



CS 7643: Deep Learning

Topics:

- Computational Graphs
 - Notation + example
- Computing Gradients
 - Forward mode vs Reverse mode AD

Dhruv Batra
Georgia Tech

Administrativa

- HW1 Released
 - Due: 09/22
- PS1 Solutions
 - Coming soon

Project

- Goal
 - Chance to try Deep Learning
 - **Combine with other classes / research / credits / anything**
 - You have our blanket permission
 - Extra credit for shooting for a publication
 - Encouraged to apply to your research (computer vision, NLP, robotics,...)
 - Must be done this semester.
- Main categories
 - **Application/Survey**
 - Compare a bunch of existing algorithms on a new application domain of your interest
 - **Formulation/Development**
 - Formulate a new model or algorithm for a new or old problem
 - **Theory**
 - Theoretically analyze an existing algorithm

Administrativa

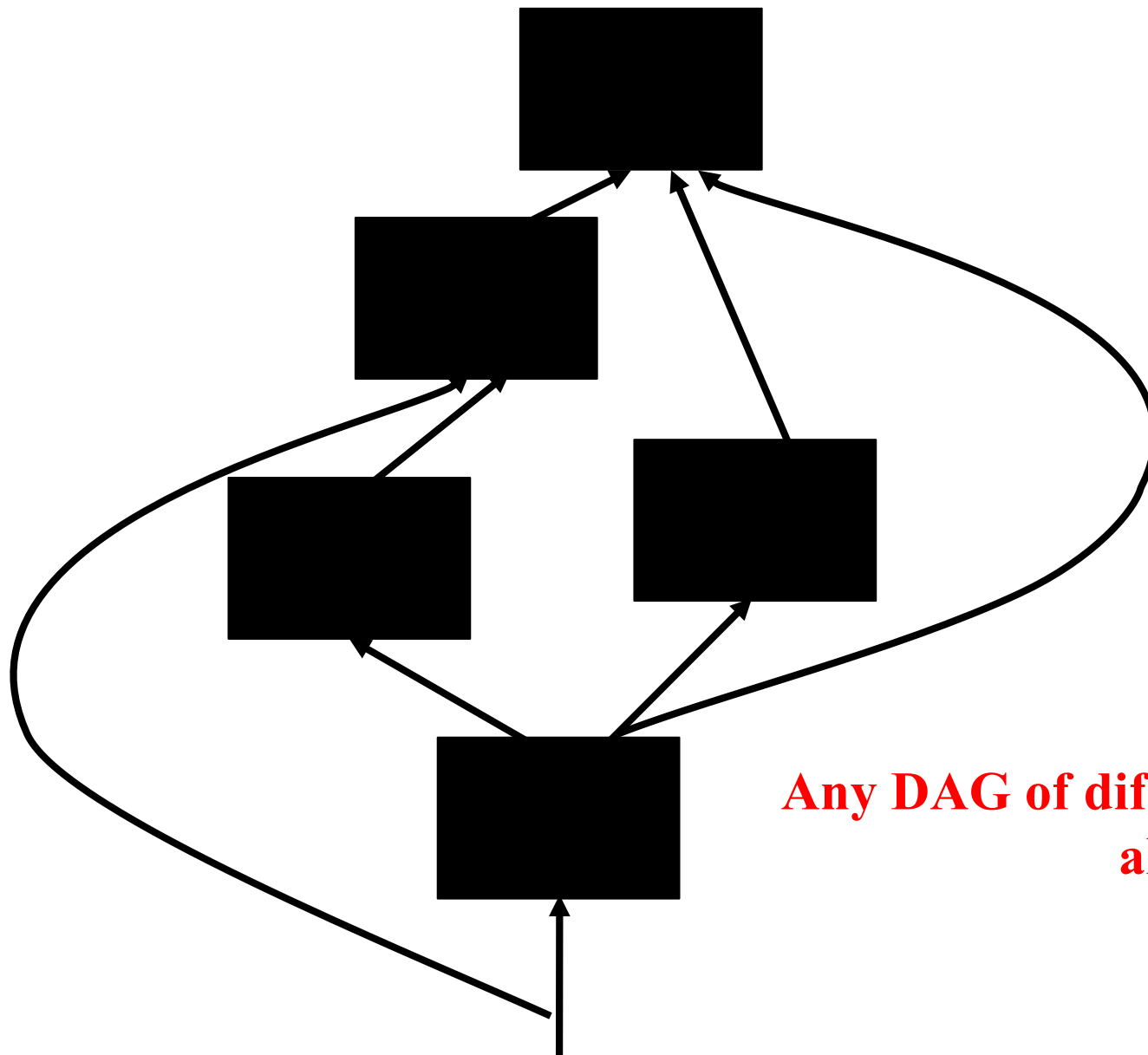
- Project Teams Google Doc
 - <https://docs.google.com/spreadsheets/d/1AaXY0JE4IAbHvoDaWlc9zsmfKMyuGS39JAn9dpeXhhQ/edit#gid=0>
 - Project Title
 - 1-3 sentence project summary TL;DR
 - Team member names + GT IDs

Recap of last time

How do we compute gradients?

- Manual Differentiation
- Symbolic Differentiation
- Numerical Differentiation
- Automatic Differentiation
 - Forward mode AD
 - Reverse mode AD
 - aka “backprop”

Computational Graph



Any DAG of differentiable modules is allowed!

Directed Acyclic Graphs (DAGs)

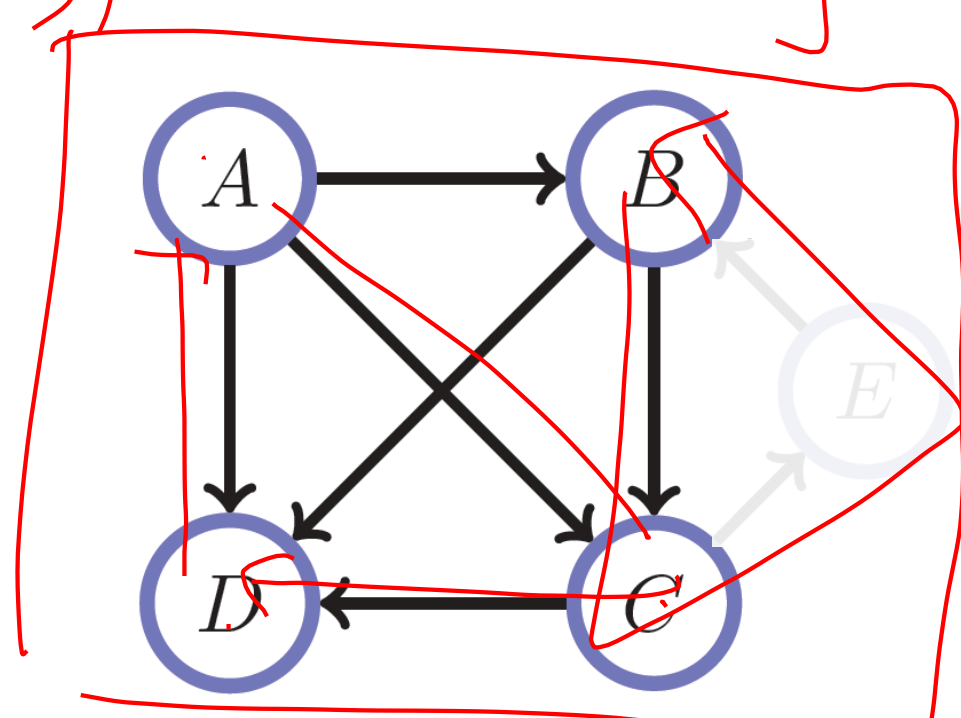
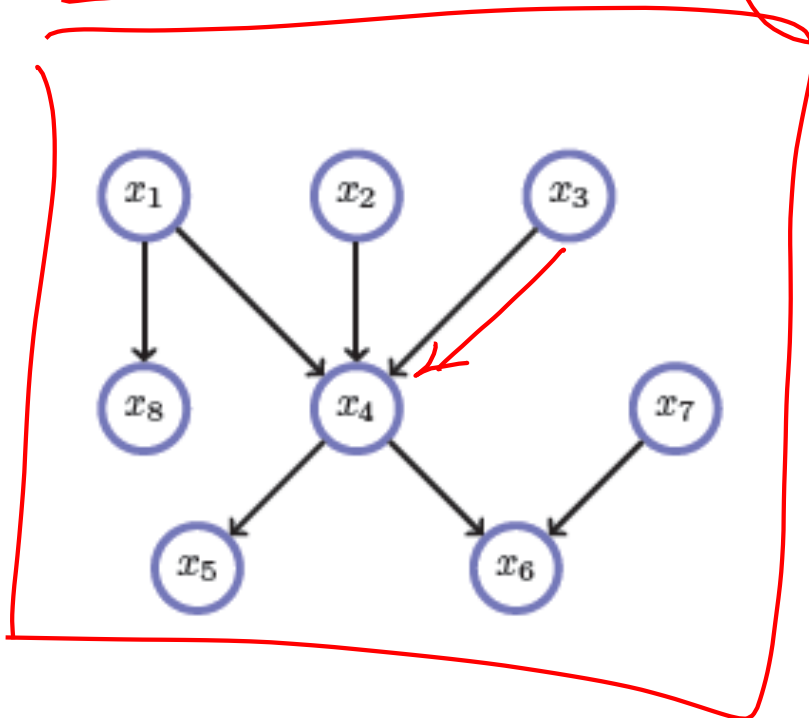
- Exactly what the name suggests
 - Directed edges
 - No (directed) cycles
 - Underlying undirected cycles okay

$$E = \{ (v_i, v_j) \}$$

$$\{ \{v_i, v_j\} \}$$

$$(v_i, v_j) \dots v_j$$

$$(D, A) \notin E$$

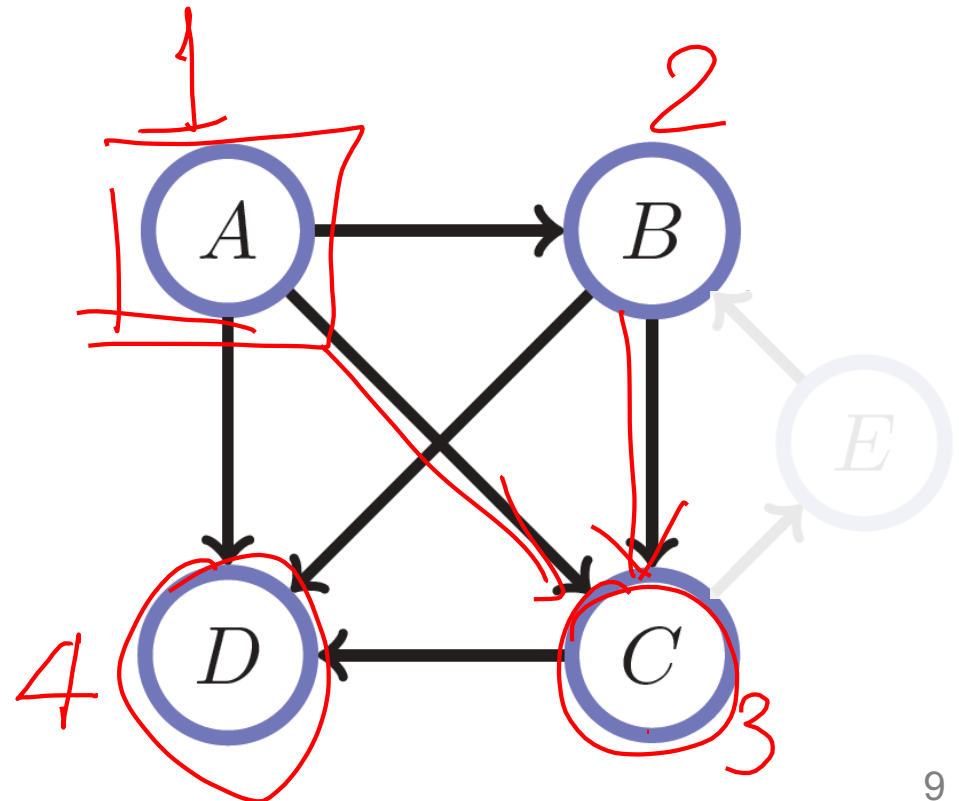
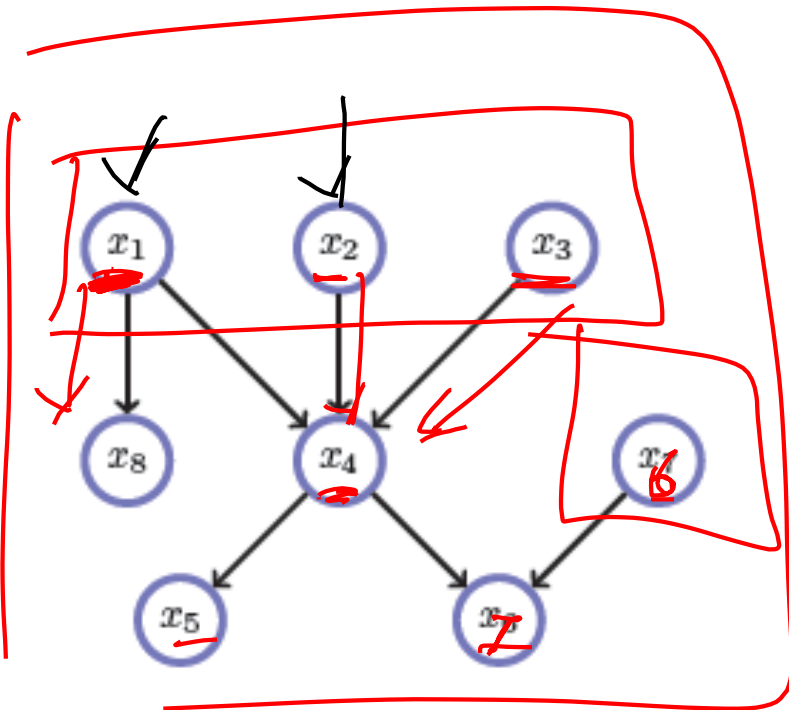


Directed Acyclic Graphs (DAGs)

- Concept
 - Topological Ordering

$$\exists \sigma: V \rightarrow [n] = \{1, \dots, n\}$$

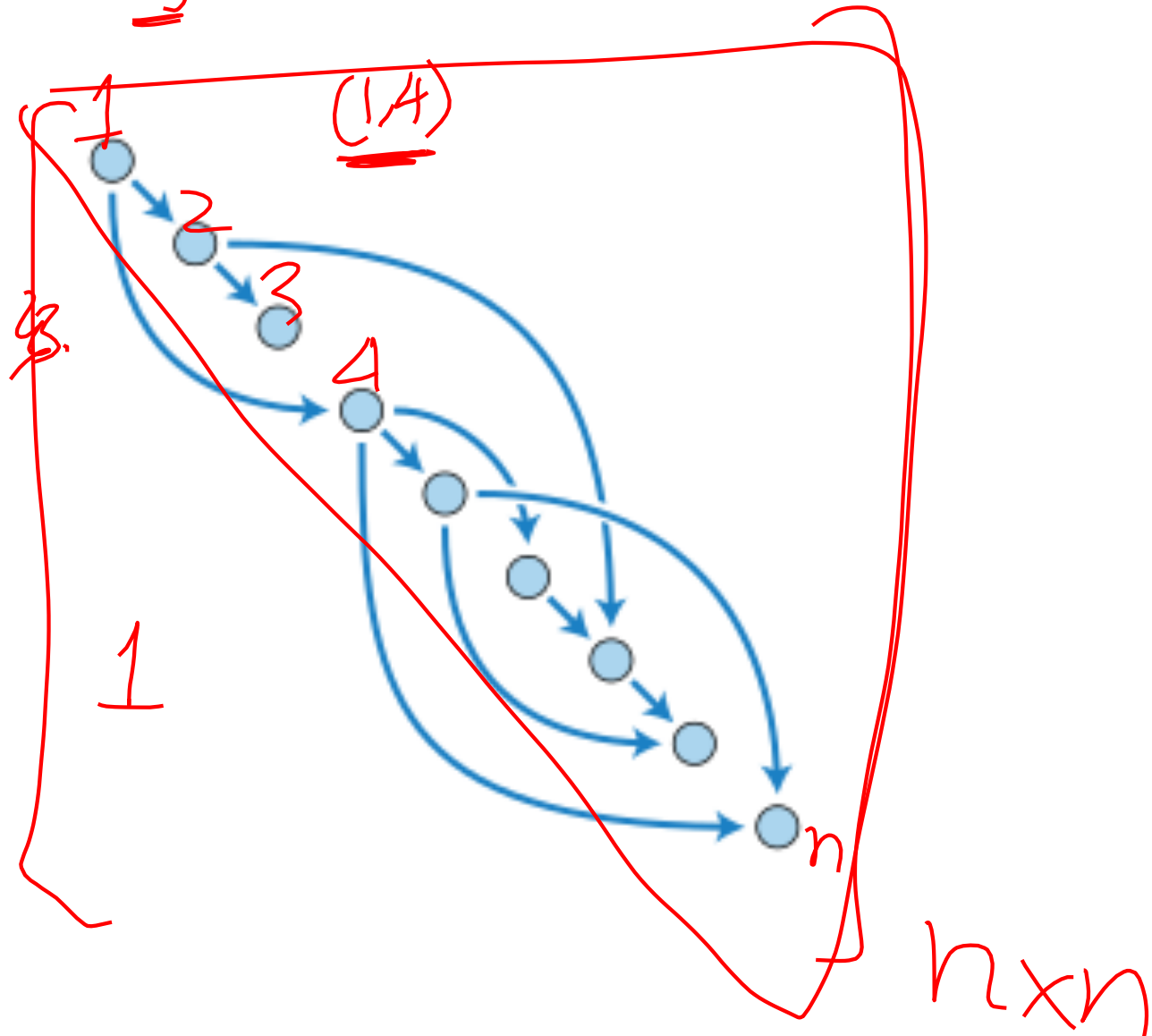
$$\text{s.t. } (v_i, v_j) \in E \implies \sigma(v_i) < \sigma(v_j)$$



Directed Acyclic Graphs (DAGs)

$$a_{ij} = 1 \quad (i, j) \in E$$

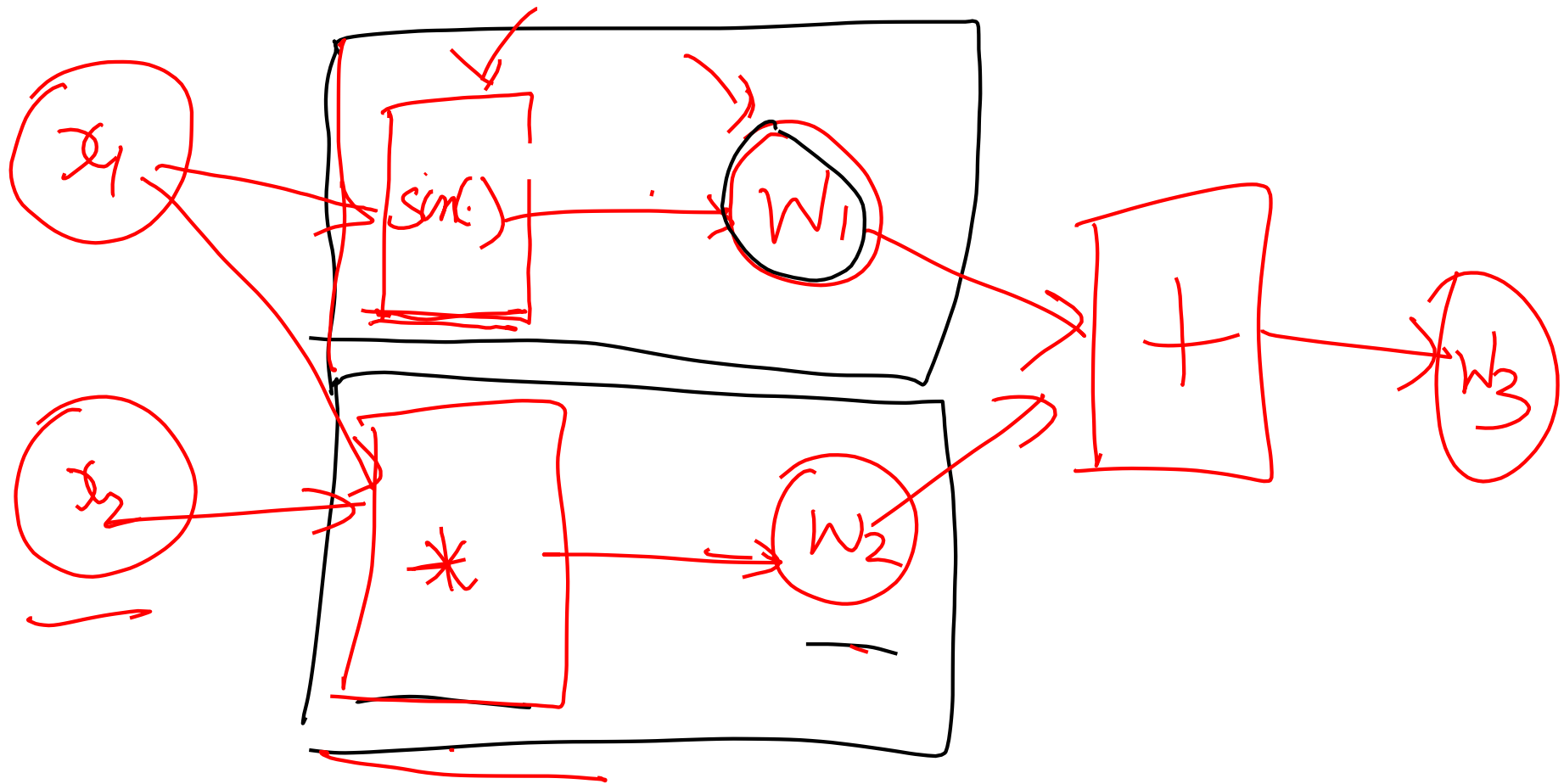
$$A =$$



Computational Graphs

- Notation #1

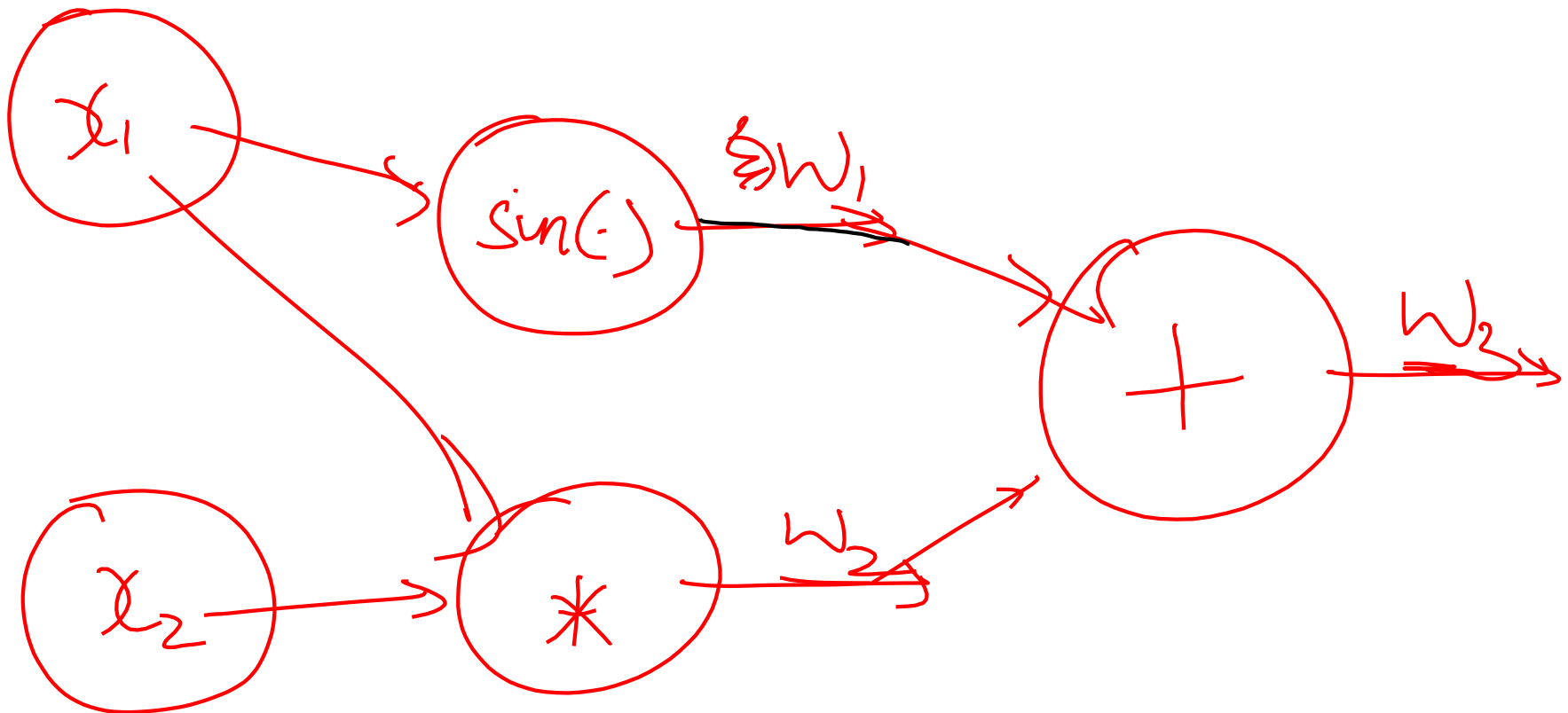
$$\underline{f(x_1, x_2)} = \underline{x_1 x_2 + \sin(x_1)}$$



