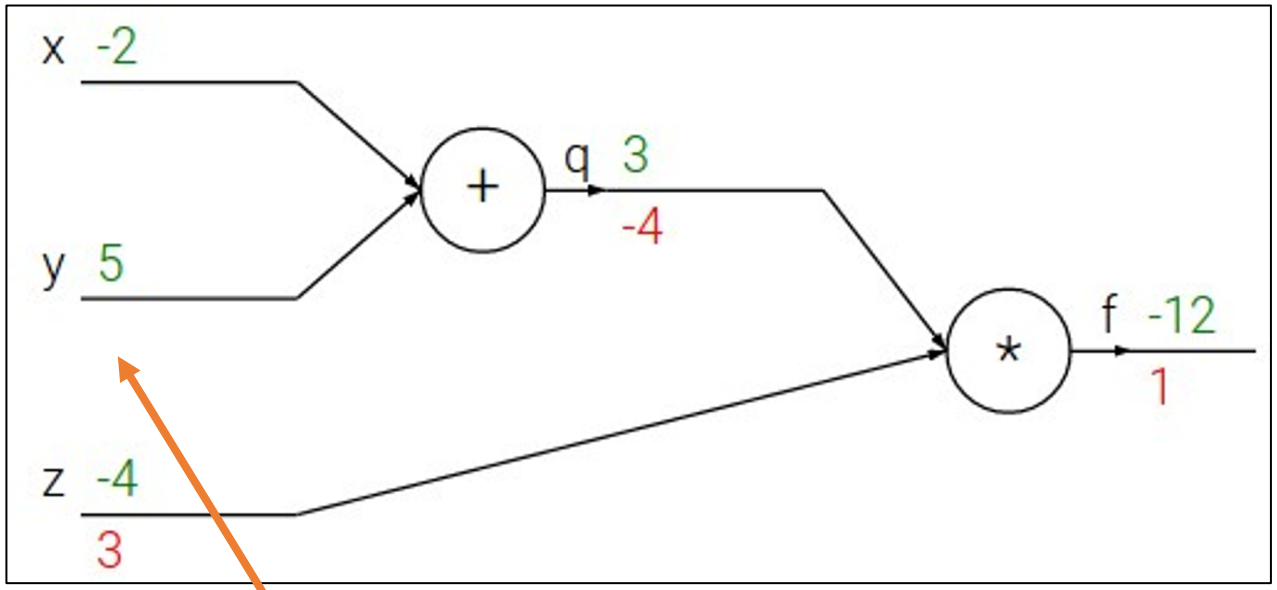
Chain Rule

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

Backpropagation: Simple Example

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

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



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

Chain Rule

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

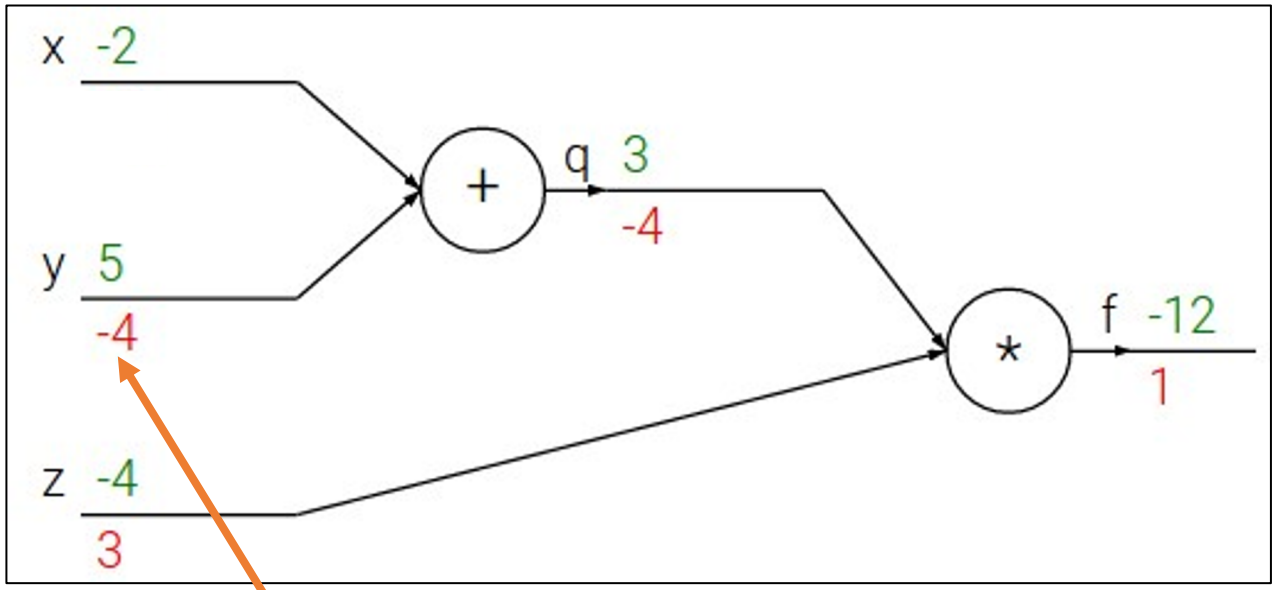
$$\frac{\partial q}{\partial y} = 1$$

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

Backpropagation: Simple Example

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

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



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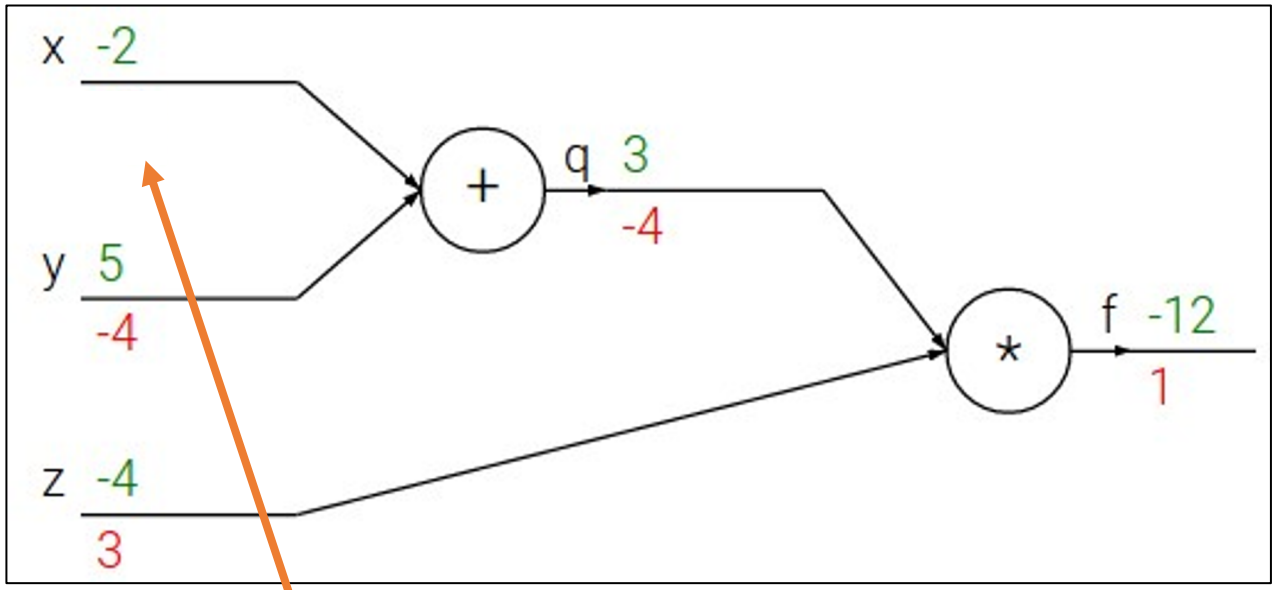

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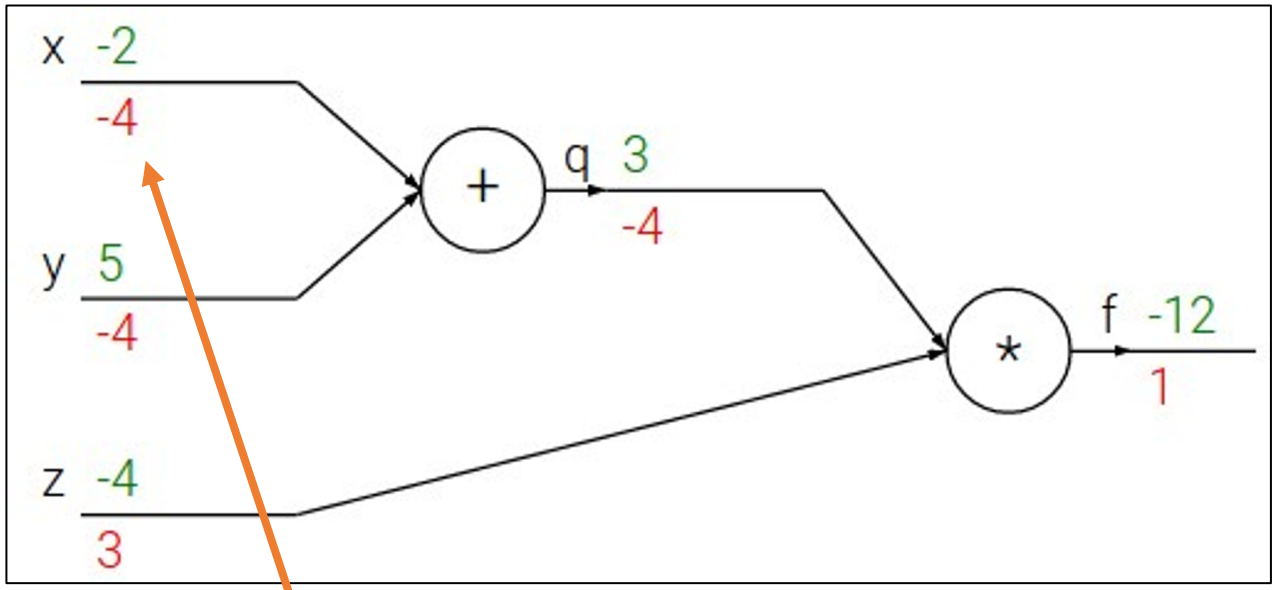

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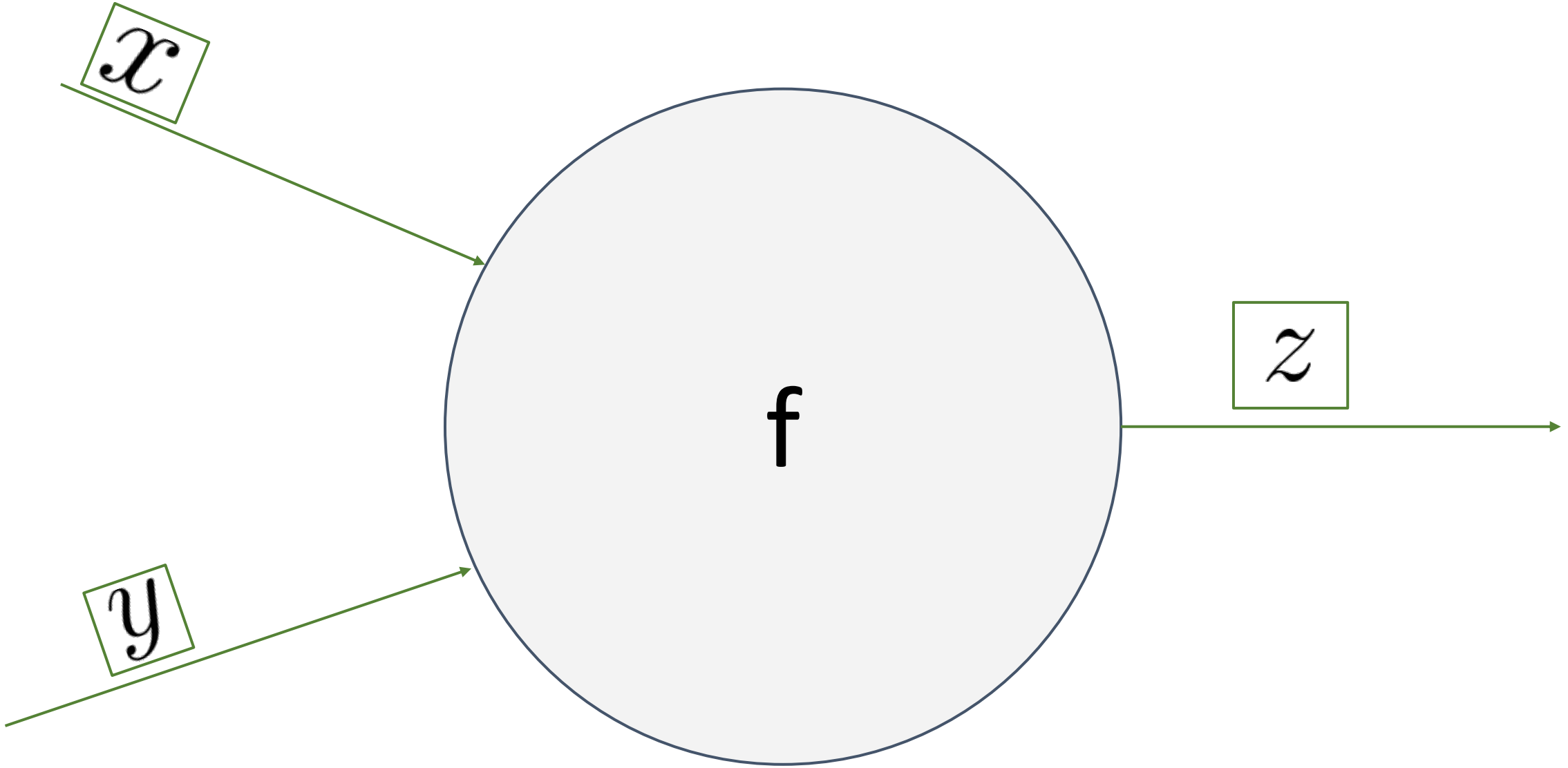
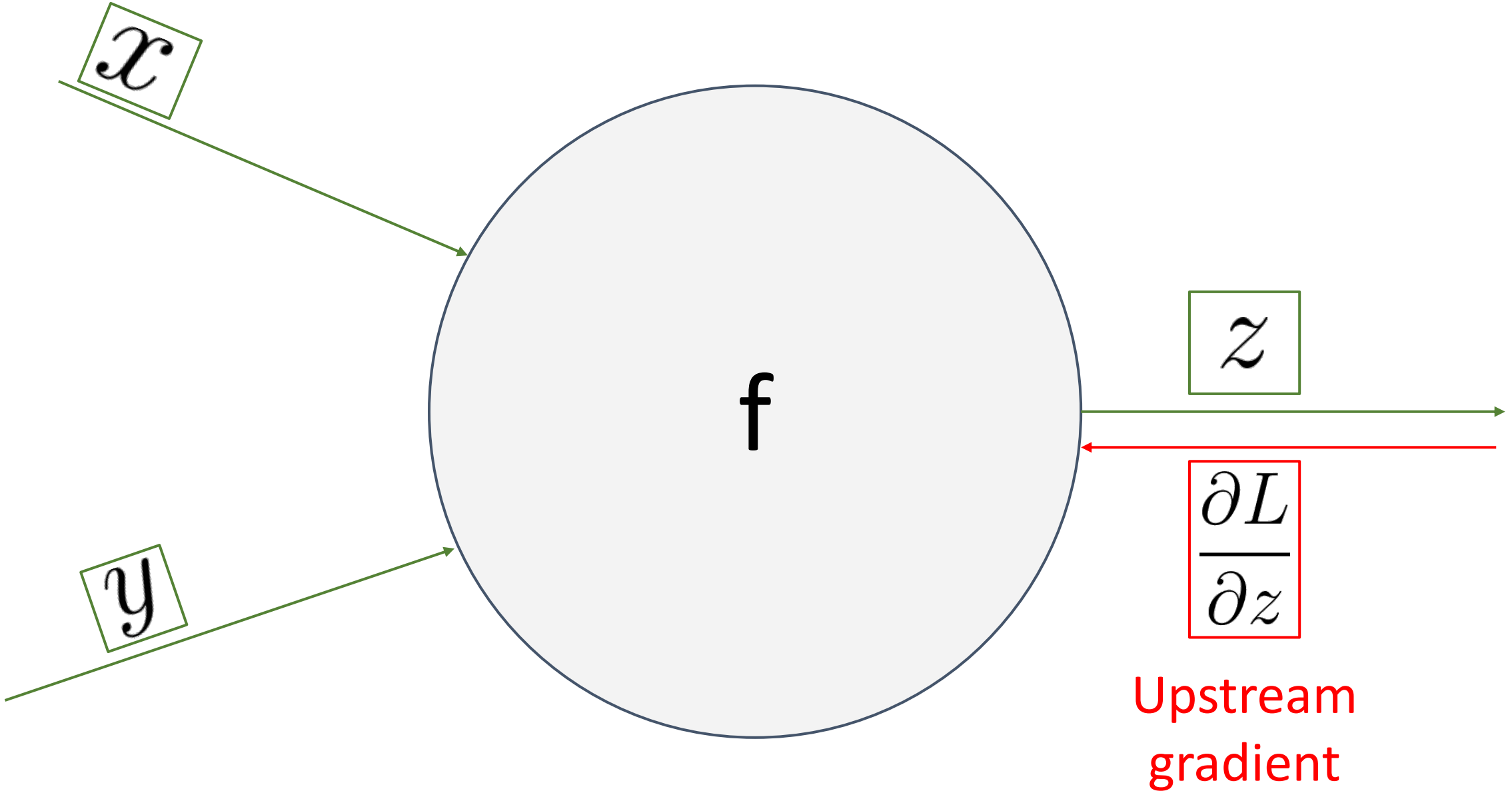
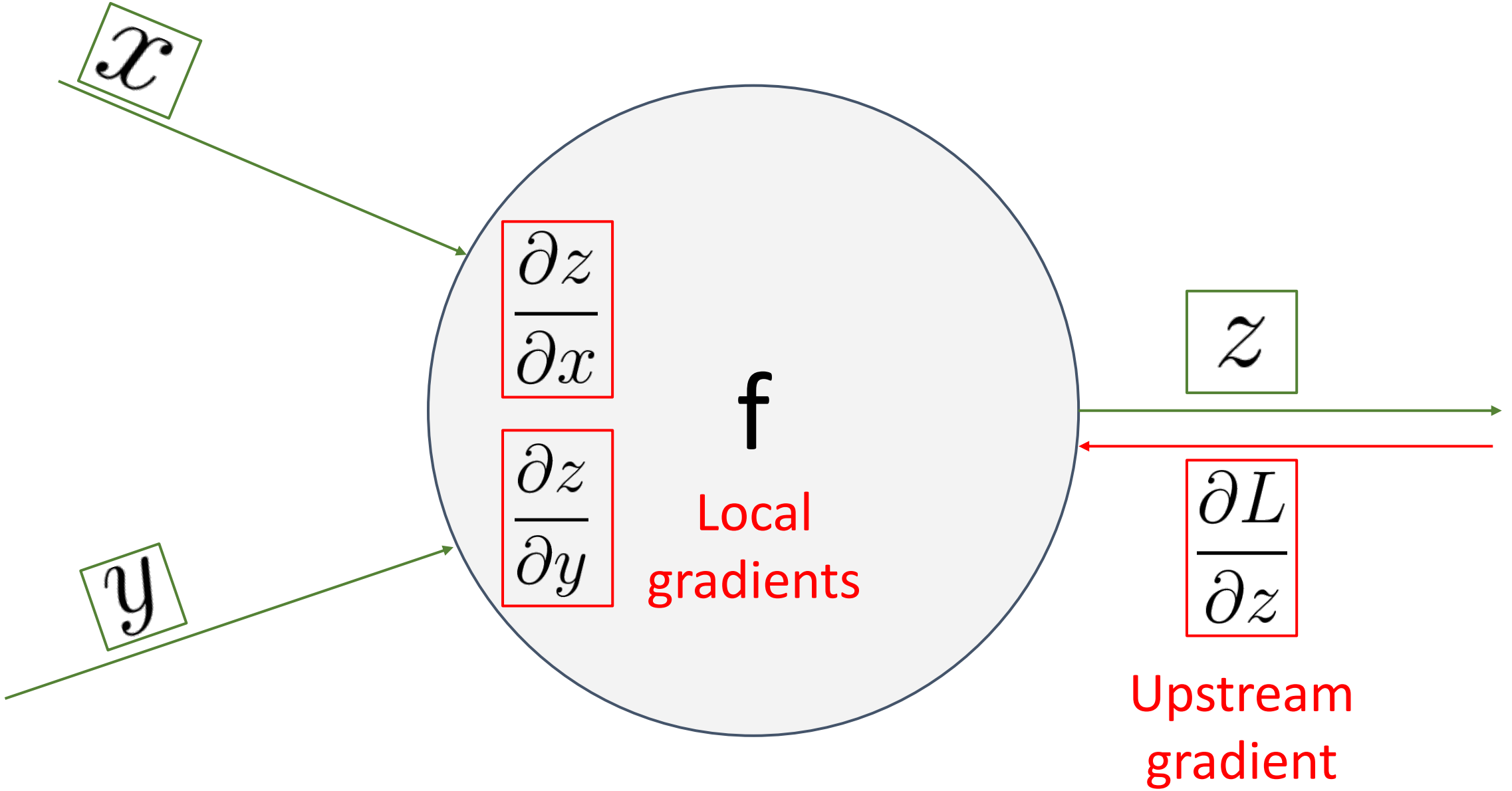
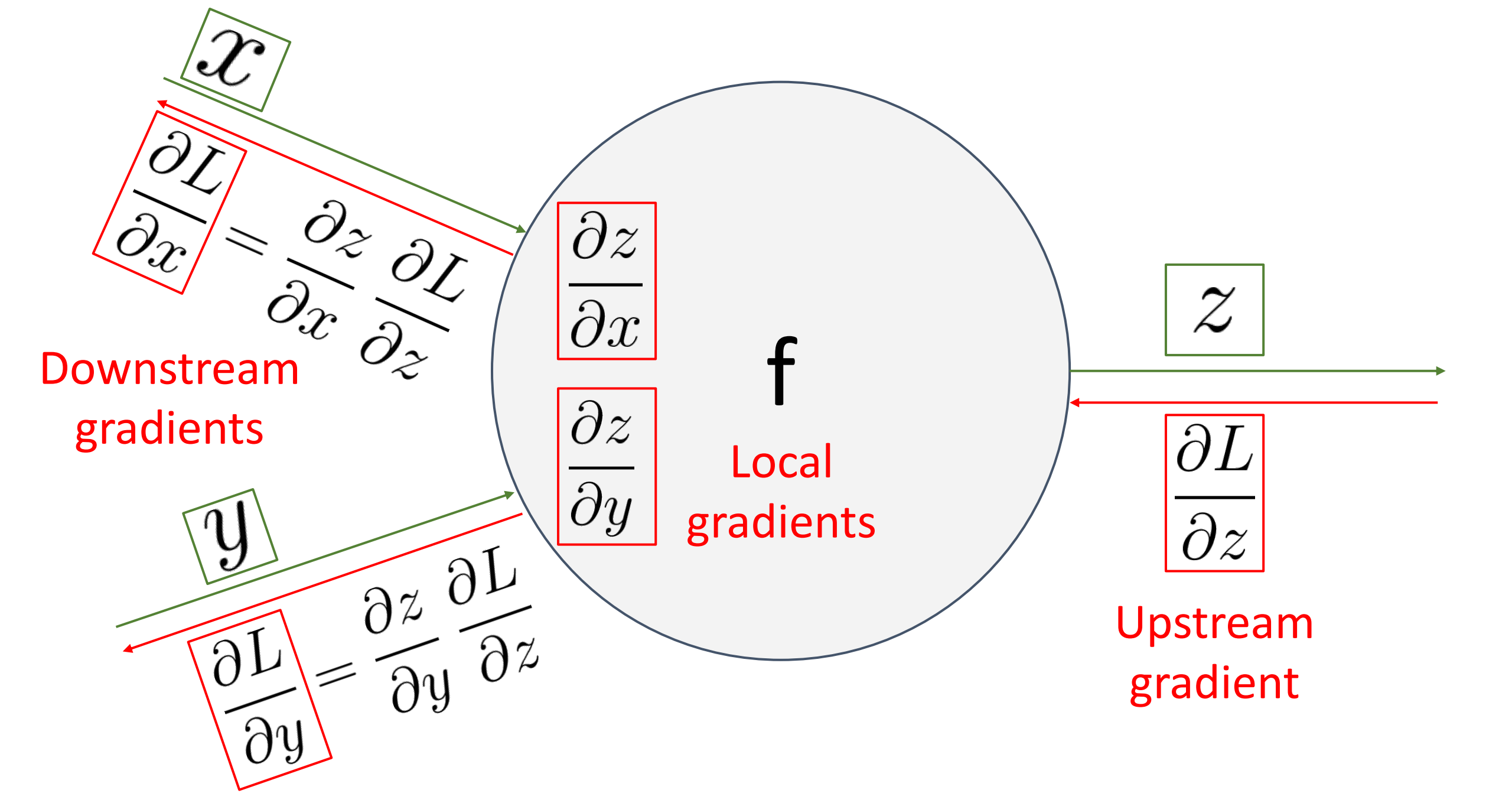
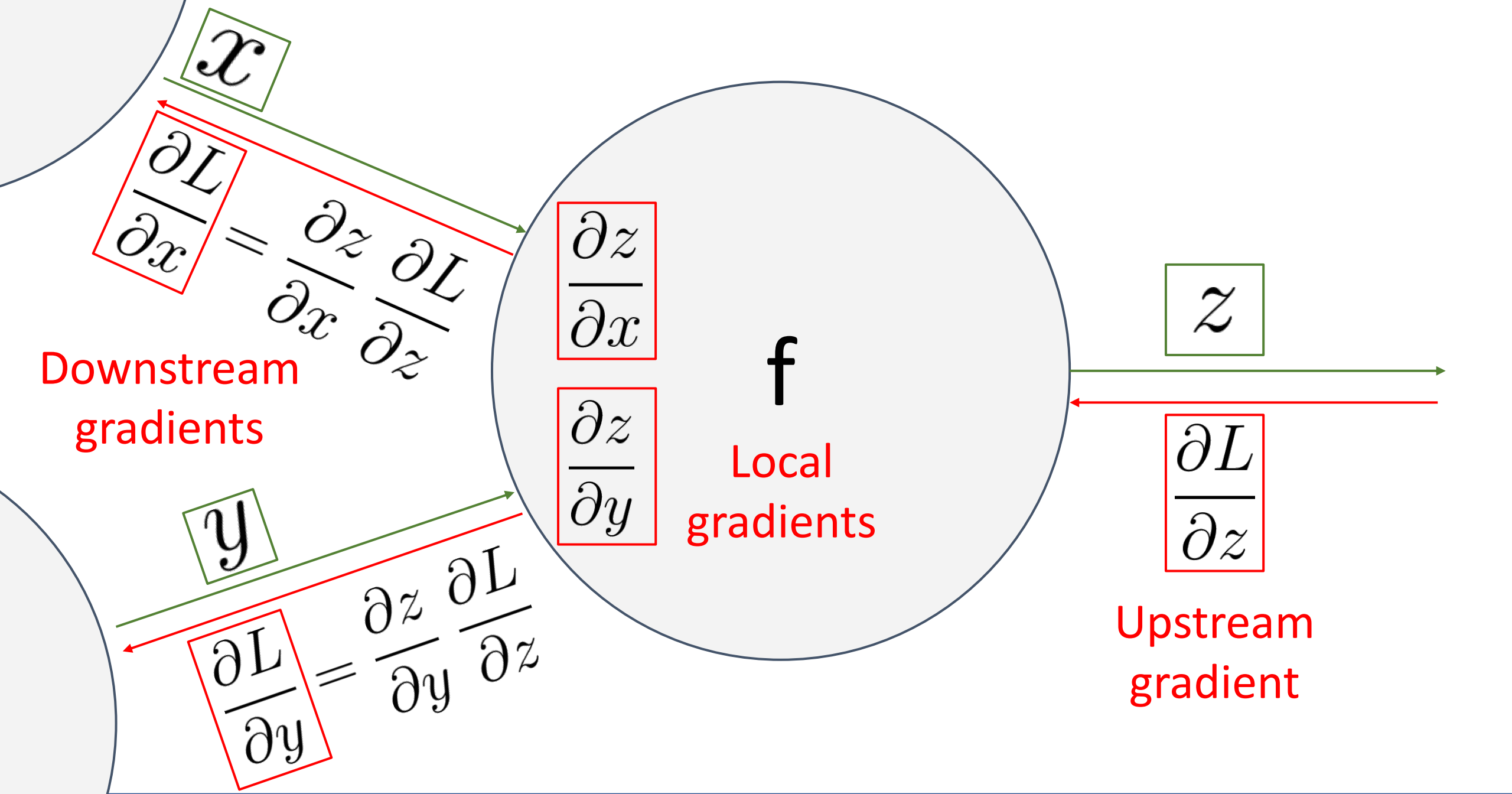

