CMB Workshop

Intro to AI and Machine Learning

Anastasios Kyrillidis
Rice CS

Overview

- Introduction to ML/AI

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- Introduction to neural networks

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- Feedforward / Fully-connected neural networks or MLPs

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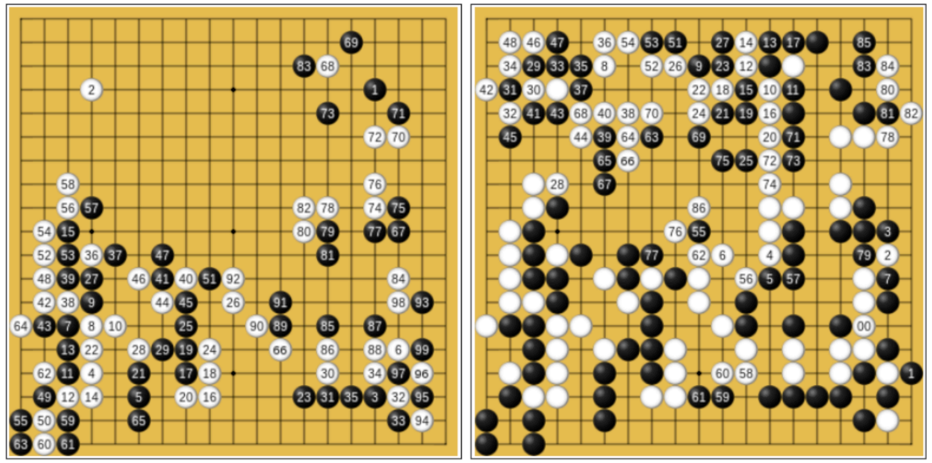
Where are we today?

GPT-3 Example

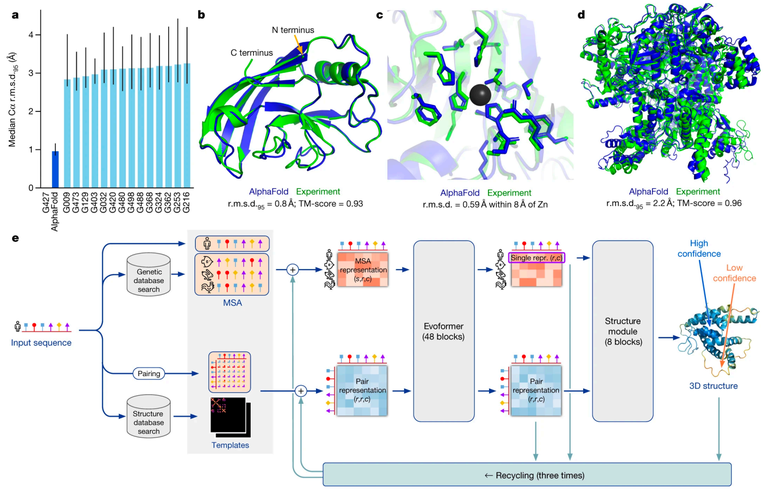
Title: United Methodists Agree to Historic Split
Subtitle: Those who oppose gay marriage will form their own denomination
Article: After two days of intense debate, the United Methodist Church has agreed to a historic split - one that is expected to end in the creation of a new denomination, one that will be "theologically and socially conservative," according to The Washington Post. The majority of delegates attending the church's annual General Conference in May voted to strengthen a ban on the ordination of LGBTQ clergy and to write new rules that will "discipline" clergy who officiate at same-sex weddings. But those who opposed these measures have a new plan: They say they will form a separate denomination by 2020, calling their church the Christian Methodist denomination.
The Post notes that the denomination, which claims 12.5 million members, was in the early 20th century the "largest Protestant denomination in the U.S.," but that it has been shrinking in recent decades. The new split will be the second in the church's history. The first occurred in 1968, when roughly 10 percent of the denomination left to form the Evangelical United Brethren Church. The Post notes that the proposed split "comes at a critical time for the church, which has been losing members for years," which has been "pushed toward the brink of a schism over the role of LGBTQ people in the church." Gay marriage is not the only issue that has divided the church. In 2016, the denomination was split over ordination of transgender clergy, with the North Pacific regional conference voting to ban them from serving as clergy, and the South Pacific regional conference voting to allow them.