Computational Graphs

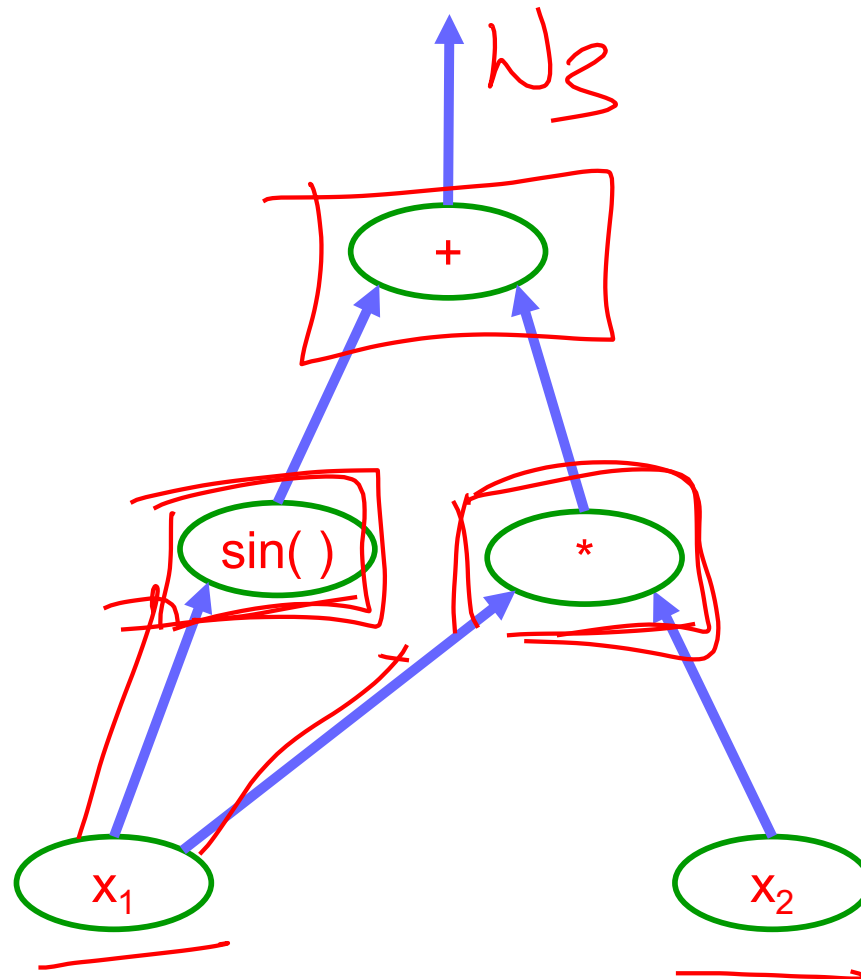
- Notation #2

$$f(x_1, x_2) = x_1 x_2 + \sin(x_1)$$



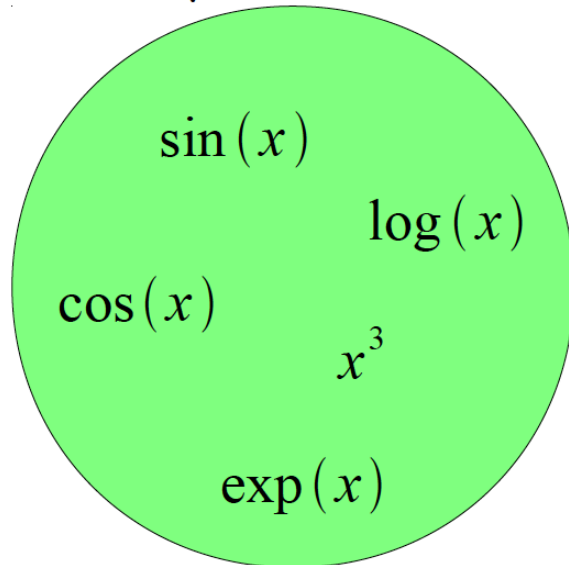
Example

$$\underline{f(x_1, x_2) = x_1 x_2 + \sin(x_1)}$$



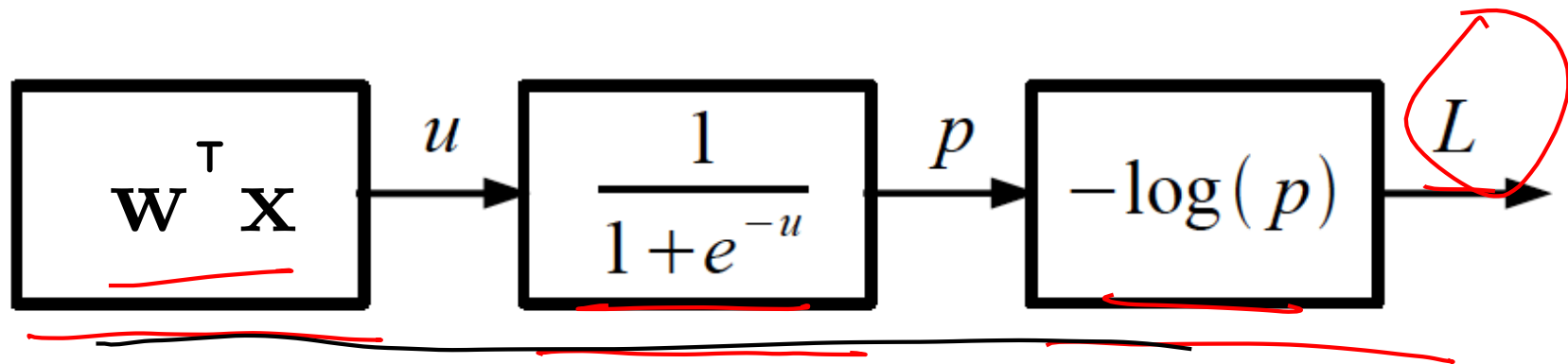
Logistic Regression as a Cascade

Given a library of simple functions



Compose into a
complicate function

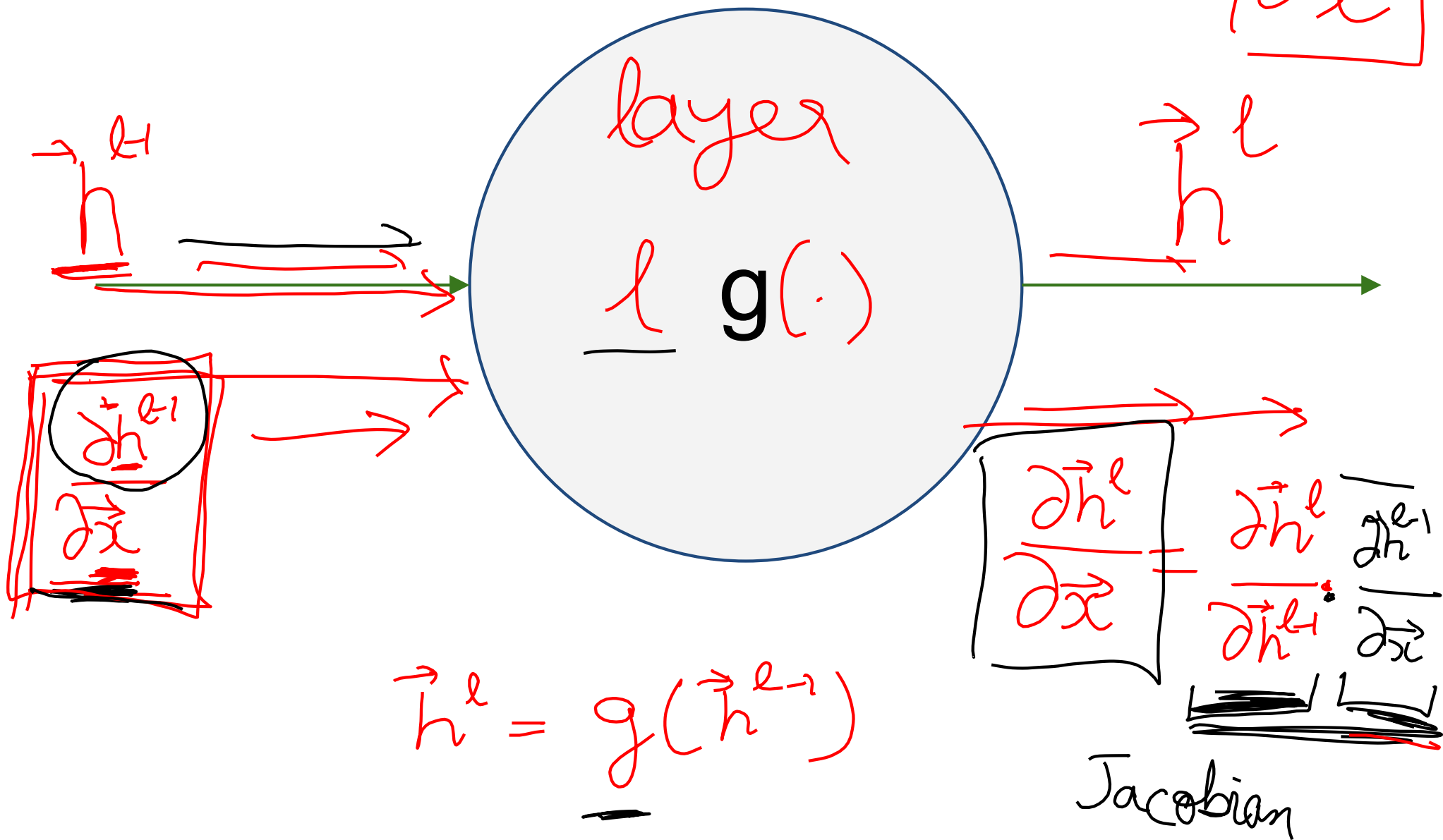
→ $-\log\left(\frac{1}{1 + e^{-\mathbf{w}^\top \mathbf{x}}}\right)$



Forward mode vs Reverse Mode

- Key Computations

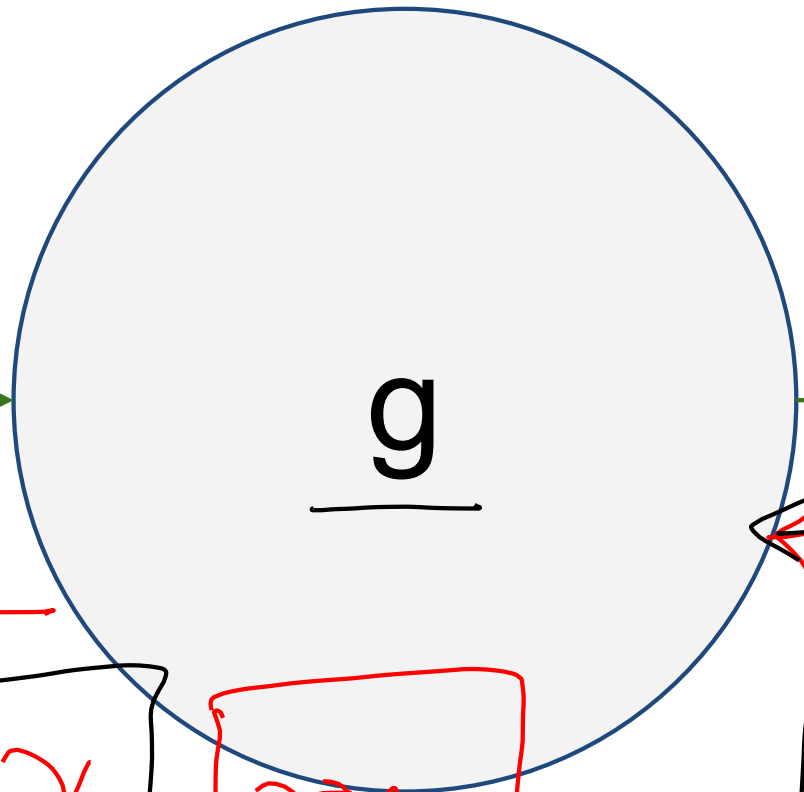
Forward mode AD



Reverse mode AD

$$\frac{\partial L}{\partial \vec{x}}$$

$$\vec{h}^{l-1}$$



$$\vec{h}^l$$



$$\frac{\partial L}{\partial \vec{h}^{l-1}}$$

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

input

$$\frac{\partial L}{\partial \vec{h}^{l-1}}$$

Jacobian

$$\frac{\partial L}{\partial \vec{h}^l}$$

Example: Forward mode AD

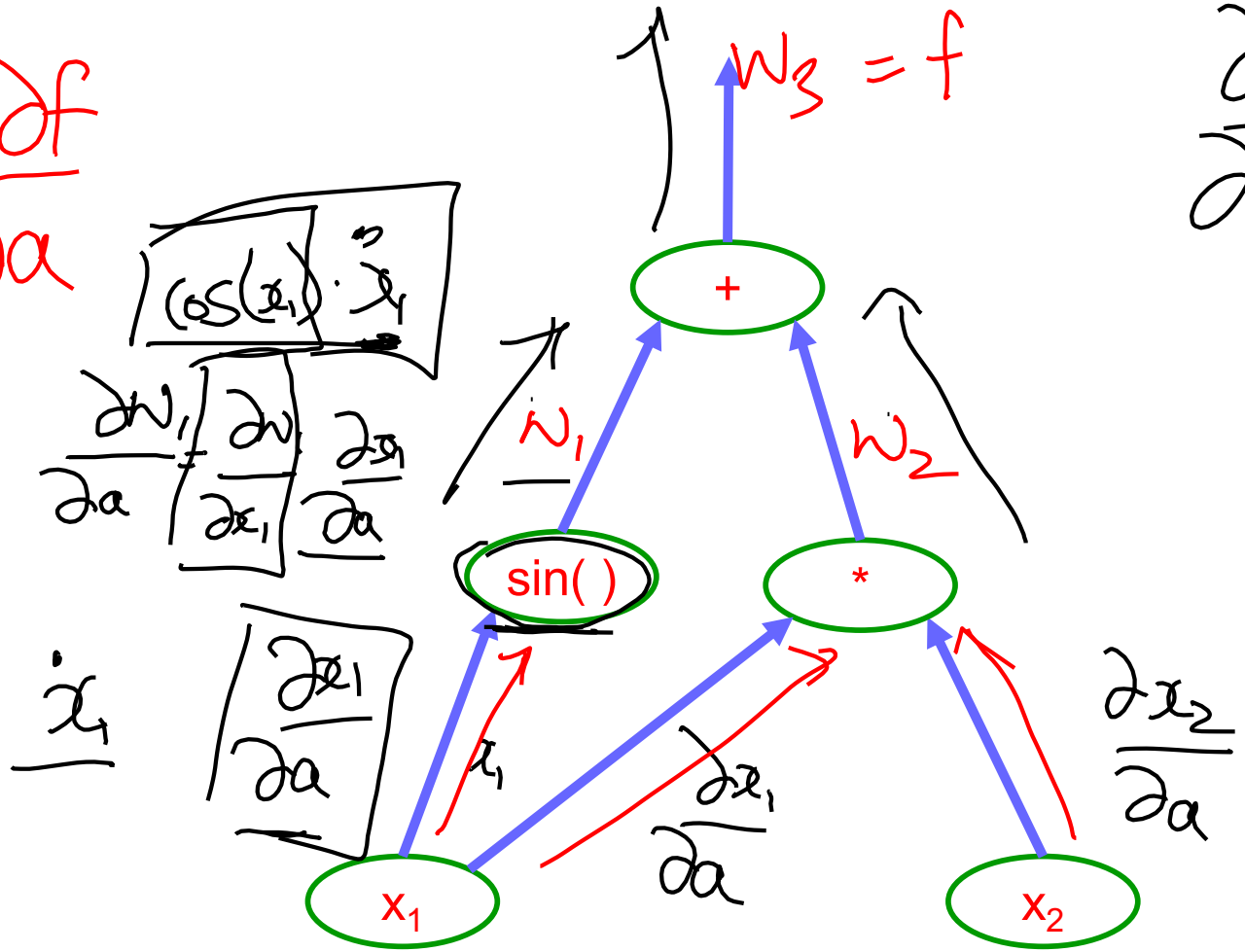
$$f(x_1, x_2) = x_1 x_2 + \sin(x_1)$$

$\left. \begin{array}{l} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \end{array} \right\}$

$\frac{\partial f}{\partial a}$

$\frac{\partial w_3}{\partial a} =$

$a = x_1$
 $a = x_2$



Example: Forward mode AD

$$f(x_1, x_2) = x_1 x_2 + \sin(x_1)$$

$\cos(x_1) + x_2$

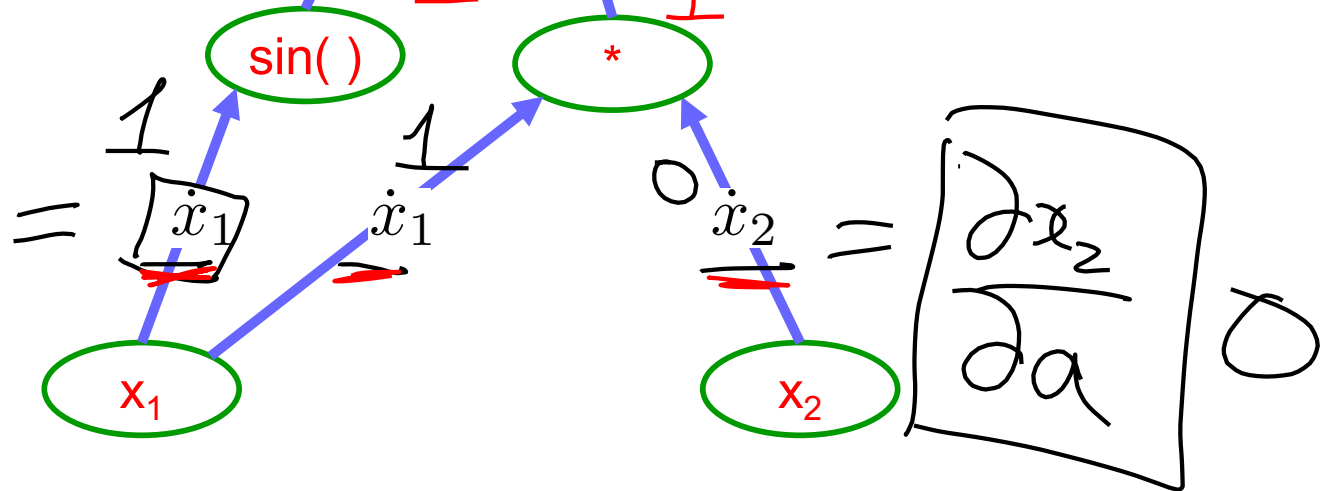
$$\dot{w}_3 = \dot{w}_1 + \dot{w}_2$$

$$\frac{\partial f}{\partial a}$$

$$\dot{w}_1 = \cos(x_1) \dot{x}_1 \quad \dot{w}_2 = \dot{x}_1 x_2 + x_1 \dot{x}_2$$

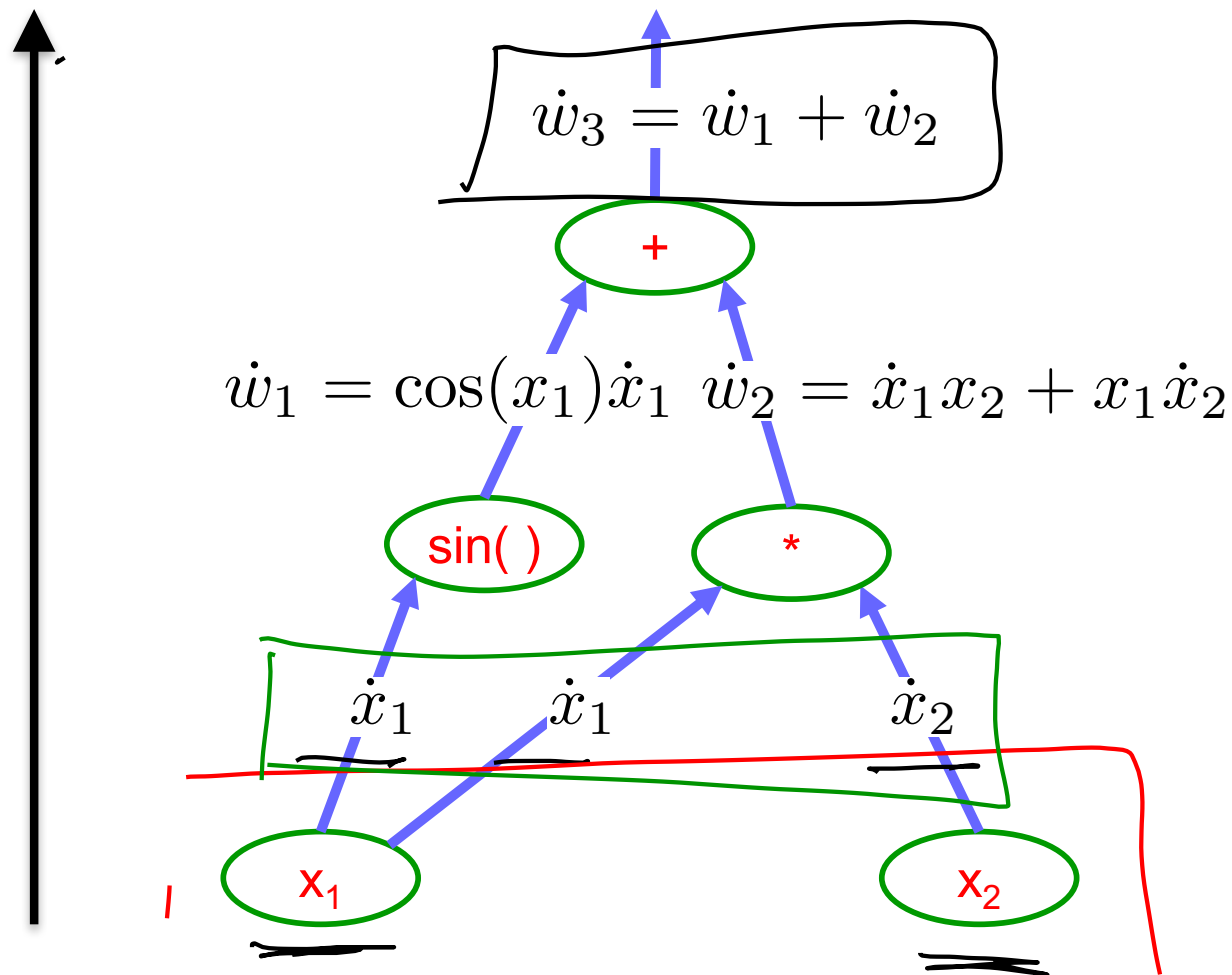
$$\frac{\partial x_1}{\partial a}$$

$$a = x_1$$



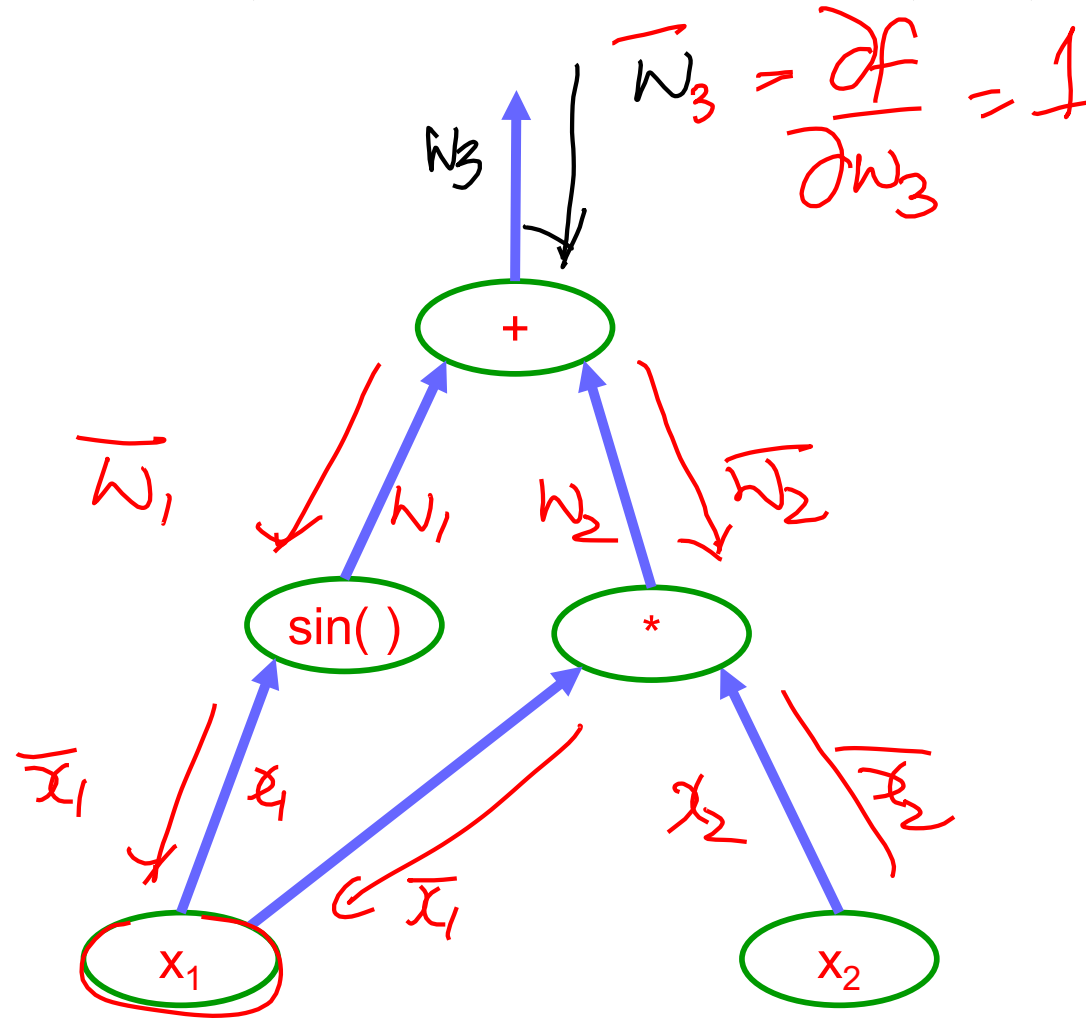
Example: Forward mode AD

$$f(x_1, x_2) = x_1 x_2 + \sin(x_1)$$



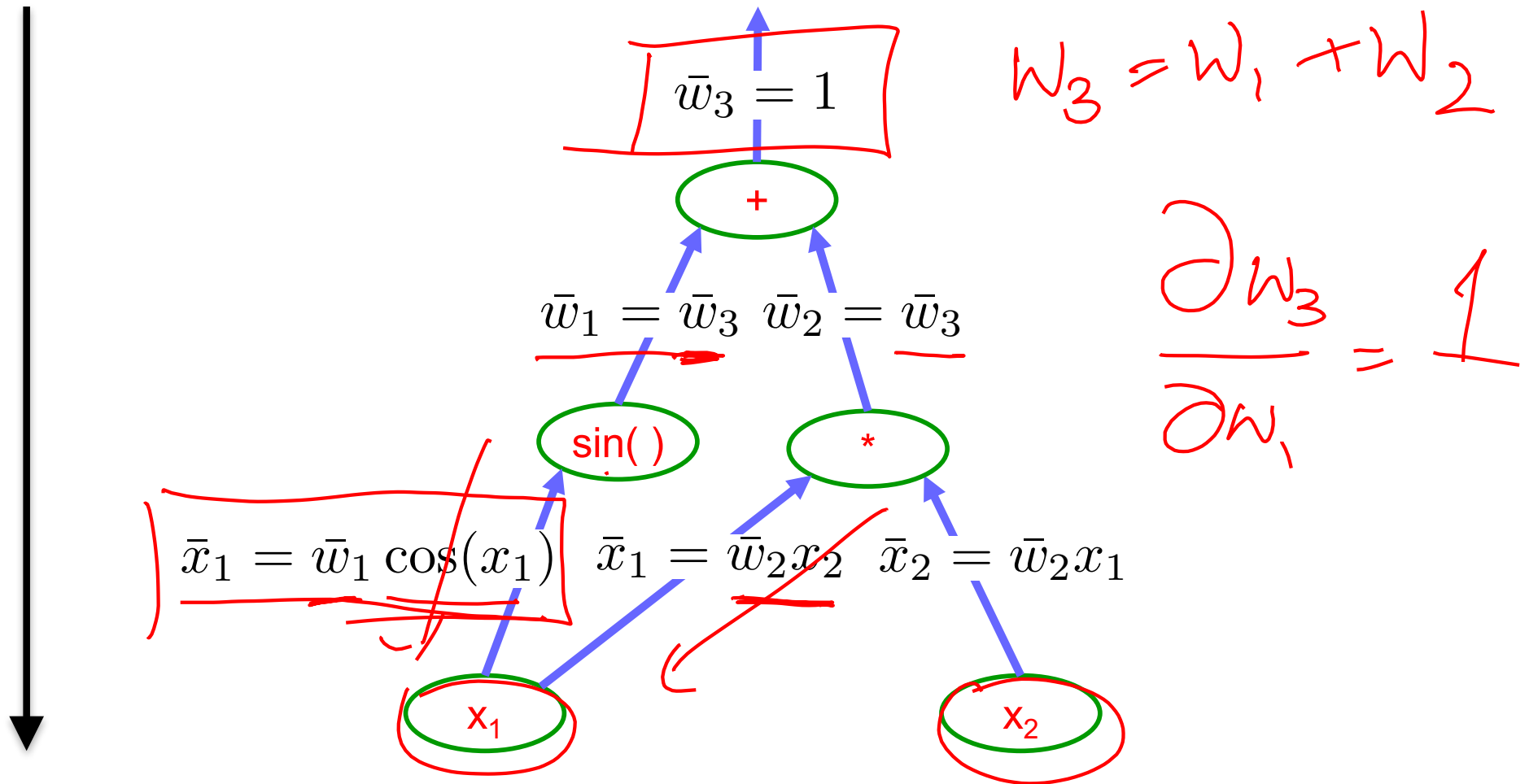
Example: Reverse mode AD

$$f(x_1, x_2) = x_1 x_2 + \sin(x_1)$$

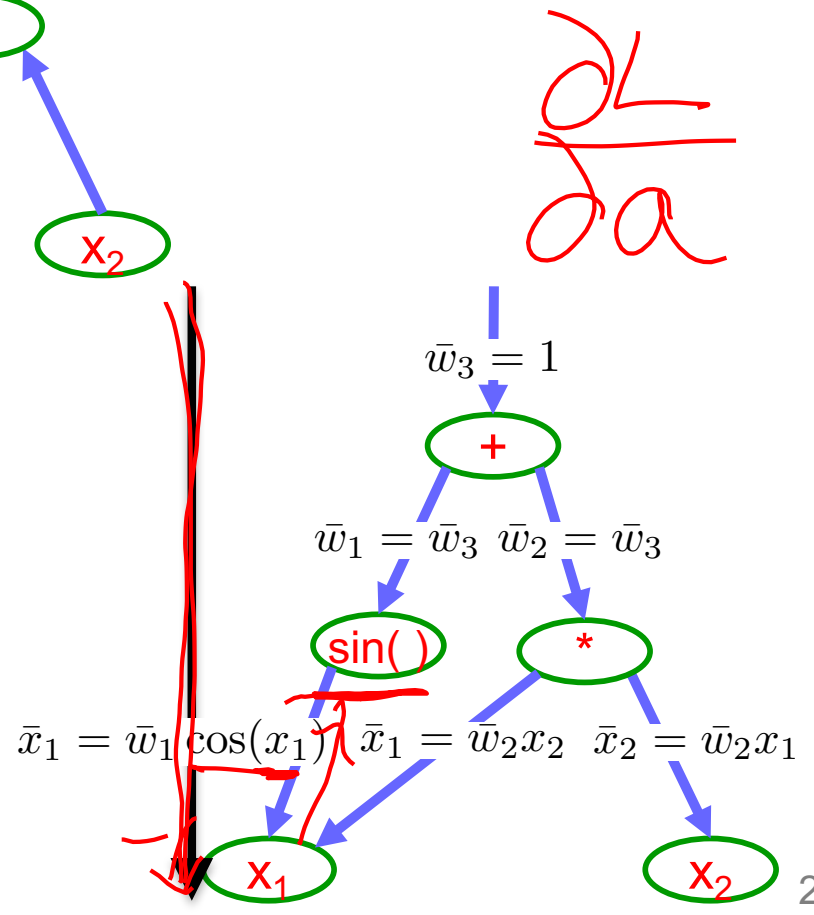
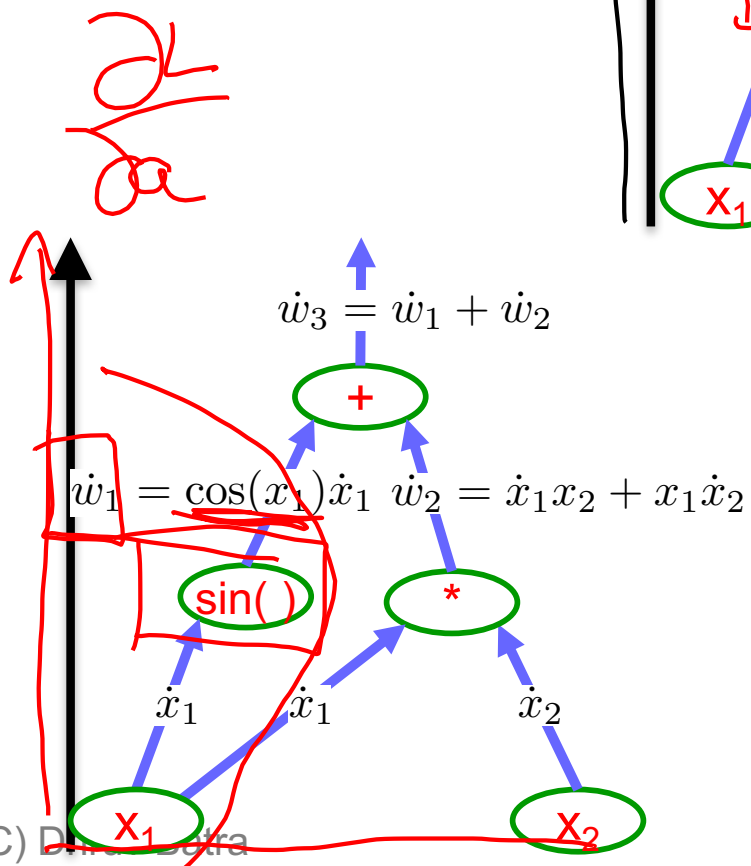
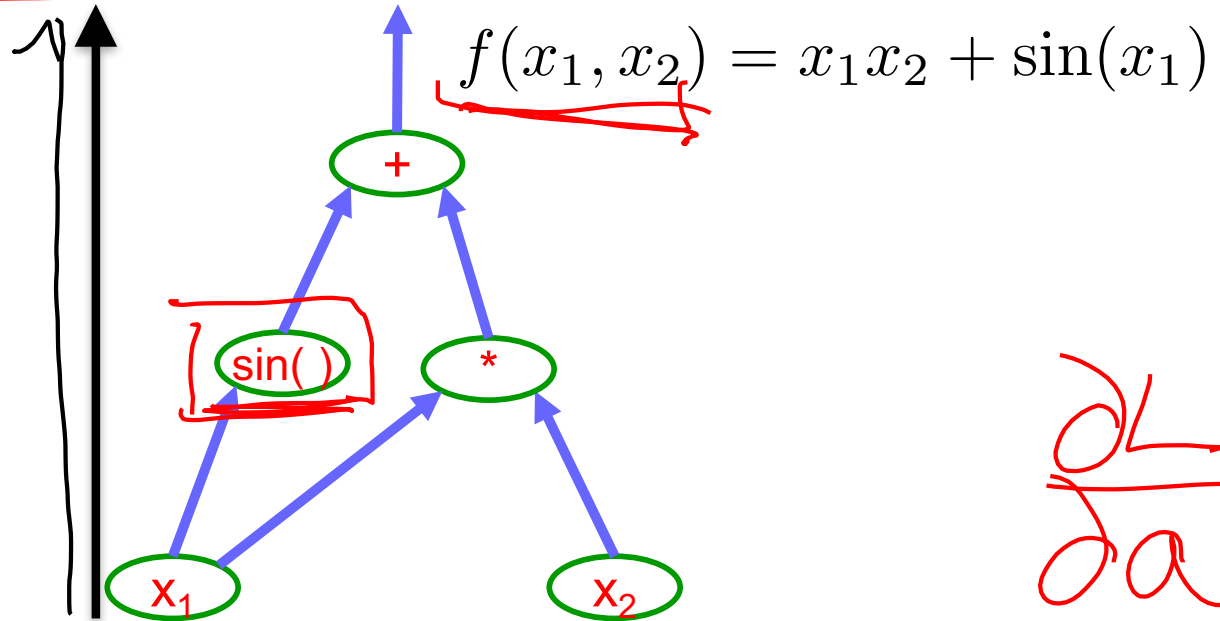