x
f
z
y

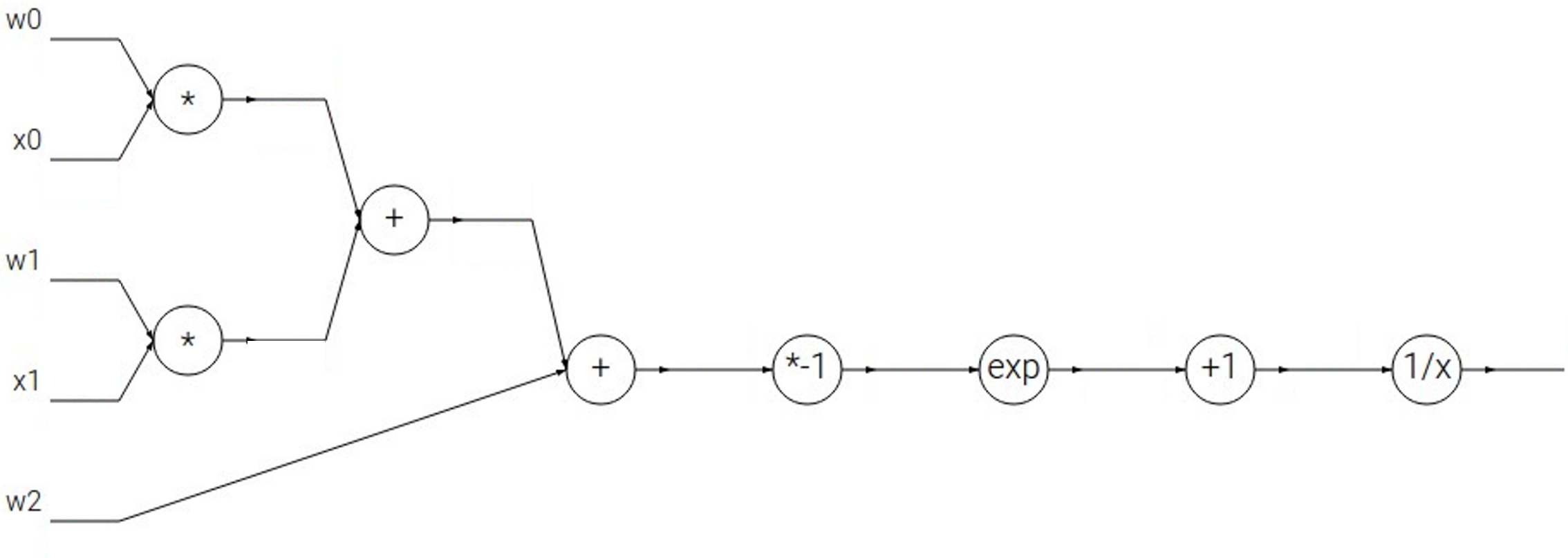

x
f
z
y
$\frac{\partial L}{\partial z}$
Upstream gradient


x
y
$\frac{\partial z}{\partial x}$
$\frac{\partial z}{\partial y}$
f
Local gradients
z
$\frac{\partial L}{\partial z}$
Upstream gradient


x
$\frac{\partial L}{\partial x} = \frac{\partial z}{\partial x}\frac{\partial L}{\partial z}$
Downstream gradients
$\frac{\partial z}{\partial x}$
$\frac{\partial z}{\partial y}$
f
Local gradients
z
$\frac{\partial L}{\partial z}$
Upstream gradient
y
$\frac{\partial L}{\partial y} = \frac{\partial z}{\partial y}\frac{\partial L}{\partial z}$


x
$\frac{\partial L}{\partial x} = \frac{\partial z}{\partial x}\frac{\partial L}{\partial z}$
Downstream gradients
y
$\frac{\partial L}{\partial y} = \frac{\partial z}{\partial y}\frac{\partial L}{\partial z}$
$\frac{\partial z}{\partial x}$
$\frac{\partial z}{\partial y}$
f
Local gradients
z
$\frac{\partial L}{\partial z}$
Upstream gradient

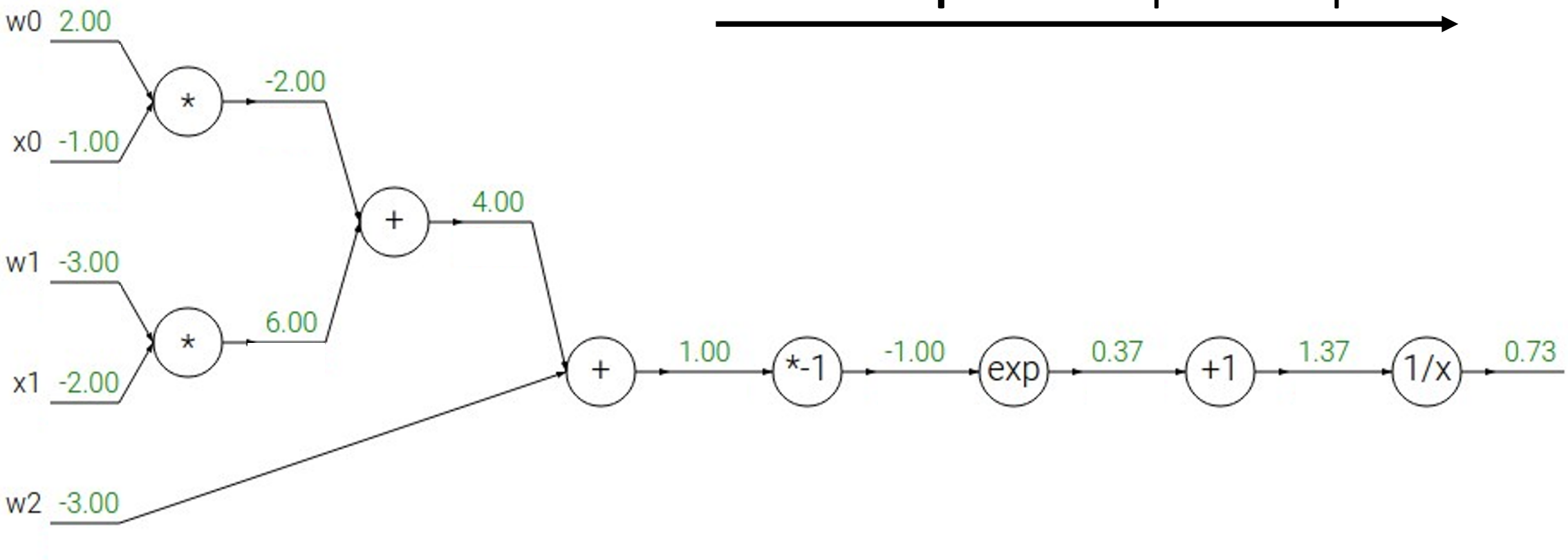
Another Example $f(x,w) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$



Another Example

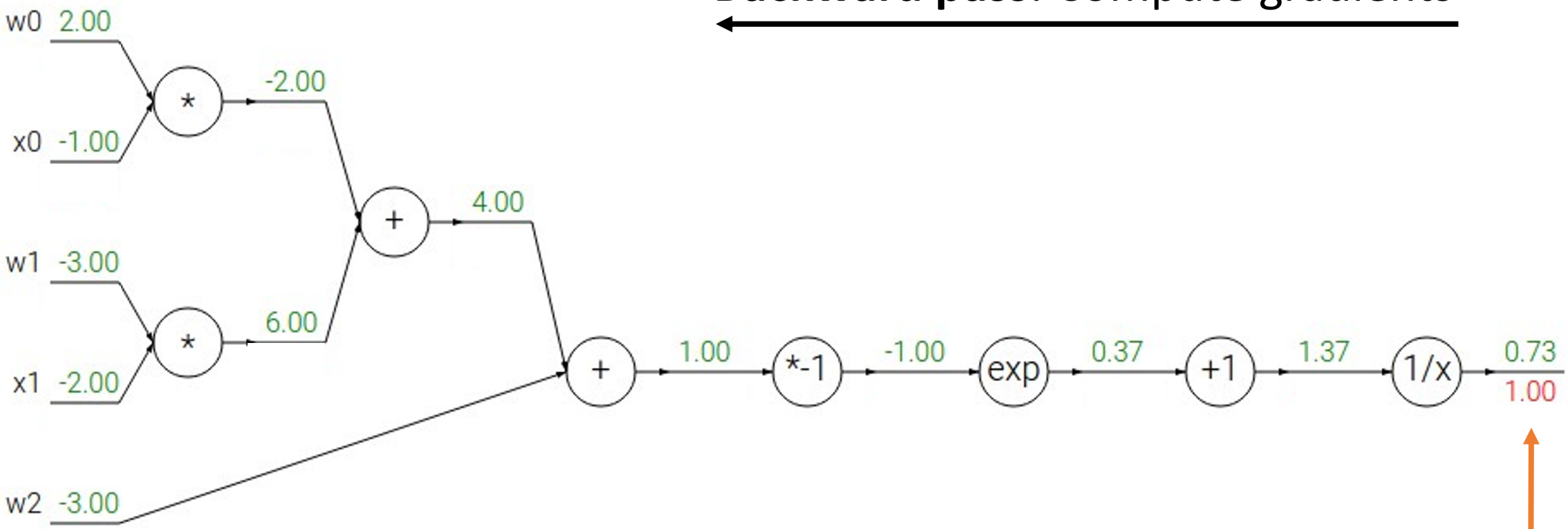
$$f(x,w) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$$

Forward pass: Compute outputs



Another Example $f(x,w) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$

Backward pass: Compute gradients



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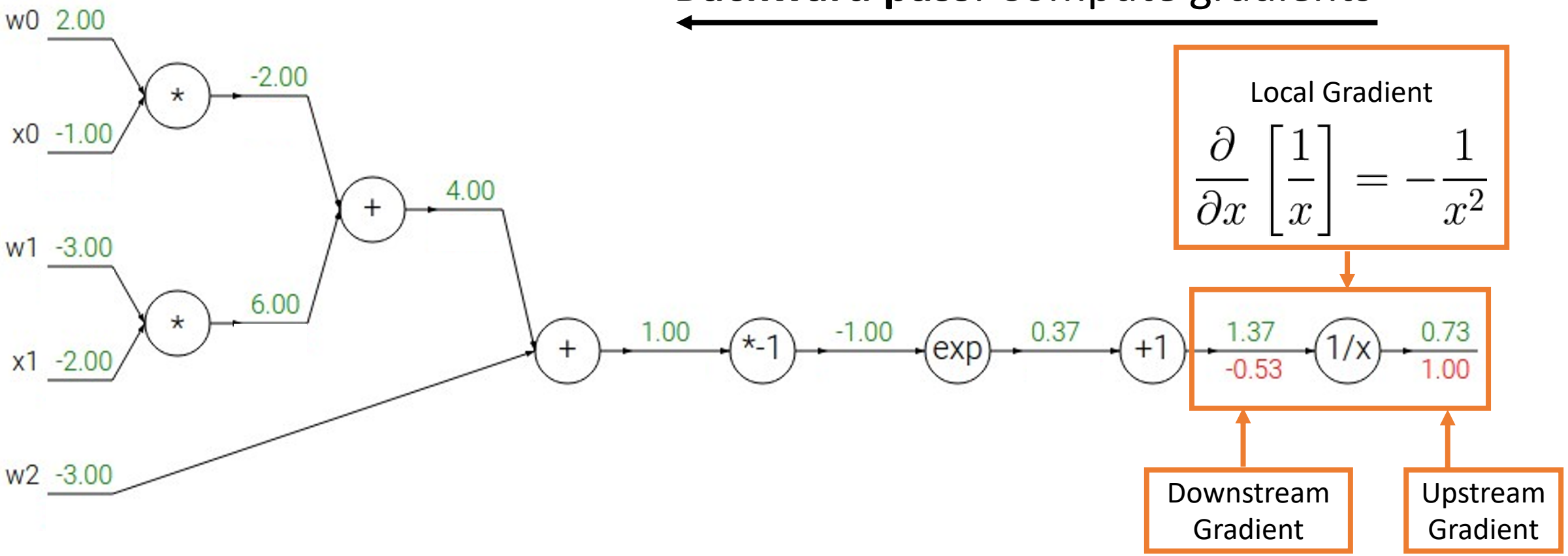

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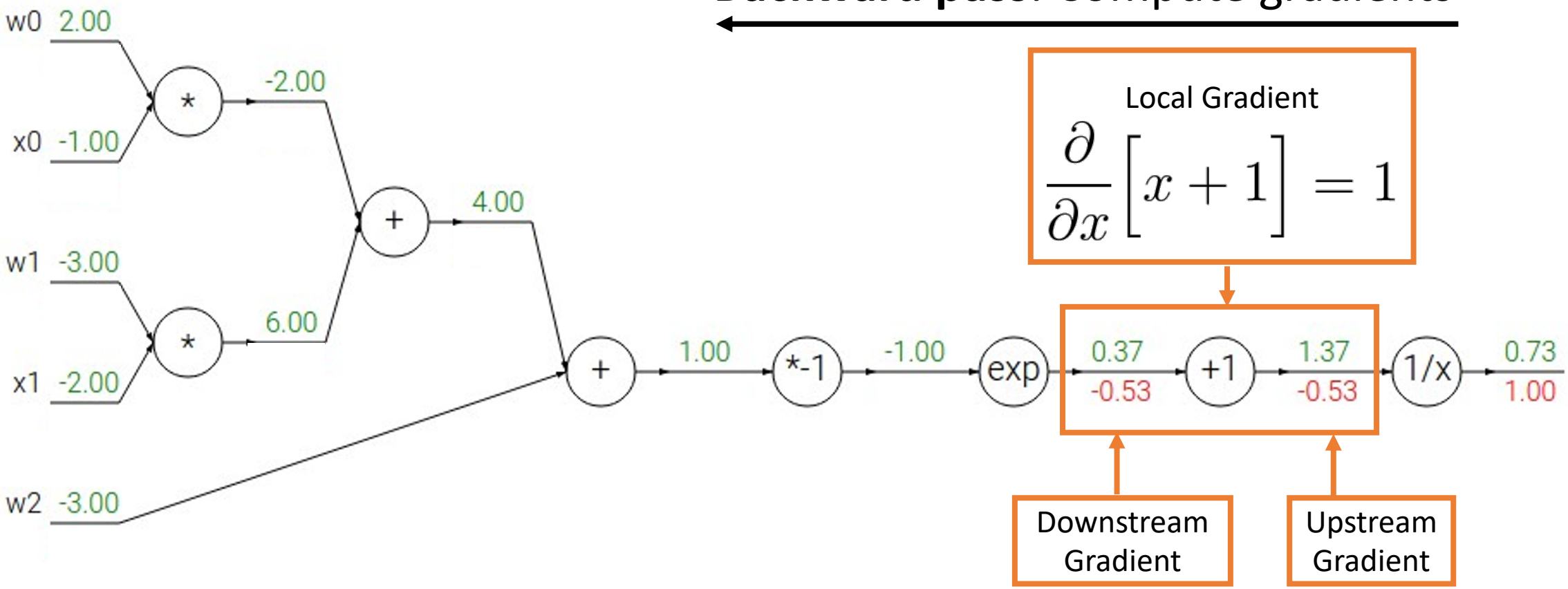

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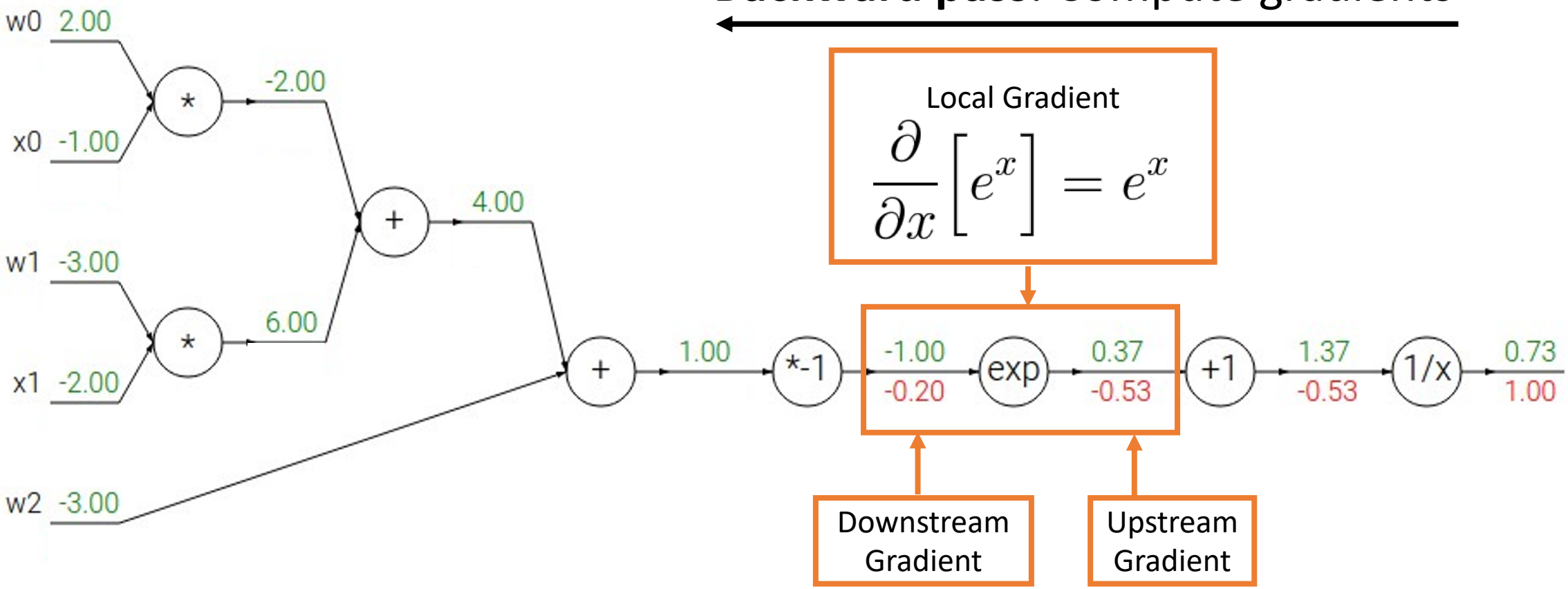
Backward pass: Compute gradients



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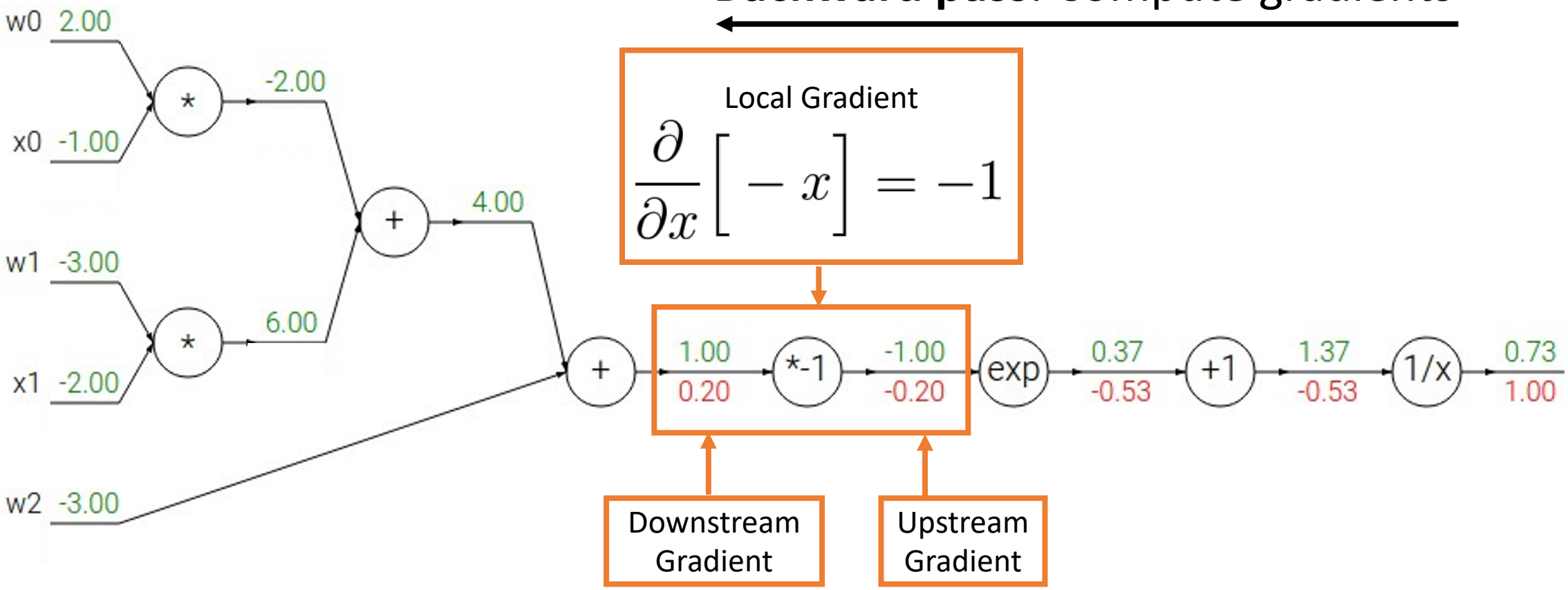
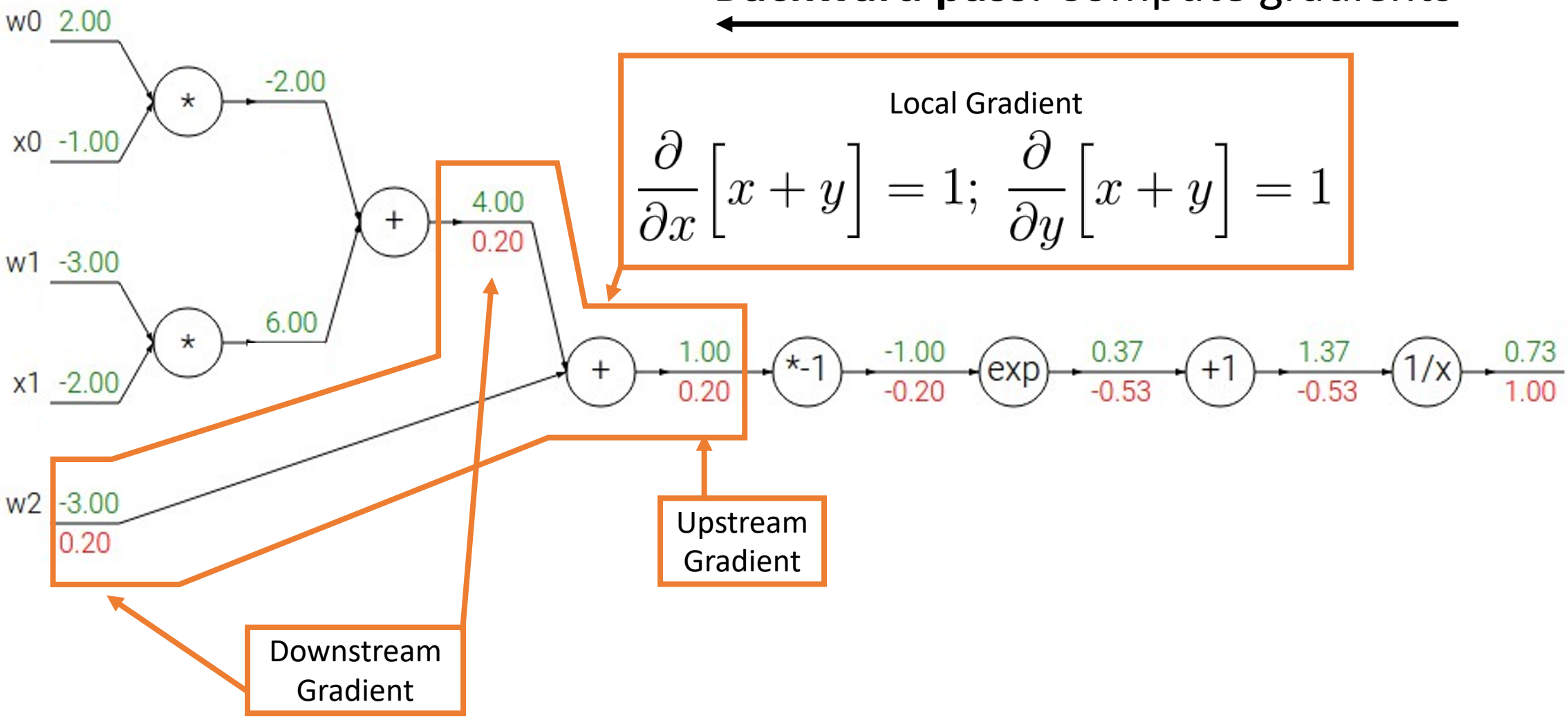
Backward pass: Compute gradients