Example: Reverse mode AD

$$f(x_1, x_2) = x_1 x_2 + \sin(x_1)$$



Forward Pass vs Forward mode AD vs Reverse Mode AD

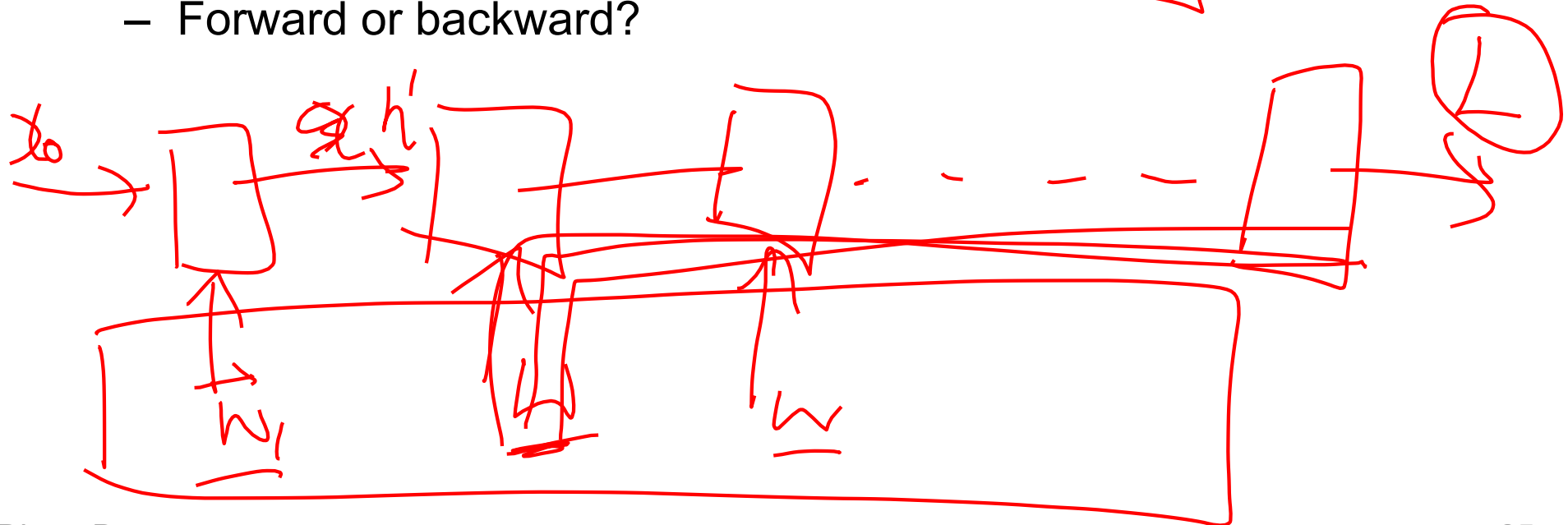
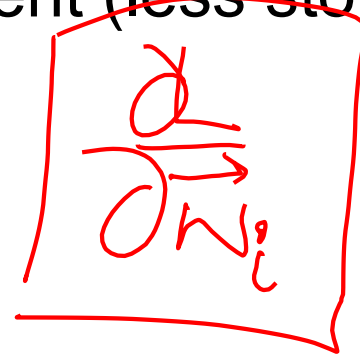
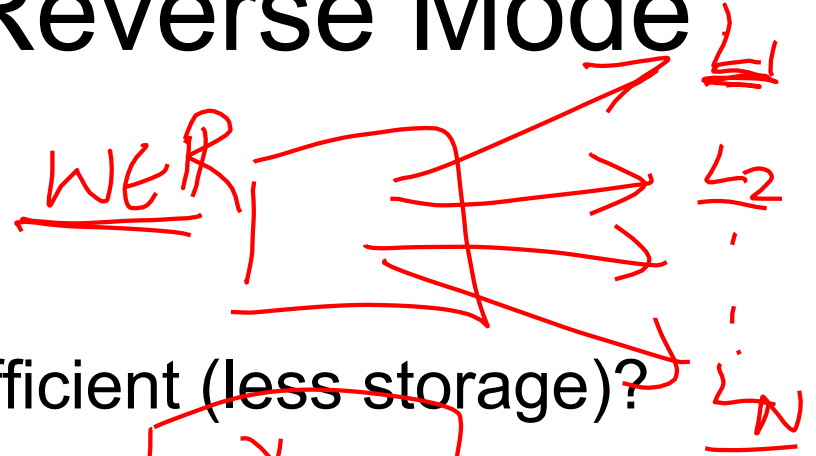


Forward mode vs Reverse Mode

- What are the differences?
- Which one is more memory efficient (less storage)?
 - Forward or backward?

Forward mode vs Reverse Mode

- What are the differences?
- Which one is more memory efficient (less storage)?
 - Forward or backward?
- Which one is faster to compute?
 - Forward or backward?

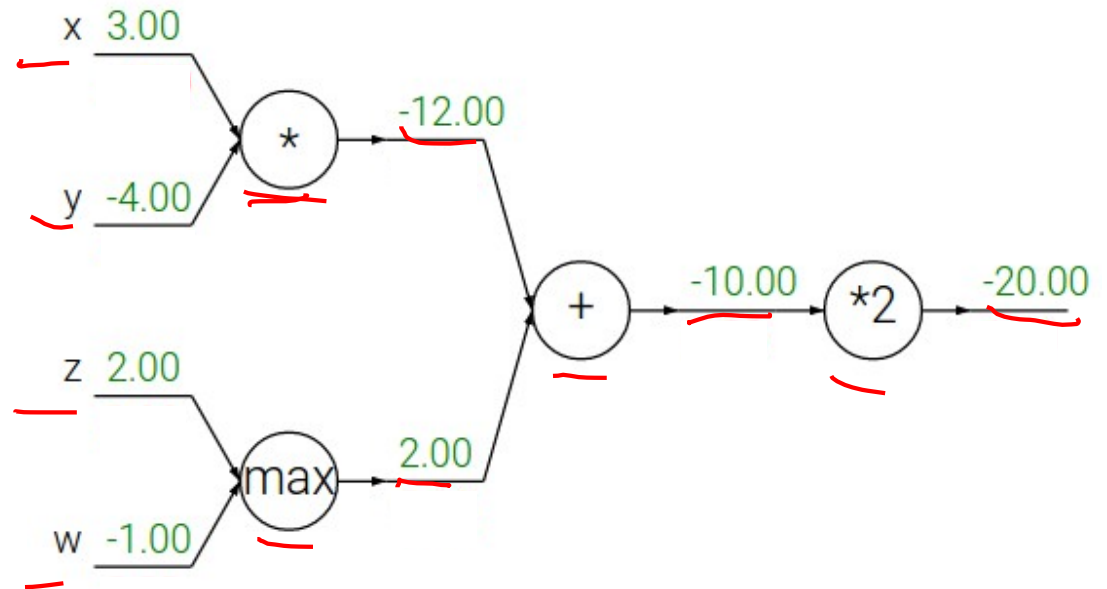


Plan for Today

- (Finish) Computing Gradients
 - Forward mode vs Reverse mode AD
 - Patterns in backprop
 - Backprop in FC+ReLU NNs
- Convolutional Neural Networks

Patterns in backward flow

$$f(\dots) = 2(xy + \max\{z, w\})$$



Patterns in backward flow

$$w_3 = w_1 + w_2$$

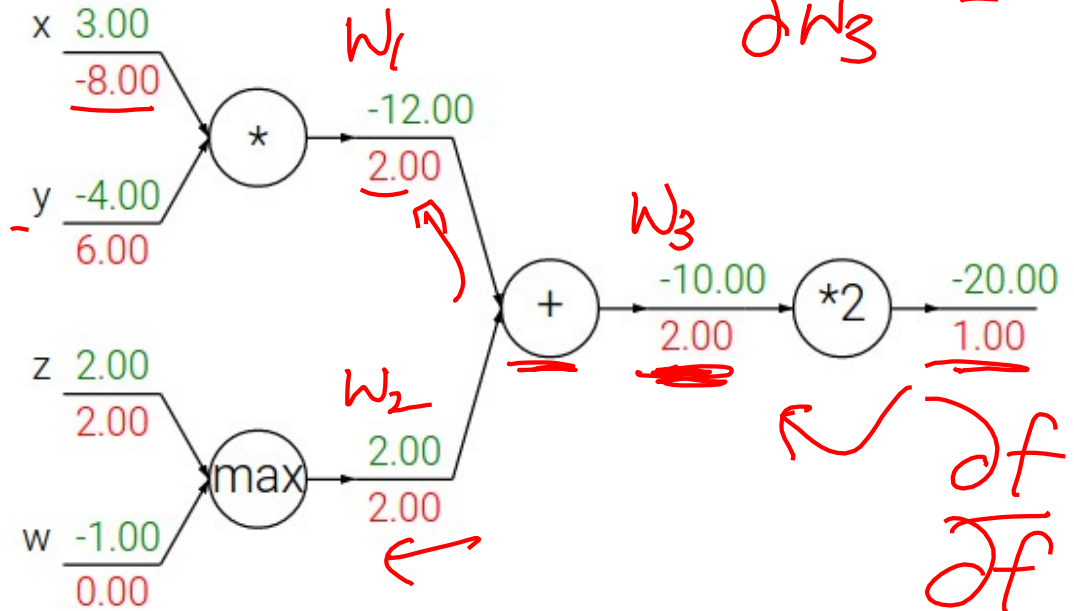
$$\frac{\partial w_3}{\partial w_1} = 1$$

$$w_1 = xy$$

$$\frac{\partial w_1}{\partial x} = y$$

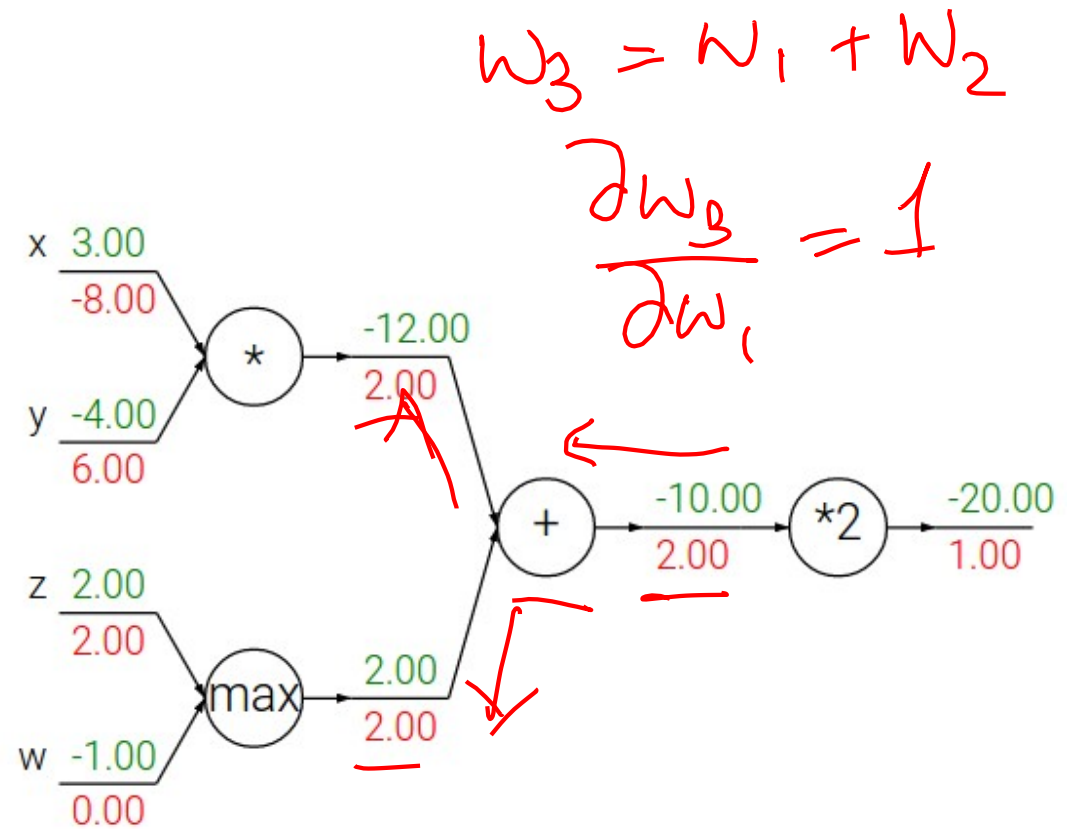
$$f = 2w_3$$

$$\frac{\partial f}{\partial w_3} = 2$$



Patterns in backward flow

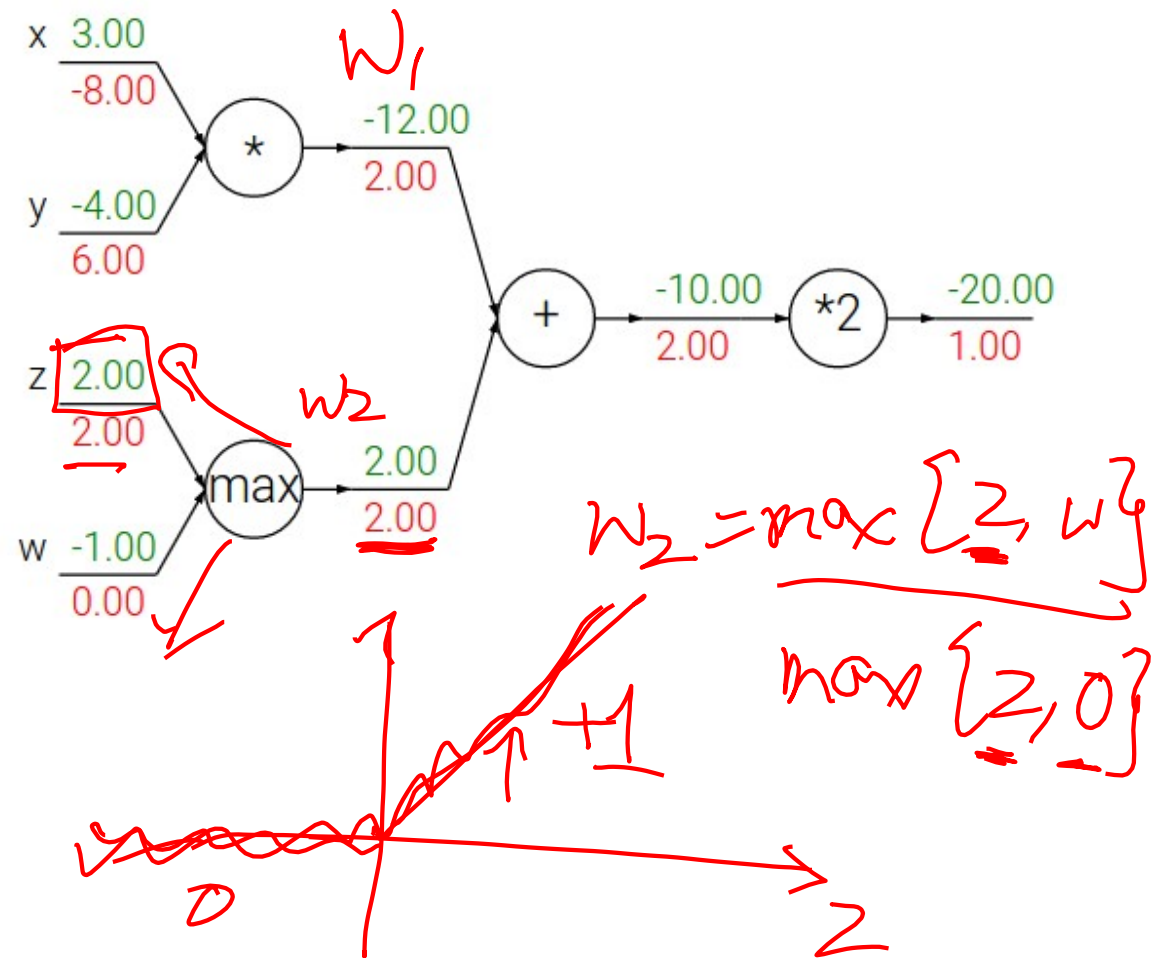
add gate: gradient distributor



Patterns in backward flow

add gate: gradient distributor

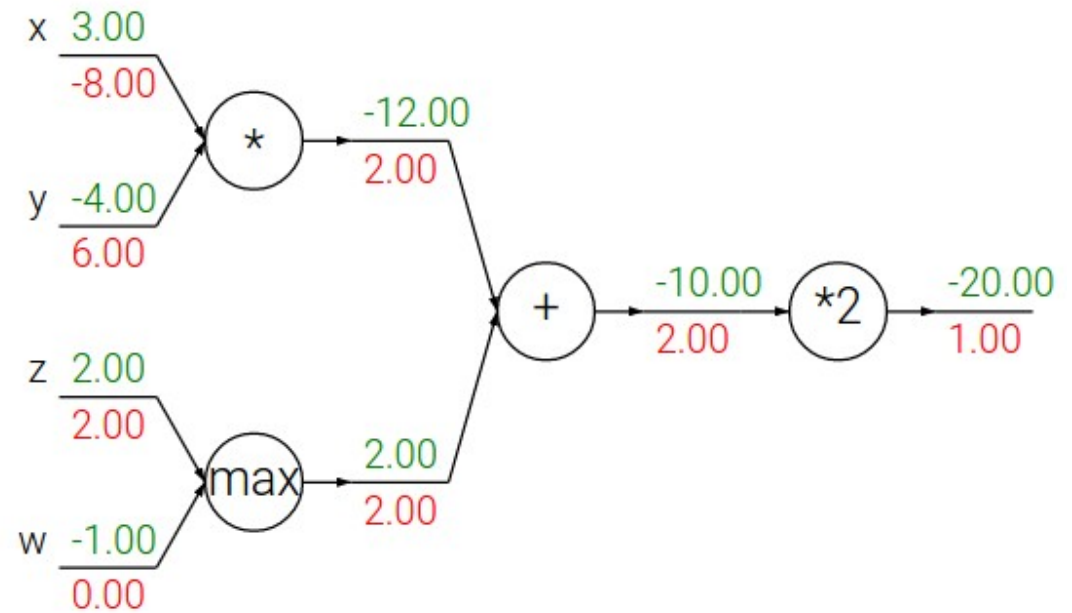
Q: What is a max gate?



Patterns in backward flow

add gate: gradient distributor

max gate: gradient router

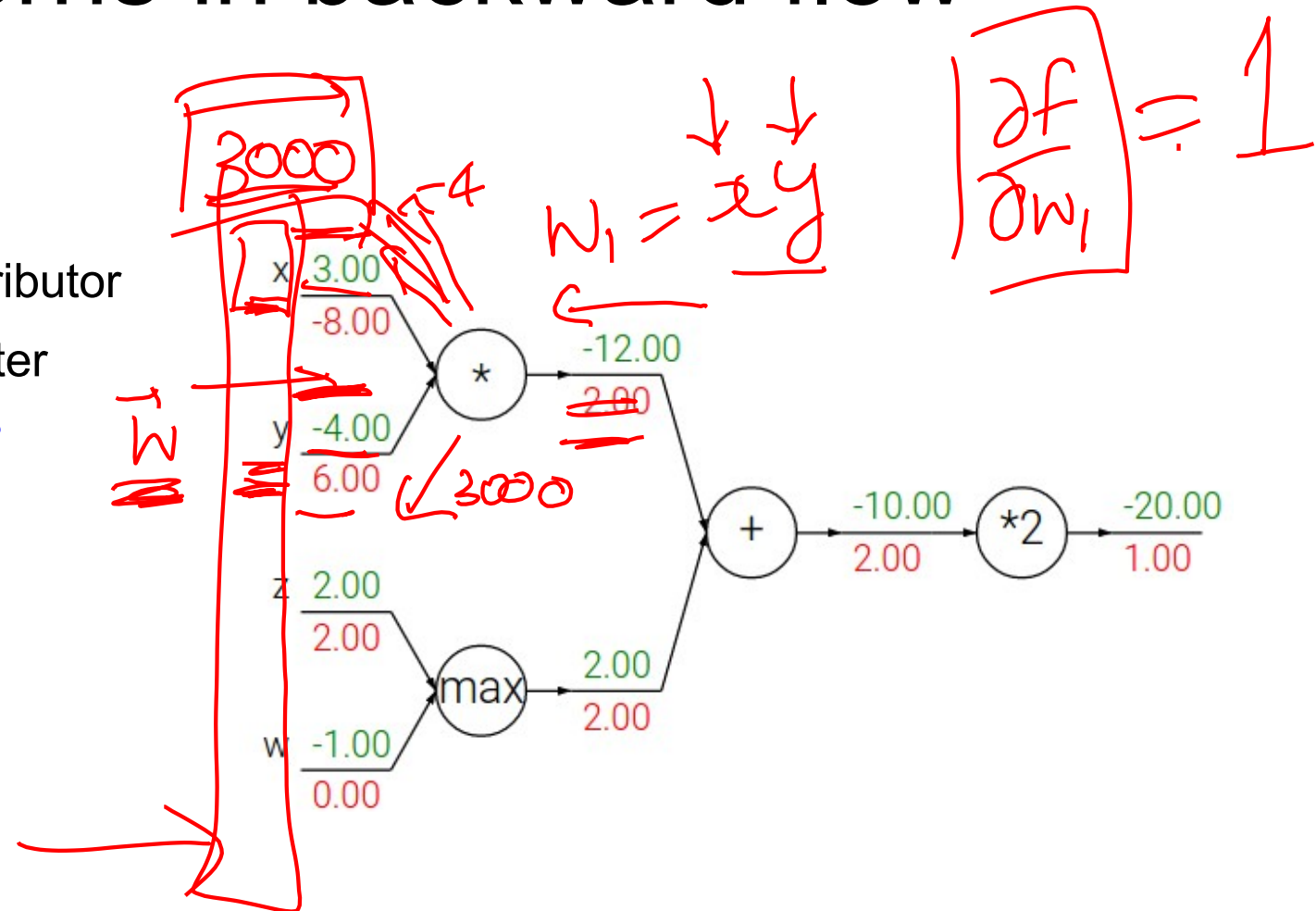


Patterns in backward flow

add gate: gradient distributor

max gate: gradient router

Q: What is a **mul** gate?