Another Example $f(x,w) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$

Backward pass: Compute gradients



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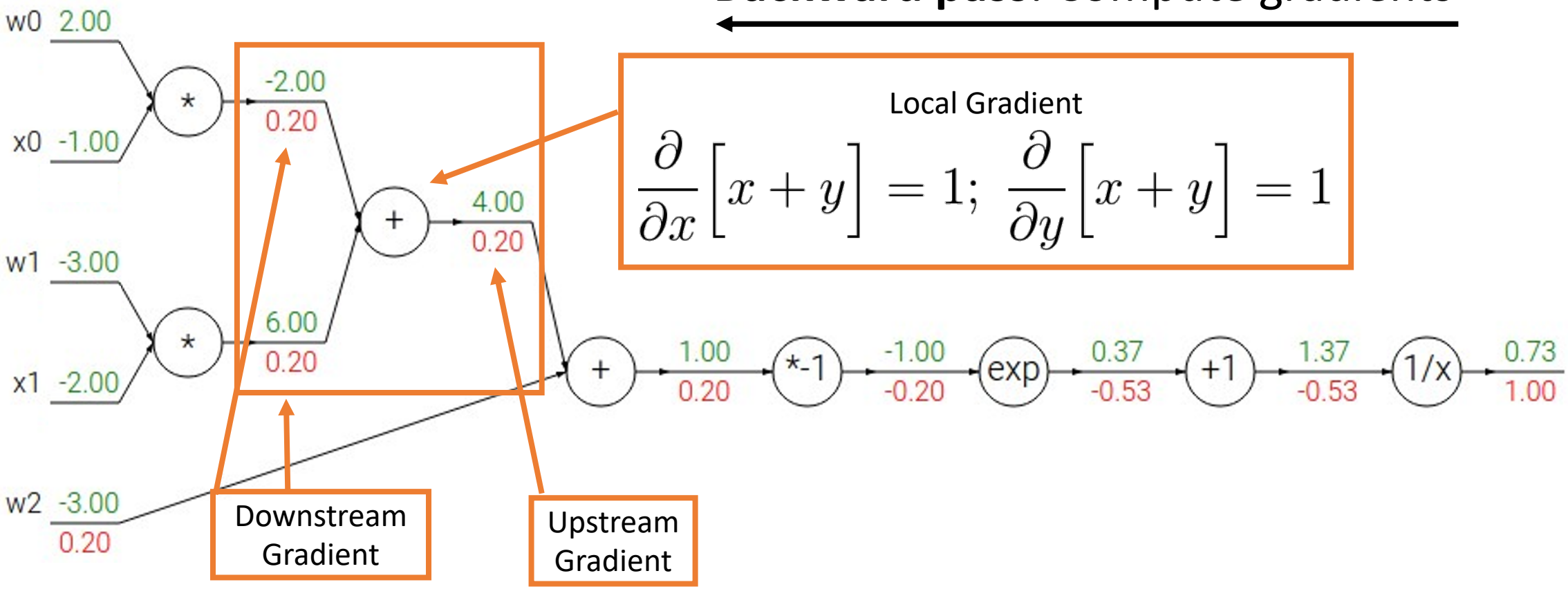
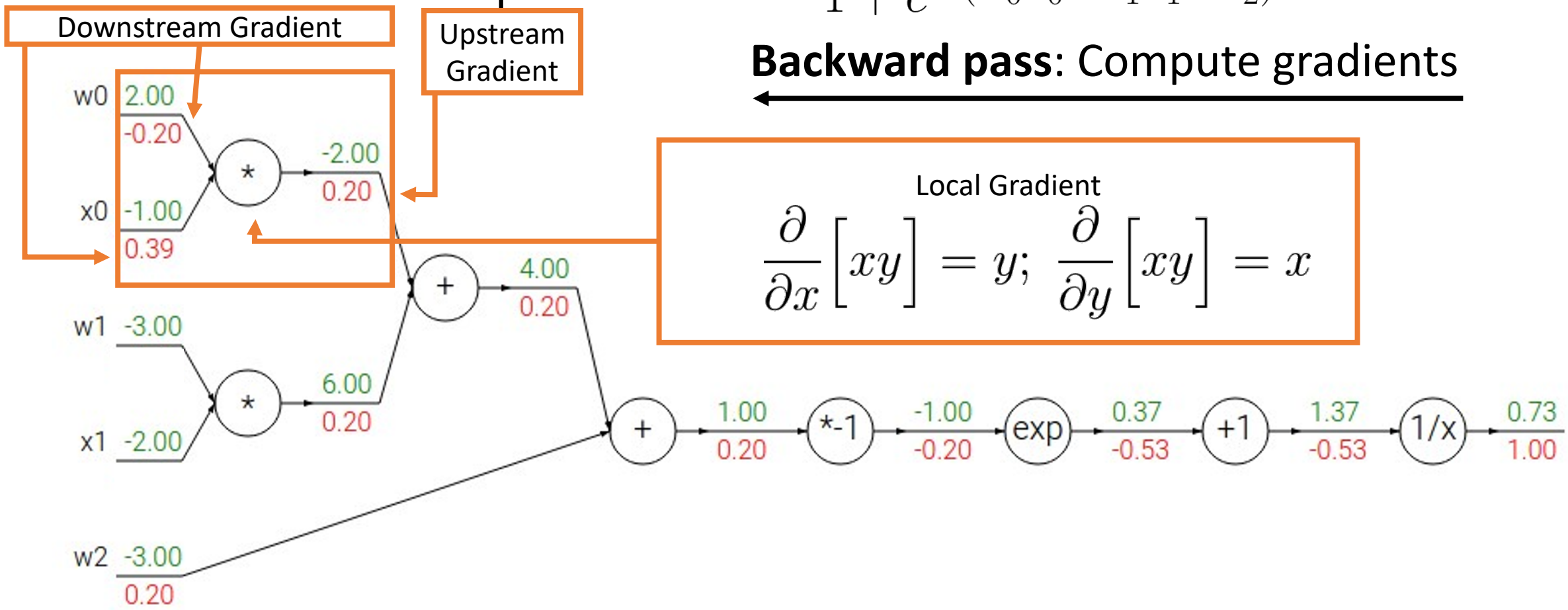


Another Example

$$f(x,w) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$$

Backward pass: Compute gradients



Another Example

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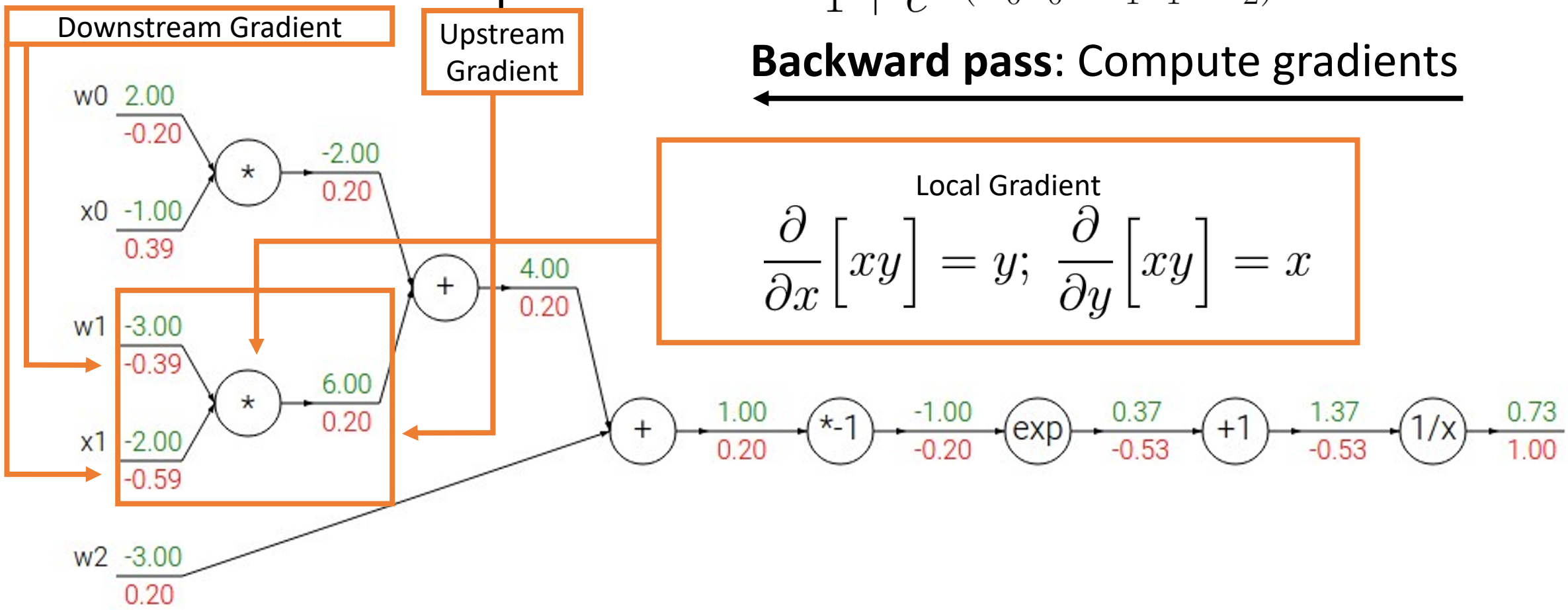
Backward pass: Compute gradients



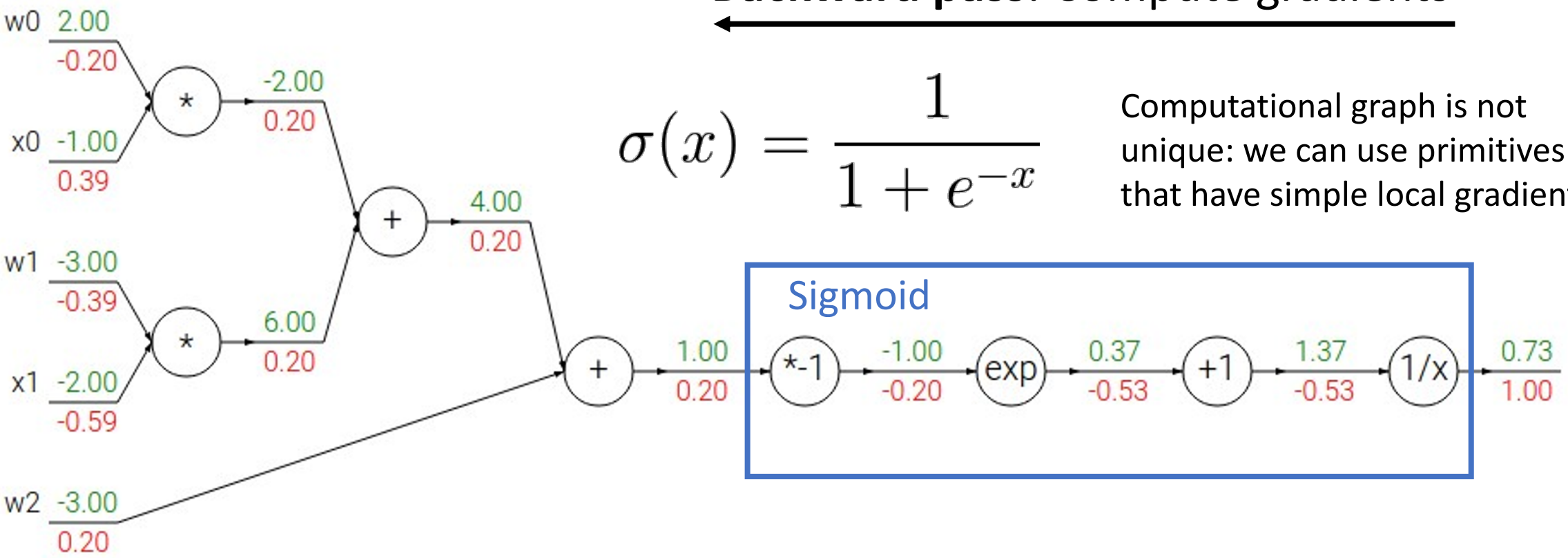
Local Gradient

$$\frac{\partial}{\partial x}[xy] = y; \quad \frac{\partial}{\partial y}[xy] = x$$

Another Example

$$f(x,w) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}} = \sigma(w_0x_0 + w_1x_1 + w_2)$$

Backward pass: Compute gradients



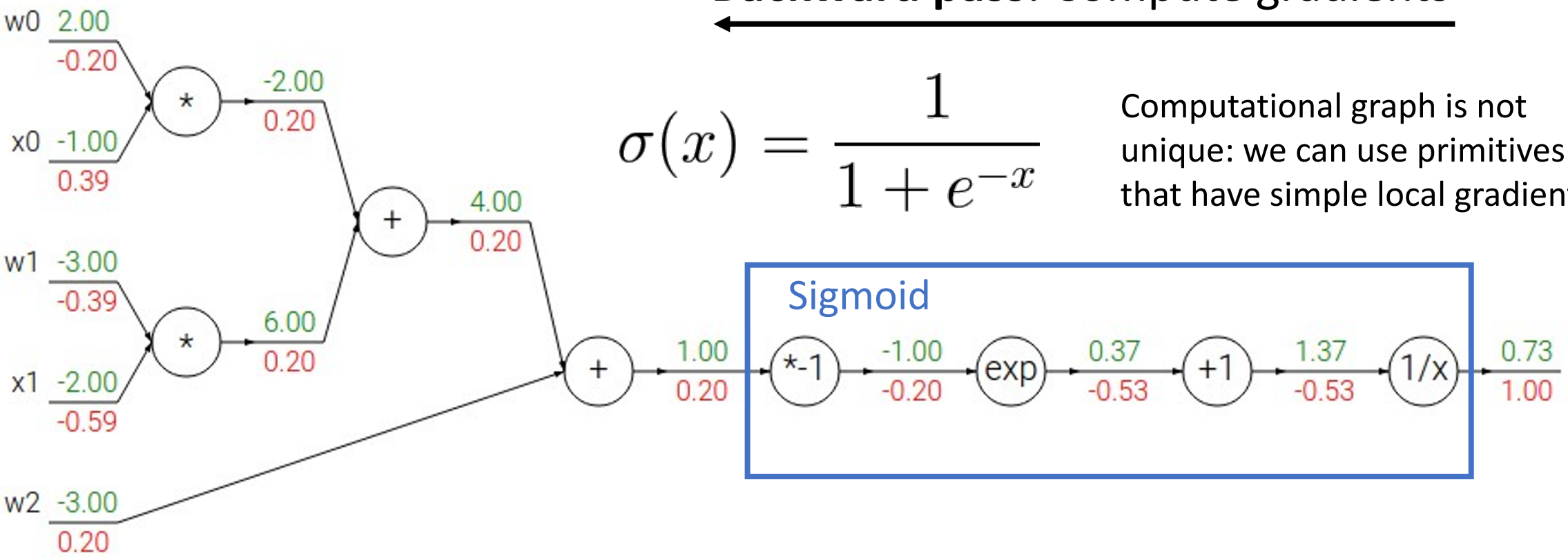
$$\sigma(x) = \frac{1}{1+e^{-x}}$$

Computational graph is not unique: we can use primitives that have simple local gradients

Another Example

$$f(x,w) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}} = \sigma(w_0x_0 + w_1x_1 + w_2)$$

Backward pass: Compute gradients



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

Computational graph is not unique: we can use primitives that have simple local gradients

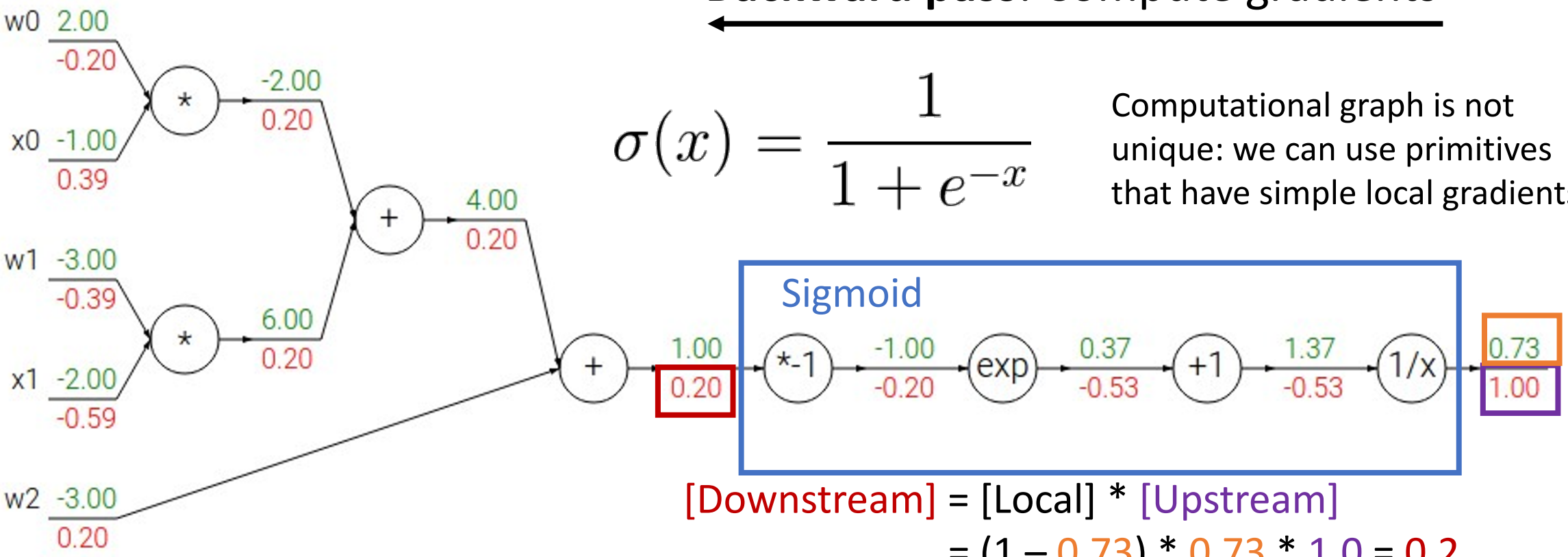
Sigmoid local gradient:

$$\frac{\partial}{\partial x}\left[\sigma(x)\right] = \frac{e^{-x}}{(1+e^{-x})^2} = \left(\frac{1+e^{-x}-1}{1+e^{-x}}\right)\left(\frac{1}{1+e^{-x}}\right) = (1-\sigma(x))\sigma(x)$$

Another Example

$$f(x,w) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}} = \sigma(w_0x_0 + w_1x_1 + w_2)$$

Backward pass: Compute gradients



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

Computational graph is not unique: we can use primitives that have simple local gradients

[Downstream] = [Local] * [Upstream]

= (1 – 0.73) * 0.73 * 1.0 = 0.2

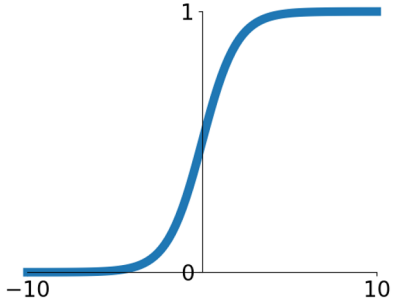
Sigmoid local gradient:

$$\frac{\partial}{\partial x}\left[\sigma(x)\right] = \frac{e^{-x}}{(1+e^{-x})^2} = \left(\frac{1+e^{-x}-1}{1+e^{-x}}\right)\left(\frac{1}{1+e^{-x}}\right) = (1-\sigma(x))\sigma(x)$$

Gradients of other Activation Functions?

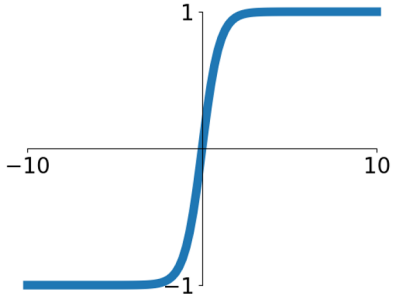
Sigmoid

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



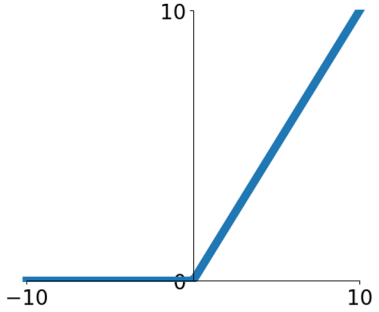
tanh

$$\tanh(x)$$



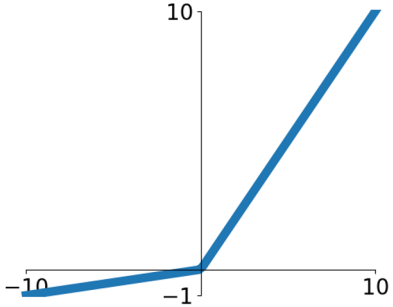
ReLU

$$\max(0, x)$$



Leaky ReLU

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

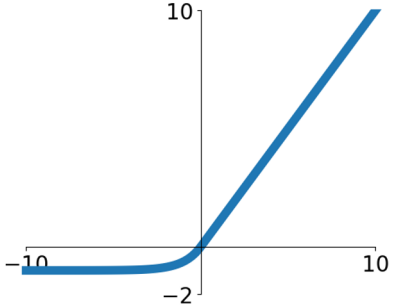


Maxout

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

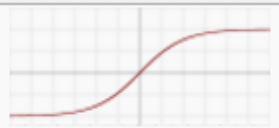
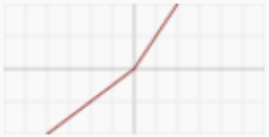
ELU

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



Gradients of activation functions?

Sigmoid local gradient: $$\frac{\partial}{\partial x}\left[\sigma(x)\right] = \frac{e^{-x}}{(1+e^{-x})^2} = \left(\frac{1+e^{-x}-1}{1+e^{-x}}\right)\left(\frac{1}{1+e^{-x}}\right) = (1-\sigma(x))\sigma(x)$$

Name	Plot	Equation	Derivative
TanH		$f(x) = \tanh(x) = \frac{2}{1+e^{-2x}} - 1$	$f'(x) = 1 - f(x)^2$
Rectified Linear Unit (ReLU)		$f(x) = \begin{cases} 0 & \text{for } x < 0 \\ x & \text{for } x \geq 0 \end{cases}$	$f'(x) = \begin{cases} 0 & \text{for } x < 0 \\ 1 & \text{for } x \geq 0 \end{cases}$
Parameteric Rectified Linear Unit (PReLU) [2]		$f(x) = \begin{cases} \alpha x & \text{for } x < 0 \\ x & \text{for } x \geq 0 \end{cases}$	$f'(x) = \begin{cases} \alpha & \text{for } x < 0 \\ 1 & \text{for } x \geq 0 \end{cases}$

https://towardsdatascience.com/activation-functions-neural-networks-1cbd9f8d91d6

Cross-Entropy Loss (Multinomial Logistic Regression)

Want to interpret raw classifier scores as **probabilities**

$$s = f(x_i; W)$$

$$P(Y = k|X = x_i) = \frac{e^{s_k}}{\sum_j e^{s_j}}$$

Softmax function

$$L_i = -\log P(Y = y_i|X = x_i)$$

	Unnormalized log-probabilities / logits	exp	Probabilities must be >= 0	normalize	Probabilities must sum to 1
cat	**3.2**	→	**24.5**	→	**0.13**
car	5.1		164.0		0.87
frog	-1.7		0.18		0.00
			unnormalized probabilities		probabilities

$L_i = -\log(0.13)$
$= \mathbf{2.04}$

Maximum Likelihood Estimation
Choose weights to maximize the likelihood of the observed data (next lecture)

Gradients of softmax?

Derivative of softmax

Let's compute $D_j S_i$ for arbitrary *i* and *j*:

$$D_j S_i = \frac{\partial S_i}{\partial a_j} = \frac{\partial \frac{e^{a_i}}{\sum_{k=1}^{N} e^{a_k}}}{\partial a_j}$$

We'll be using the quotient rule of derivatives. For $f(x) = \frac{g(x)}{h(x)}$:

$$f'(x) = \frac{g'(x)h(x) - h'(x)g(x)}{[h(x)]^2}$$

In our case, we have:

$$g_i = e^{a_i}$$

$$h_i = \sum_{k=1}^{N} e^{a_k}$$

$$D_j S_i = \begin{cases} S_i(1 - S_j) & i = j \\ -S_j S_i & i \neq j \end{cases}$$

es, but if anyone is taking more prid
why you'll find various "condensed"
s using the Kronecker delta function

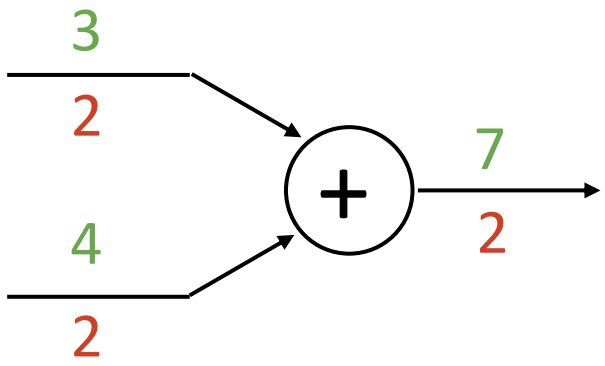
$$\delta_{ij} = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases}$$

$$D_j S_i = S_i(\delta_{ij} - S_j)$$

https://eli.thegreenplace.net/2016/the-softmax-function-and-its-derivative/

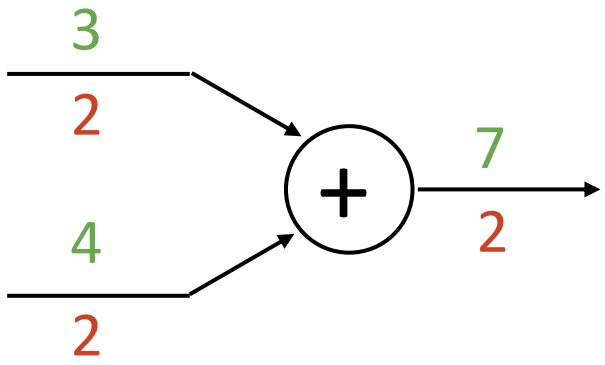
Patterns in Gradient Flow

add gate: gradient distributor

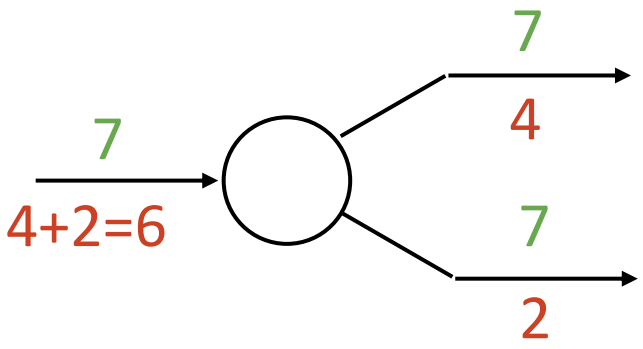


Patterns in Gradient Flow

add gate: gradient distributor

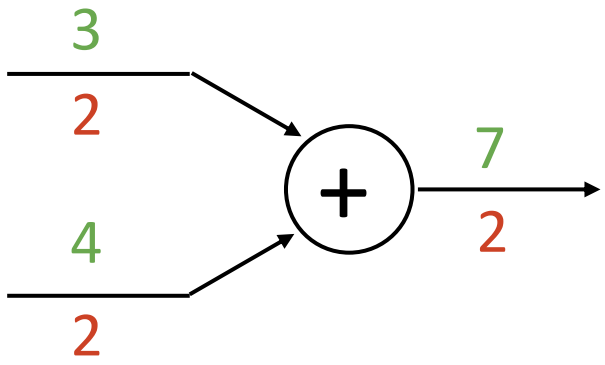


copy gate: gradient adder

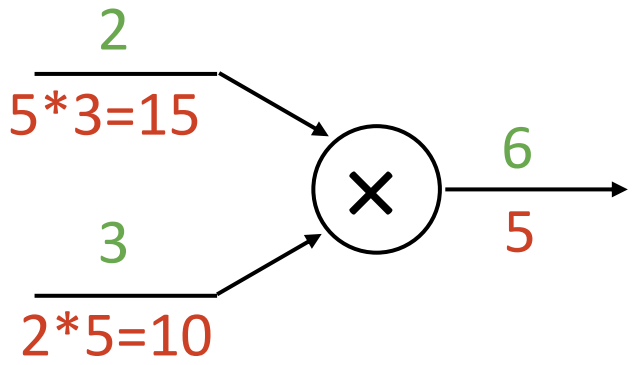


Patterns in Gradient Flow

add gate: gradient distributor



mul gate: "swap multiplier"



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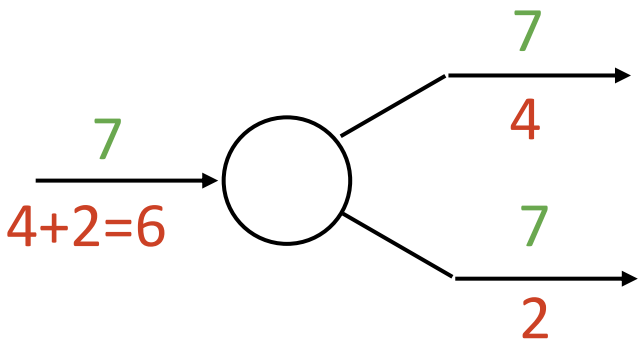