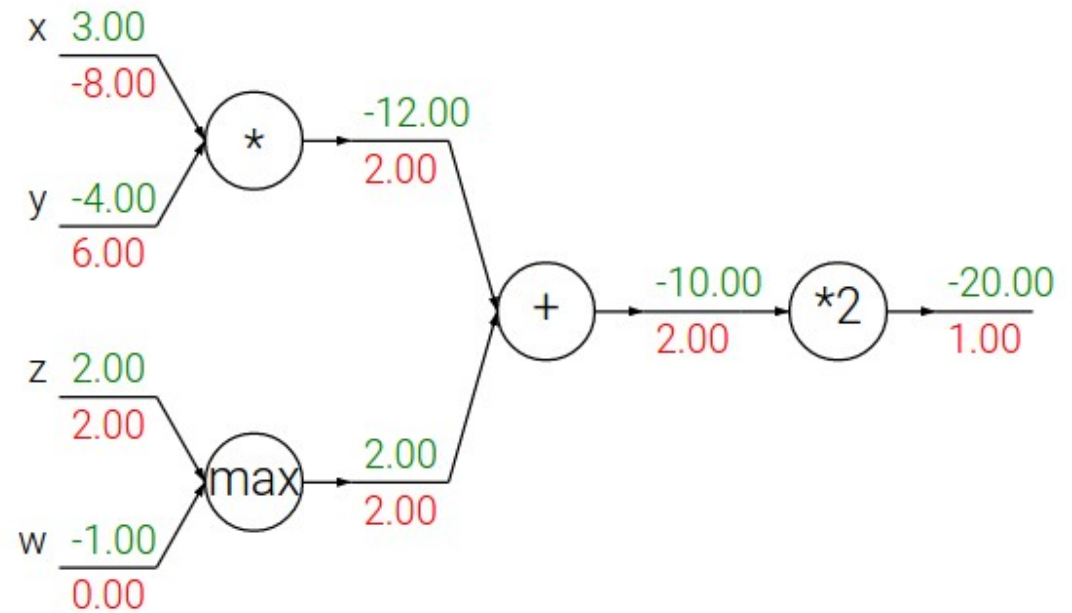


Patterns in backward flow

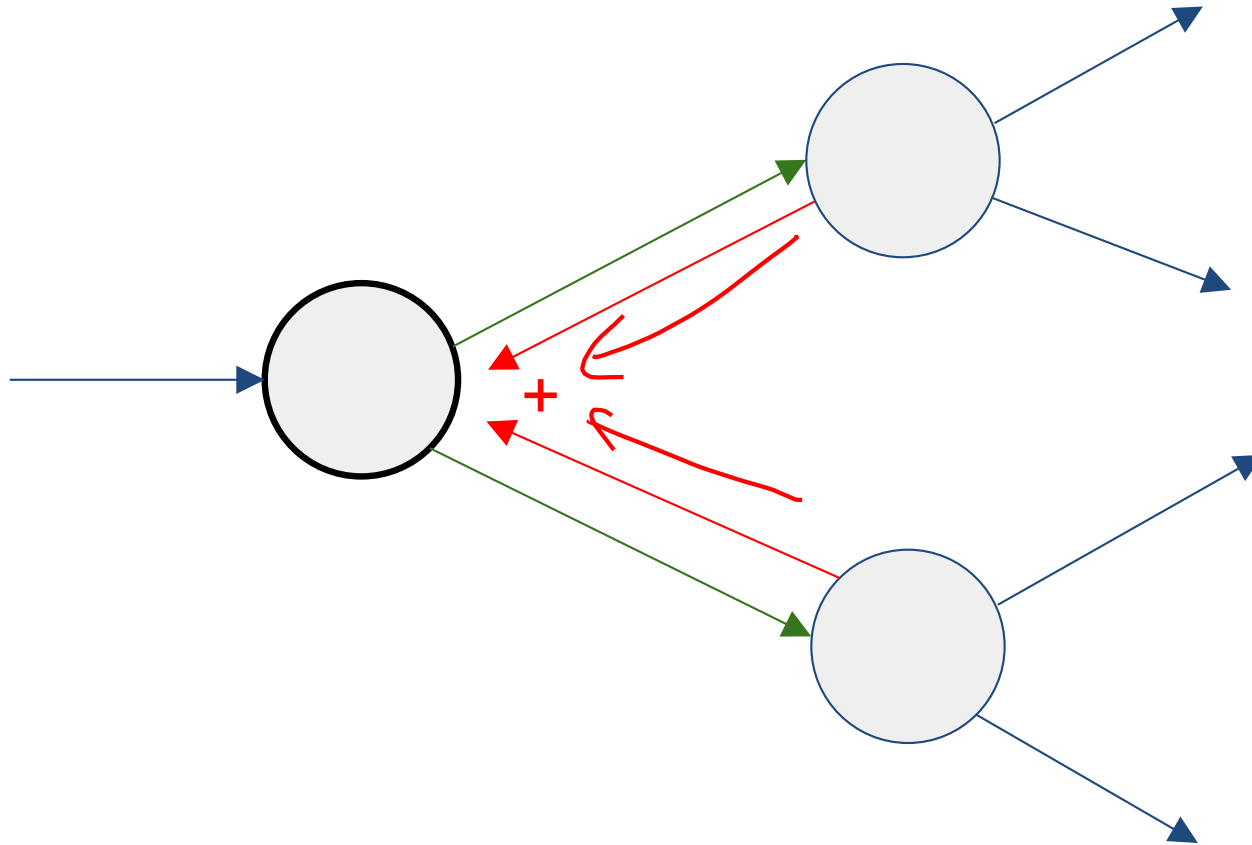
add gate: gradient distributor

max gate: gradient router

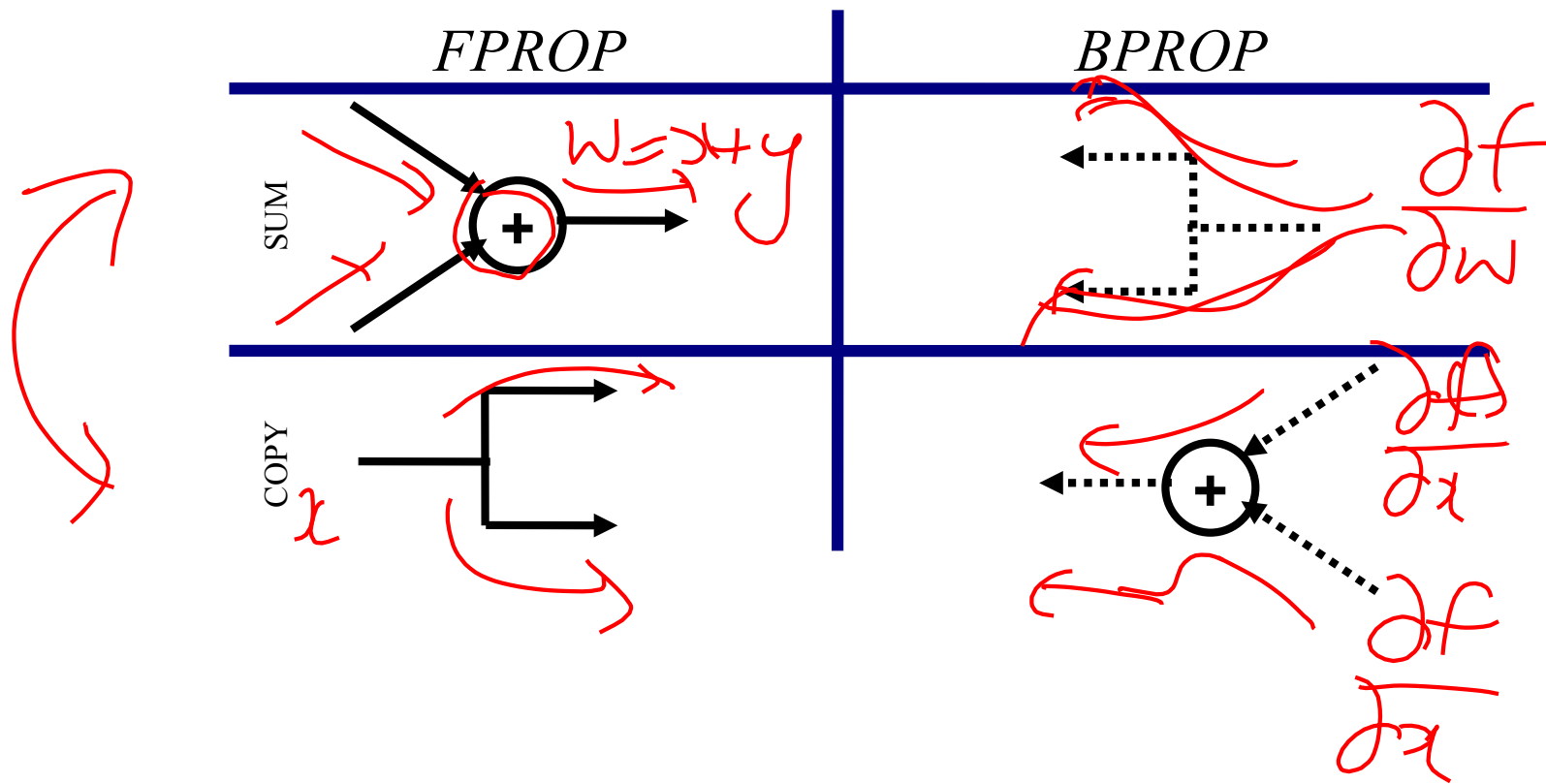
mul gate: gradient switcher



Gradients add at branches

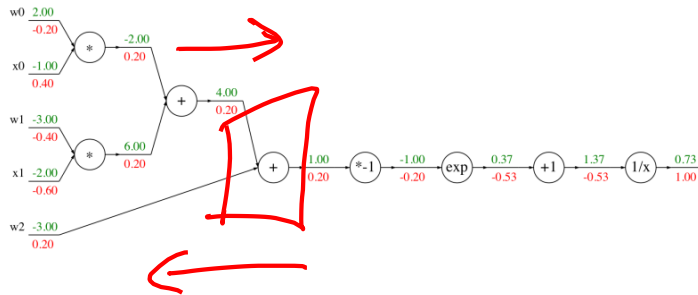


Duality in Fprop and Bprop



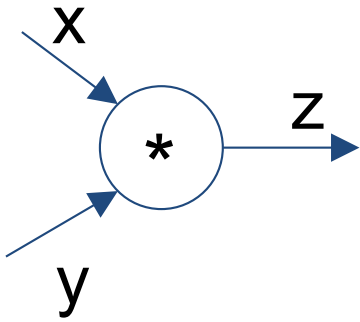
Modularized implementation: forward / backward API

Graph (or Net) object (*rough psuedo 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
```

Modularized implementation: forward / backward API



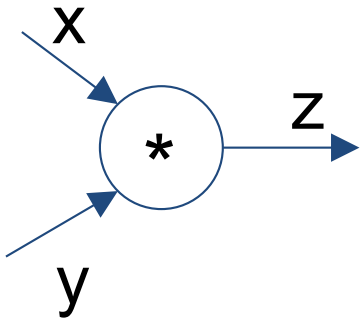
(x,y,z are scalars)

```
class MultiplyGate(object):  
    def forward(x,y):  
        z = x*y  
        return z  
    def backward(dz):  
        # dx = ... #todo  
        # dy = ... #todo  
        return [dx, dy]
```

$$\frac{\partial L}{\partial z}$$

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

Modularized implementation: forward / backward API



(x,y,z are scalars)

```
class MultiplyGate(object):  
    def forward(x,y):  
        z = x*y  
        self.x = x # must keep these around!  
        self.y = y  
        return z  
    def backward(dz):  
        dx = self.y * dz # [dz/dx * dL/dz]  
        dy = self.x * dz # [dz/dy * dL/dz]  
        return [dx, dy]
```

Example: Caffe layers

Branch: master | [caffe / src / caffe / layers /](#) | [Create new file](#) | [Upload files](#) | [Find file](#) | [History](#)

shelhamer committed on GitHub Merge pull request #4630 from BiGene/load_hdf5_fix Latest commit e687a71 21 days ago

..

absval_layer.cpp	dismantle layer headers	a year ago
absval_layer.cu	dismantle layer headers	a year ago
accuracy_layer.cpp	dismantle layer headers	a year ago
argmax_layer.cpp	dismantle layer headers	a year ago
base_conv_layer.cpp	enable dilated deconvolution	a year ago
base_data_layer.cpp	Using default from proto for prefetch	3 months ago
base_data_layer.cu	Switched multi-GPU to NCCL	3 months ago
batch_norm_layer.cpp	Add missing spaces besides equal signs in batch_norm_layer.cpp	4 months ago
batch_norm_layer.cu	dismantle layer headers	a year ago
batch_reindex_layer.cpp	dismantle layer headers	a year ago
batch_reindex_layer.cu	dismantle layer headers	a year ago
bias_layer.cpp	Remove incorrect cast of gemm int arg to Dtype in BiasLayer	a year ago
bias_layer.cu	Separation and generalization of ChannelwiseAffineLayer into BiasLayer	a year ago
bnl_layer.cpp	dismantle layer headers	a year ago
bnl_layer.cu	dismantle layer headers	a year ago
concat_layer.cpp	dismantle layer headers	a year ago
concat_layer.cu	dismantle layer headers	a year ago
contrastive_loss_layer.cpp	dismantle layer headers	a year ago
contrastive_loss_layer.cu	dismantle layer headers	a year ago
conv_layer.cpp	add support for 2D dilated convolution	a year ago
conv_layer.cu	dismantle layer headers	a year ago
crop_layer.cpp	remove redundant operations in Crop layer (#5138)	2 months ago
crop_layer.cu	remove redundant operations in Crop layer (#5138)	2 months ago
cudnn_conv_layer.cpp	dismantle layer headers	a year ago
cudnn_conv_layer.cu	Add cuDNN v5 support, drop cuDNN v3 support	11 months ago

[Caffe](#) is licensed under [BSD 2-Clause](#)

cudnn_lcn_layer.cpp	dismantle layer headers	a year ago
cudnn_lcn_layer.cu	dismantle layer headers	a year ago
cudnn_lrn_layer.cpp	dismantle layer headers	a year ago
cudnn_lrn_layer.cu	dismantle layer headers	a year ago
cudnn_pooling_layer.cpp	dismantle layer headers	a year ago
cudnn_pooling_layer.cu	dismantle layer headers	a year ago
cudnn_relu_layer.cpp	Add cuDNN v5 support, drop cuDNN v3 support	11 months ago
cudnn_relu_layer.cu	Add cuDNN v5 support, drop cuDNN v3 support	11 months ago
cudnn_sigmoid_layer.cpp	Add cuDNN v5 support, drop cuDNN v3 support	11 months ago
cudnn_sigmoid_layer.cu	Add cuDNN v5 support, drop cuDNN v3 support	11 months ago
cudnn_softmax_layer.cpp	dismantle layer headers	a year ago
cudnn_softmax_layer.cu	dismantle layer headers	a year ago
cudnn_tanh_layer.cpp	Add cuDNN v5 support, drop cuDNN v3 support	11 months ago
cudnn_tanh_layer.cu	Add cuDNN v5 support, drop cuDNN v3 support	11 months ago
data_layer.cpp	Switched multi-GPU to NCCL	3 months ago