Patterns in Gradient Flow

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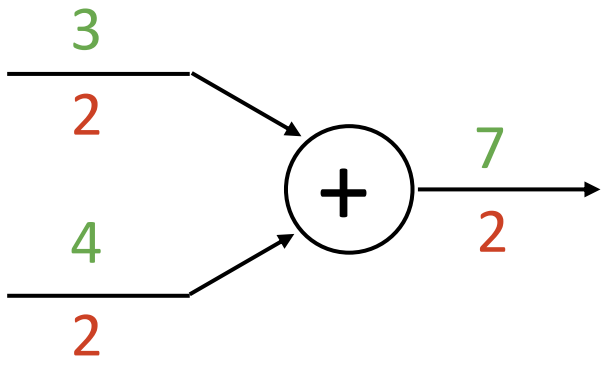

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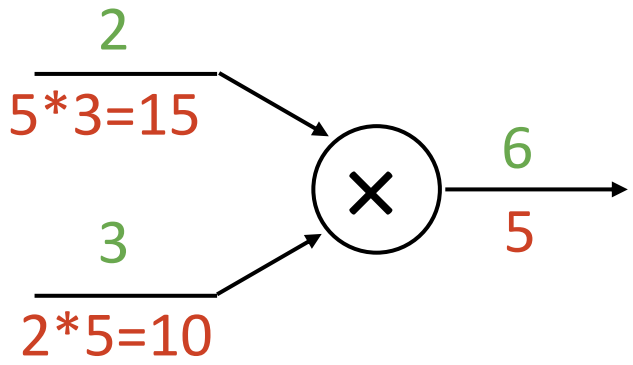

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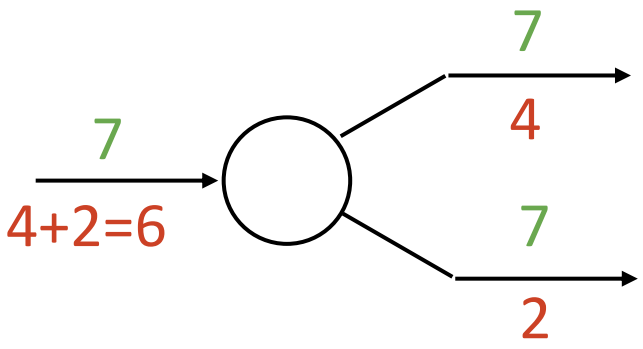
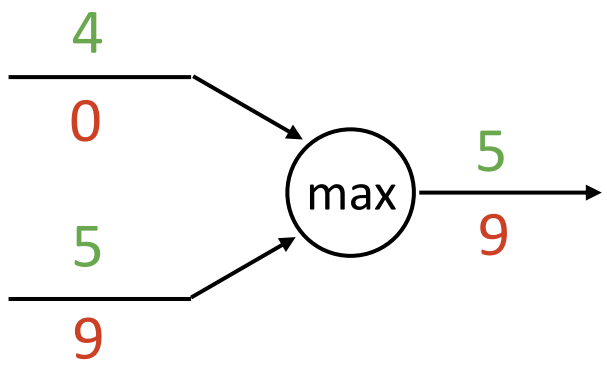


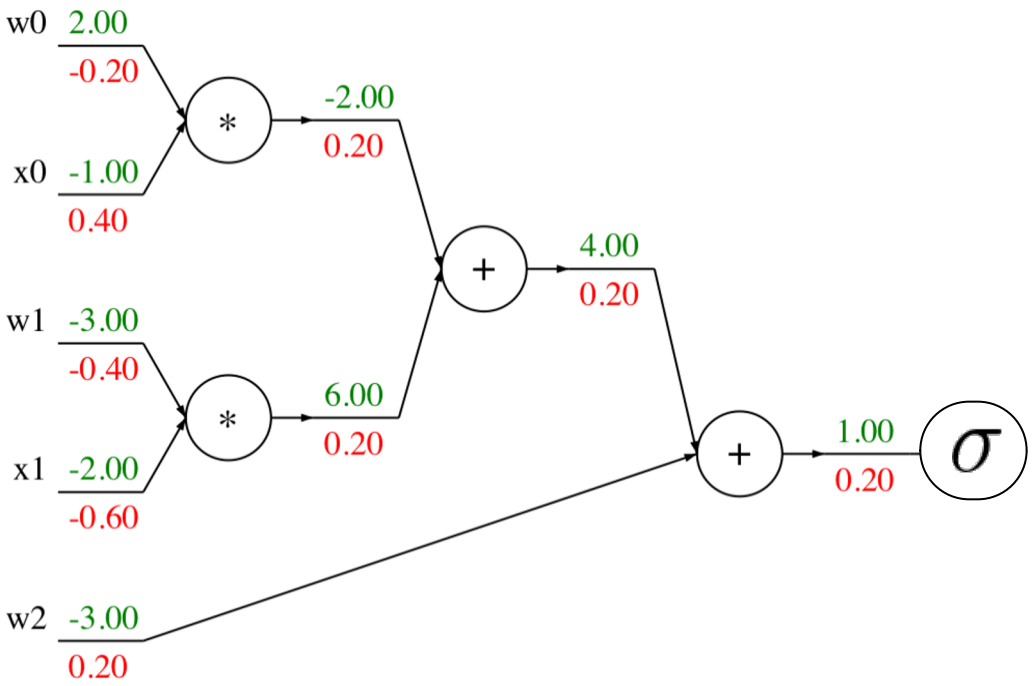
max gate: gradient router



Backprop Implementation: "Flat" gradient code:

Forward pass:
Compute output

```
def f(w0, x0, w1, x1, w2):
  s0 = w0 * x0
  s1 = w1 * x1
  s2 = s0 + s1
  s3 = s2 + w2
  L = sigmoid(s3)
```



Backprop Implementation: "Flat" gradient code:

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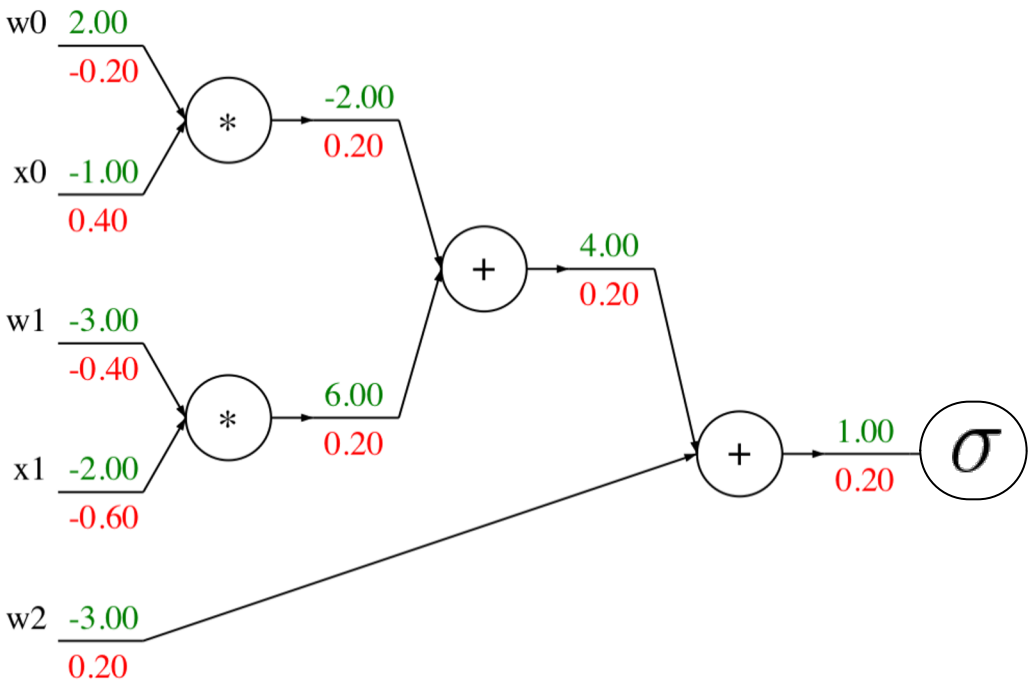
Compute output




```
def f(w0, x0, w1, x1, w2):
  s0 = w0 * x0
  s1 = w1 * x1
  s2 = s0 + s1
  s3 = s2 + w2
  L = sigmoid(s3)
```

Backward pass:
Compute grads

```
grad_L = 1.0
grad_s3 = grad_L * (1 - L) * L
grad_w2 = grad_s3
grad_s2 = grad_s3
grad_s0 = grad_s2
grad_s1 = grad_s2
grad_w1 = grad_s1 * x1
grad_x1 = grad_s1 * w1
grad_w0 = grad_s0 * x0
grad_x0 = grad_s0 * w0
```

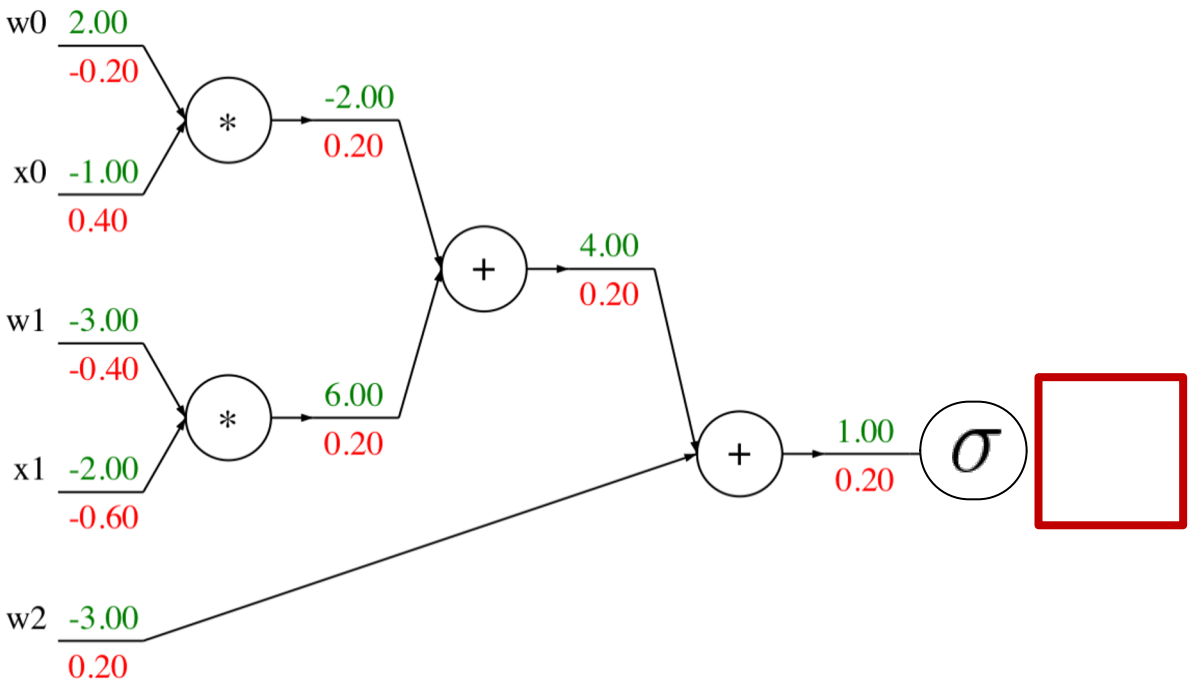
Backprop Implementation: "Flat" gradient code:

Forward pass: Compute output

```
def f(w0, x0, w1, x1, w2):
  s0 = w0 * x0
  s1 = w1 * x1
  s2 = s0 + s1
  s3 = s2 + w2
  L = sigmoid(s3)
```

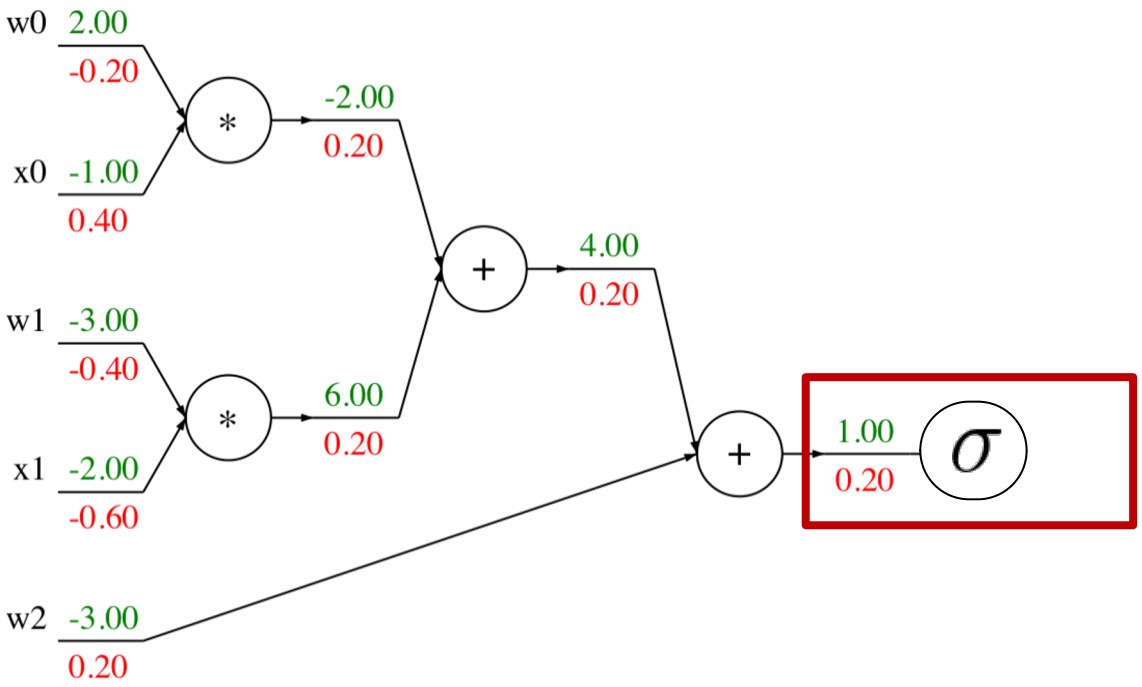
Base case

```
  grad_L = 1.0
  grad_s3 = grad_L * (1 - L) * L
  grad_w2 = grad_s3
  grad_s2 = grad_s3
  grad_s0 = grad_s2
  grad_s1 = grad_s2
  grad_w1 = grad_s1 * x1
  grad_x1 = grad_s1 * w1
  grad_w0 = grad_s0 * x0
  grad_x0 = grad_s0 * w0
```



Backprop Implementation: "Flat" gradient code:

Forward pass:
Compute output

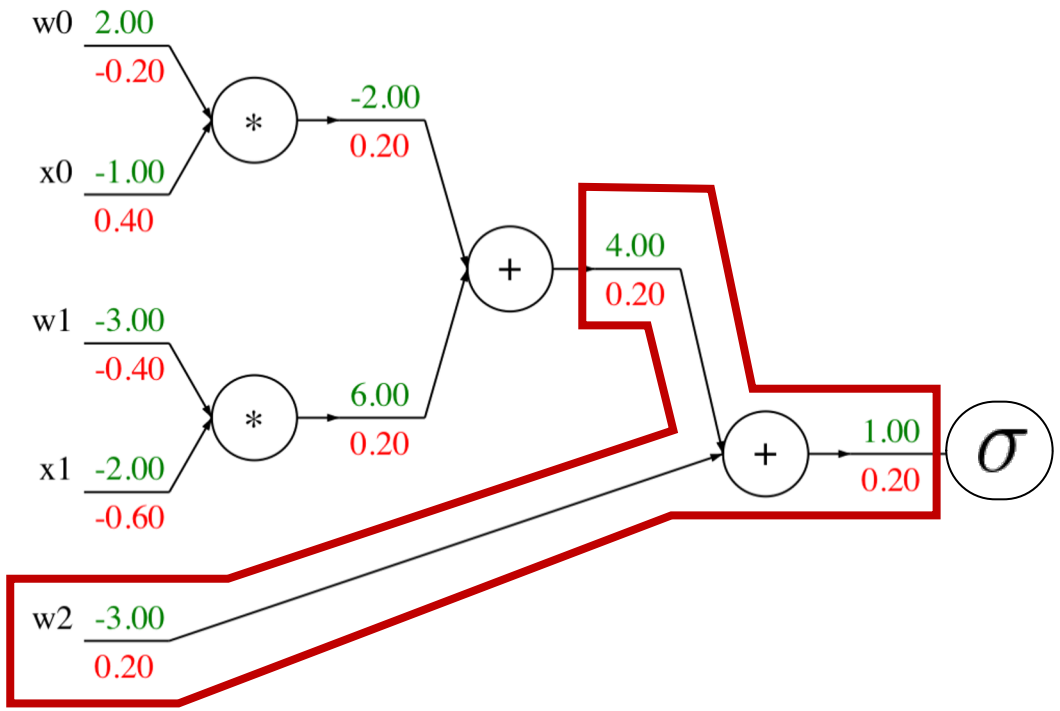



```
def f(w0, x0, w1, x1, w2):
  s0 = w0 * x0
  s1 = w1 * x1
  s2 = s0 + s1
  s3 = s2 + w2
  L = sigmoid(s3)
```

Sigmoid

```
  grad_L = 1.0
  grad_s3 = grad_L * (1 - L) * L
  grad_w2 = grad_s3
  grad_s2 = grad_s3
  grad_s0 = grad_s2
  grad_s1 = grad_s2
  grad_w1 = grad_s1 * x1
  grad_x1 = grad_s1 * w1
  grad_w0 = grad_s0 * x0
  grad_x0 = grad_s0 * w0
```

Backprop Implementation: "Flat" gradient code:



Forward pass:
Compute output

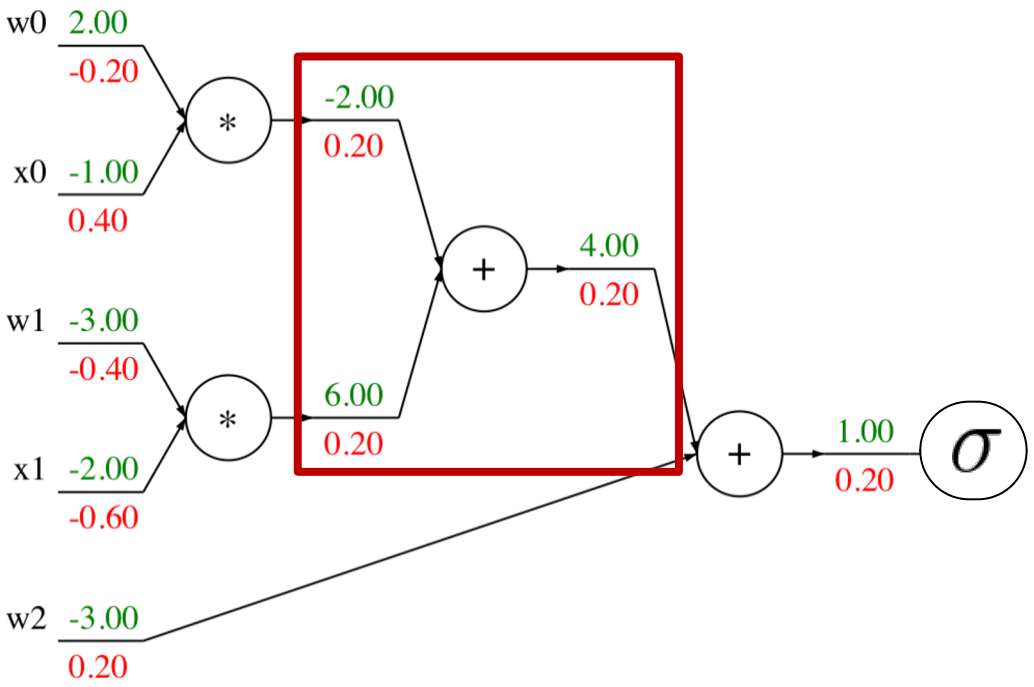
```
def f(w0, x0, w1, x1, w2):
  s0 = w0 * x0
  s1 = w1 * x1
  s2 = s0 + s1
  s3 = s2 + w2
  L = sigmoid(s3)
```

Add

```
  grad_L = 1.0
  grad_s3 = grad_L * (1 - L) * L
  grad_w2 = grad_s3
  grad_s2 = grad_s3
  grad_s0 = grad_s2
  grad_s1 = grad_s2
  grad_w1 = grad_s1 * x1
  grad_x1 = grad_s1 * w1
  grad_w0 = grad_s0 * x0
  grad_x0 = grad_s0 * w0
```

Backprop Implementation: "Flat" gradient code:

Forward pass:
Compute output

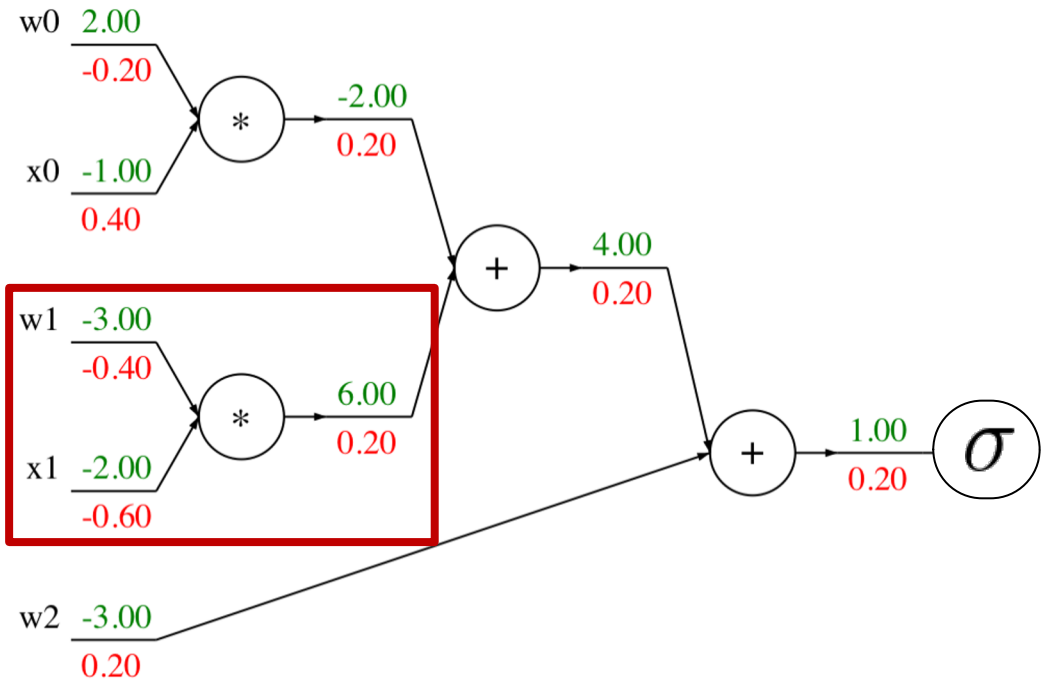



```
def f(w0, x0, w1, x1, w2):
  s0 = w0 * x0
  s1 = w1 * x1
  s2 = s0 + s1
  s3 = s2 + w2
  L = sigmoid(s3)
```

Add

```
  grad_L = 1.0
  grad_s3 = grad_L * (1 - L) * L
  grad_w2 = grad_s3
  grad_s2 = grad_s3
  grad_s0 = grad_s2
  grad_s1 = grad_s2
  grad_w1 = grad_s1 * x1
  grad_x1 = grad_s1 * w1
  grad_w0 = grad_s0 * x0
  grad_x0 = grad_s0 * w0
```

Backprop Implementation: "Flat" gradient code:



Forward pass: Compute output

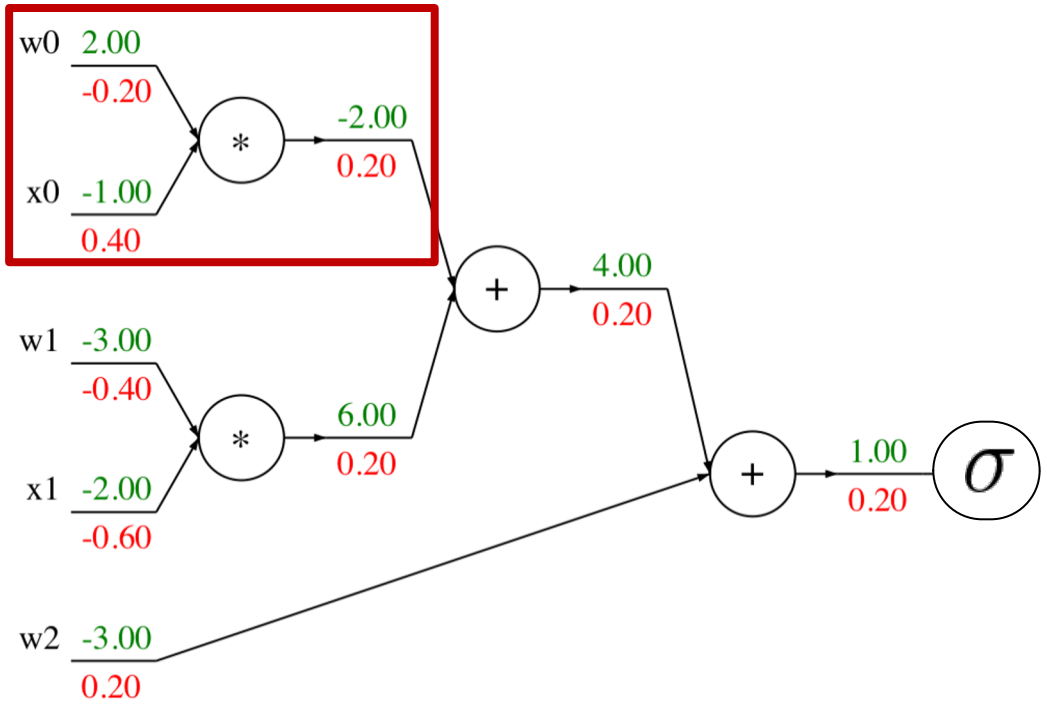
```
def f(w0, x0, w1, x1, w2):
  s0 = w0 * x0
  s1 = w1 * x1
  s2 = s0 + s1
  s3 = s2 + w2
  L = sigmoid(s3)
```

```
  grad_L = 1.0
  grad_s3 = grad_L * (1 - L) * L
  grad_w2 = grad_s3
  grad_s2 = grad_s3
  grad_s0 = grad_s2
  grad_s1 = grad_s2
  grad_w1 = grad_s1 * x1
  grad_x1 = grad_s1 * w1
  grad_w0 = grad_s0 * x0
  grad_x0 = grad_s0 * w0
```

Multiply

Backprop Implementation: "Flat" gradient code:

Forward pass: Compute output

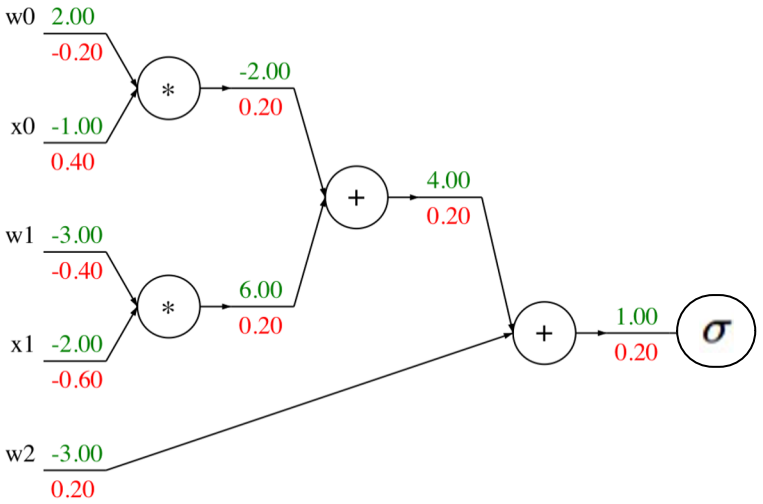



```
def f(w0, x0, w1, x1, w2):
  s0 = w0 * x0
  s1 = w1 * x1
  s2 = s0 + s1
  s3 = s2 + w2
  L = sigmoid(s3)
```

```
  grad_L = 1.0
  grad_s3 = grad_L * (1 - L) * L
  grad_w2 = grad_s3
  grad_s2 = grad_s3
  grad_s0 = grad_s2
  grad_s1 = grad_s2
  grad_w1 = grad_s1 * x1
  grad_x1 = grad_s1 * w1
  grad_w0 = grad_s0 * x0
  grad_x0 = grad_s0 * w0
```