deconv_layer.cpp	enable dilated deconvolution	a year ago
deconv_layer.cu	dismantle layer headers	a year ago
dropout_layer.cpp	supporting N-D Blobs in Dropout layer Reshape	a year ago
dropout_layer.cu	dismantle layer headers	a year ago
dummy_data_layer.cpp	dismantle layer headers	a year ago
eltwise_layer.cpp	dismantle layer headers	a year ago
eltwise_layer.cu	dismantle layer headers	a year ago
elu_layer.cpp	ELU layer with basic tests	a year ago
elu_layer.cu	ELU layer with basic tests	a year ago
embed_layer.cpp	dismantle layer headers	a year ago
embed_layer.cu	dismantle layer headers	a year ago
euclidean_loss_layer.cpp	dismantle layer headers	a year ago
euclidean_loss_layer.cu	dismantle layer headers	a year ago
exp_layer.cpp	Solving issue with exp layer with base e	a year ago
exp_layer.cu	dismantle layer headers	a year ago

Caffe Sigmoid Layer

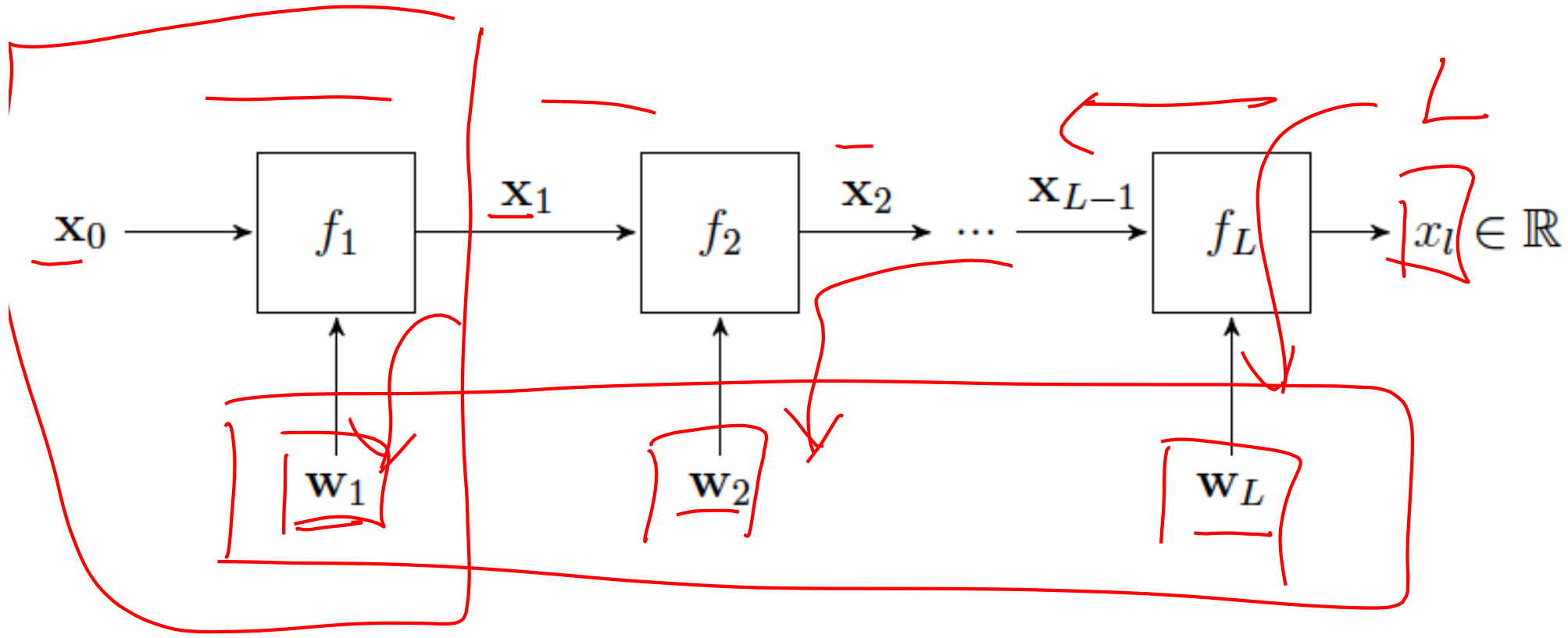
```
1 #include <cmath>
2 #include <vector>
3
4 #include "caffe/layers/sigmoid_layer.hpp"
5
6 namespace caffe {
7
8 template <typename Dtype>
9 inline Dtype sigmoid(Dtype x) {
10     return 1. / (1. + exp(-x));
11 }
12
13 template <typename Dtype>
14 void SigmoidLayer<Dtype>::Forward_cpu(const vector<Blob<Dtype>*>& bottom,
15     const vector<Blob<Dtype>*>& top) {
16     const Dtype* bottom_data = bottom[0]->cpu_data();
17     Dtype* top_data = top[0]->mutable_cpu_data();
18     const int count = bottom[0]->count();
19     for (int i = 0; i < count; ++i) {
20         top_data[i] = sigmoid(bottom_data[i]);
21     }
22 }
23
24 template <typename Dtype>
25 void SigmoidLayer<Dtype>::Backward_cpu(const vector<Blob<Dtype>*>& top,
26     const vector<bool>& propagate_down,
27     const vector<Blob<Dtype>*>& bottom) {
28     if (propagate_down[0]) {
29         const Dtype* top_data = top[0]->cpu_data();
30         const Dtype* top_diff = top[0]->cpu_diff();
31         Dtype* bottom_diff = bottom[0]->mutable_cpu_diff();
32         const int count = bottom[0]->count();
33         for (int i = 0; i < count; ++i) {
34             const Dtype sigmoid_x = top_data[i];
35             bottom_diff[i] = top_diff[i] * sigmoid_x * (1. - sigmoid_x);
36         }
37     }
38 }
39
40 #ifdef CPU_ONLY
41 STUB_GPU(SigmoidLayer);
42 #endif
43
44 INSTANTIATE_CLASS(SigmoidLayer);
45
46 } // namespace caffe
```

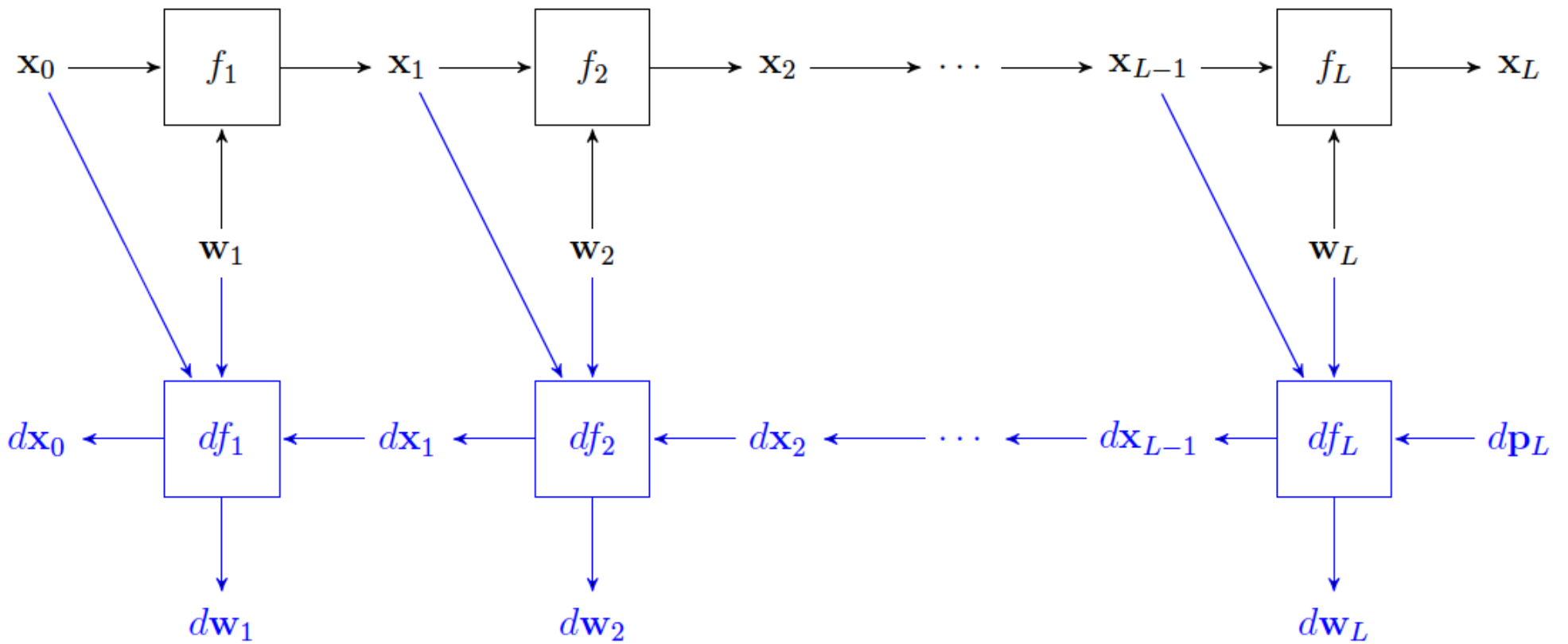
$$\sigma(x) = \frac{1}{1 + e^{-x}}$$

$$(1 - \sigma(x)) \sigma(x) * \text{top_diff} \text{ (chain rule)}$$

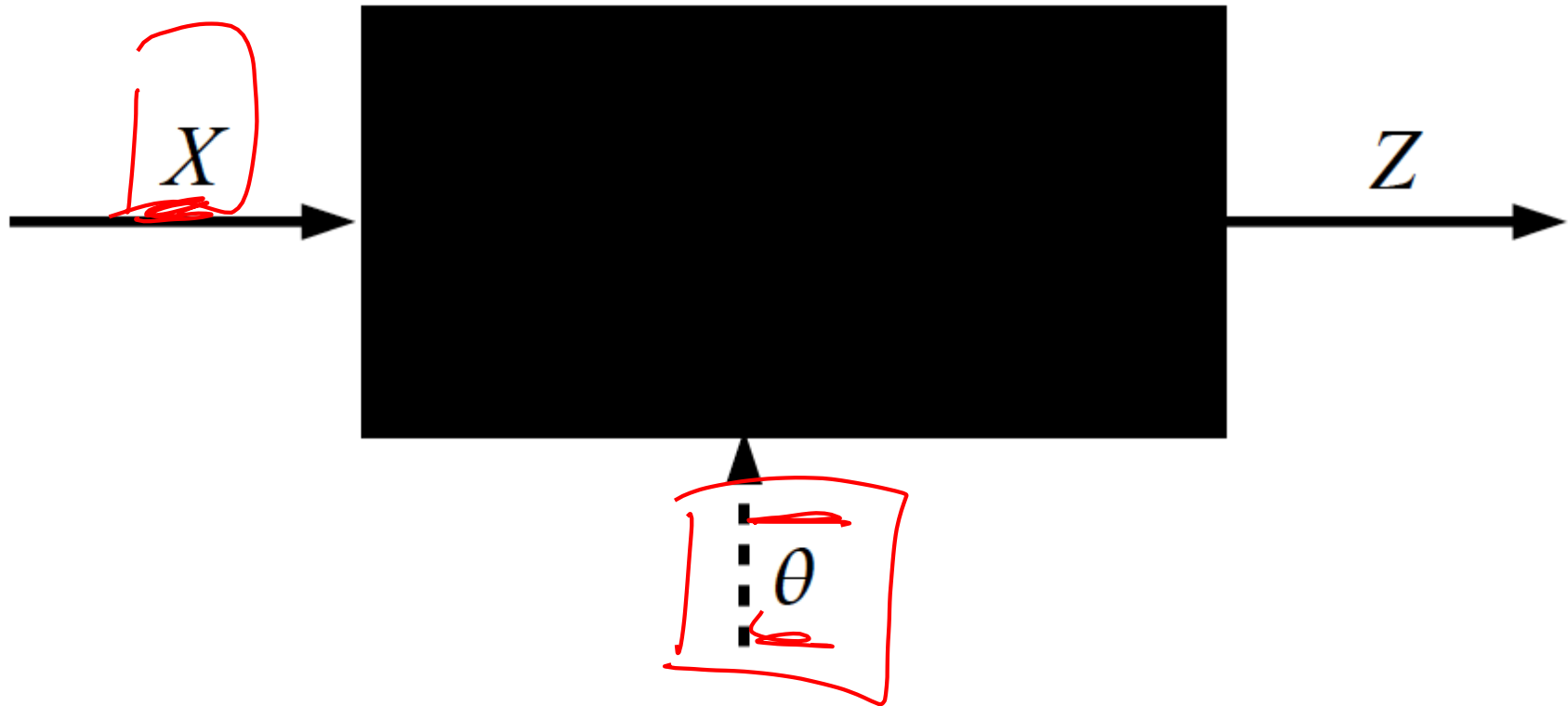
[Caffe](#) is licensed under [BSD 2-Clause](#)

$$\frac{\partial L}{\partial w_l}$$



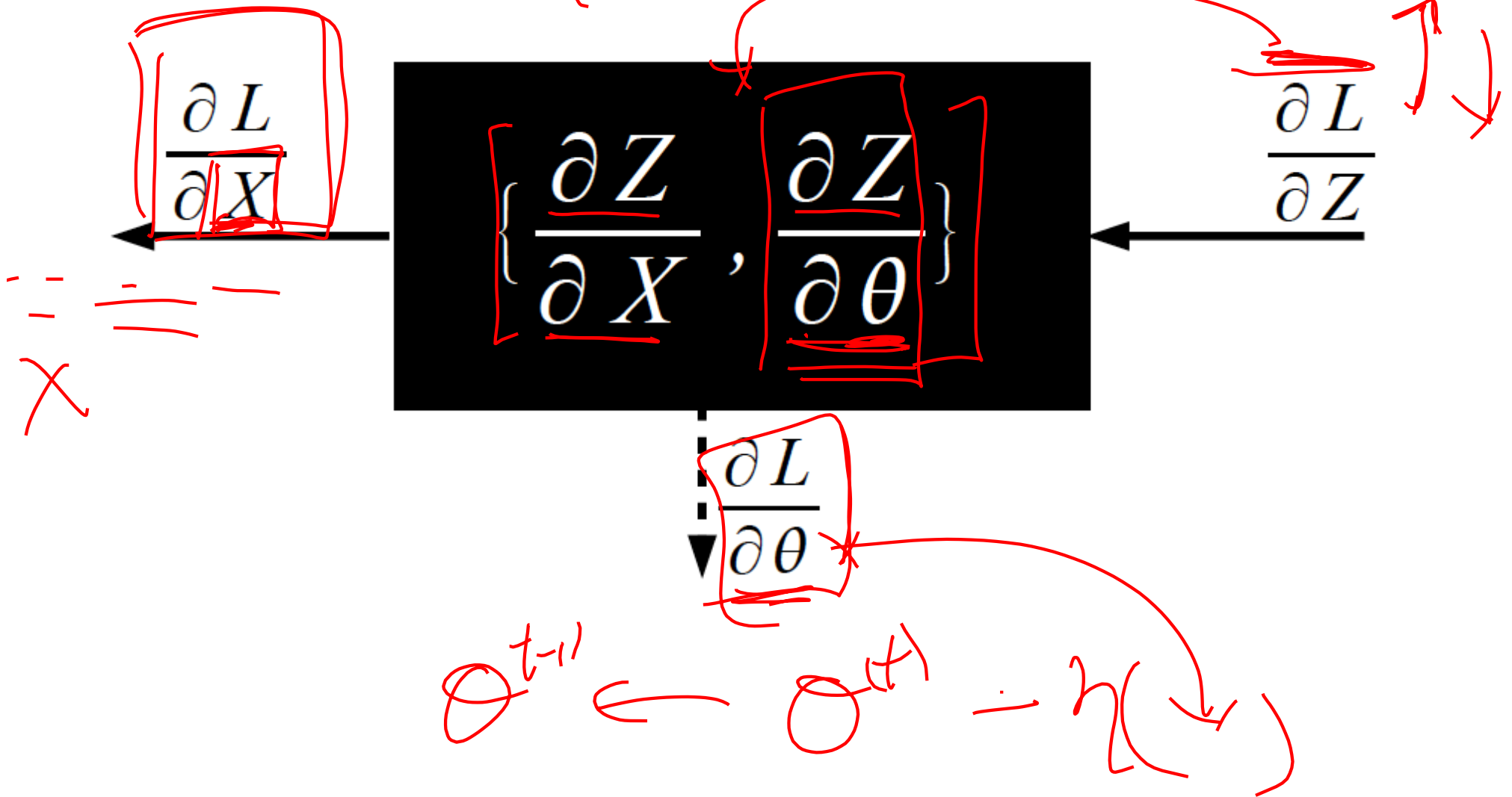


Key Computation in DL: Forward-Prop

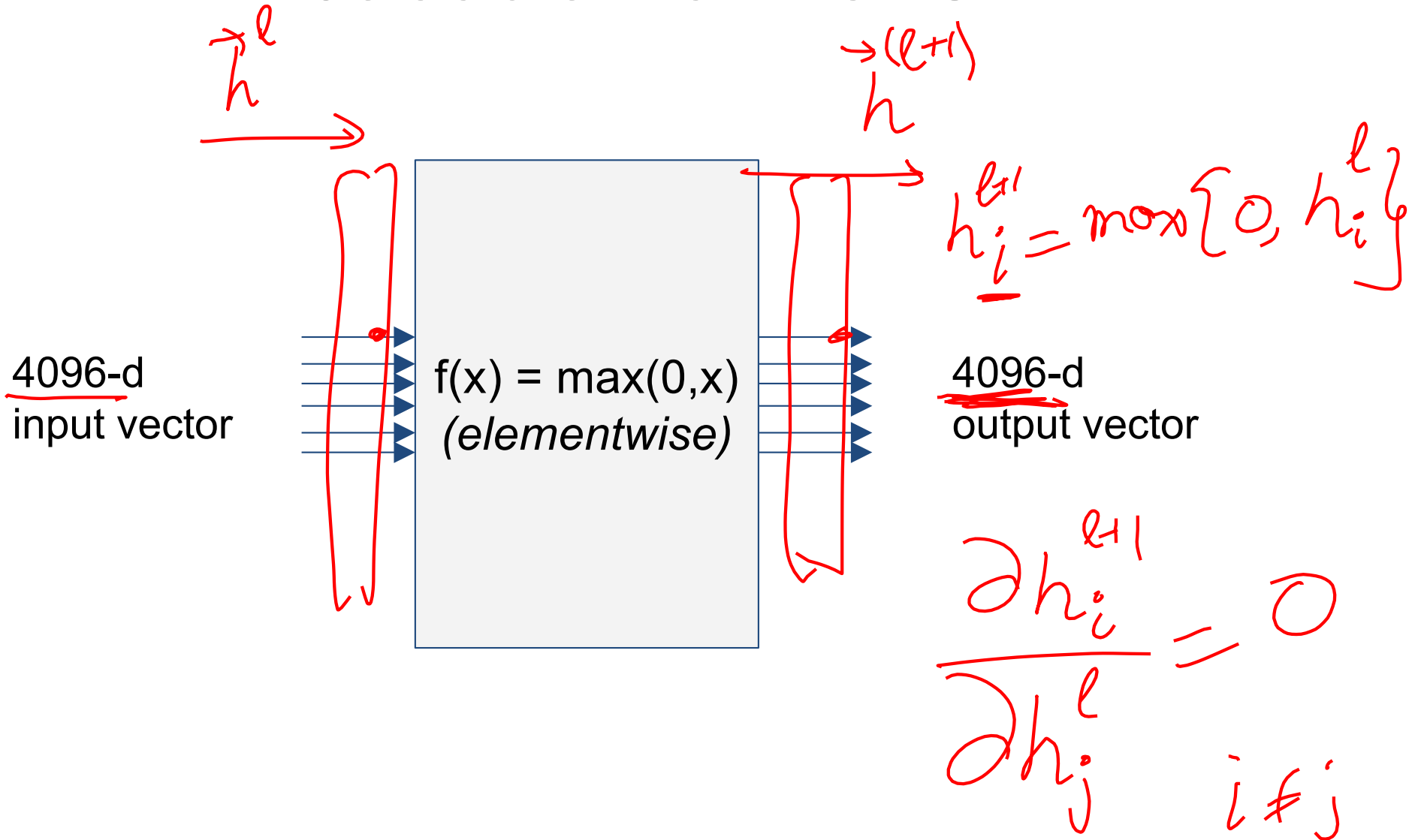


Key Computation in DL: Back-Prop

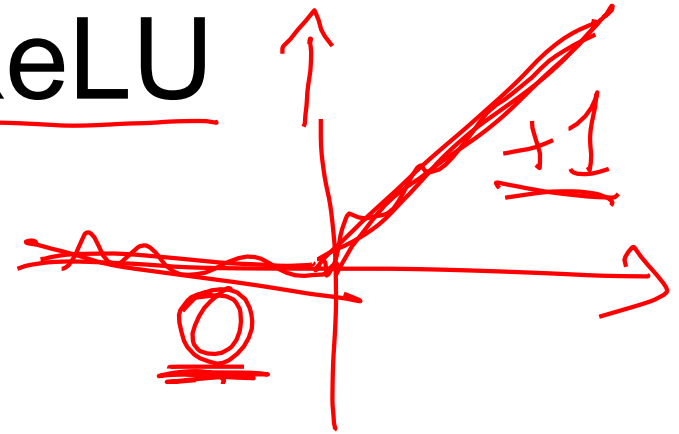
$$X^{(t+1)} \leftarrow X^{(t)} - \eta$$



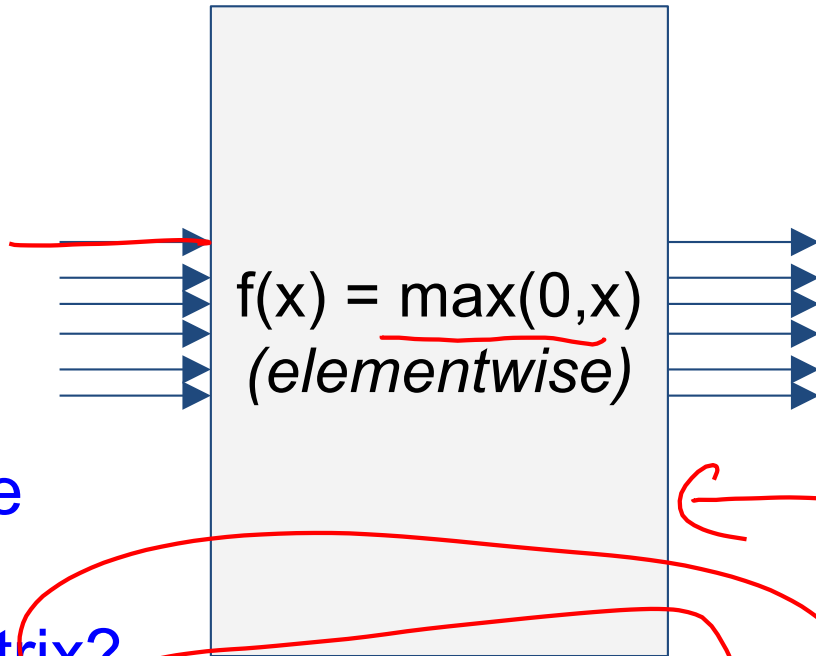
Jacobian of ReLU



Jacobian of ReLU

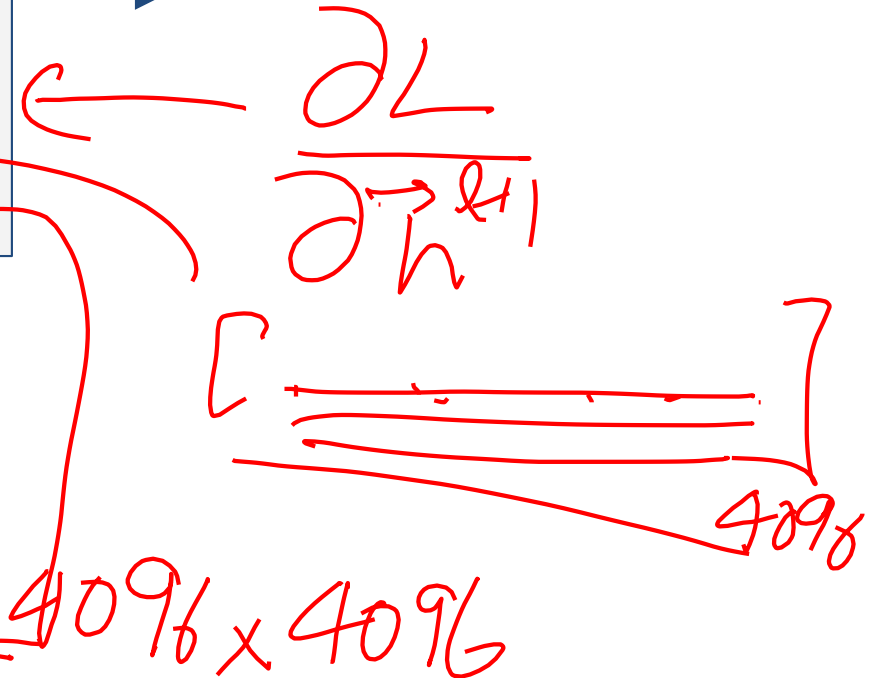


4096-d
input vector

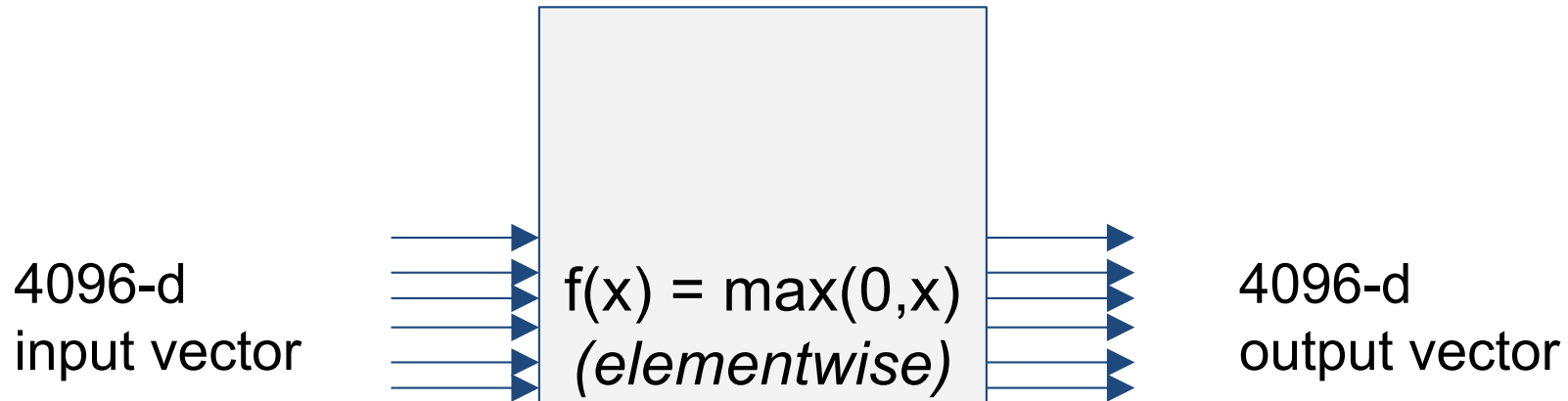


4096-d
output vector

Q: what is the
size of the
Jacobian matrix?

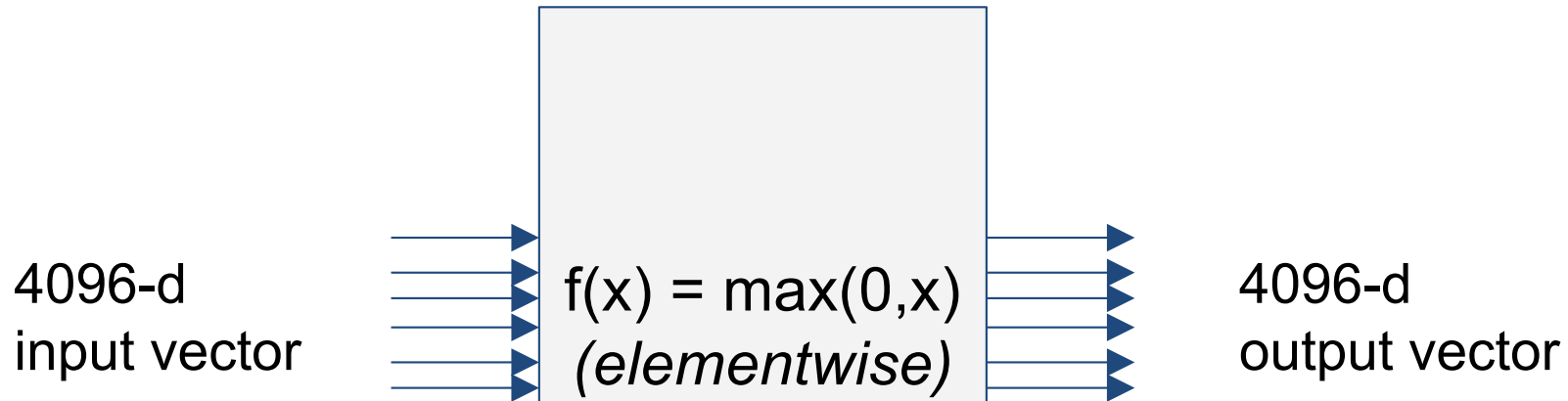


Jacobian of ReLU



Q: what is the size of the Jacobian matrix?
[4096 x 4096!]

Jacobian of ReLU



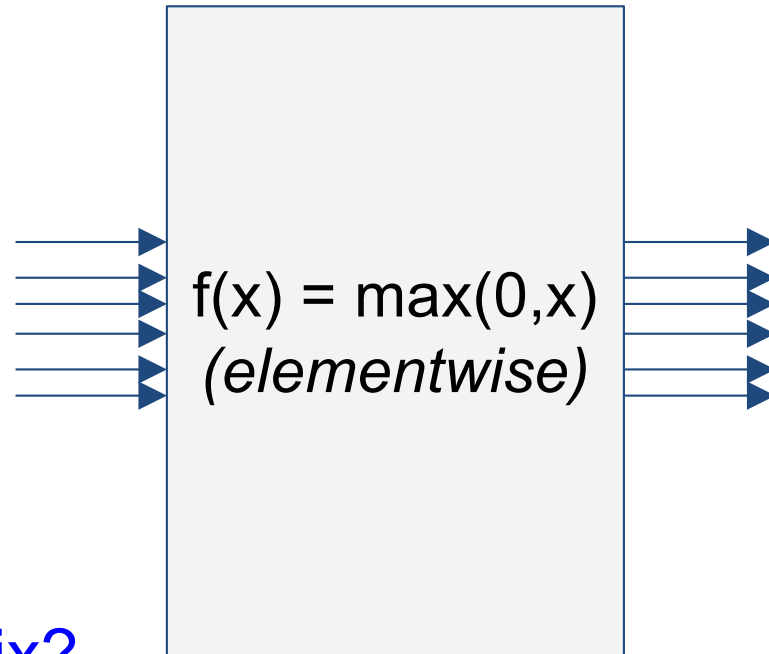
Q: what is the
size of the
Jacobian matrix?
[4096 x 4096!]

in practice we process an
entire minibatch (e.g. 100)
of examples at one time:

i.e. Jacobian would technically be a
[409,600 x 409,600] matrix :\
(Note: the original image contains a typo '\')

Jacobian of ReLU

4096-d
input vector

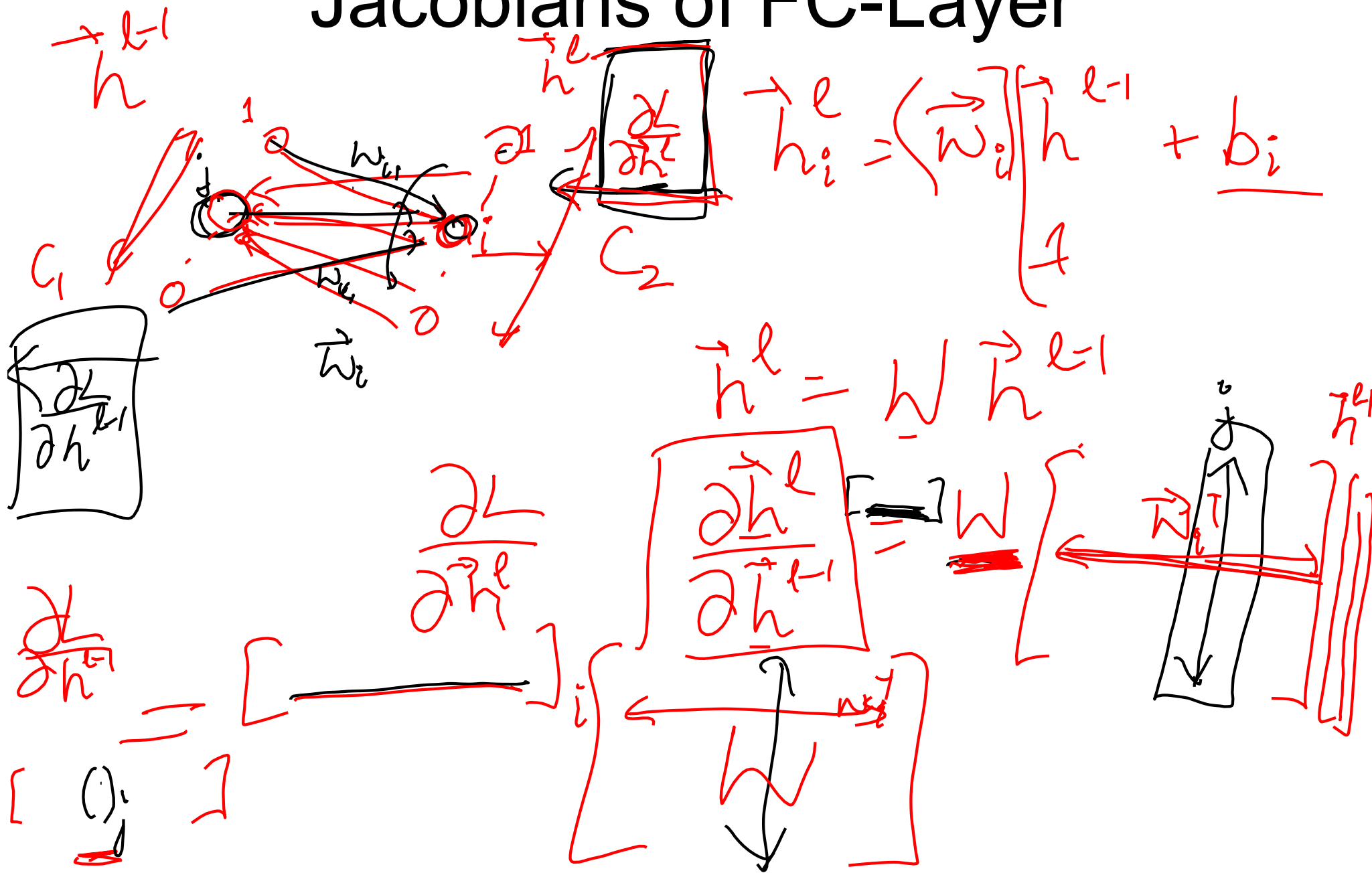


4096-d
output vector

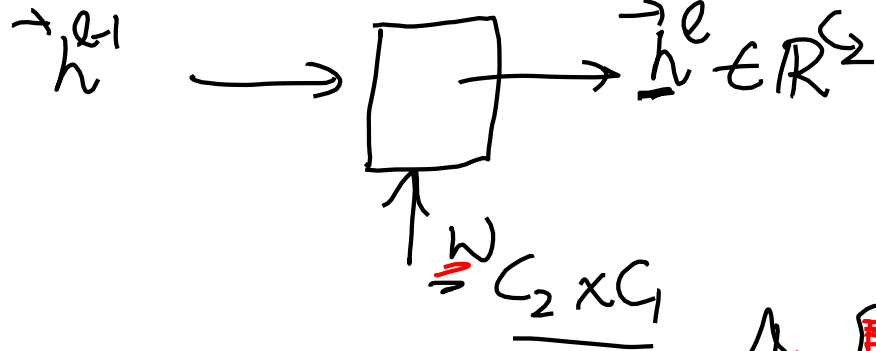
Q: what is the
size of the
Jacobian matrix?
[4096 x 4096!]

Q2: what does it
look like?

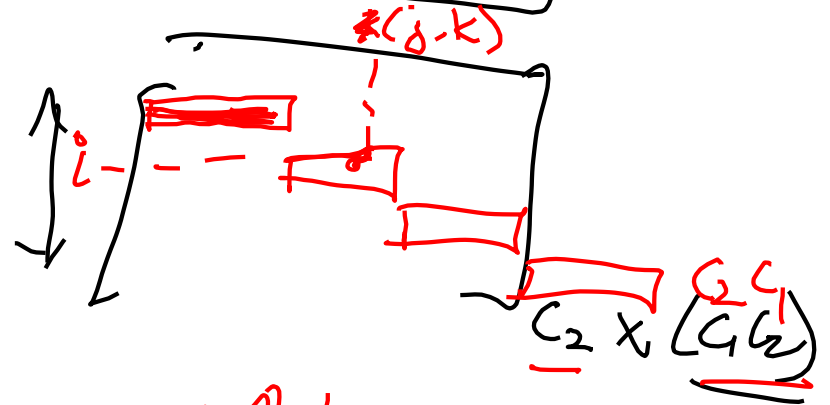
Jacobians of FC-Layer



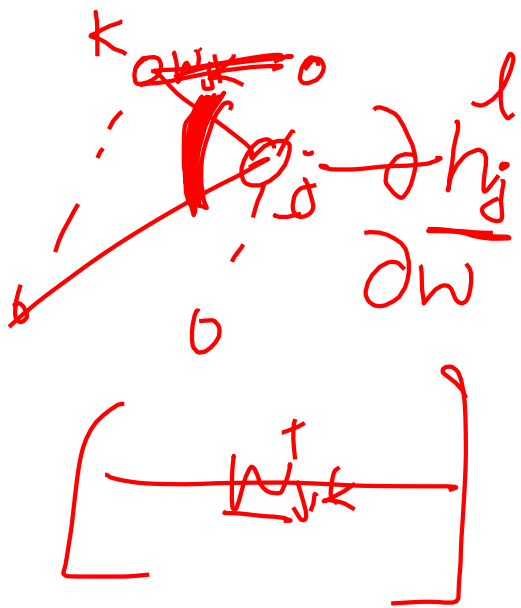
Jacobians of FC-Layer



$$\frac{\partial \vec{h}^l}{\partial W}$$



$$\frac{\partial h_i^l}{\partial w_{j,k}}$$



$$h_j^l = \vec{w}_j^T \vec{h}^{l-1}$$

$$\frac{\partial h_j^l}{\partial \vec{w}_j} = (\vec{h}^{l-1})^T$$

Jacobians of FC-Layer



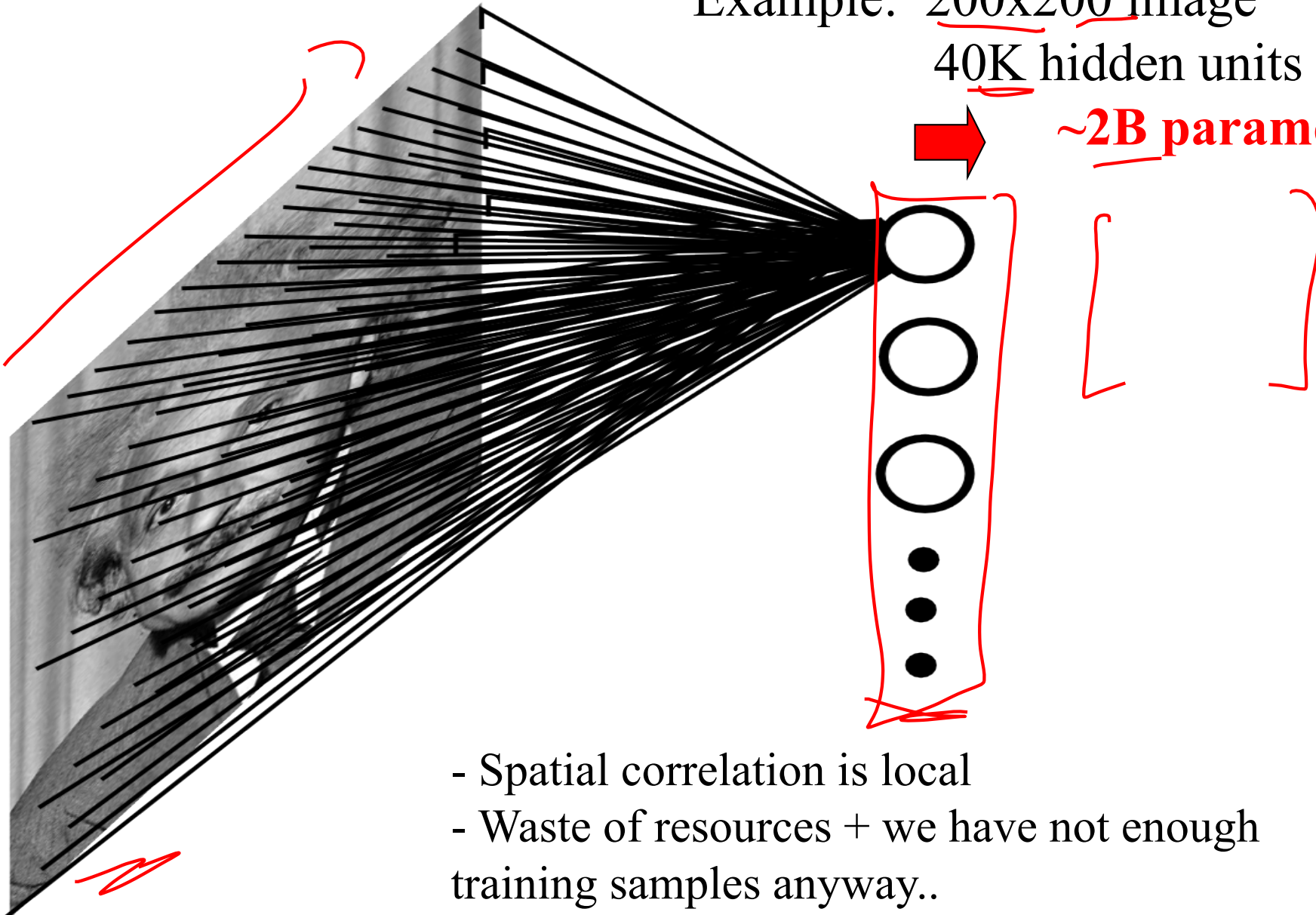
Convolutional Neural Networks

(without the brain stuff)

Fully Connected Layer 4×10^4

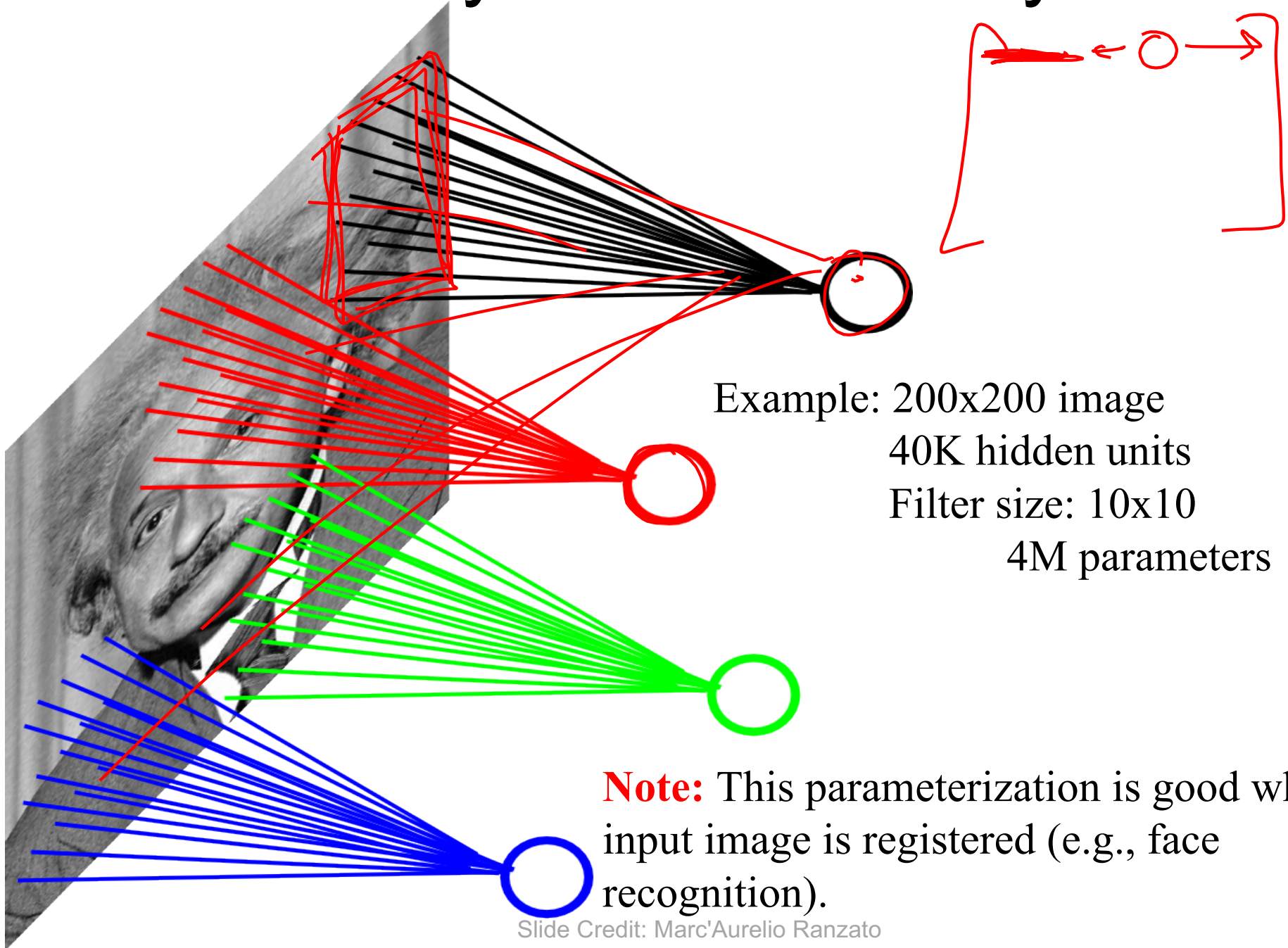
Example: 200x200 image
40K hidden units

~2B parameters!!!

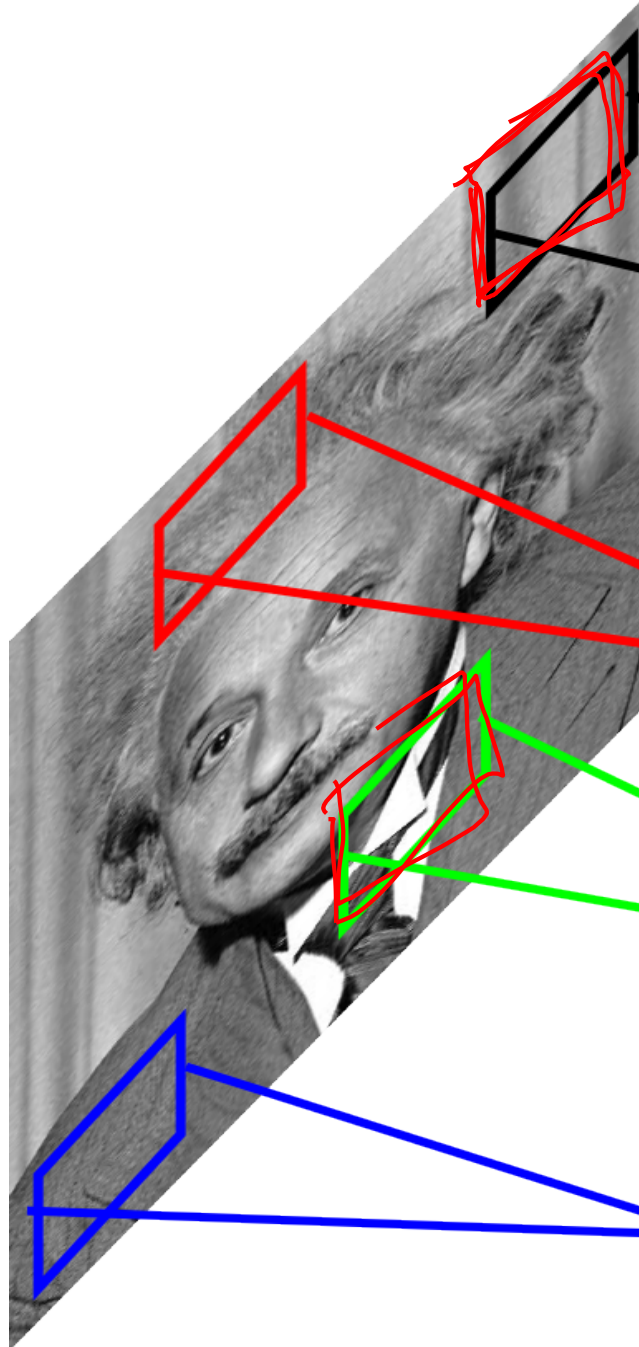


- Spatial correlation is local
- Waste of resources + we have not enough training samples anyway..

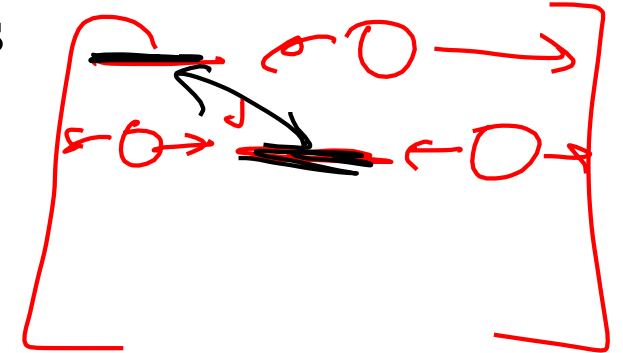
Locally Connected Layer



Locally Connected Layer



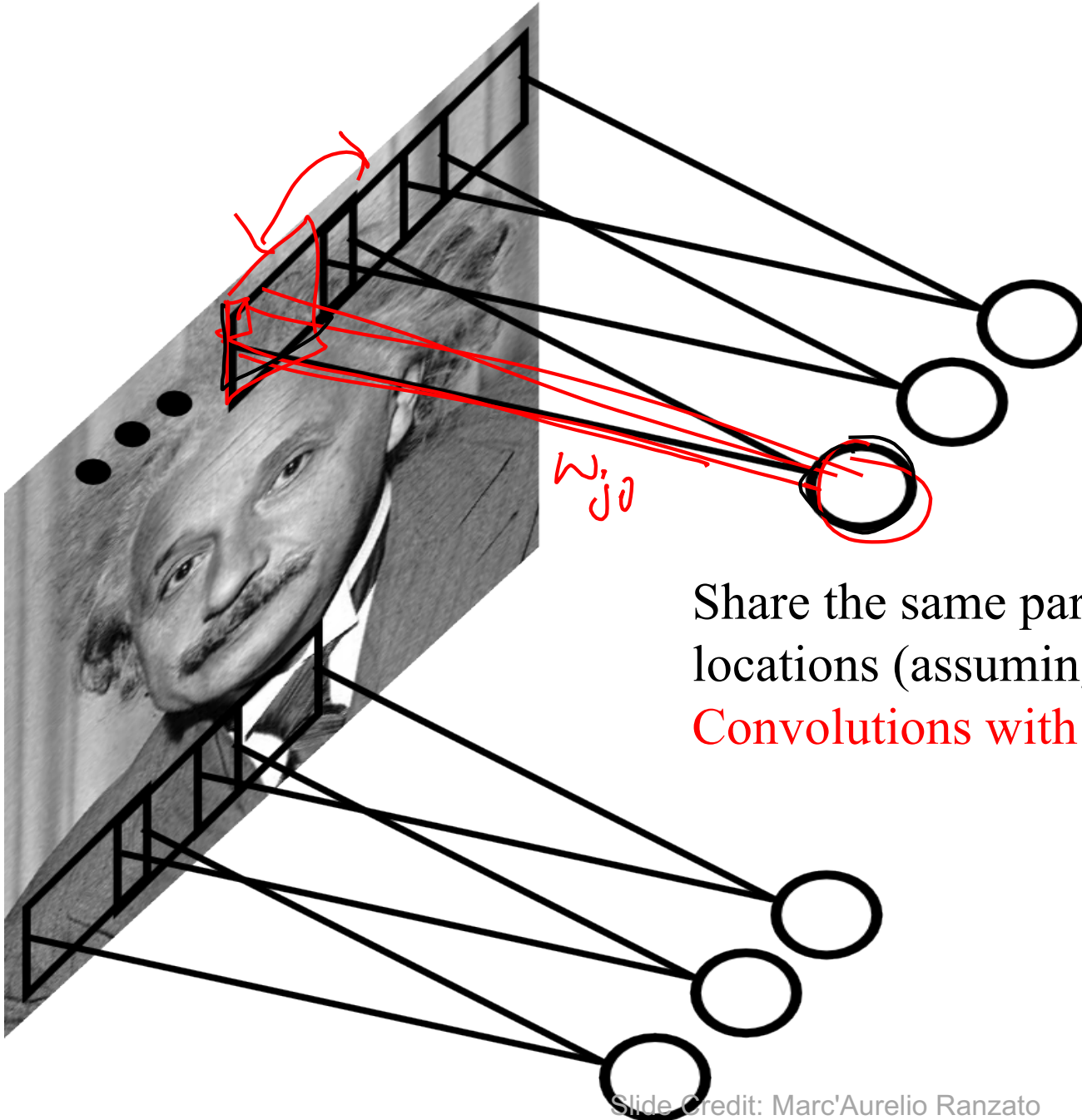
STATIONARITY? Statistics is similar at different locations



Example: 200x200 image
40K hidden units
Filter size: 10x10
4M parameters

Note: This parameterization is good when input image is registered (e.g., face recognition).

Convolutional Layer



Share the same parameters across different locations (assuming input is stationary):

Convolutions with learned kernels

Convolutions for mathematicians

$$x(t) \quad y(t) \quad w(t)$$

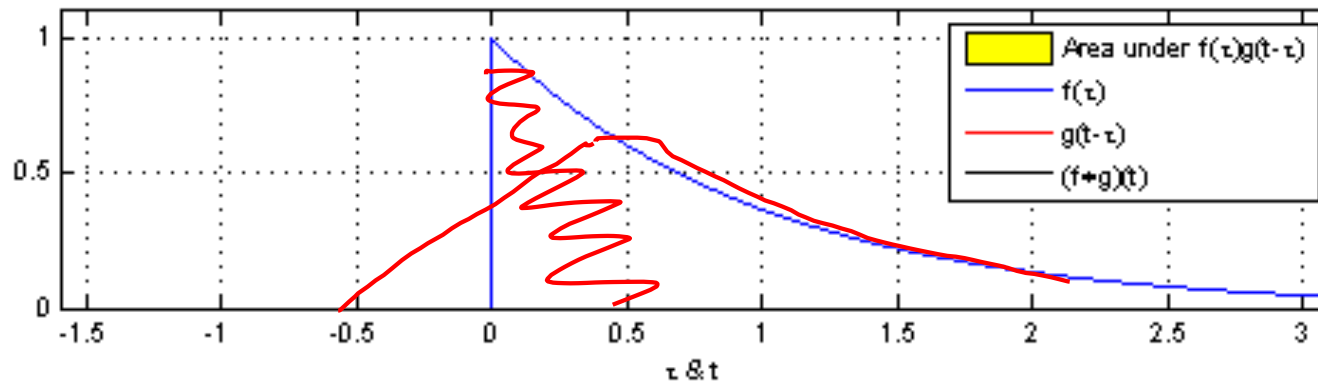
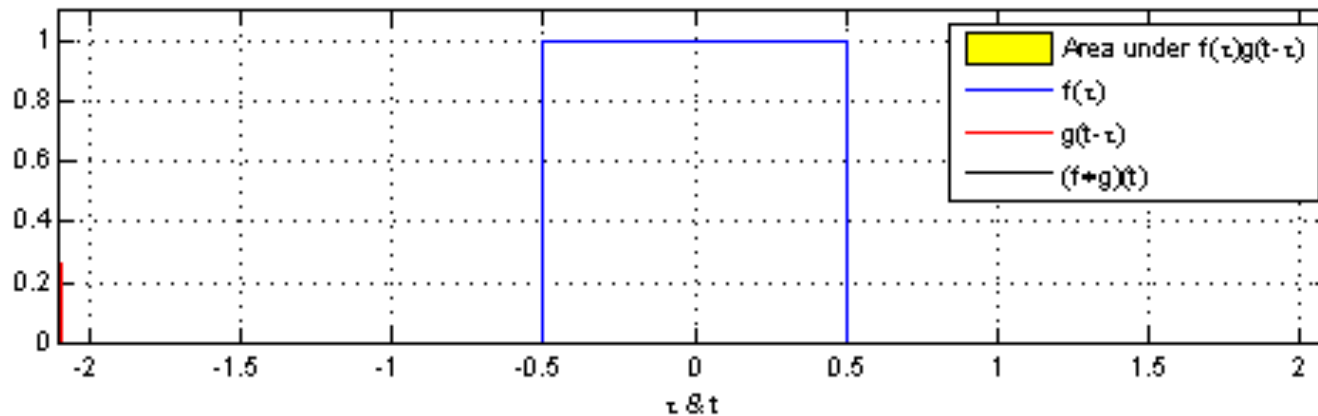
$$y(t) = (x * w)(t) = \int_{a=-\infty}^{\infty} \underbrace{x(t-a)} \underbrace{w(a)} da$$

$$= \int \underbrace{x(a)} \underbrace{w(t-a)} da$$

$$w(a) \rightarrow f(w(-a))$$

$$w(-a) \rightarrow w(t-a-t)$$

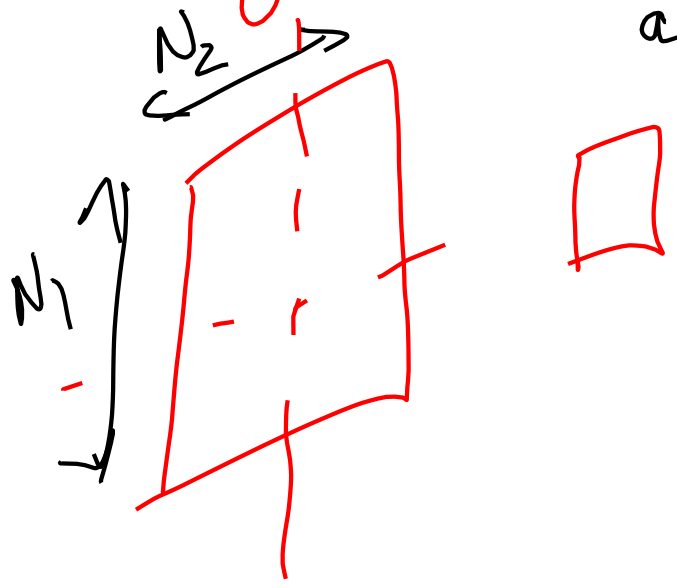
$$y(t_1, t_2) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} x(a-t_1, b-t_2) w(a, b) da db$$



"Convolution of box signal with itself2" by Convolution_of_box_signal_with_itself.gif: Brian Amberg derivative work: Tinos (talk) - Convolution_of_box_signal_with_itself.gif. Licensed under CC BY-SA 3.0 via Commons - https://commons.wikimedia.org/wiki/File:Convolution_of_box_signal_with_itself2.gif#/media/File:Convolution_of_box_signal_with_itself2.gif

Convolutions for computer scientists

$$y[x, c] = \sum_{a = -\frac{N-1}{2}}^{\frac{N-1}{2}} \sum_{b = -\frac{N-1}{2}}^{+\frac{N-1}{2}} x[\underline{x-a}, \underline{c-b}] w[a, b]$$



Convolutions for programmers

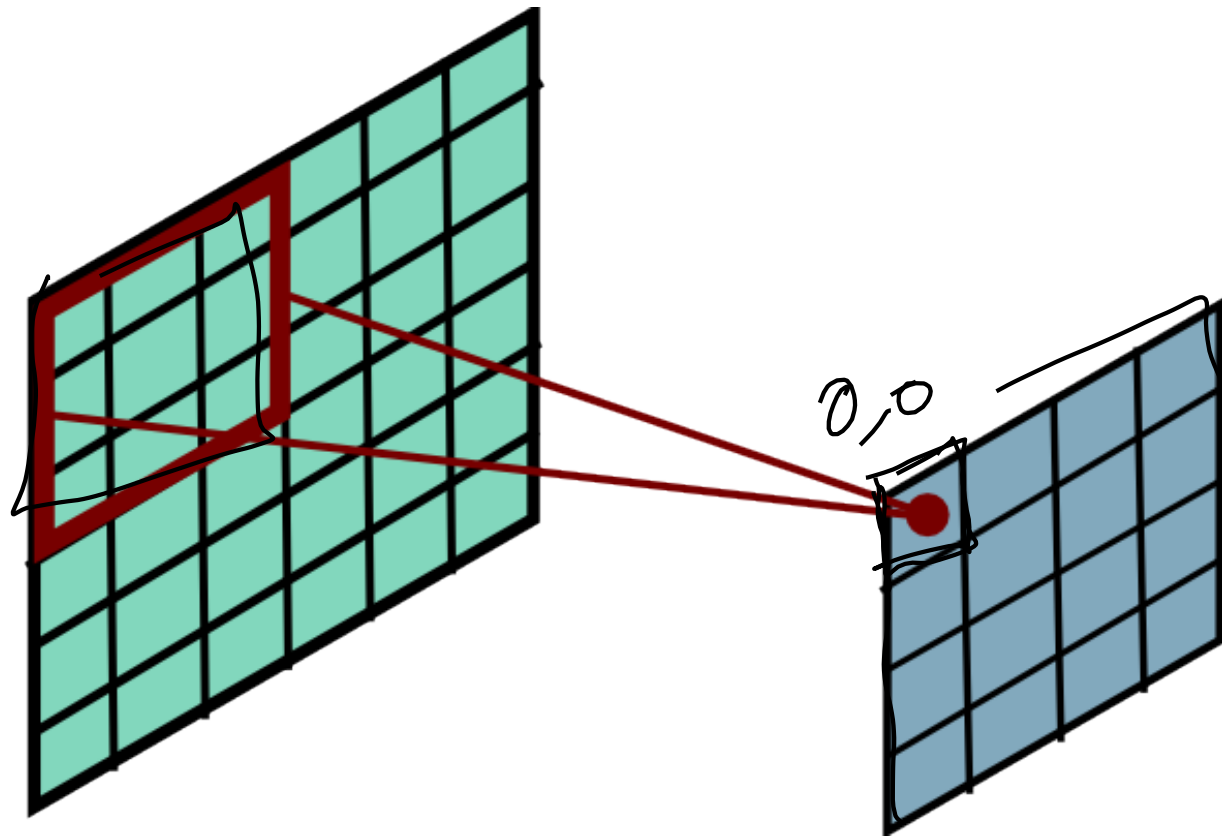
$$y[r, c] = \sum_{a=0}^{N_1-1} \sum_{b=0}^{N_2-1} x[r+a, c+b] w[a, b]$$