Multiply

Backprop Implementation: Modular API

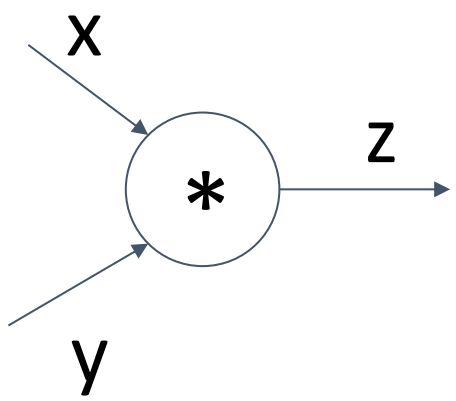


Graph (or Net) object *(rough pseudo code)*

```
class ComputationalGraph(object):
    #...
    def forward(inputs):
        # 1. [pass inputs to input gates...]
        # 2. forward the computational graph:
        for gate in self.graph.nodes_topologically_sorted():
            gate.forward()
        return loss # the final gate in the graph outputs the loss
    def backward():
        for gate in reversed(self.graph.nodes_topologically_sorted()):
            gate.backward() # little piece of backprop (chain rule applied)
        return inputs_gradients
```

Example: PyTorch Autograd Functions

Write something similar in HW3



(x,y,z are scalars)

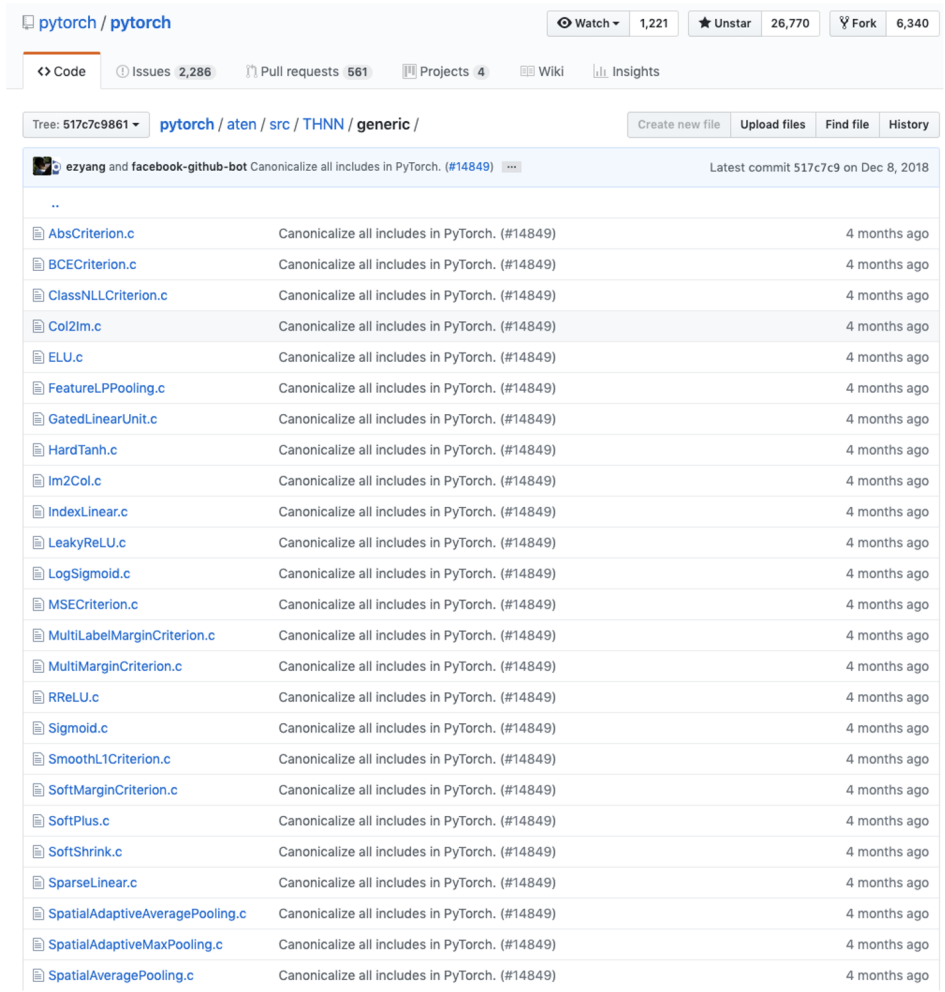
```
class Multiply(torch.autograd.Function):
  @staticmethod
  def forward(ctx, x, y):
    ctx.save_for_backward(x, y)
    z = x * y
    return z
  @staticmethod
  def backward(ctx, grad_z):
    x, y = ctx.saved_tensors
    grad_x = y * grad_z   # dz/dx * dL/dz
    grad_y = x * grad_z   # dz/dy * dL/dz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

Need to stash some values for use in backward

Upstream gradient

Multiply upstream and local gradients

Example: PyTorch operators



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

..

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
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SpatialAdaptiveMaxPooling.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
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VolumetricFullDilatedConvolution.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
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VolumetricUpSamplingTrilinear.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago
linear_upsampling.h	Implement nn.functional.interpolate based on upsample. (#8591)	9 months ago
pooling_shape.h	Use integer math to compute output size of pooling operations (#14405)	4 months ago
unfold.c	Canonicalize all includes in PyTorch. (#14849)	4 months ago

PyTorch sigmoid layer

```
#ifndef TH_GENERIC_FILE
#define TH_GENERIC_FILE "THNN/generic/Sigmoid.c"
#else

void THNN_(Sigmoid_updateOutput)(
          THNNState *state,
          THTensor *input,
          THTensor *output)
{
  THTensor_(sigmoid)(output, input);
}

void THNN_(Sigmoid_updateGradInput)(
          THNNState *state,
          THTensor *gradOutput,
          THTensor *gradInput,
          THTensor *output)
{
  THNN_CHECK_NELEMENT(output, gradOutput);
  THTensor_(resizeAs)(gradInput, output);
  TH_TENSOR_APPLY3(scalar_t, gradInput, scalar_t, gradOutput, scalar_t, output,
    scalar_t z = *output_data;
    *gradInput_data = *gradOutput_data * (1. - z) * z;
  );
}

#endif
```

Source

PyTorch sigmoid layer

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}

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          THTensor *gradOutput,
          THTensor *gradInput,
          THTensor *output)
{
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  THTensor_(resizeAs)(gradInput, output);
  TH_TENSOR_APPLY3(scalar_t, gradInput, scalar_t, gradOutput, scalar_t, output,
    scalar_t z = *output_data;
    *gradInput_data = *gradOutput_data * (1. - z) * z;
  );
}

#endif
```

Forward

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

Source

PyTorch sigmoid layer

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          THTensor *gradOutput,
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    scalar_t z = *output_data;
    *gradInput_data = *gradOutput_data * (1. - z) * z;
  );
}

#endif
```

Forward

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

```
static void sigmoid_kernel(TensorIterator& iter) {
  AT_DISPATCH_FLOATING_TYPES(iter.dtype(), "sigmoid_cpu", [&]() {
    unary_kernel_vec(
        iter,
        [=](scalar_t a) -> scalar_t { return (1 / (1 + std::exp((-a)))); },
        [=](Vec256<scalar_t> a) {
          a = Vec256<scalar_t>((scalar_t)(0)) - a;
          a = a.exp();
          a = Vec256<scalar_t>((scalar_t)(1)) + a;
          a = a.reciprocal();
          return a;
        });
  });
}
```

Forward actually defined elsewhere...

```
return (1 / (1 + std::exp((-a))));
```

Source

PyTorch sigmoid layer

```
#ifndef TH_GENERIC_FILE
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#else

void THNN_(Sigmoid_updateOutput)(
          THNNState *state,
          THTensor *input,
          THTensor *output)
{
  THTensor_(sigmoid)(output, input);
}

void THNN_(Sigmoid_updateGradInput)(
          THNNState *state,
          THTensor *gradOutput,
          THTensor *gradInput,
          THTensor *output)
{
  THNN_CHECK_NELEMENT(output, gradOutput);
  THTensor_(resizeAs)(gradInput, output);
  TH_TENSOR_APPLY3(scalar_t, gradInput, scalar_t, gradOutput, scalar_t, output,
    scalar_t z = *output_data;
    *gradInput_data = *gradOutput_data * (1. - z) * z;
  );
}