The image shows a handwritten convolution equation with several annotations. A bracket above the equation groups the two summation indices, N_1-1 and N_2-1 . Below the first summation, the expression $a=0$ is written. Below the second summation, the expression $b=0$ is written. A bracket under these two expressions indicates the starting point of the summations. In the term $x[r+a, c+b]$, there is a small 'g' above the 'c' and a horizontal line under the 'r'. In the term $w[a, b]$, there is a horizontal line under the 'a' and a horizontal line under the 'b'. A curved arrow points from the $c+b$ term in the x function to the a, b terms in the w function.

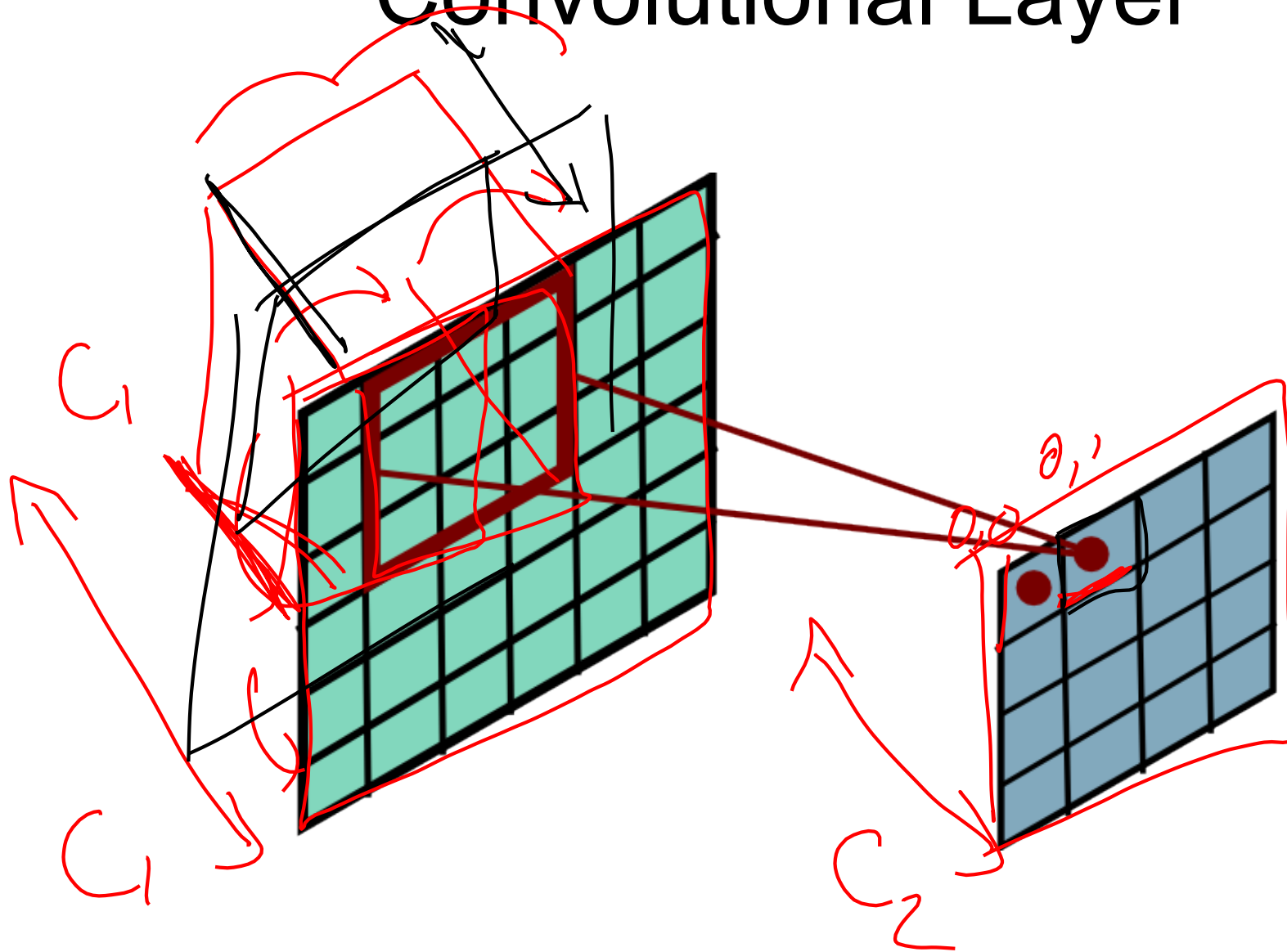
Convolution Explained

- <http://setosa.io/ev/image-kernels/>
- <https://github.com/bruckner/deepViz>

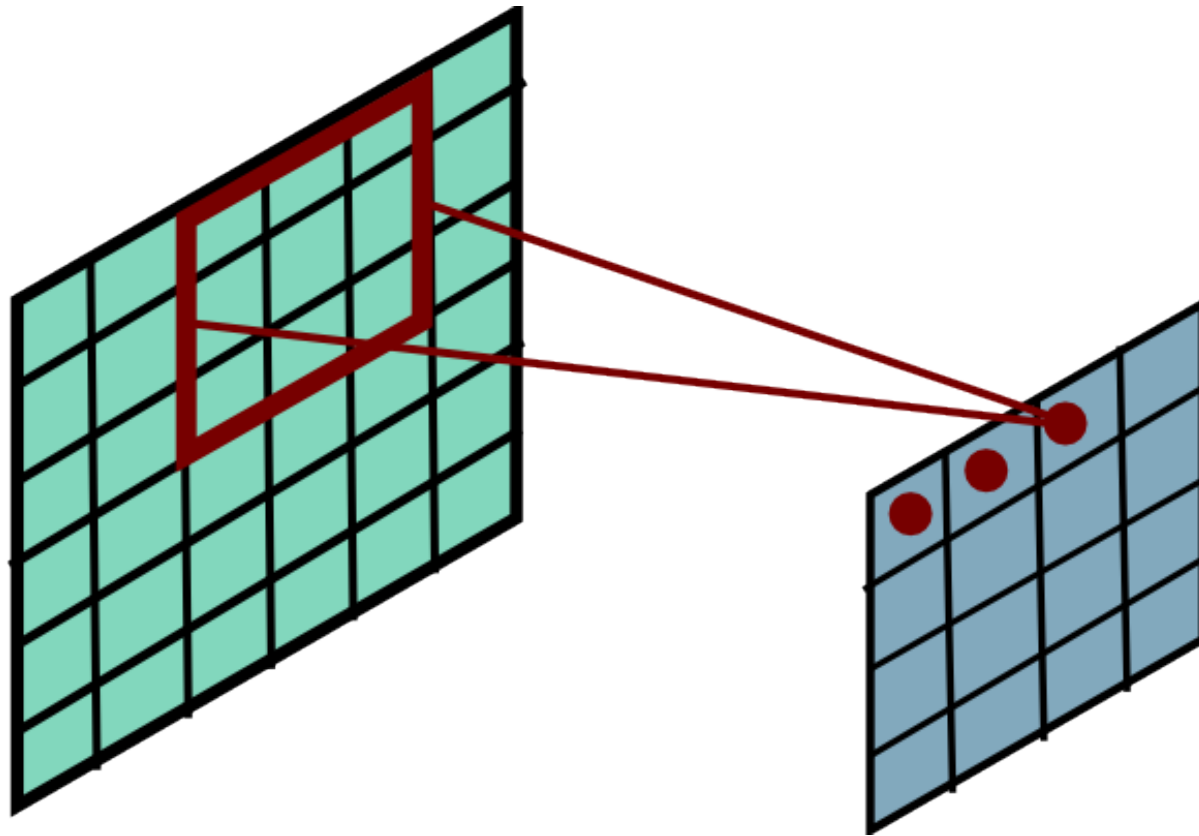
Convolutional Layer



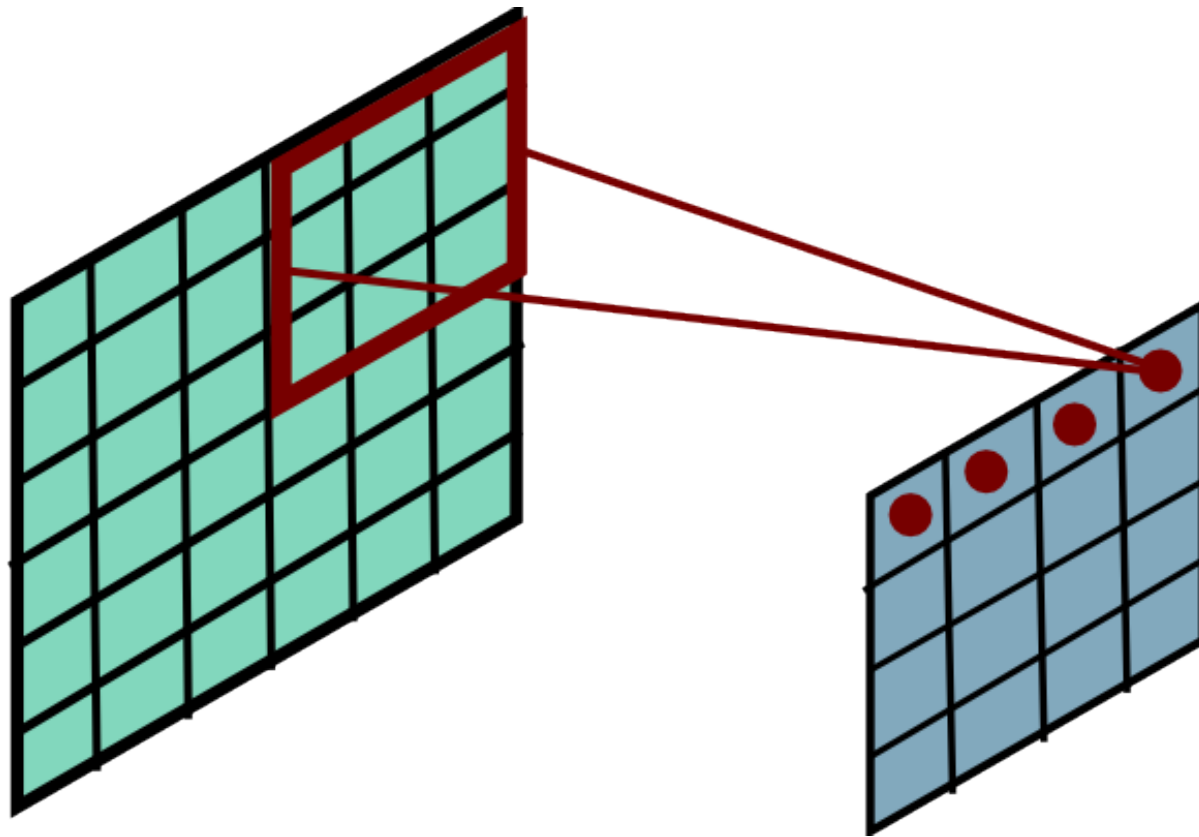
Convolutional Layer



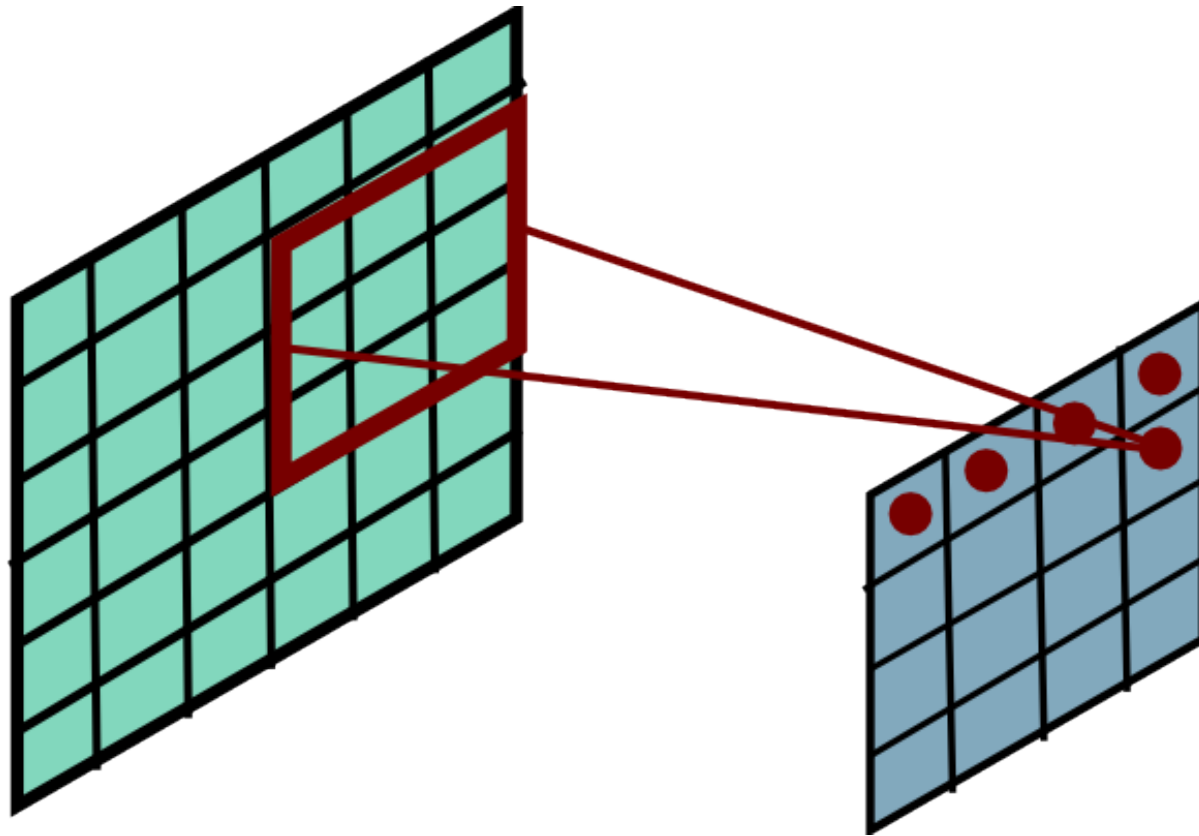
Convolutional Layer



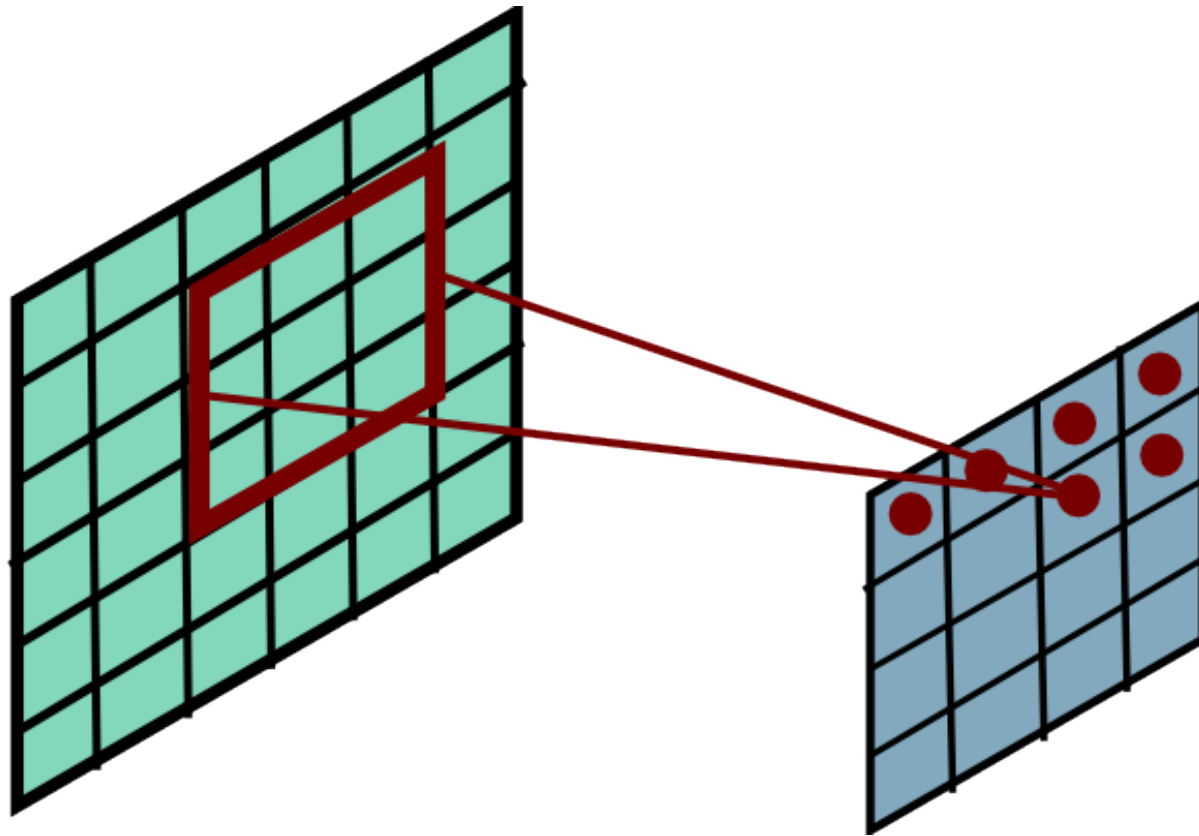
Convolutional Layer



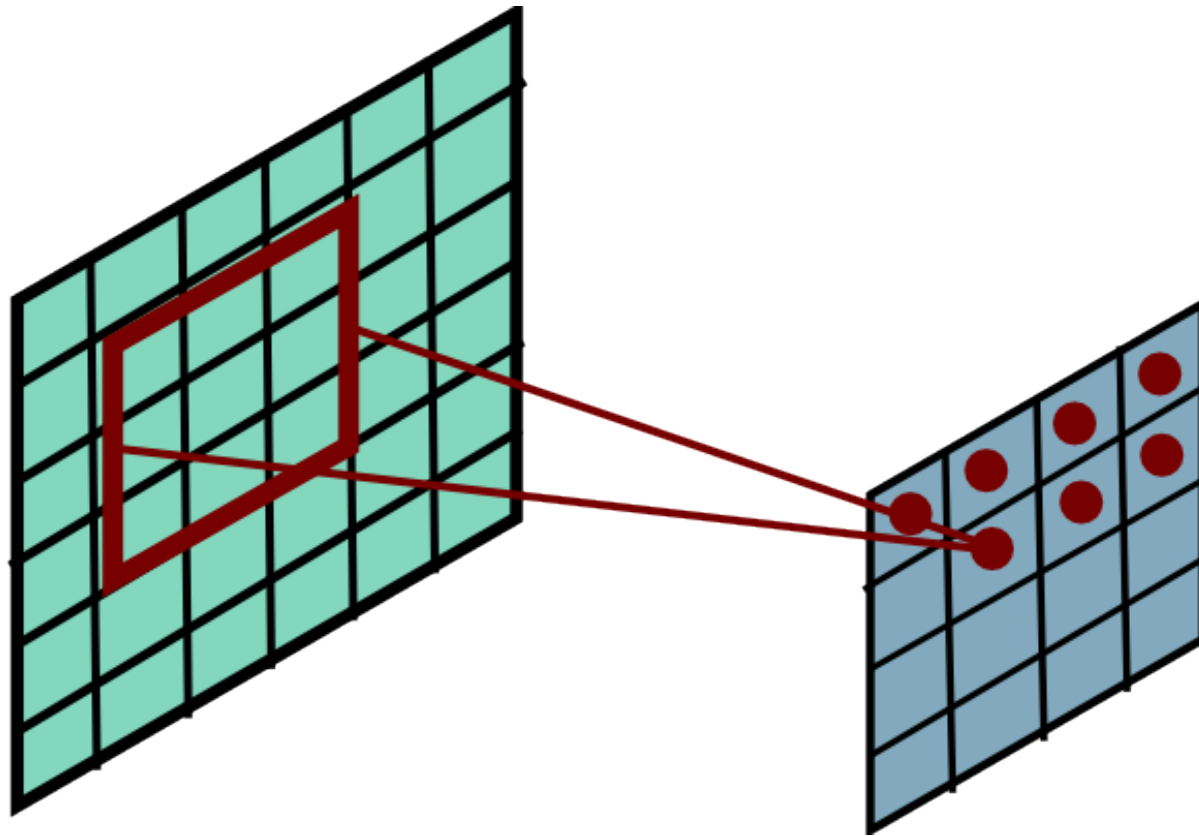
Convolutional Layer



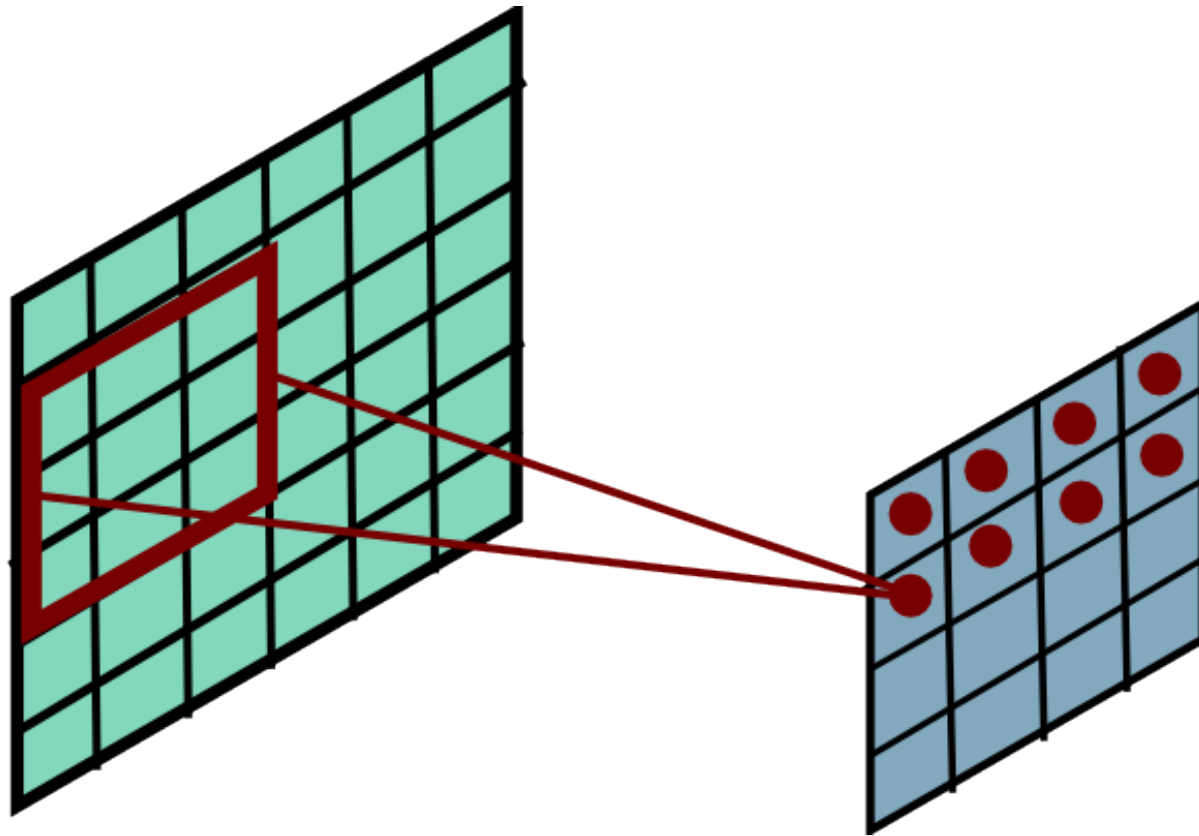
Convolutional Layer



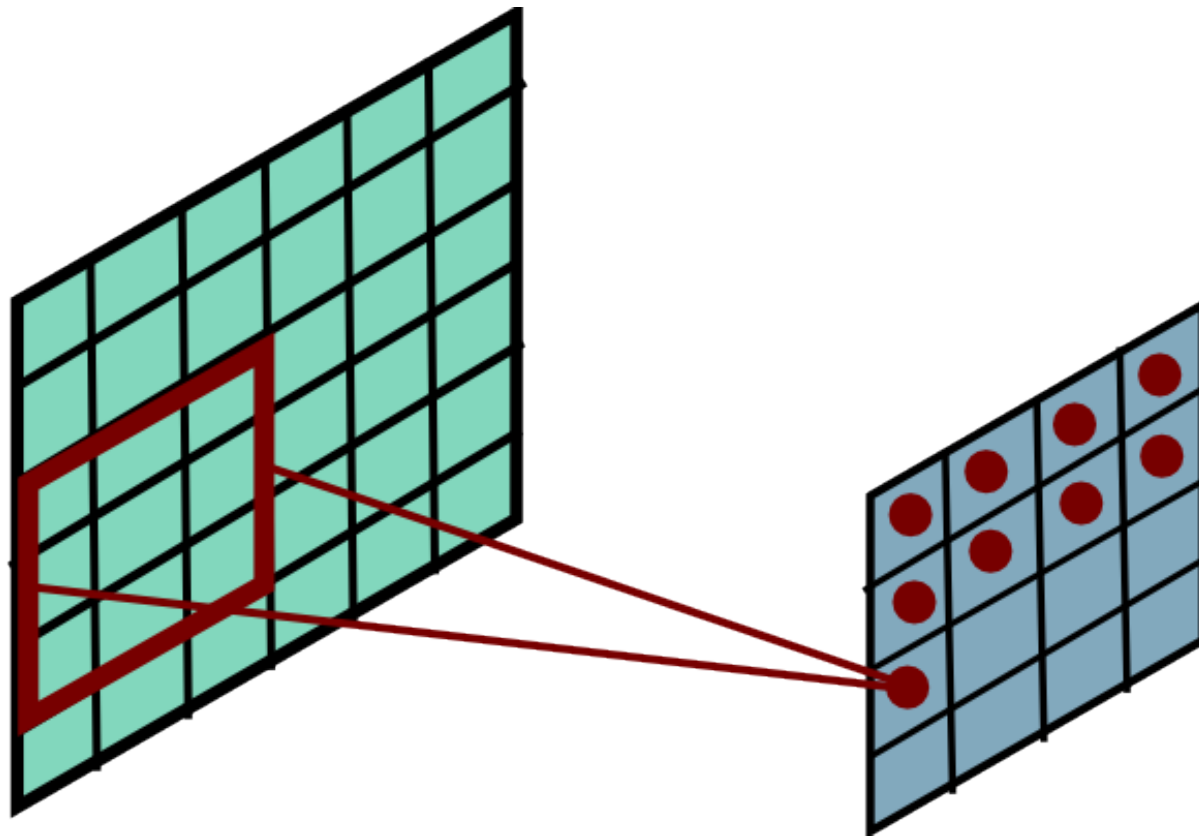
Convolutional Layer



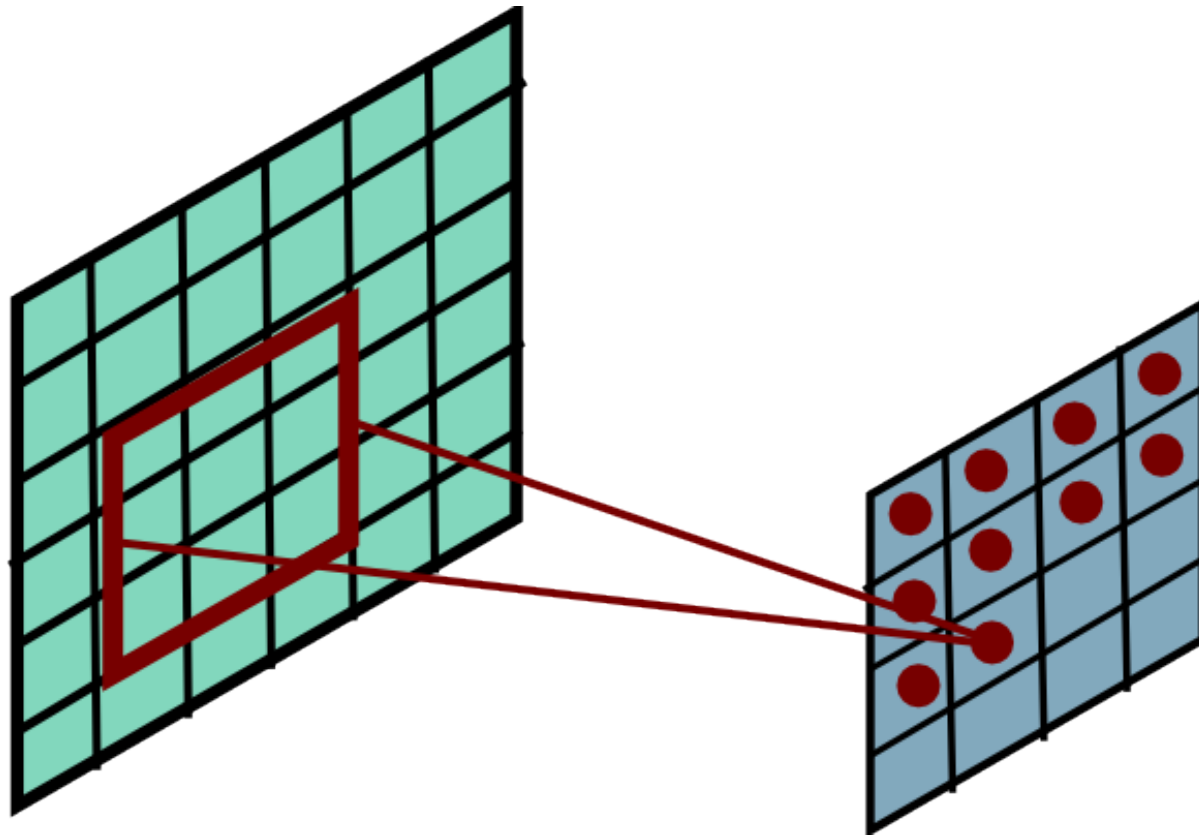
Convolutional Layer



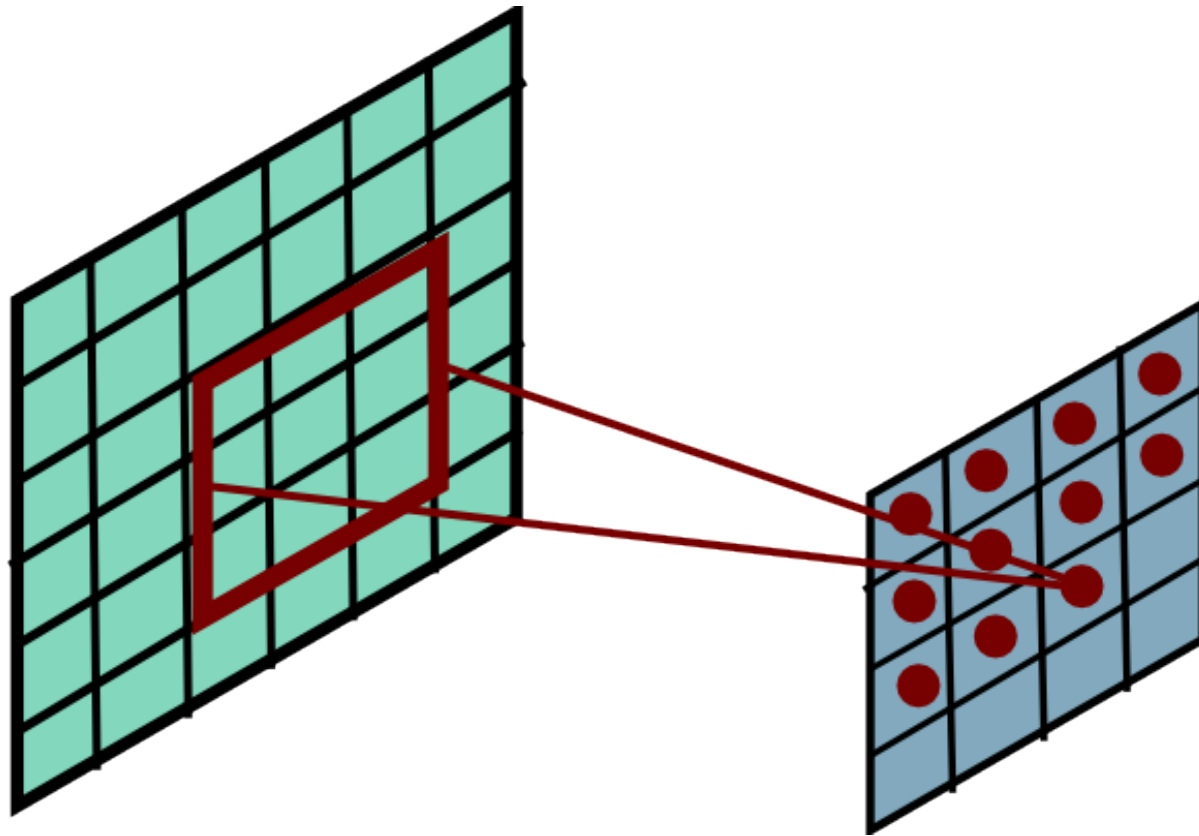
Convolutional Layer



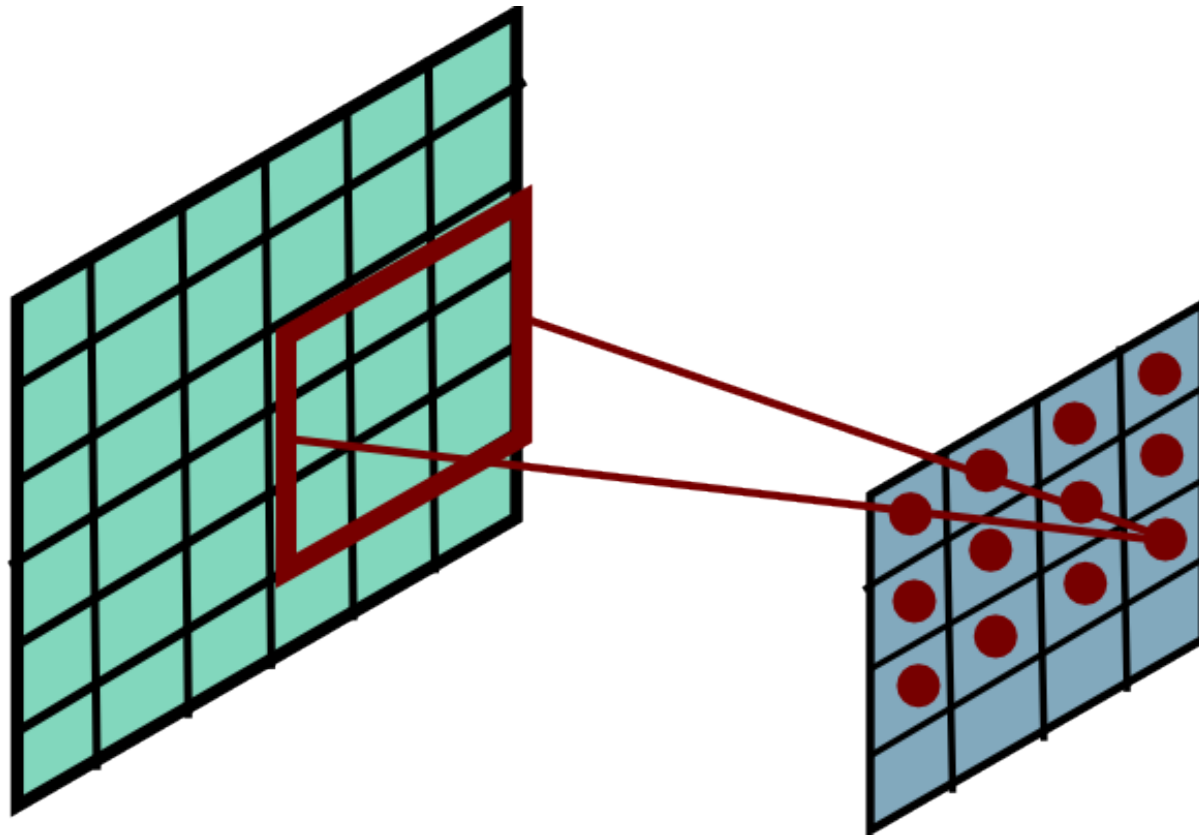
Convolutional Layer



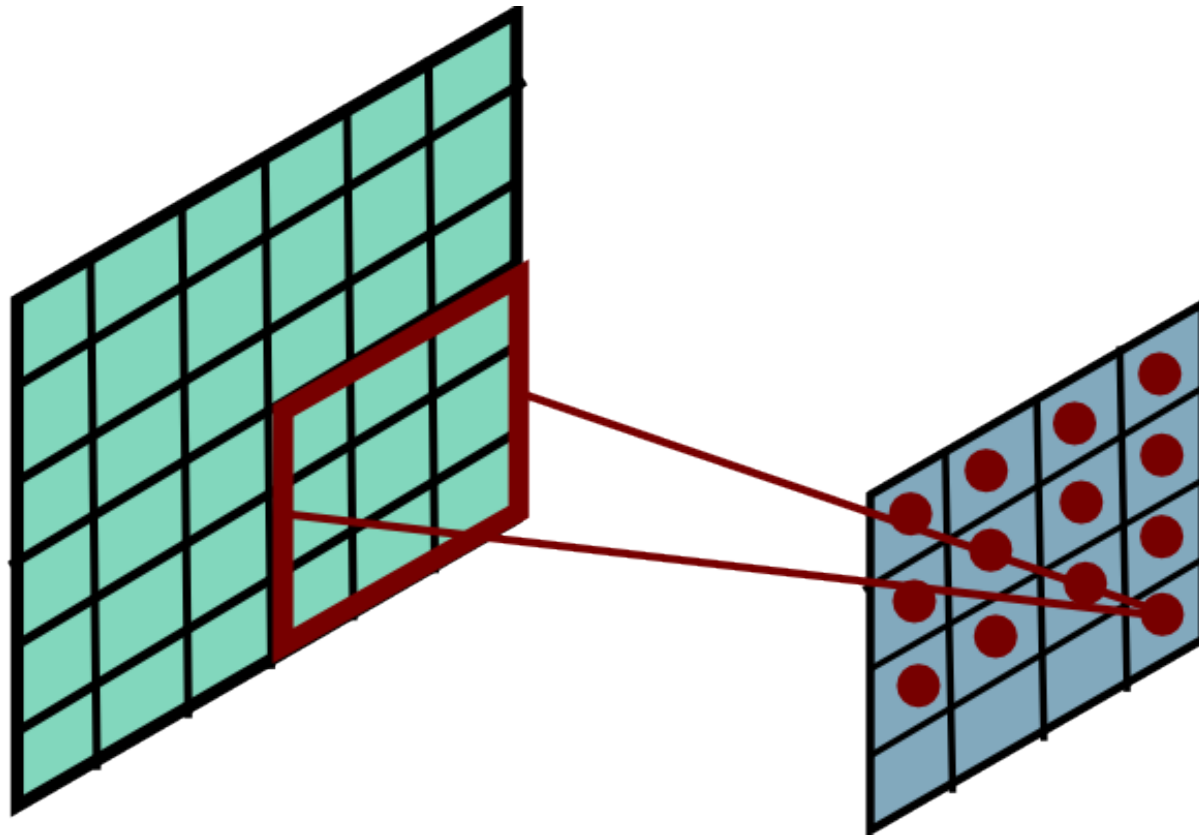
Convolutional Layer



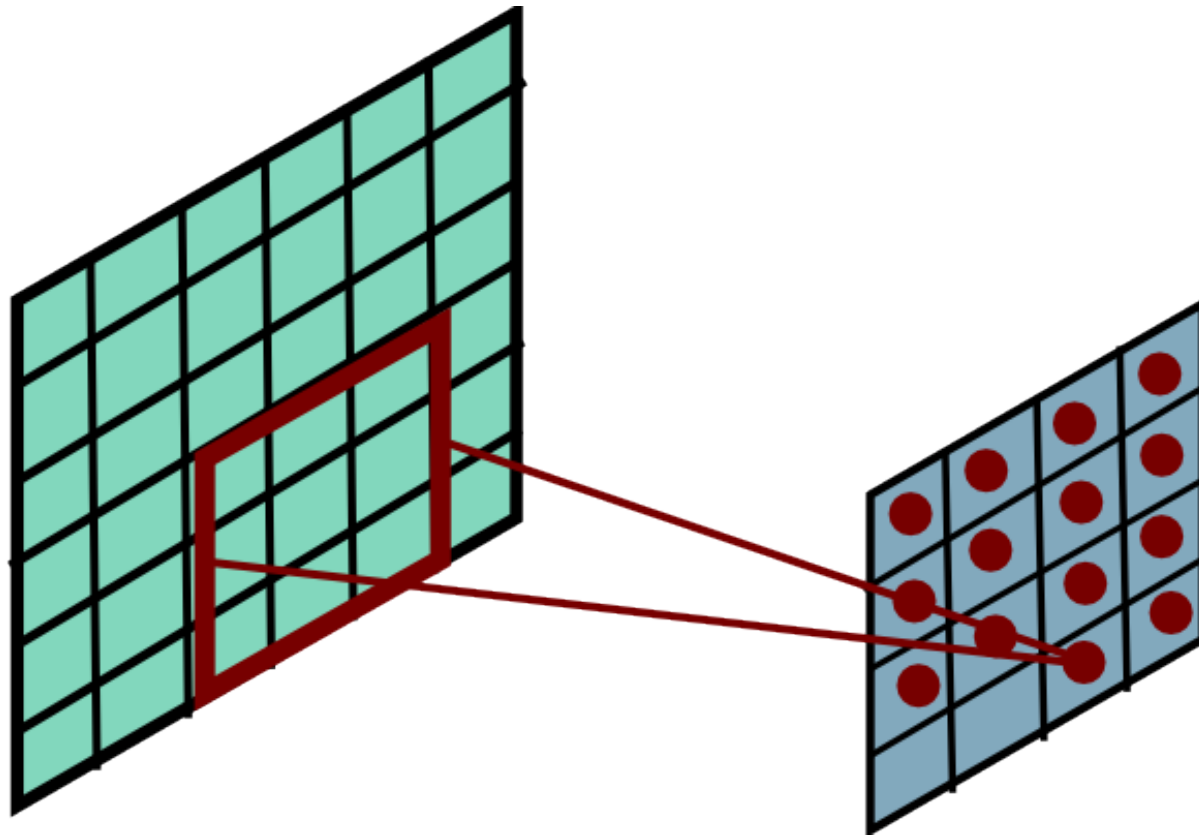
Convolutional Layer



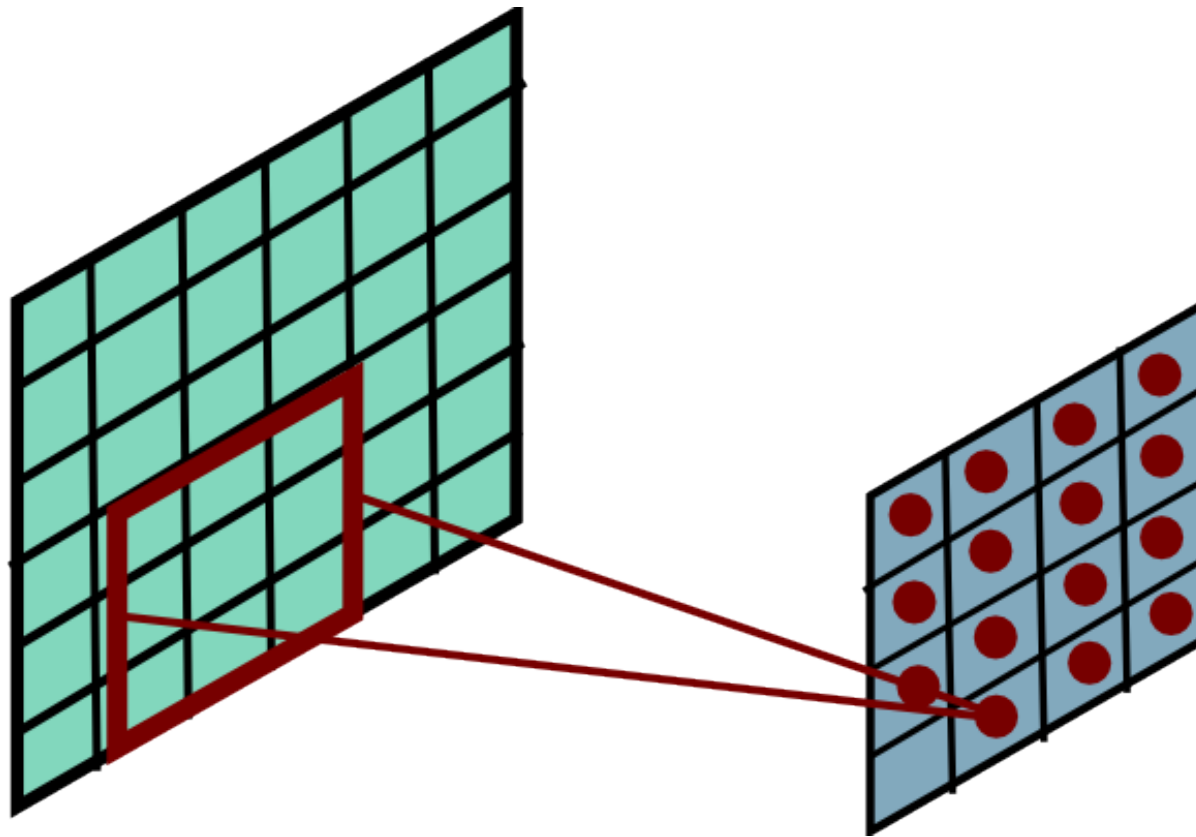
Convolutional Layer



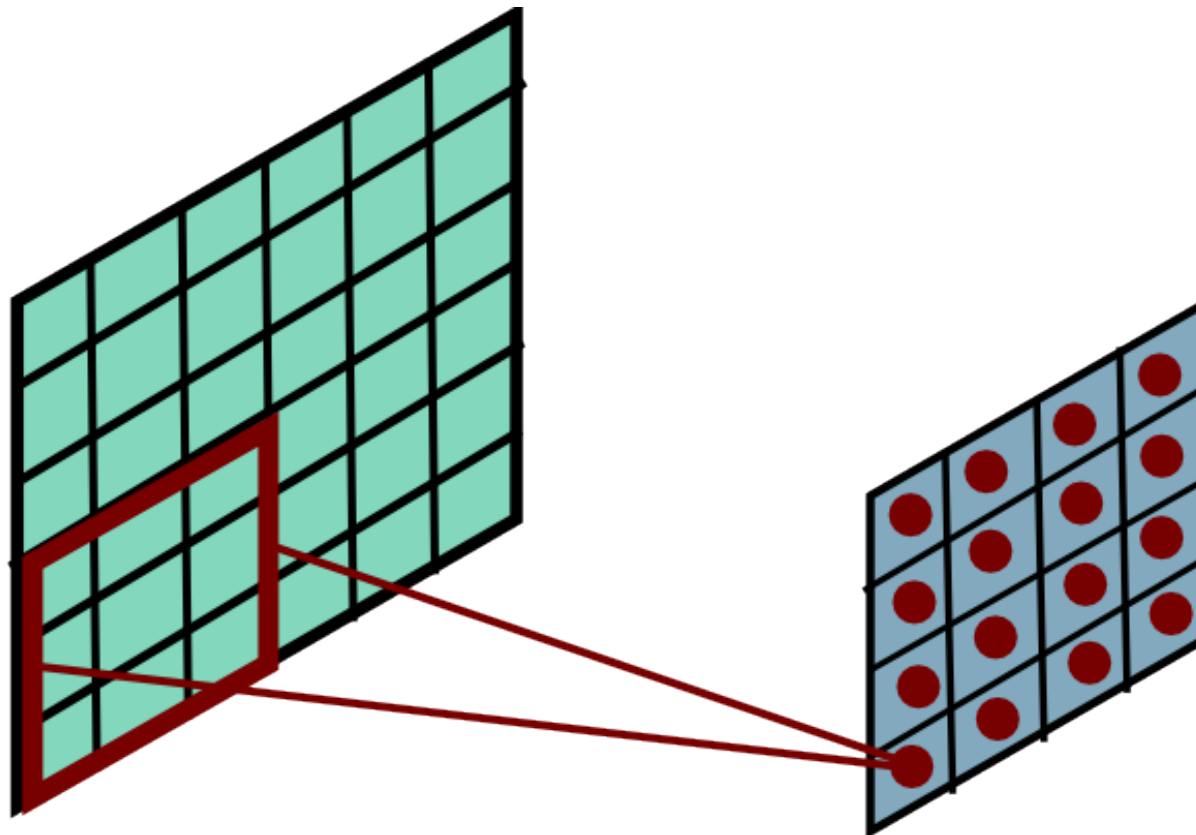
Convolutional Layer



Convolutional Layer

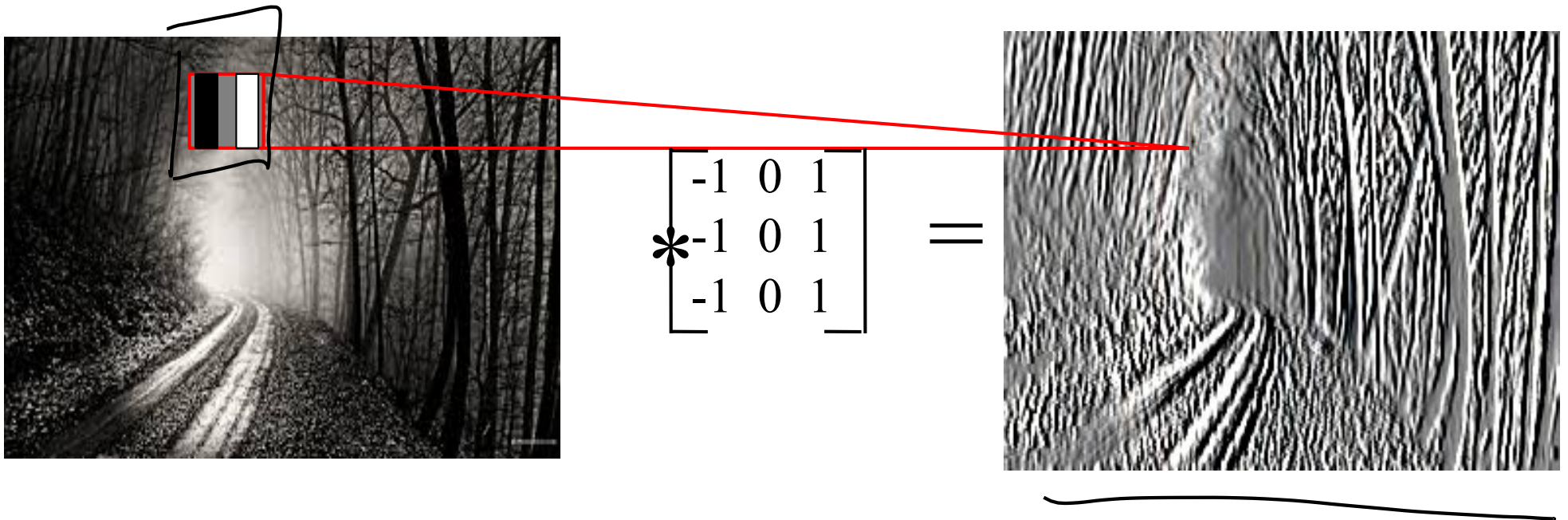


Convolutional Layer

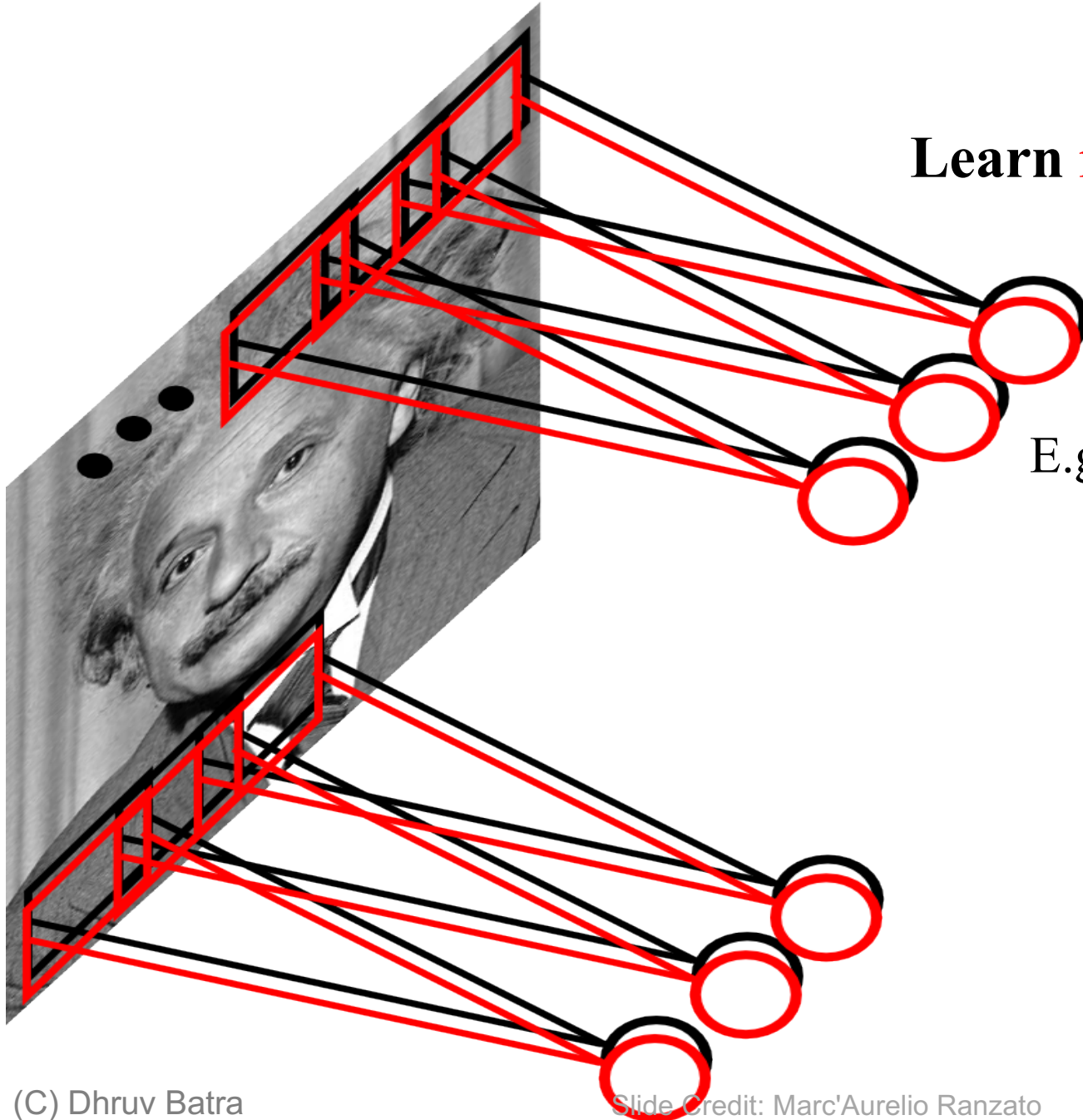


Mathieu et al. “Fast training of CNNs through FFTs” ICLR 2014

Convolutional Layer



Convolutional Layer



Learn **multiple filters**.

E.g.: 200x200 image

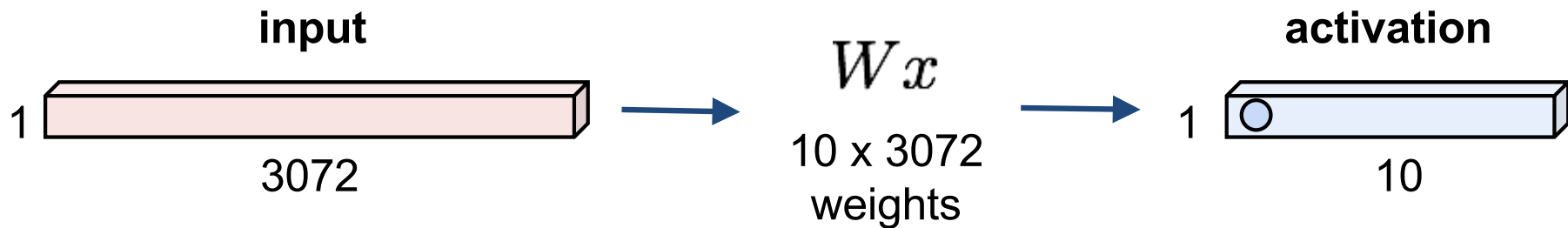
100 Filters

Filter size: 10x10

10K parameters

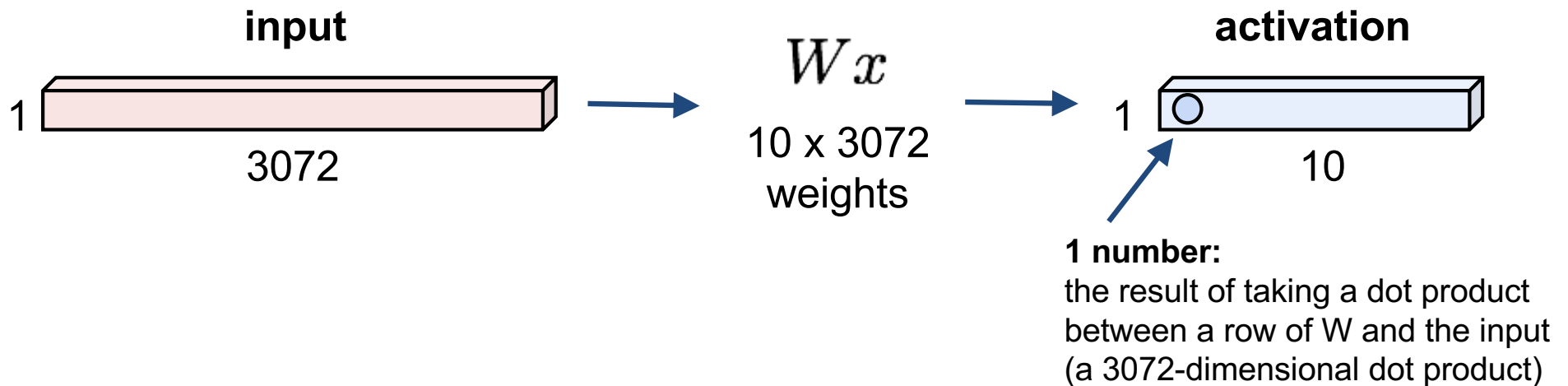
Fully Connected Layer

32x32x3 image -> stretch to 3072 x 1



Fully Connected Layer

32x32x3 image -> stretch to 3072 x 1





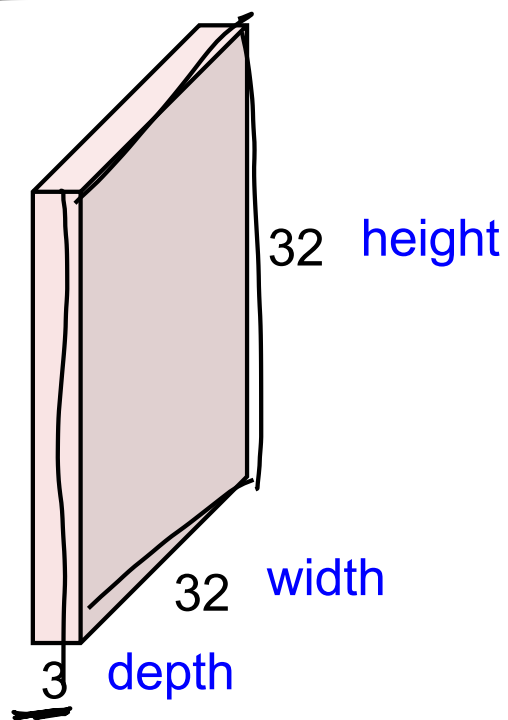
Convolutional Layer



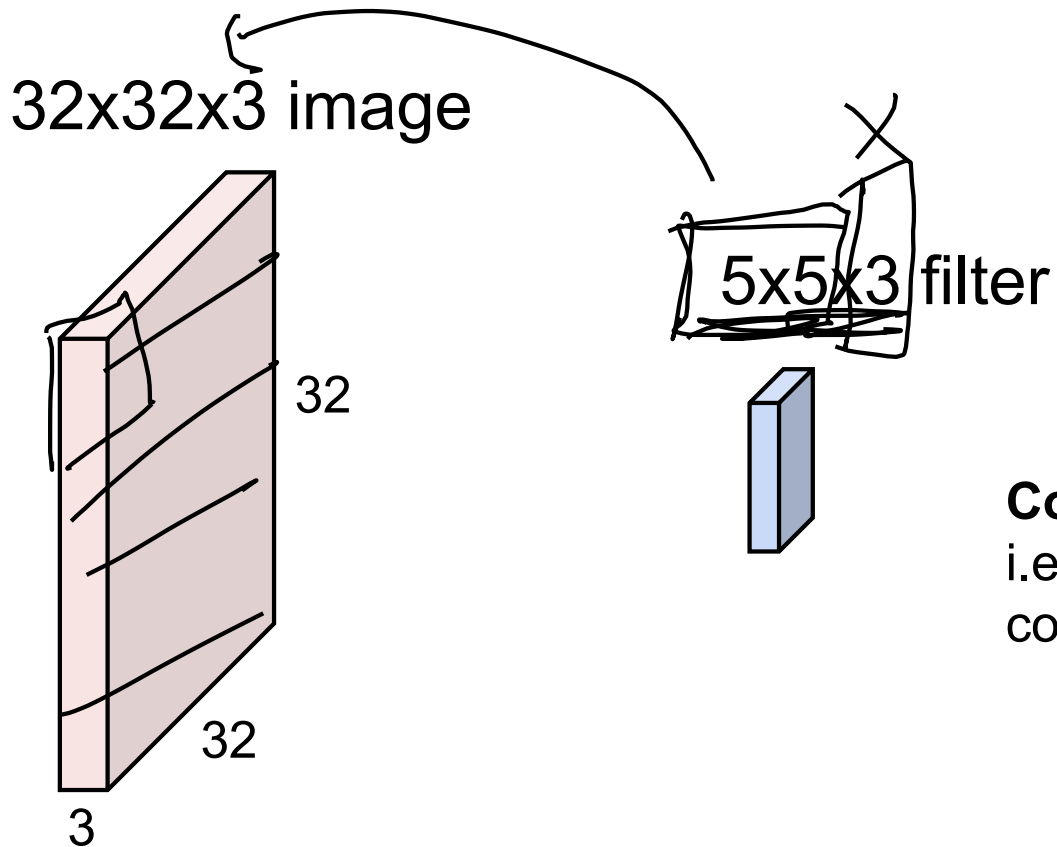
Convolutional Layer

Convolution Layer

32x32x3 image -> preserve spatial structure



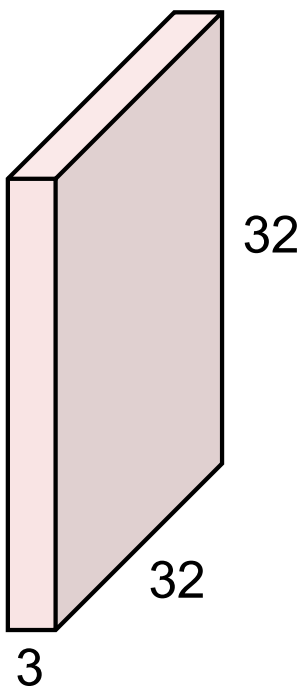
Convolution Layer



Convolve the filter with the image
i.e. “slide over the image spatially,
computing dot products”

Convolution Layer

32x32x3 image



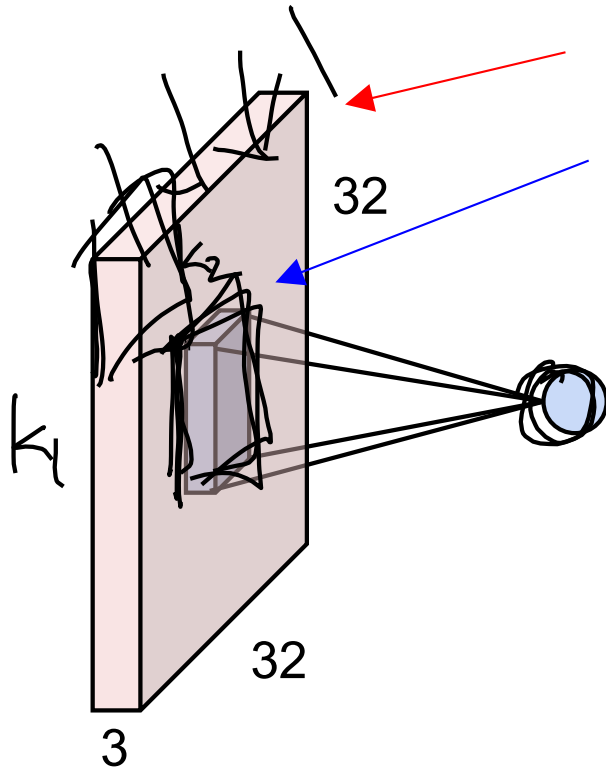
Filters always extend the full depth of the input volume

5x5x3 filter



Convolve the filter with the image
i.e. “slide over the image spatially,
computing dot products”

Convolution Layer



32x32x3 image

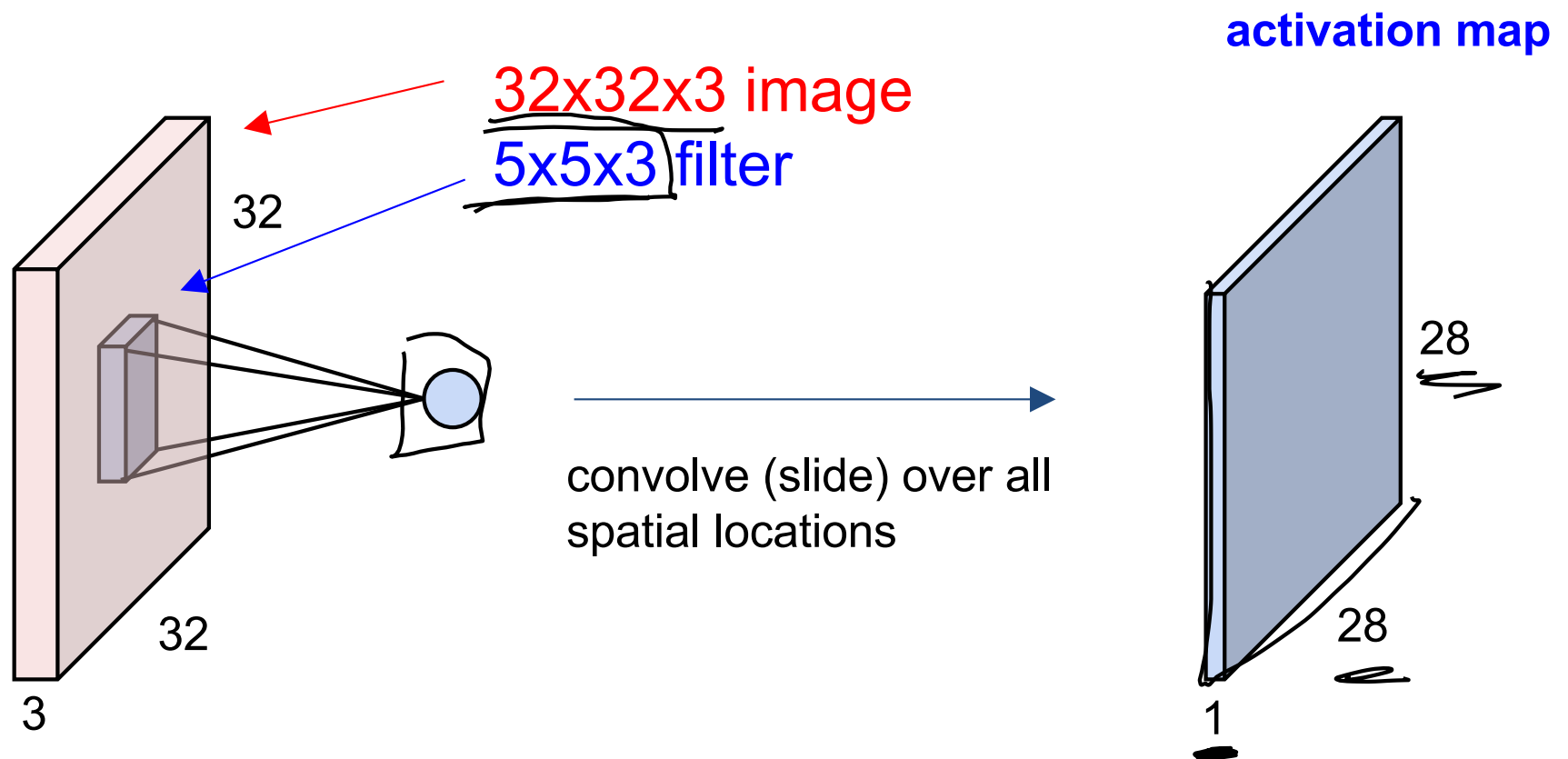
5x5x3 filter w

1 number:

the result of taking a dot product between the filter and a small 5x5x3 chunk of the image (i.e. $5*5*3 = 75$ -dimensional dot product + bias)

$$\underline{\underline{w^T x + b}}$$

Convolution Layer

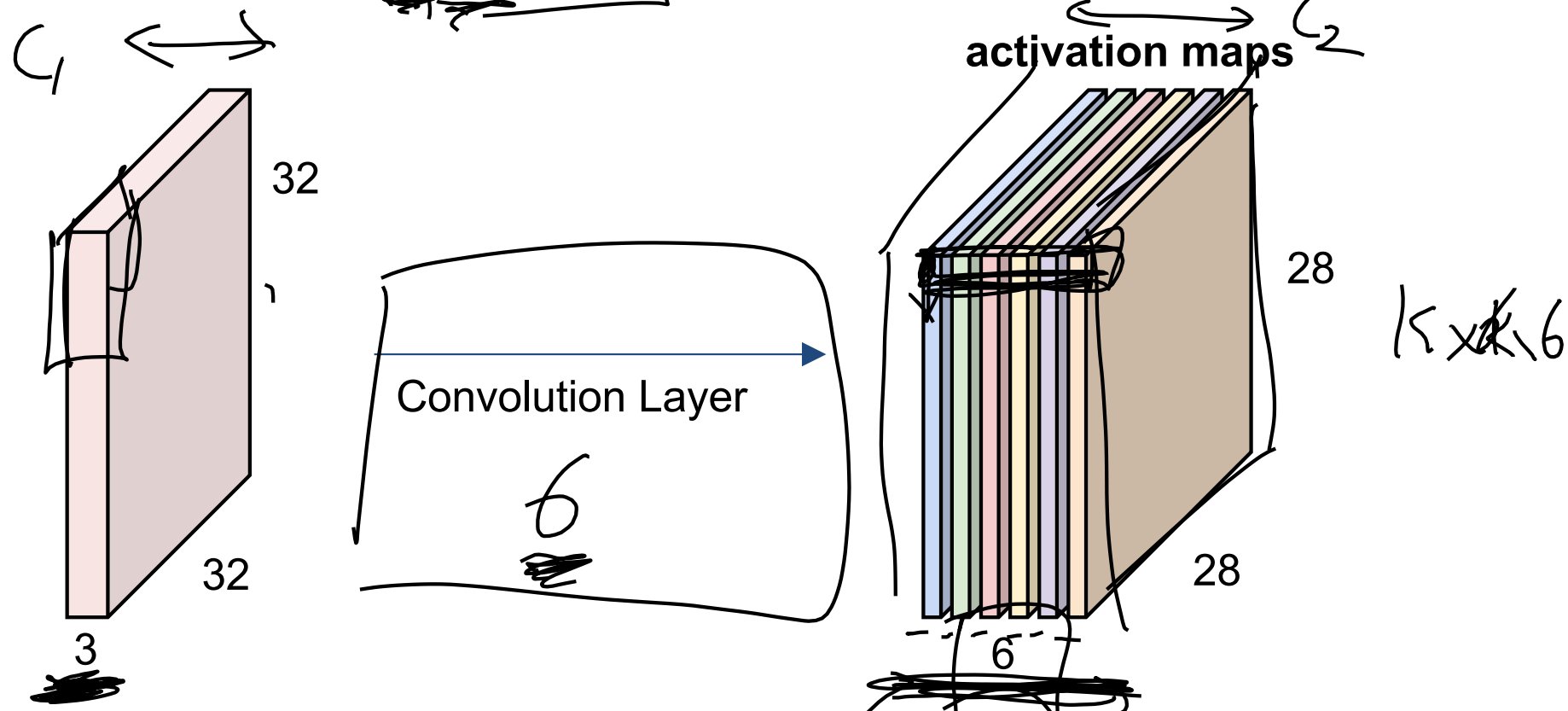


Convolution Layer

consider a second, **green** filter



For example, if we had 6 5×5 filters, we'll get 6 separate activation maps:



We stack these up to get a "new image" of size $28 \times 28 \times 6$!