#endif
```

Forward

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

Backward

$$(1-\sigma(x))\,\sigma(x)$$

Source

So far: backprop with scalars

What about vector-valued functions?

Recap: 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?

Recap: Vector Derivatives

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

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?

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

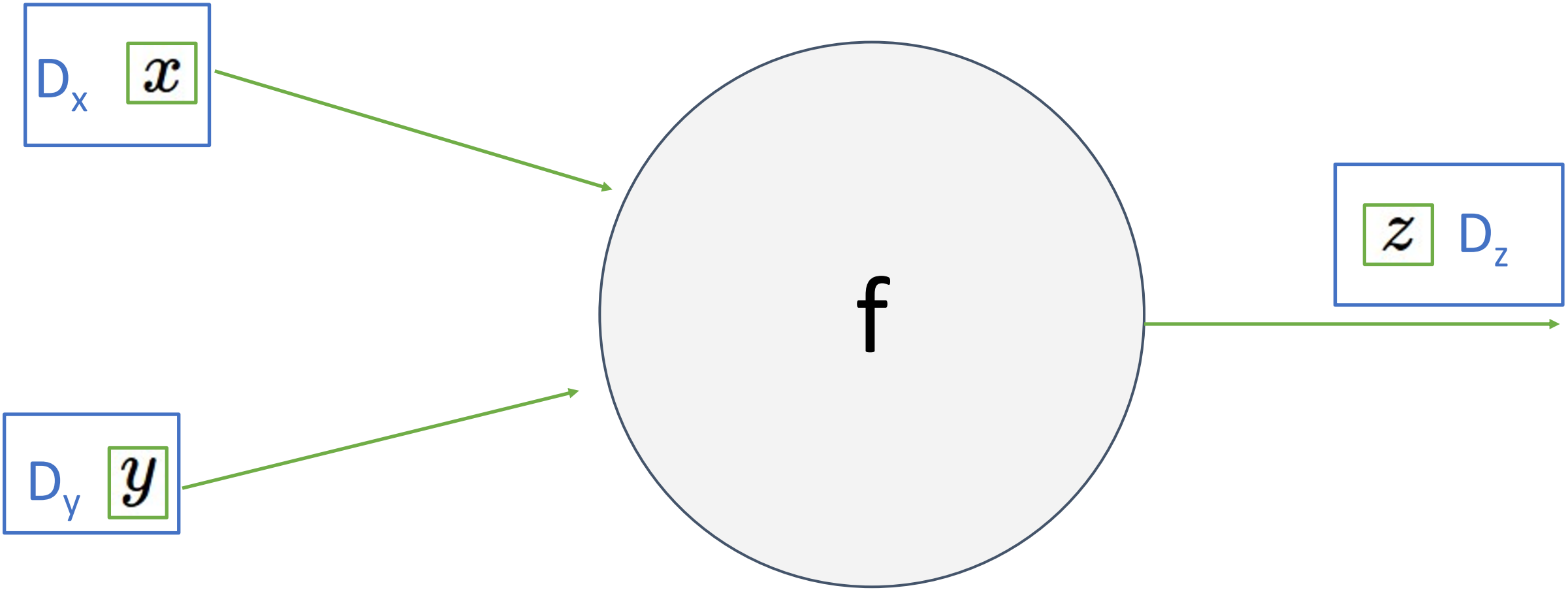
$x \in \mathbb{R}^N, y \in \mathbb{R}^M$

Derivative is **Jacobian**:

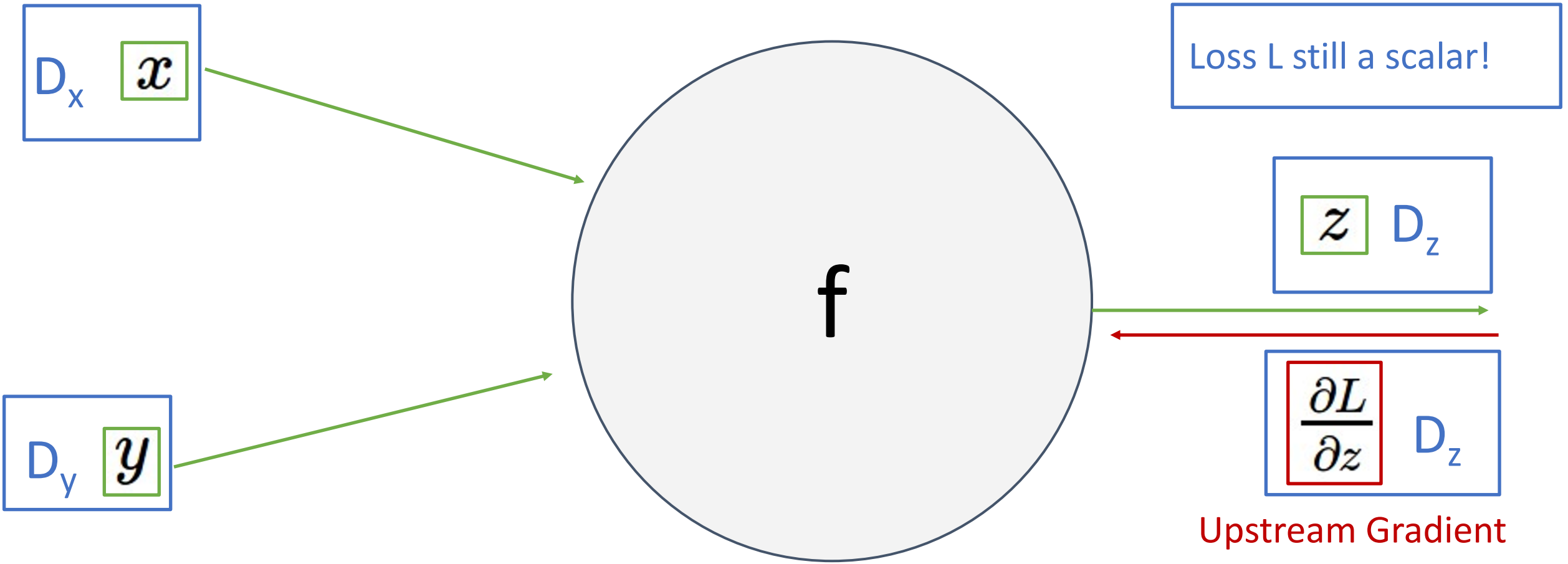
$$\frac{\partial y}{\partial x} \in \mathbb{R}^{N \times M} \quad \left(\frac{\partial y}{\partial x}\right)_{n,m} = \frac{\partial y_m}{\partial x_n}$$

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

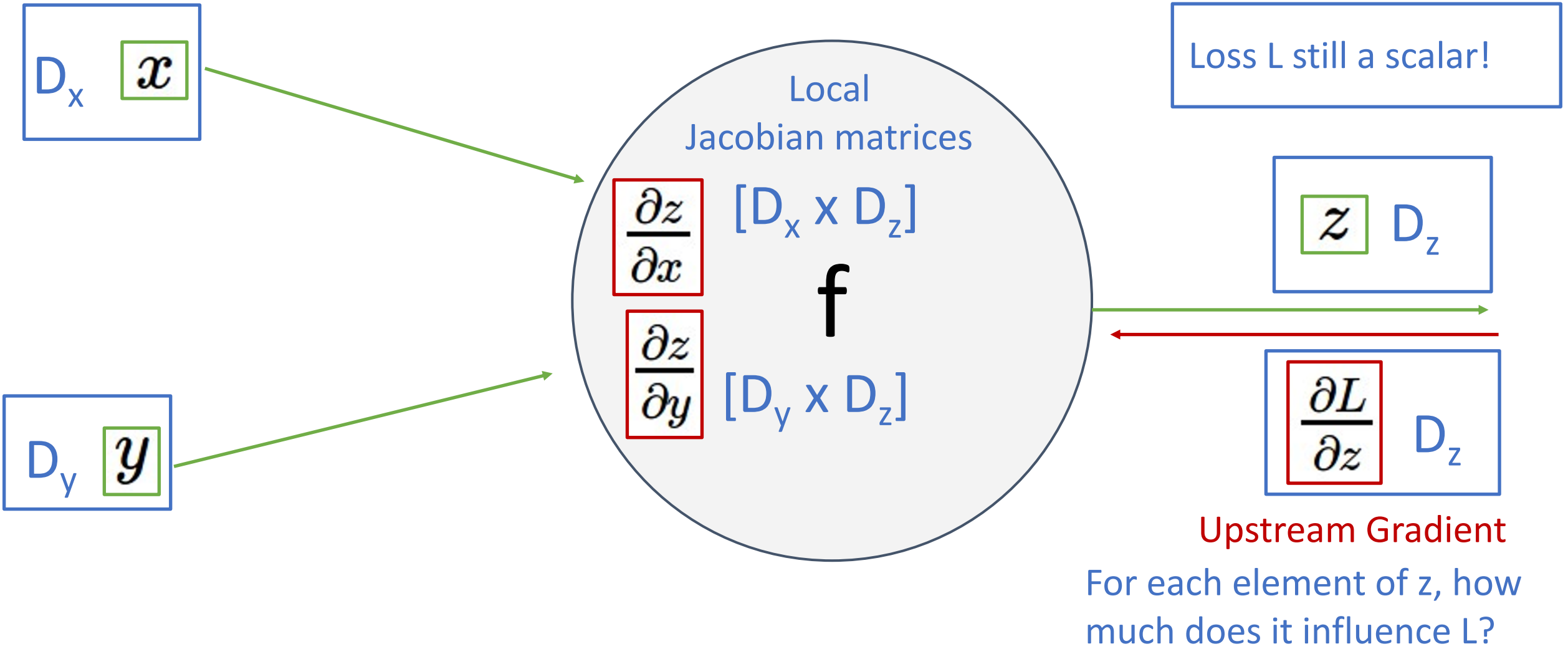
Backprop with Vectors



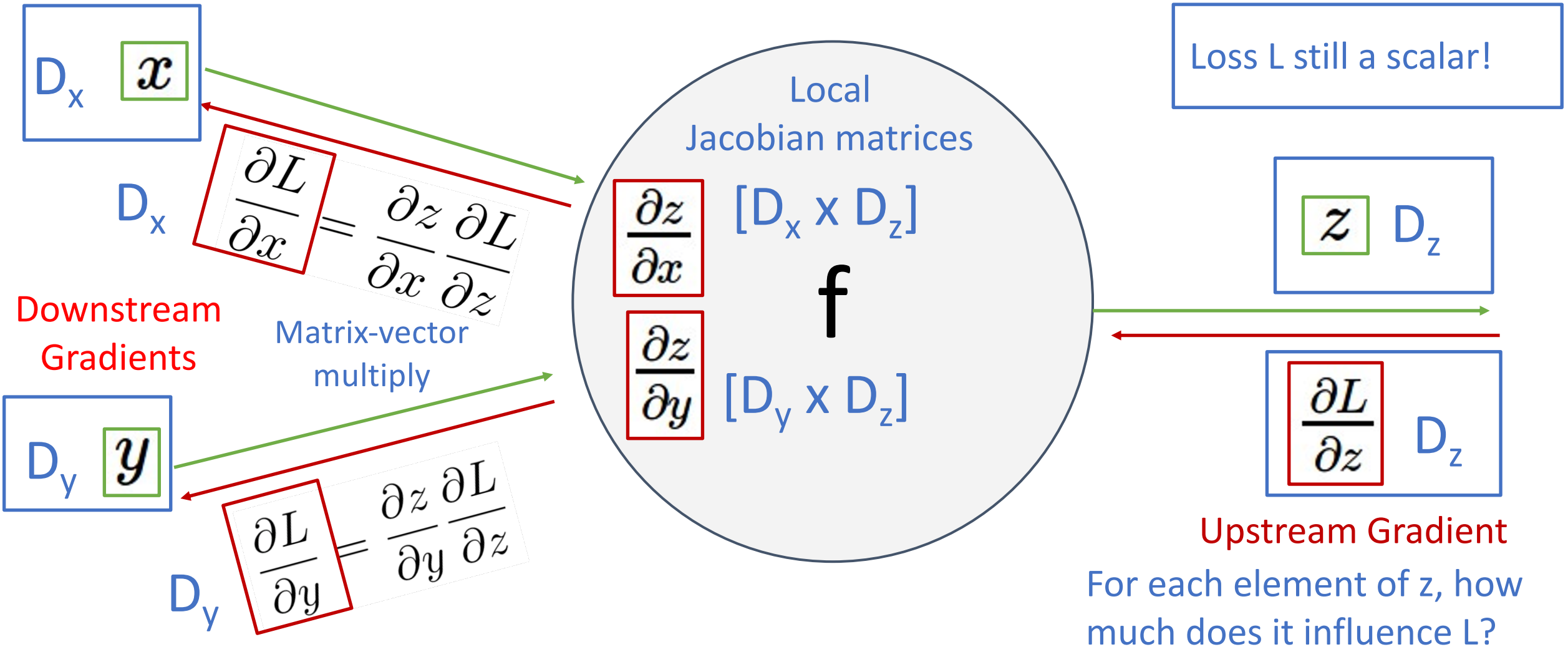
Backprop with Vectors



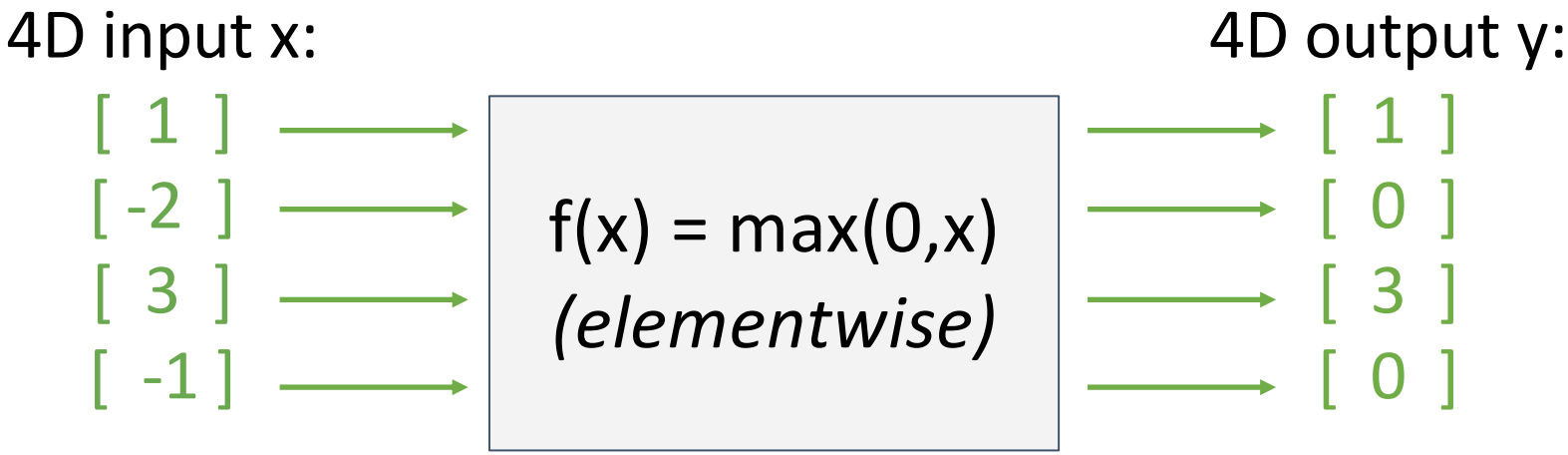
Backprop with Vectors



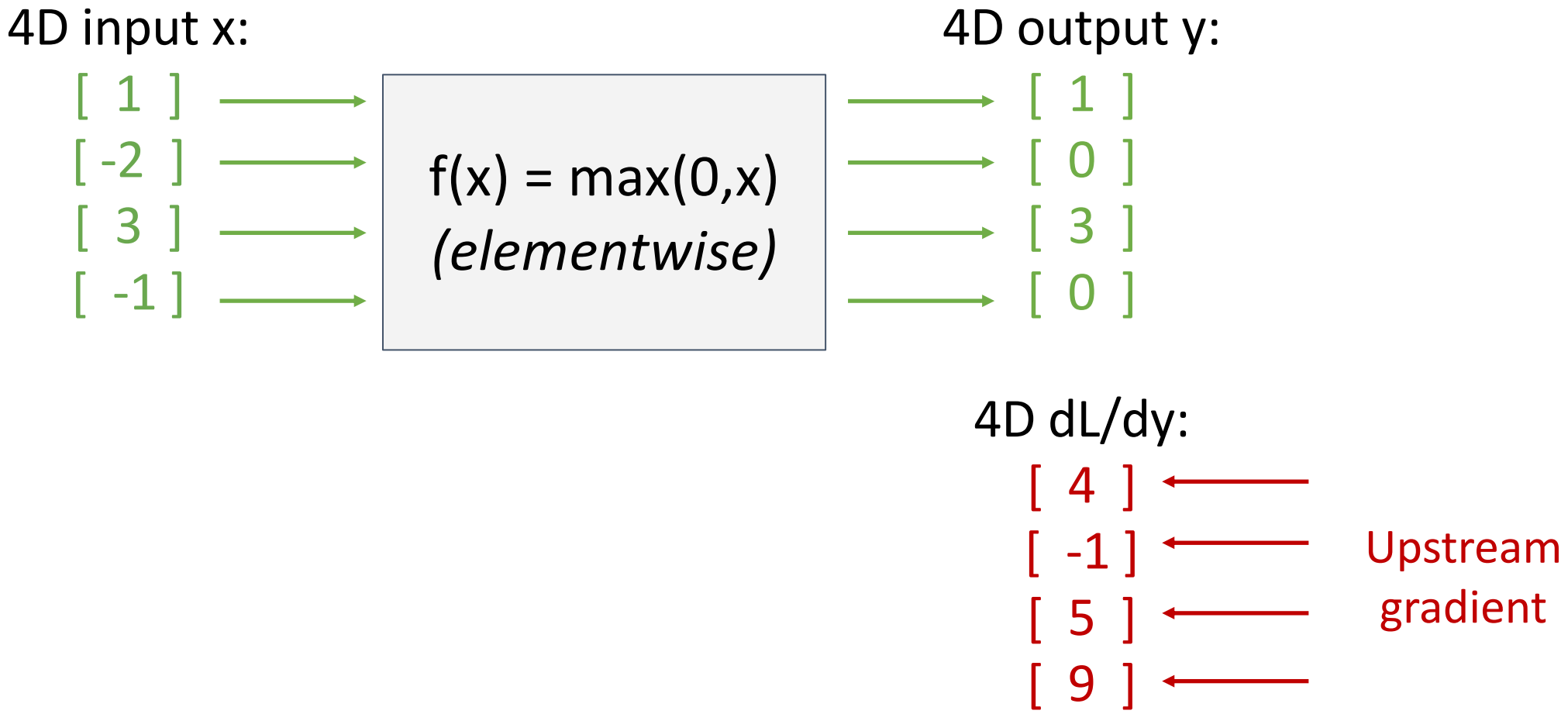
Backprop with Vectors



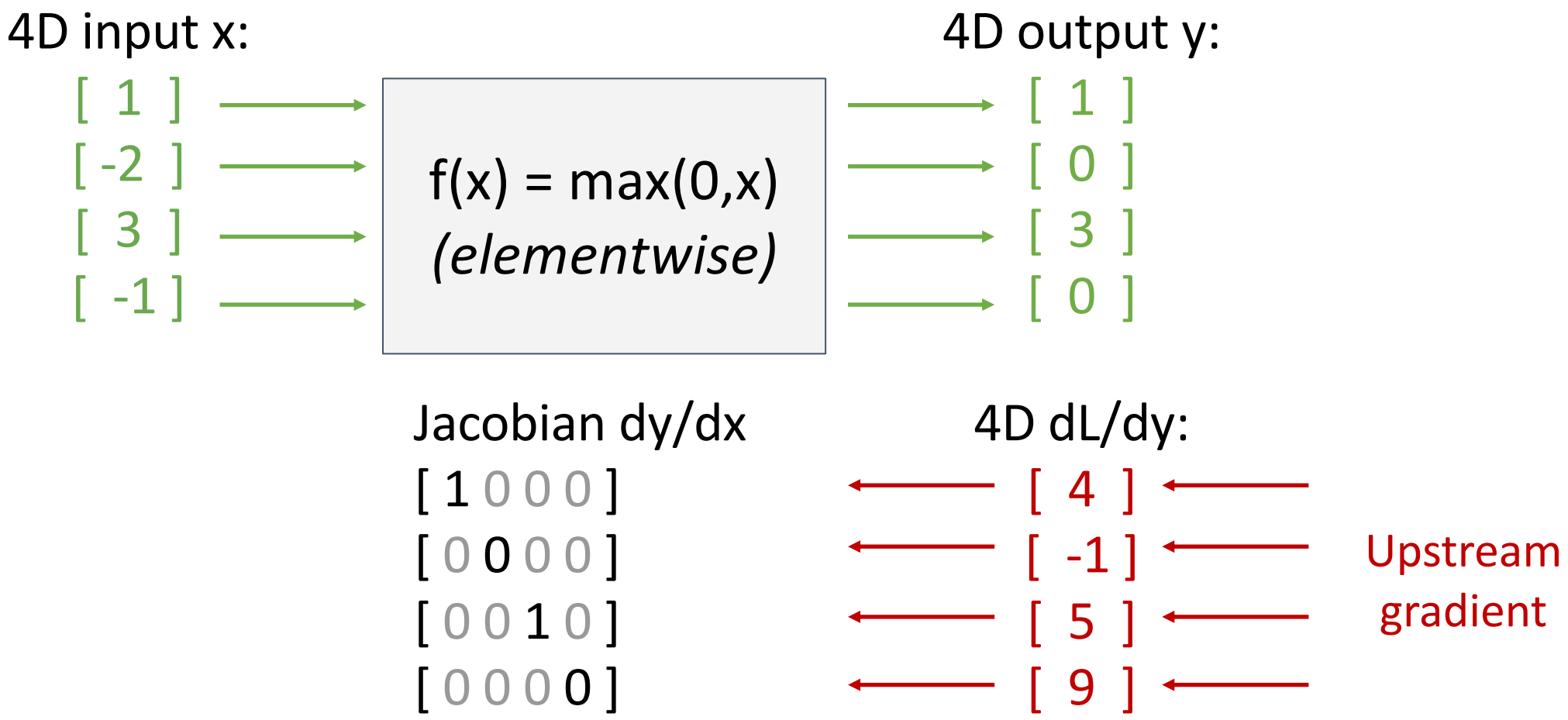
Backprop with Vectors



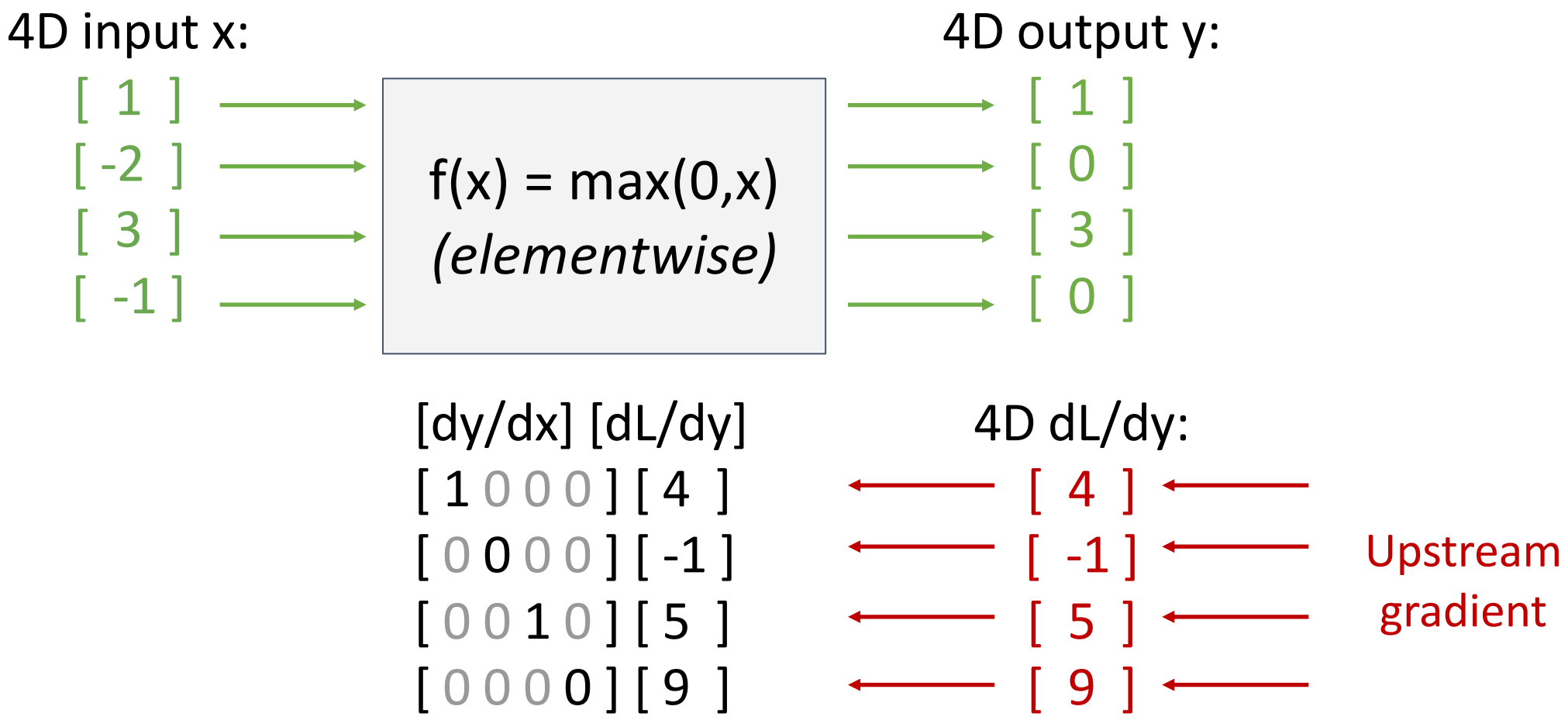
Backprop with Vectors



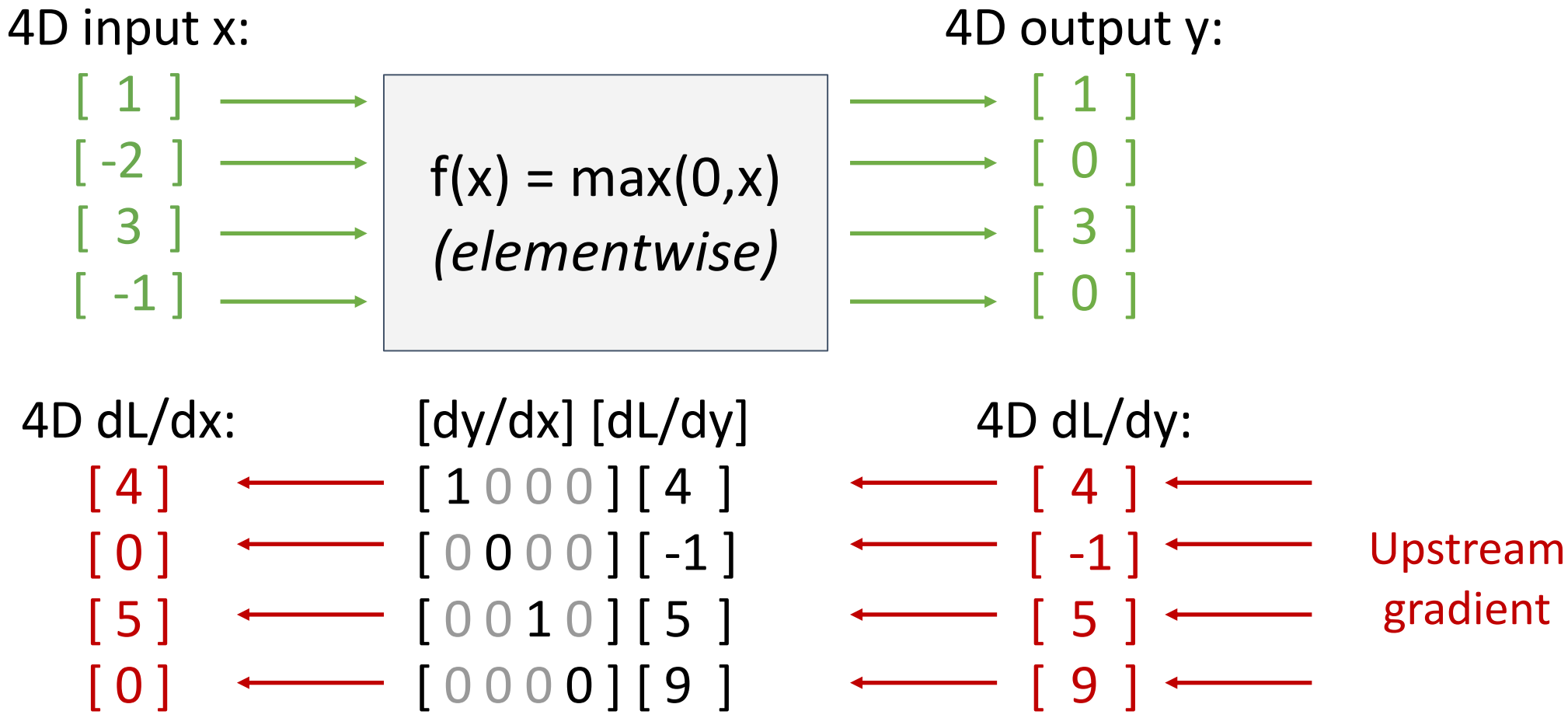
Backprop with Vectors



Backprop with Vectors

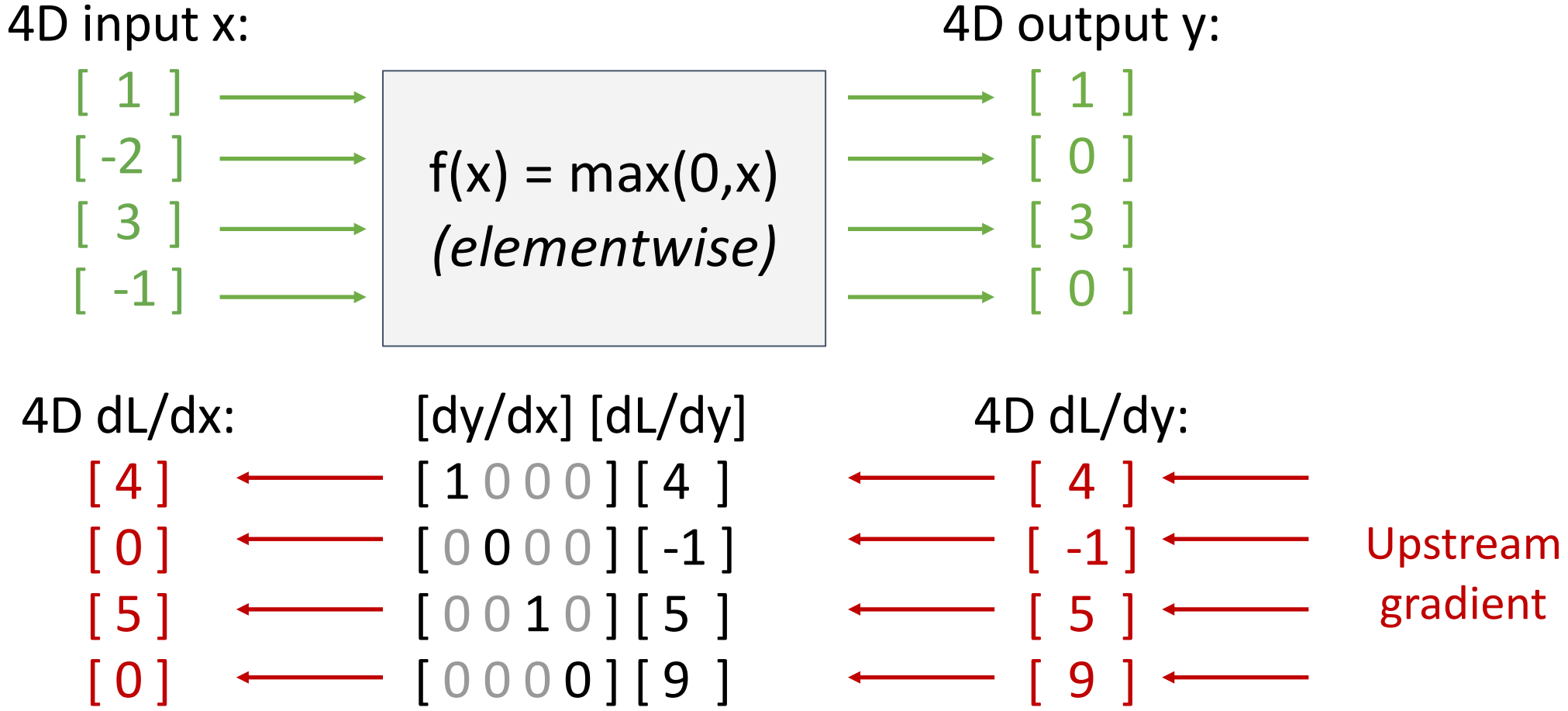


Backprop with Vectors



Backprop with Vectors

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



Backprop with Vectors

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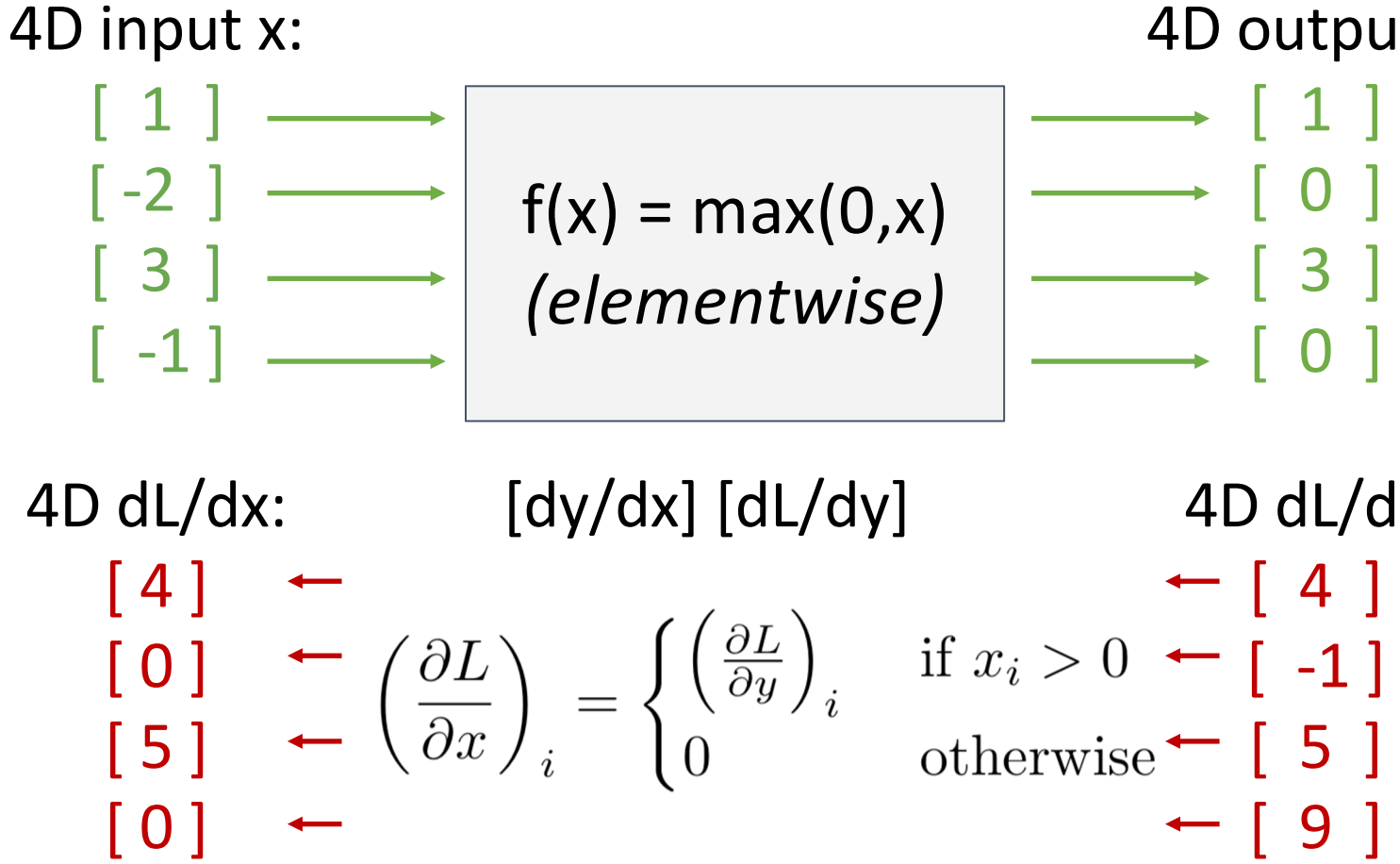
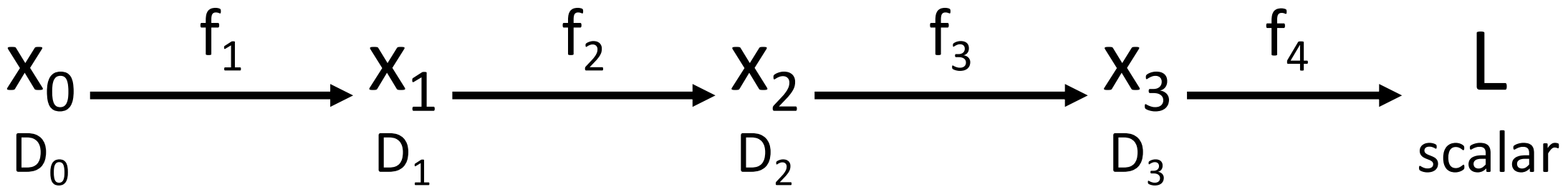


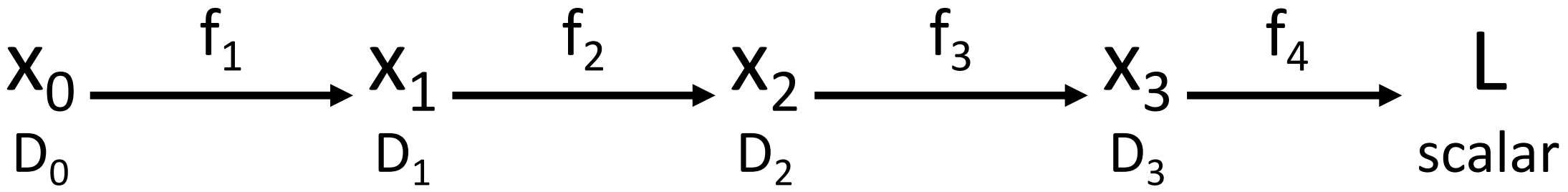
Backpropagation: Another View



Chain rule

$$\frac{\partial L}{\partial x_0} = \left(\frac{\partial x_1}{\partial x_0}\right)\left(\frac{\partial x_2}{\partial x_1}\right)\left(\frac{\partial x_3}{\partial x_2}\right)\left(\frac{\partial L}{\partial x_3}\right)$$

Backpropagation: Another View



Matrix multiplication is **associative**: we can compute products in any order

Chain rule

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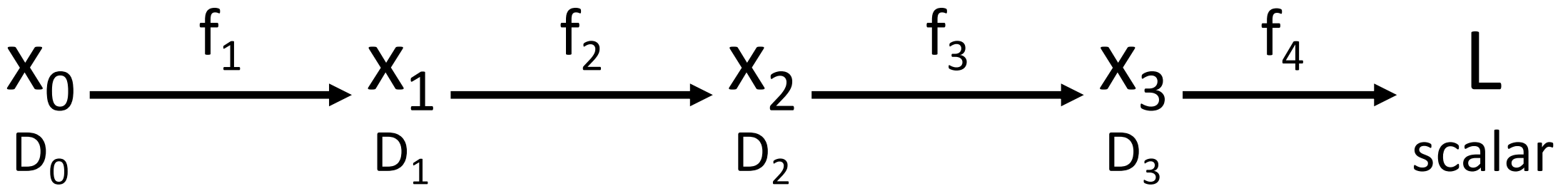
$D_0 \times D_1$ $D_1 \times D_2$ $D_2 \times D_3$ D_3

Reverse-Mode Automatic Differentiation



Matrix multiplication is **associative**: we can compute products in any order

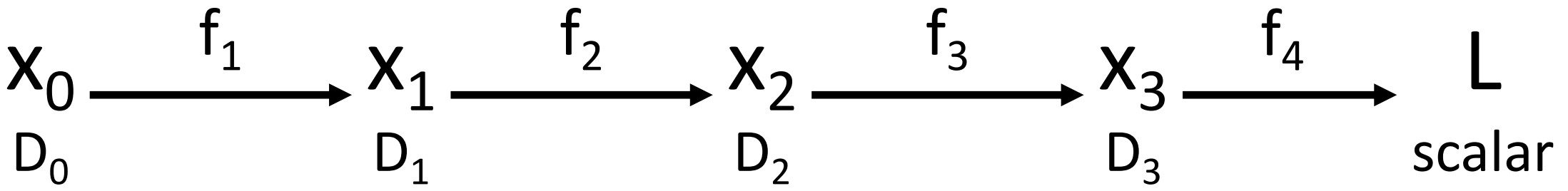
Computing products right-to-left avoids matrix-matrix products; only needs matrix-vector

Chain rule

$$\frac{\partial L}{\partial x_0} = \left(\frac{\partial x_1}{\partial x_0}\right)\left(\frac{\partial x_2}{\partial x_1}\right)\left(\frac{\partial x_3}{\partial x_2}\right)\left(\frac{\partial L}{\partial x_3}\right)$$

$D_0 \times D_1$ $D_1 \times D_2$ $D_2 \times D_3$ D_3

Reverse-Mode Automatic Differentiation



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Computing products right-to-left avoids matrix-matrix products; only needs matrix-vector

Chain rule

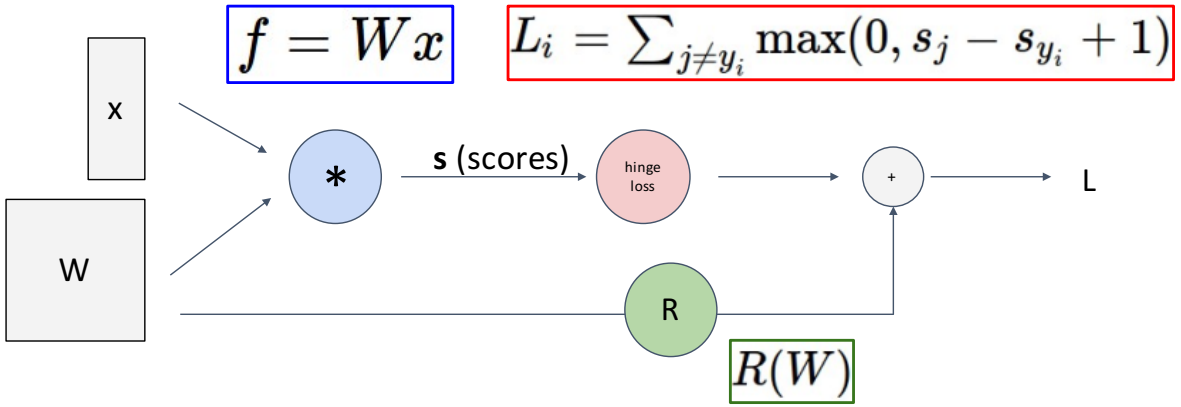
$$\frac{\partial L}{\partial x_0} = \left(\frac{\partial x_1}{\partial x_0}\right)\left(\frac{\partial x_2}{\partial x_1}\right)\left(\frac{\partial x_3}{\partial x_2}\right)\left(\frac{\partial L}{\partial x_3}\right)$$

Compute grad of scalar output w/respect to all vector inputs

$D_0 \times D_1$ $D_1 \times D_2$ $D_2 \times D_3$ D_3

Summary

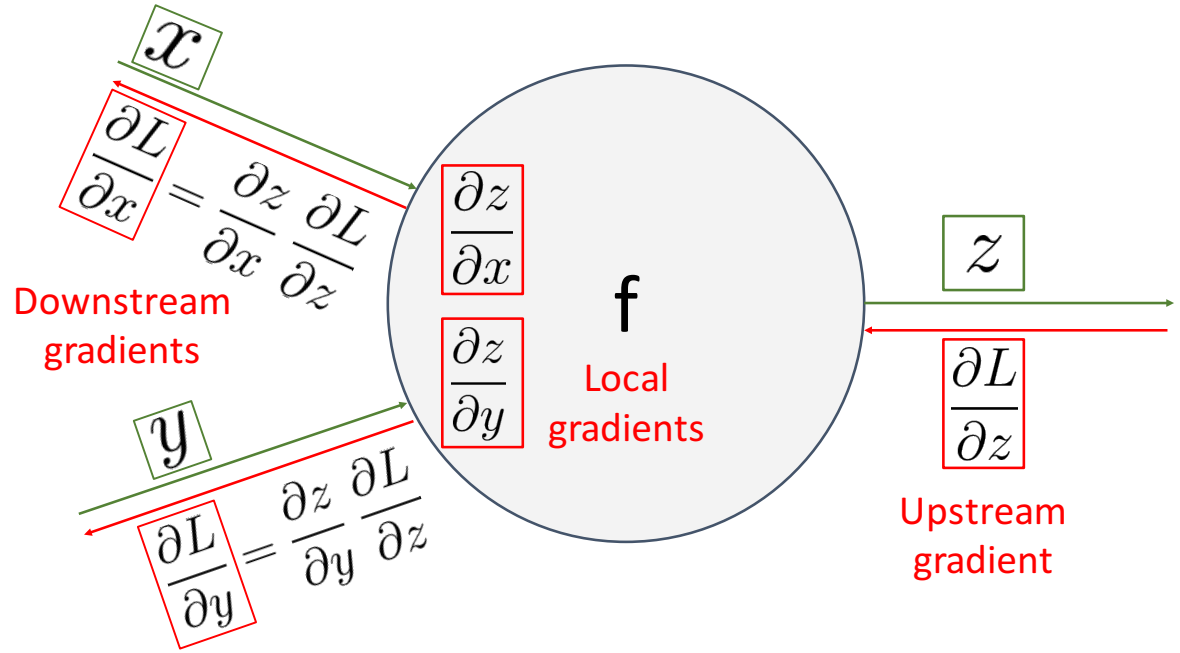
Represent complex expressions as **computational graphs**



Forward pass computes outputs

Backward pass computes gradients

During the backward pass, each node in the graph receives **upstream gradients** and multiplies them by **local gradients** to compute **downstream gradients**



Summary

Backprop can be implemented with “flat” code where the backward pass looks like forward pass reversed (Use this for A2!)

```
def f(w0, x0, w1, x1, w2):
  s0 = w0 * x0
  s1 = w1 * x1
  s2 = s0 + s1
  s3 = s2 + w2
  L = sigmoid(s3)

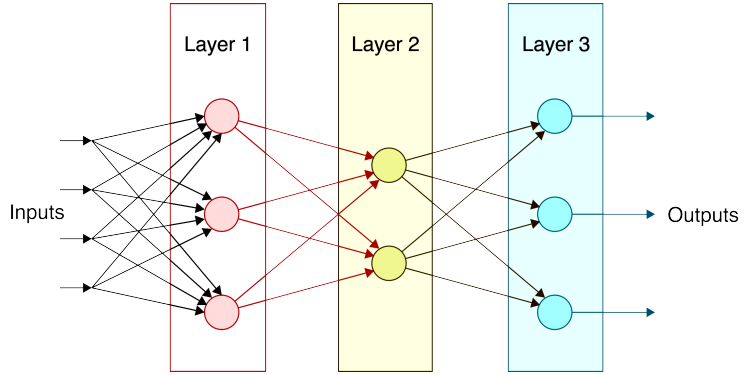
  grad_L = 1.0
  grad_s3 = grad_L * (1 - L) * L
  grad_w2 = grad_s3
  grad_s2 = grad_s3
  grad_s0 = grad_s2
  grad_s1 = grad_s2
  grad_w1 = grad_s1 * x1
  grad_x1 = grad_s1 * w1
  grad_w0 = grad_s0 * x0
  grad_x0 = grad_s0 * w0
```

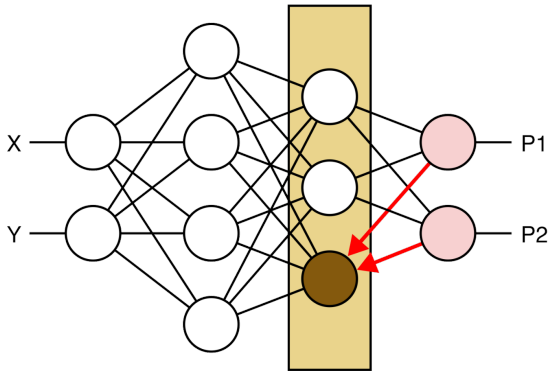
Backprop can be implemented with a modular API, as a set of paired forward/backward functions (We will do this on A3!)

```
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
```

Deep neural networks

- Loss functions
- Regularization
- Weights and layers
- Activation functions
- Backpropagation
- Training and optimization





Lecture 4: Optimization

Loss Functions quantify preferences

- We have some dataset of (x, y)
- We have a **score function:**
- We have a **loss function**:

Q: How do we find the best W?

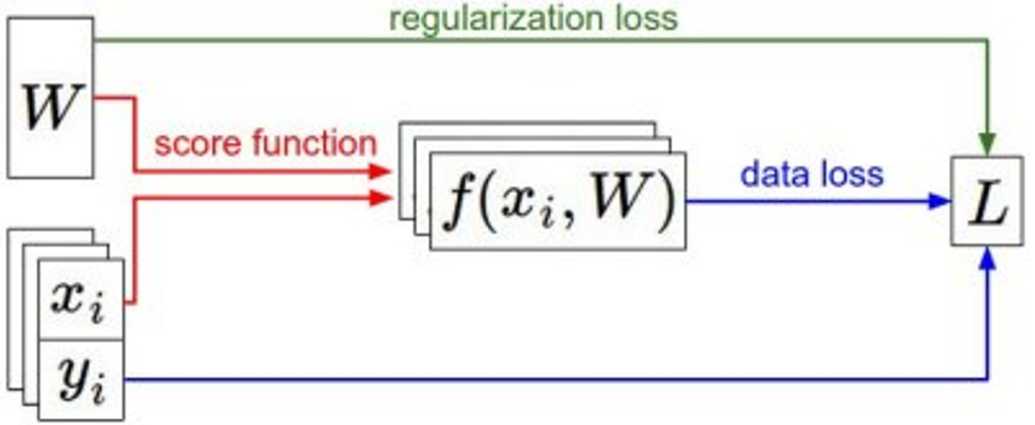
$$s = f(x; W) = Wx$$

Linear classifier

$$L_i = -\log\left(\frac{e^{sy_i}}{\sum_j e^{s_j}}\right)$$ Softmax

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

$$L = \frac{1}{N}\sum_{i=1}^{N} L_i + R(W)$$ Full loss



Follow the slope

In 1-dimension, the **derivative** of a function gives the slope:

$$\frac{df(x)}{dx} = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

In multiple dimensions, the **gradient** is the vector of (partial derivatives) along each dimension

The slope in any direction is the **dot product** of the direction with the gradient
The direction of steepest descent is the **negative gradient**

Loss is a function of W: **Analytic Gradient**

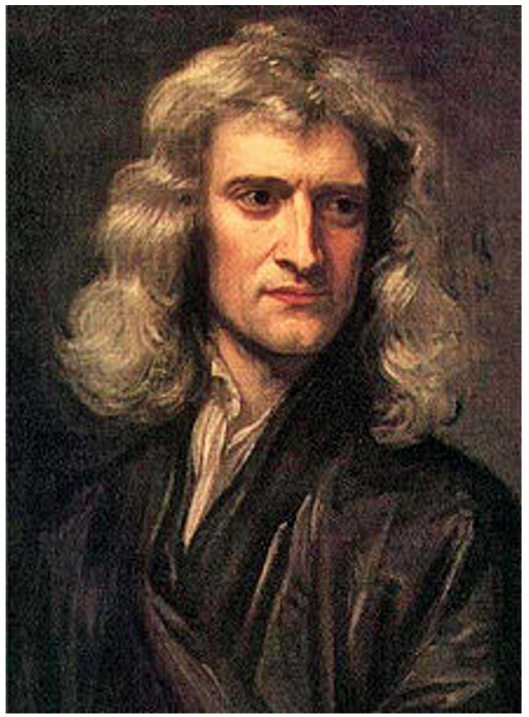
$$L = \frac{1}{N}\sum_{i=1}^{N} L_i + \sum_k W_k^2$$

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

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

want $\nabla_W L$

Use calculus to compute an **analytic gradient**



This image is in the public domain

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Computing Gradients

- **Numeric gradient**: approximate, slow, easy to write
- **Analytic gradient**: exact, fast, error-prone

In practice: Always use analytic gradient, but check implementation with numerical gradient. This is called a **gradient check.**

Computing Gradients

- **Numeric gradient**: approximate, slow, easy to write
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In practice: Always use analytic gradient, but check implementation with numerical gradient. This is called a **gradient check.**

```
def grad_check_sparse(f, x, analytic_grad, num_checks=10, h=1e-7):
  """
  sample a few random elements and only return numerical
  in this dimensions.
  """
```

Computing Gradients

- **Numeric gradient**: approximate, slow, easy to write
- **Analytic gradient**: exact, fast, error-prone

`torch.autograd.gradcheck(`*`func`*`,` *`inputs`*`,` *`eps=1e-06`*`,` *`atol=1e-05`*`,` *`rtol=0.001`*`,`
`raise_exception=True``,` *`check_sparse_nnz=False`*`,` *`nondet_tol=0.0`*`)` [SOURCE]

Check gradients computed via small finite differences against analytical gradients w.r.t. tensors in `inputs` that are of floating point type and with `requires_grad=True`.

The check between numerical and analytical gradients uses `allclose()`.

Computing Gradients

- **Numeric gradient**: approximate, slow, easy to write
- **Analytic gradient**: exact, fast, error-prone

`torch.autograd.gradgradcheck(`*`func`*`, `*`inputs`*`, `*`grad_outputs=None`*`, `*`eps=1e-06`*`, `*`atol=1e-05`*`, `*`rtol=0.001`*`, `*`gen_non_contig_grad_outputs=False`*`, `*`raise_exception=True`*`, `*`nondet_tol=0.0`*`)` [SOURCE]

Check gradients of gradients computed via small finite differences against analytical gradients w.r.t. tensors in `inputs` and `grad_outputs` that are of floating point type and with `requires_grad=True`.

This function checks that backpropagating through the gradients computed to the given `grad_outputs` are correct.

Gradient Descent

Iteratively step in the direction of
the negative gradient
(direction of local steepest descent)

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

Hyperparameters:

- Weight initialization method
- Number of steps
- Learning rate

Gradient Descent

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(direction of local steepest descent)

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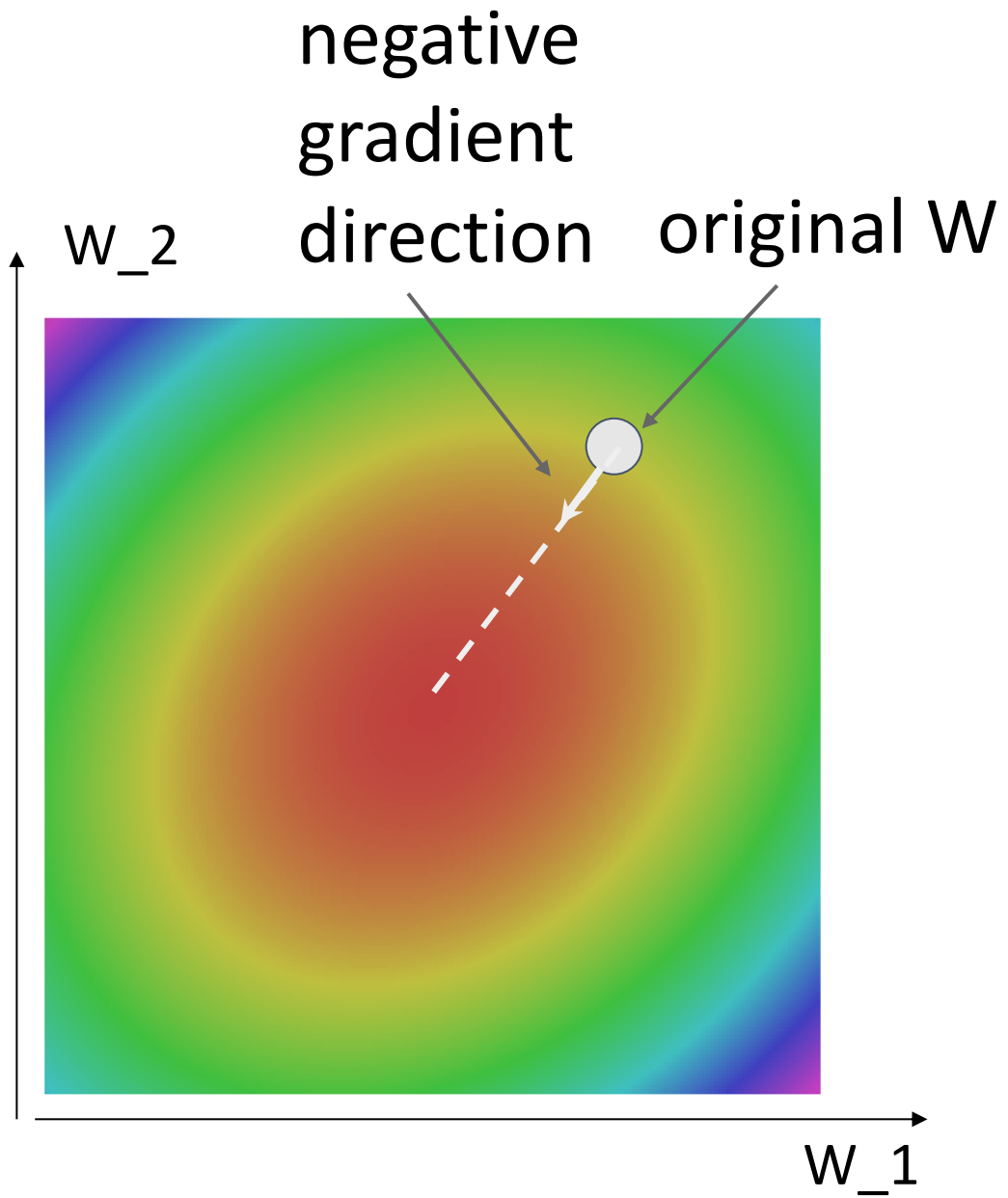

Batch Gradient Descent

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

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

Full sum expensive when N is large!

Stochastic Gradient Descent (SGD)

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

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

Full sum expensive when N is large!

Approximate sum using a **minibatch** of examples
32 / 64 / 128 common

```
# 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

Stochastic Gradient Descent (SGD)

$$L(W) = \mathbb{E}_{(x,y)\sim p_{data}}[L(x, y, W)] + \lambda R(W)$$

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

Think of loss as an expectation over the full **data distribution** p_{data}

Approximate expectation via sampling

Stochastic Gradient Descent (SGD)

$$L(W) = \mathbb{E}_{(x,y)\sim p_{data}}[L(x, y, W)] + \lambda R(W)$$

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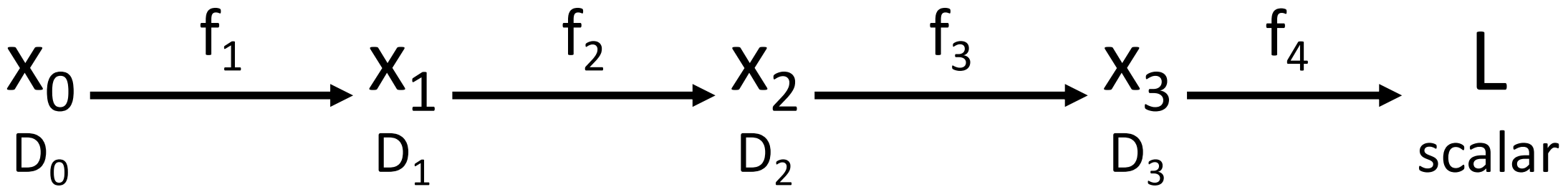
Think of loss as an expectation over the full **data distribution** p_{data}

Approximate expectation via sampling

$$\nabla_W L(W) = \nabla_W \mathbb{E}_{(x,y)\sim p_{data}}[L(x, y, W)] + \lambda \nabla_W R(W))$$

$$\approx \sum_{i=1}^{N} \nabla_W L_W(x_i, y_i, W) + \nabla_W R(W)$$

Recall: Reverse-Mode Automatic Differentiation



Matrix multiplication is **associative**: we can compute products in any order

Computing products right-to-left avoids matrix-matrix products; only needs matrix-vector

Chain rule

$$\frac{\partial L}{\partial x_0} = \left(\frac{\partial x_1}{\partial x_0}\right)\left(\frac{\partial x_2}{\partial x_1}\right)\left(\frac{\partial x_3}{\partial x_2}\right)\left(\frac{\partial L}{\partial x_3}\right)$$

Compute grad of scalar output w/respect to all vector inputs

$D_0 \times D_1$ $D_1 \times D_2$ $D_2 \times D_3$ D_3

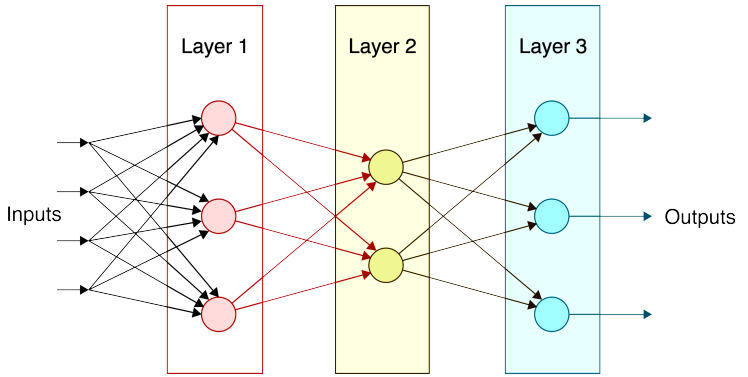
Mini-batch evaluation with matrices (HW3)

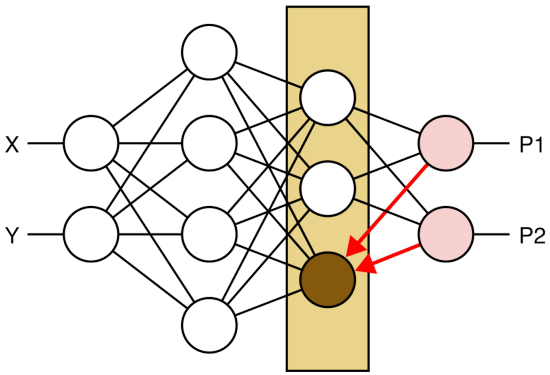
- DNNs are described as passing ***vectors*** between layers
- Why not pass all samples in a mini-batch as a ***matrix***?
- What used to be column vectors are now rows
- Need to adjust weight-vector multiplies

  $\boldsymbol{s} = \boldsymbol{W}\,\boldsymbol{x}$

  becomes

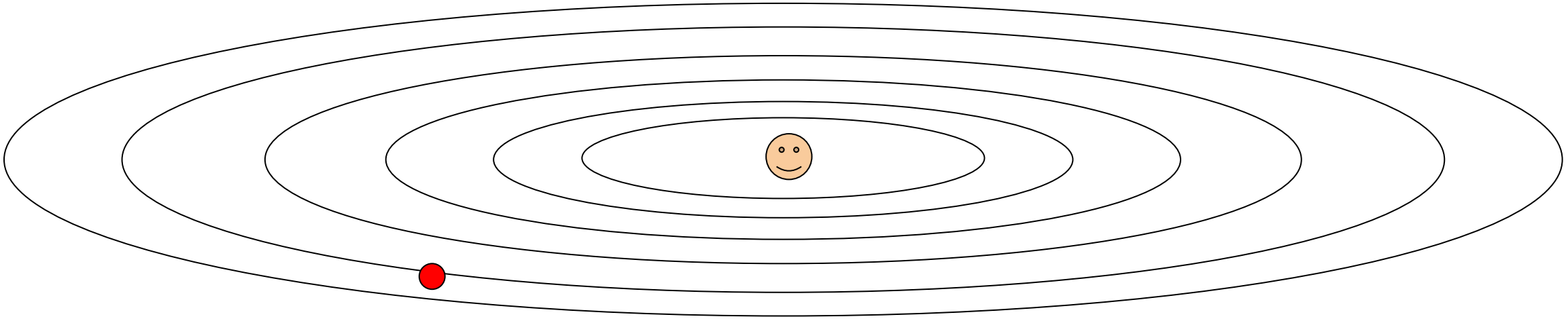
  $\boldsymbol{S} = \boldsymbol{X}\,\boldsymbol{W}^{\mathrm{T}}$
- Need to adjust gradients (Jacobians) as well
- *Fix this description after doing homework…*





Problems with SGD

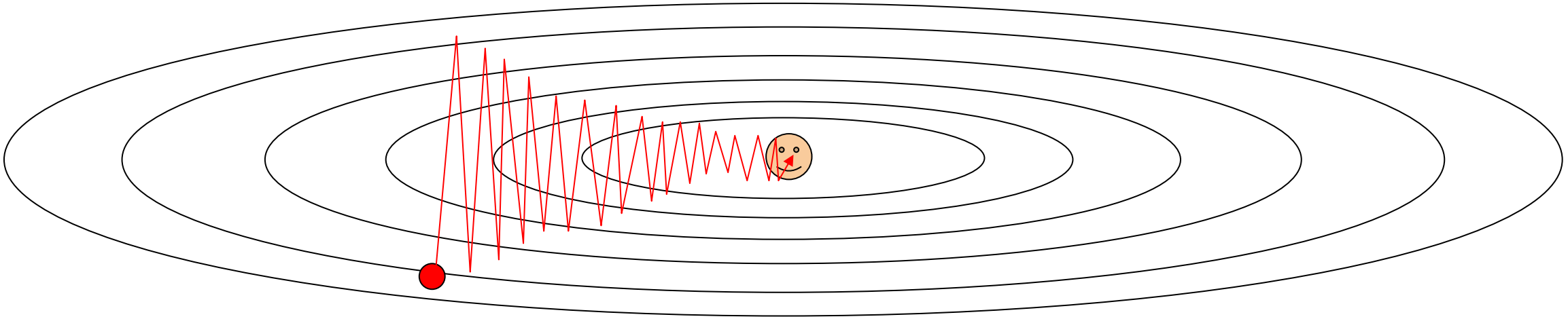
What if loss changes quickly in one direction and slowly in another?
What does gradient descent do?



Loss function has high **condition number**: ratio of largest to smallest singular value of the Hessian matrix is large

Problems with SGD

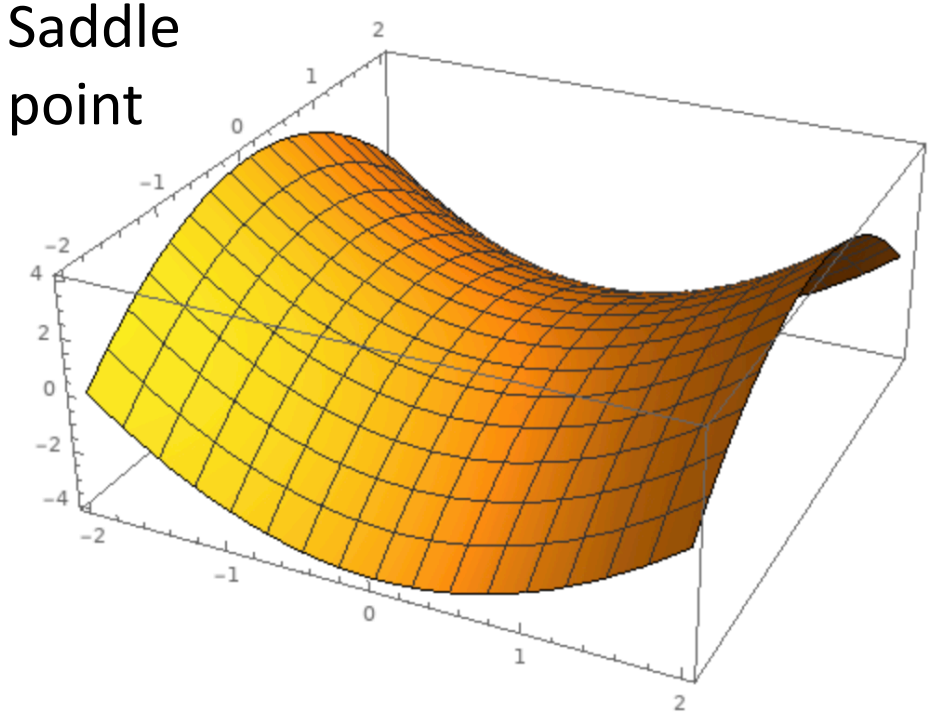
What if loss changes quickly in one direction and slowly in another?
What does gradient descent do?
Very slow progress along shallow dimension, jitter along steep direction



Loss function has high **condition number**: ratio of largest to smallest singular value of the Hessian matrix is large

Problems with SGD

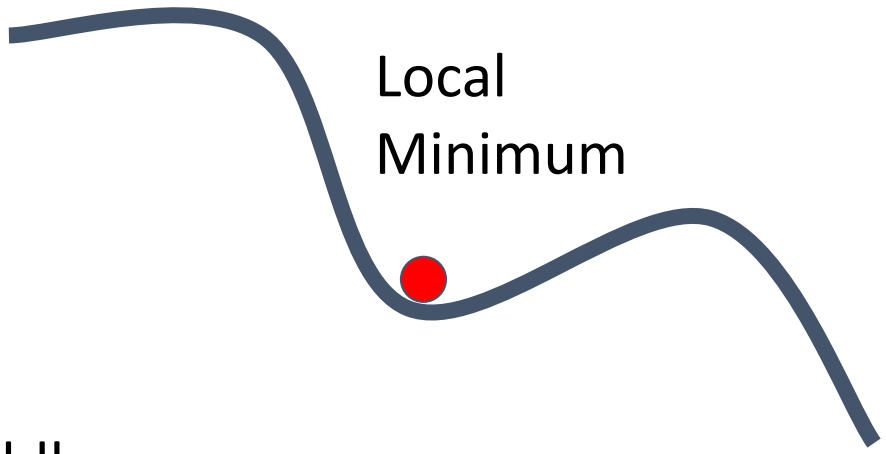
What if the loss function has a **local minimum** or **saddle point**?

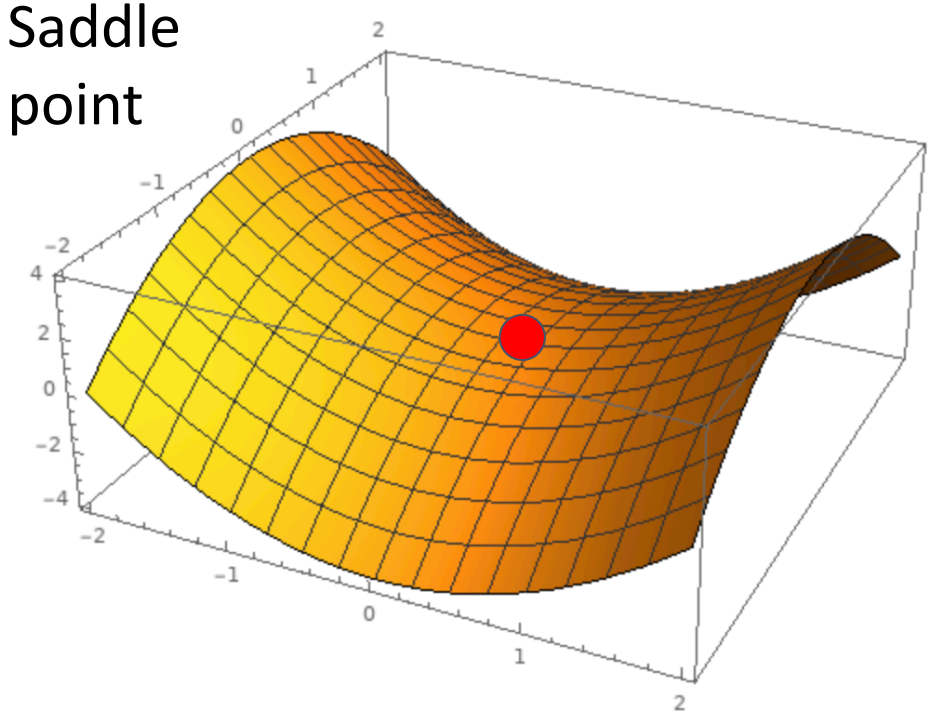


Problems with SGD

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

Zero gradient, gradient descent gets stuck



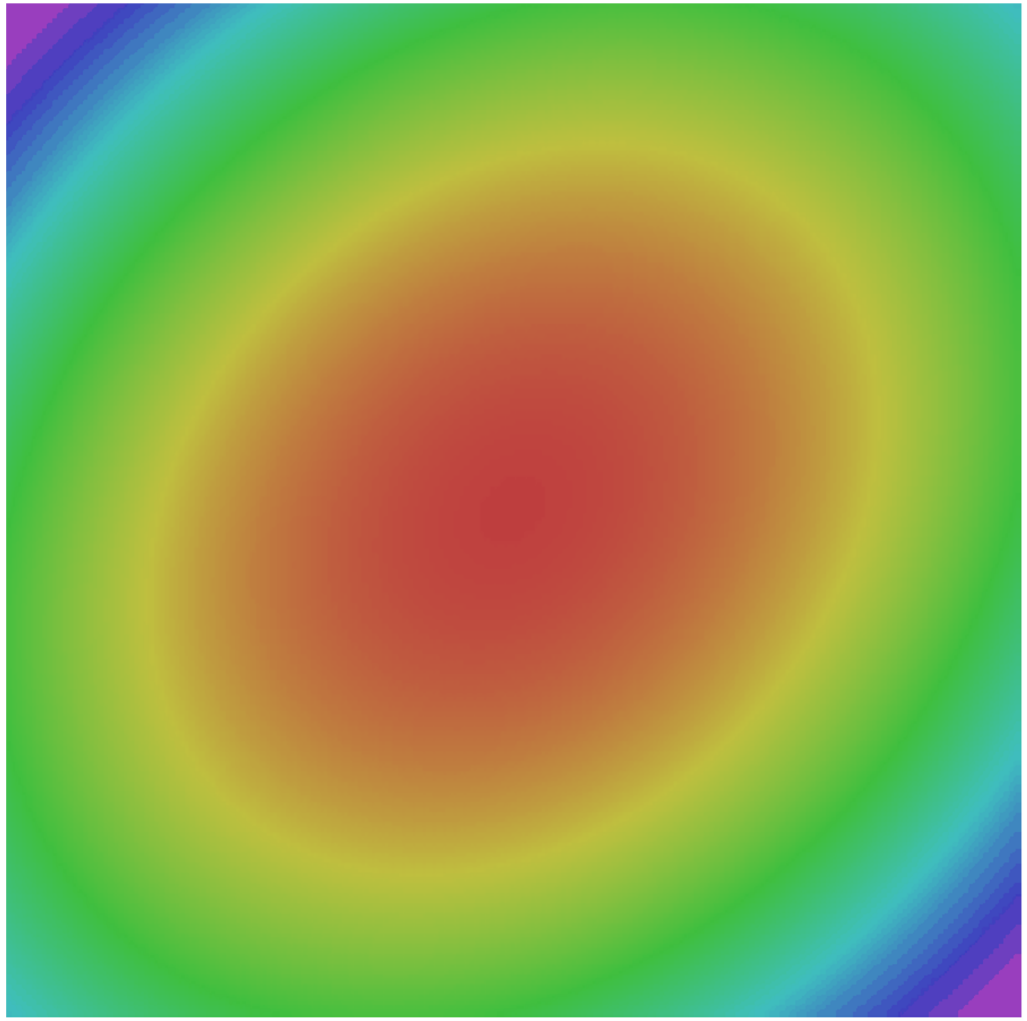


Problems with SGD

Our gradients come from minibatches so they can be noisy!

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

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



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
```

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

SGD + Momentum

SGD+Momentum

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

$$x_{t+1} = x_t + v_{t+1}$$

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

SGD+Momentum

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

$$x_{t+1} = x_t - \alpha v_{t+1}$$

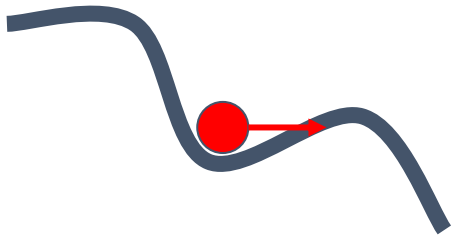
```
v = 0
for t in range(num_steps):
  dw = compute_gradient(w)
  v = rho * v + dw
  w -= learning_rate * v
```

You may see SGD+Momentum formulated different ways, but they are equivalent - give same sequence of x

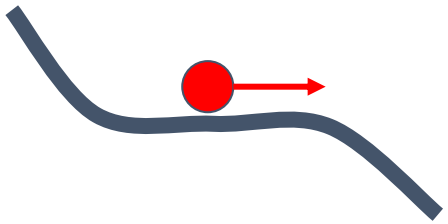
Sutskever et al, "On the importance of initialization and momentum in deep learning", ICML 2013

SGD + Momentum

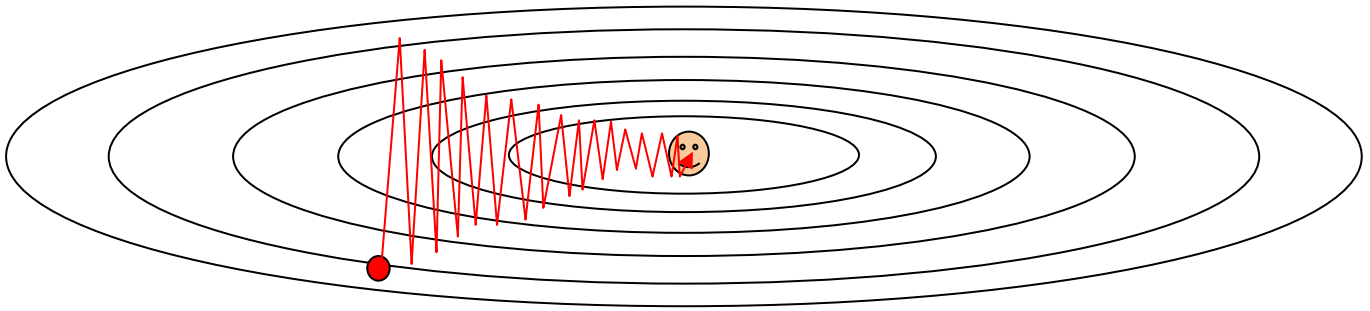
Local Minima



Saddle points



Poor Conditioning



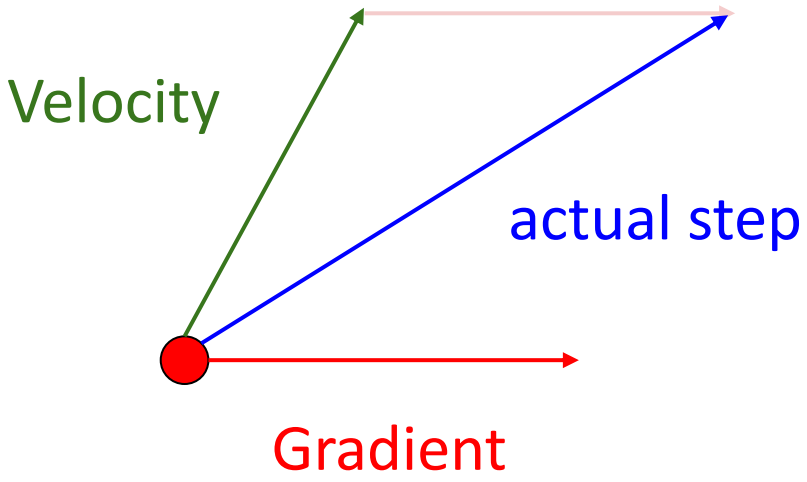
Gradient Noise

SGD SGD+Momentum

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

SGD + Momentum

Momentum update:

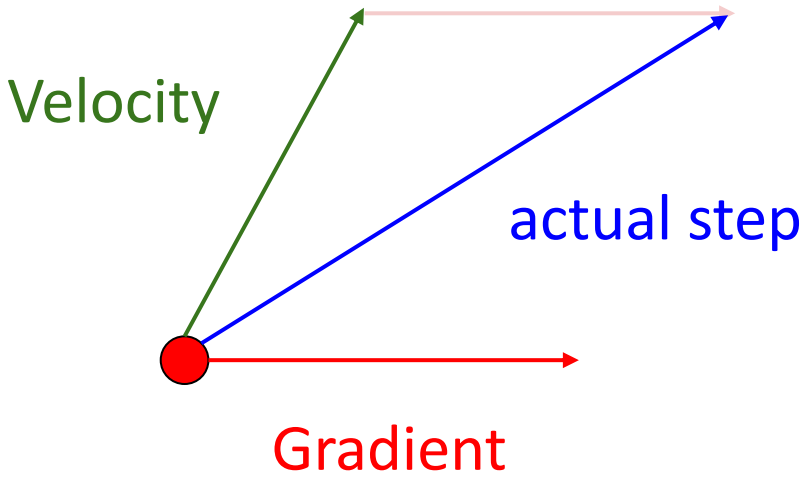


Combine gradient at current point with velocity to get step used to update weights

Nesterov, “A method of solving a convex programming problem with convergence rate O(1/k^2)”, 1983
Nesterov, “Introductory lectures on convex optimization: a basic course”, 2004
Sutskever et al, “On the importance of initialization and momentum in deep learning”, ICML 2013

Nesterov Momentum

Momentum update:



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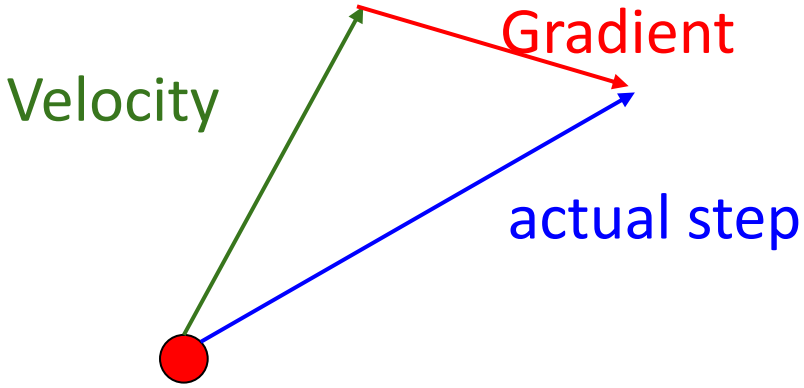

"Look ahead" to the point where updating using velocity would take us; compute gradient there and mix it with velocity to get actual update direction

Nesterov, "A method of solving a convex programming problem with convergence rate O(1/k^2)", 1983
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Sutskever et al, "On the importance of initialization and momentum in deep learning", ICML 2013

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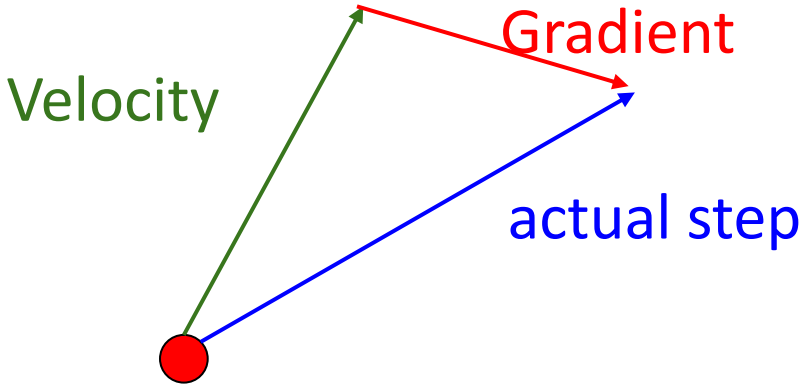

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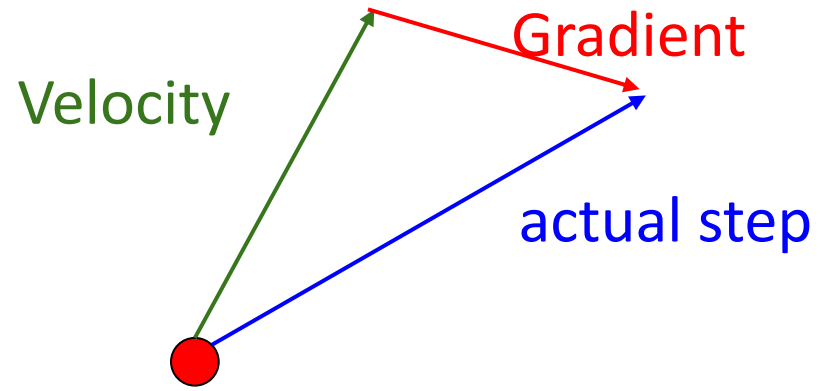
$$x_{t+1} = x_t + v_{t+1}$$

Annoying, usually we want update in terms of $x_t, \nabla f(x_t)$



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$$x_{t+1} = x_t + v_{t+1}$$

Annoying, usually we want update in terms of $x_t, \nabla f(x_t)$

Change of variables $\tilde{x}_t = x_t + \rho v_t$ and rearrange:

$$v_{t+1} = \rho v_t - \alpha \nabla f(\tilde{x}_t)$$
$$\tilde{x}_{t+1} = \tilde{x}_t - \rho v_t + (1+\rho) v_{t+1}$$
$$= \tilde{x}_t + v_{t+1} + \rho(v_{t+1} - v_t)$$

```
v = 0
for t in range(num_steps):
  dw = compute_gradient(w)
  old_v = v
  v = rho * v - learning_rate * dw
  w -= rho * old_v - (1 + rho) * v
```

Nesterov Momentum

SGD

SGD+Momentum

Nesterov

AdaGrad

```
grad_squared = 0
for t in range(num_steps):
  dw = compute_gradient(w)
  grad_squared += dw * dw
  w -= learning_rate * dw / (grad_squared.sqrt() + 1e-7)
```

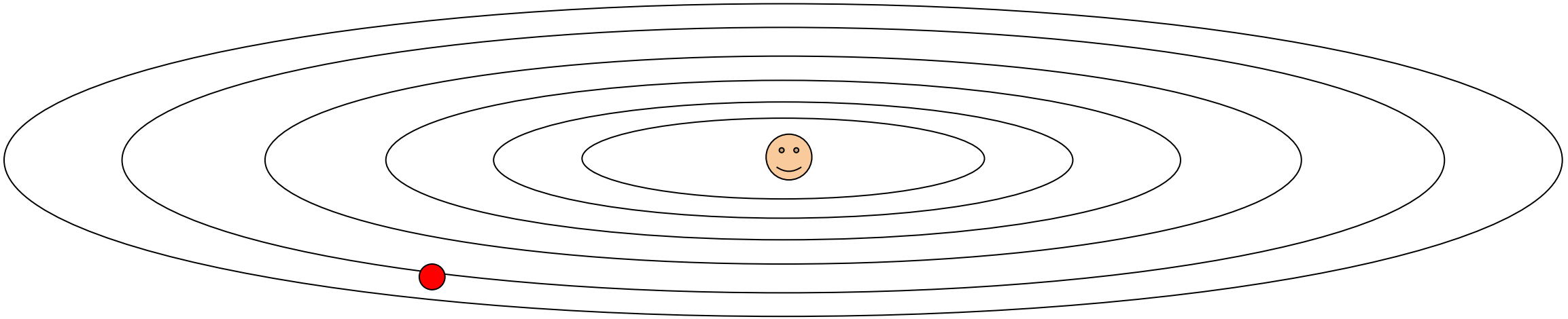
Added element-wise scaling of the gradient based on the historical sum of squares in each dimension

"Per-parameter learning rates"
or "adaptive learning rates"

Duchi et al, "Adaptive subgradient methods for online learning and stochastic optimization", JMLR 2011

AdaGrad

```
grad_squared = 0
for t in range(num_steps):
  dw = compute_gradient(w)
  grad_squared += dw * dw
  w -= learning_rate * dw / (grad_squared.sqrt() + 1e-7)
```



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AdaGrad

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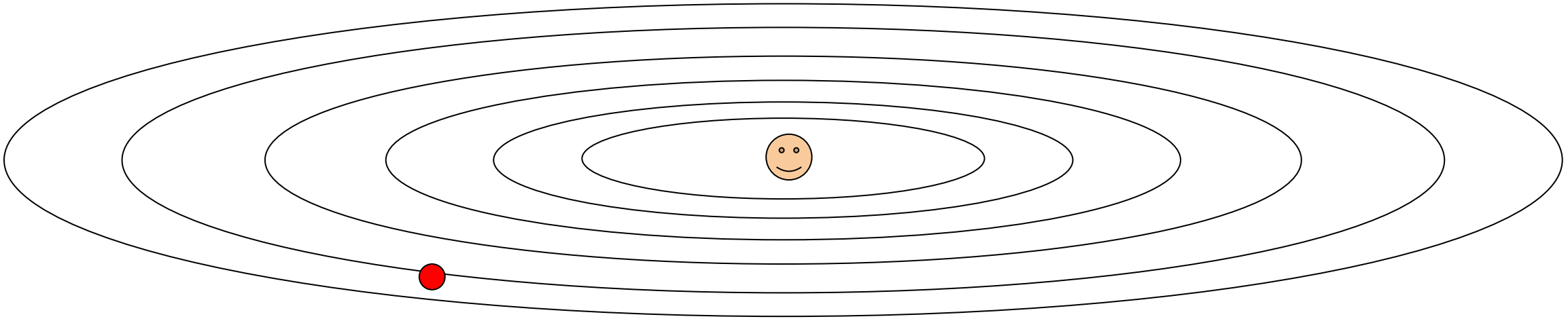
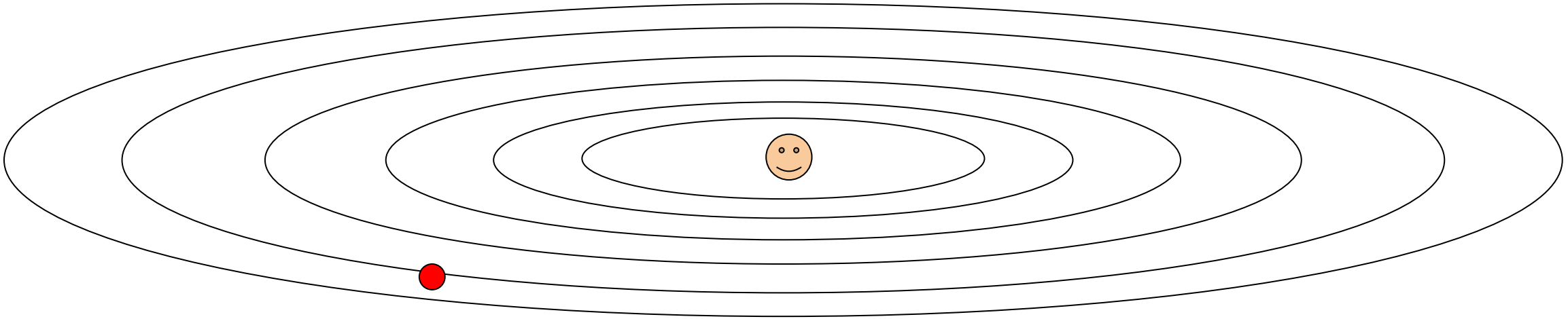
  dw = compute_gradient(w)
  grad_squared += dw * dw
  w -= learning_rate * dw / (grad_squared.sqrt() + 1e-7)
```



Q: What happens with AdaGrad?

AdaGrad

```
grad_squared = 0
for t in range(num_steps):
  dw = compute_gradient(w)
  grad_squared += dw * dw
  w -= learning_rate * dw / (grad_squared.sqrt() + 1e-7)
```



Q: What happens with AdaGrad?

Progress along “steep” directions is damped;
progress along “flat” directions is accelerated

RMSProp: "Leaky Adagrad"

```
grad_squared = 0
for t in range(num_steps):
  dw = compute_gradient(w)
  grad_squared += dw * dw
  w -= learning_rate * dw / (grad_squared.sqrt() + 1e-7)
```

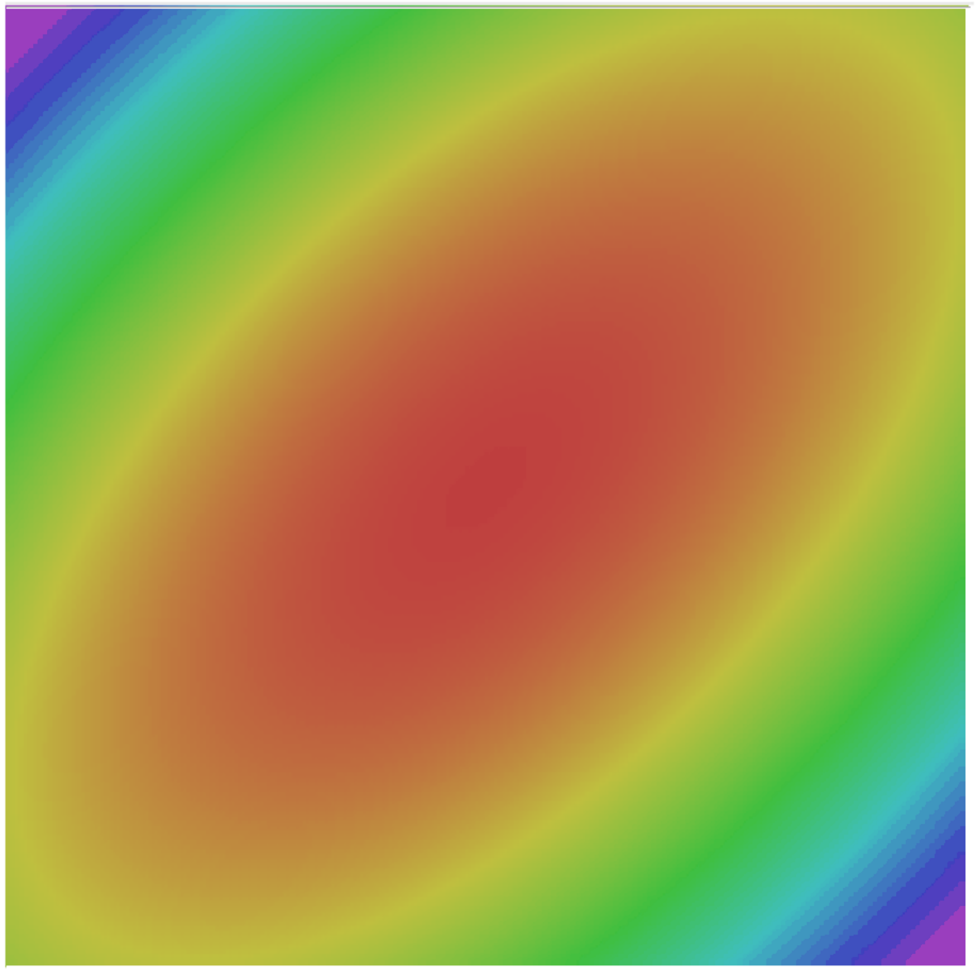
AdaGrad

```
grad_squared = 0
for t in range(num_steps):
  dw = compute_gradient(w)
  grad_squared = decay_rate * grad_squared + (1 - decay_rate) * dw * dw
  w -= learning_rate * dw / (grad_squared.sqrt() + 1e-7)
```

RMSProp

Tieleman and Hinton, 2012

RMSProp



SGD

SGD+Momentum

RMSProp

Adam (almost): RMSProp + Momentum

```
moment1 = 0
moment2 = 0
for t in range(num_steps):
  dw = compute_gradient(w)
  moment1 = beta1 * moment1 + (1 - beta1) * dw
  moment2 = beta2 * moment2 + (1 - beta2) * dw * dw
  w -= learning_rate * moment1 / (moment2.sqrt() + 1e-7)
```

Kingma and Ba, "Adam: A method for stochastic optimization", ICLR 2015

Adam (almost): RMSProp + Momentum

```
moment1 = 0
moment2 = 0
for t in range(num_steps):
  dw = compute_gradient(w)
  moment1 = beta1 * moment1 + (1 - beta1) * dw
  moment2 = beta2 * moment2 + (1 - beta2) * dw * dw
  w -= learning_rate * moment1 / (moment2.sqrt() + 1e-7)
```

Adam

Momentum

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

SGD+Momentum

Kingma and Ba, "Adam: A method for stochastic optimization", ICLR 2015

Adam (almost): RMSProp + Momentum

```
moment1 = 0
moment2 = 0
for t in range(num_steps):
  dw = compute_gradient(w)
  moment1 = beta1 * moment1 + (1 - beta1) * dw
  moment2 = beta2 * moment2 + (1 - beta2) * dw * dw
  w -= learning_rate * moment1 / (moment2.sqrt() + 1e-7)
```

Adam

Momentum

AdaGrad / RMSProp

```
grad_squared = 0
for t in range(num_steps):
  dw = compute_gradient(w)
  grad_squared = decay_rate * grad_squared + (1 - decay_rate) * dw * dw
  w -= learning_rate * dw / (grad_squared.sqrt() + 1e-7)
```

RMSProp

Kingma and Ba, "Adam: A method for stochastic optimization", ICLR 2015

Adam (almost): RMSProp + Momentum

```
moment1 = 0
moment2 = 0
for t in range(num_steps):
  dw = compute_gradient(w)
  moment1 = beta1 * moment1 + (1 - beta1) * dw
  moment2 = beta2 * moment2 + (1 - beta2) * dw * dw
  w -= learning_rate * moment1 / (moment2.sqrt() + 1e-7)
```

Adam

Momentum

AdaGrad / RMSProp

Bias correction

Q: What happens at t=0?
(Assume beta2 = 0.999)

Kingma and Ba, "Adam: A method for stochastic optimization", ICLR 2015

Adam (almost): RMSProp + Momentum

```
moment1 = 0
moment2 = 0
for t in range(num_steps):
  dw = compute_gradient(w)
  moment1 = beta1 * moment1 + (1 - beta1) * dw
  moment2 = beta2 * moment2 + (1 - beta2) * dw * dw
  moment1_unbias = moment1 / (1 - beta1 ** t)
  moment2_unbias = moment2 / (1 - beta2 ** t)
  w -= learning_rate * moment1_unbias / (moment2_unbias.sqrt() + 1e-7)
```

Momentum

AdaGrad / RMSProp

Bias correction

Bias correction for the fact that first and second moment estimates start at zero

Kingma and Ba, "Adam: A method for stochastic optimization", ICLR 2015

Adam (almost): RMSProp + Momentum

```
moment1 = 0
moment2 = 0
for t in range(num_steps):
  dw = compute_gradient(w)
  moment1 = beta1 * moment1 + (1 - beta1) * dw
  moment2 = beta2 * moment2 + (1 - beta2) * dw * dw
  moment1_unbias = moment1 / (1 - beta1 ** t)
  moment2_unbias = moment2 / (1 - beta2 ** t)
  w -= learning_rate * moment1_unbias / (moment2_unbias.sqrt() + 1e-7)
```

Bias correction for the fact that first and second moment estimates start at zero

Adam with beta1 = 0.9, beta2 = 0.999, and learning_rate = 1e-3, 5e-4, 1e-4 is a great starting point for many models!

Kingma and Ba, "Adam: A method for stochastic optimization", ICLR 2015

Adam: Very Common in Practice!

for input to the CNN; each colored pixel in the image yields a 7D one-hot vector. Following common practice, the network is trained end-to-end using stochastic gradient descent with the Adam optimizer [22]. We anneal the learning rate to 0 using a half cosine schedule without restarts [28].

Bakhtin, van der Maaten, Johnson, Gustafson, and Girshick, NeurIPS 2019

We train all models using Adam [23] with learning rate 10^{-4} and batch size 32 for 1 million iterations; training takes about 3 days on a single Tesla P100. For each mini-batch we first update f, then update D_{img} and D_{obj}.

Johnson, Gupta, and Fei-Fei, CVPR 2018

ganized into three residual blocks. We train for 25 epochs using Adam [27] with learning rate 10^{-4} and 32 images per batch on 8 Tesla V100 GPUs. We set the `cubify` thresh-

Gkioxari, Malik, and Johnson, ICCV 2019

sampled with each bit drawn uniformly at random. For gradient descent, we use Adam [29] with a learning rate of 10^{-3} and default hyperparameters. All models are trained with batch size 12. Models are trained for 200 epochs, or 400 epochs if being trained on multiple noise layers.

Zhu, Kaplan, Johnson, and Fei-Fei, ECCV 2018

16 dimensional vectors. We iteratively train the Generator and Discriminator with a batch size of 64 for 200 epochs using Adam [22] with an initial learning rate of 0.001.

Gupta, Johnson, et al, CVPR 2018

Adam with beta1 = 0.9,
beta2 = 0.999, and learning_rate = 1e-3, 5e-4, 1e-4
is a great starting point for many models!

Adam

SGD

SGD+Momentum

RMSProp

Adam

Optimization Algorithm Comparison

Algorithm	Tracks first moments (Momentum)	Tracks second moments (Adaptive learning rates)	Leaky second moments	Bias correction for moment estimates
SGD	✗	✗	✗	✗
SGD+Momentum	✓	✗	✗	✗
Nesterov	✓	✗	✗	✗
AdaGrad	✗	✓	✗	✗
RMSProp	✗	✓	✓	✗
Adam	✓	✓	✓	✓

In practice:

- **Adam** is a good default choice in many cases
  SGD+Momentum can outperform Adam but may require more tuning

- If you can afford to do full batch updates then try out **L-BFGS** (and don't forget to disable all sources of noise)

Deep neural networks

- Loss functions
- Regularization
- Weights and layers
- Activation functions
- Backpropagation
- Training and optimization