Example: GANS

Game Playing



Structural Biology



Underlying principles in ML: Supervised Learning

Foundation of modern ML: supervised learning

- One of the most fundamental problems in data science
  - Given a bunch of (x, y) pairs
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- Given an image, tell if has a cat or not
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- Given an image, tell if has a cat or not
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- Given a document (email) in a court case, figure which subjects relevant to
- Given information about a patient surgery, predict death
- Given head trauma patient info, predict ICP crisis
- Given an set of surgical vital signs, label "good surgery" or not
- Many others!

Underlying principles in ML: Type of outputs

- Classification:
  - Outcome to predict is in $\{+1, -1\}$ ("yes" or "no")
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- Regression:
  - Outcome to predict is a real number
  - Ex: Given an ad, predict number of clickthrus per hour

(e.g., Linear regression)

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  - Training, validation, testing
  - Training: used to learn the model (min the loss)
  - Validation: used to see if the model is OK
  - Maybe params are wrong... or bad features, or wrong model
  - Use testing to predict accuracy in deployment
  - You often find test accuracy much lower than validation (over-fitting)

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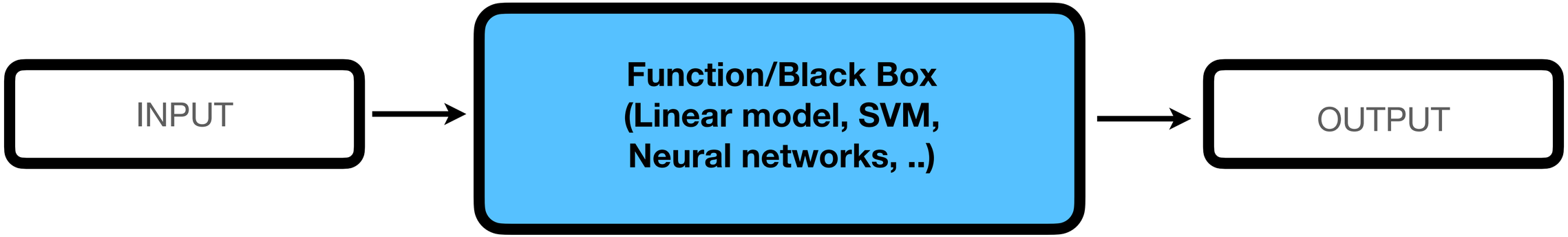

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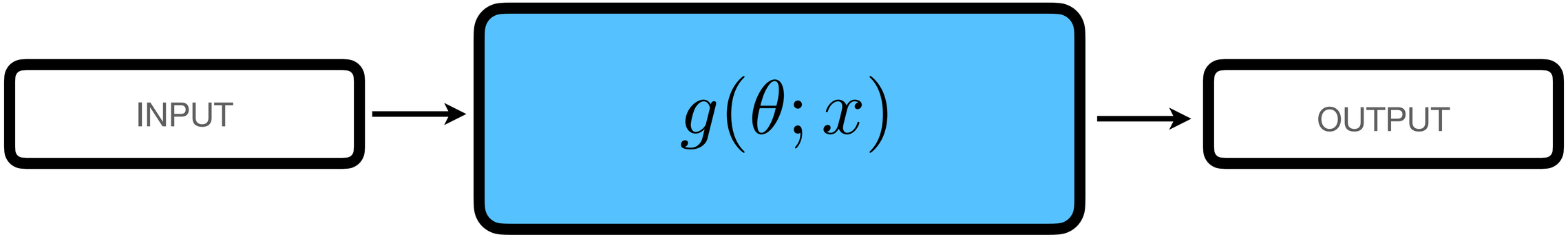

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- Finally, the loss function defines..

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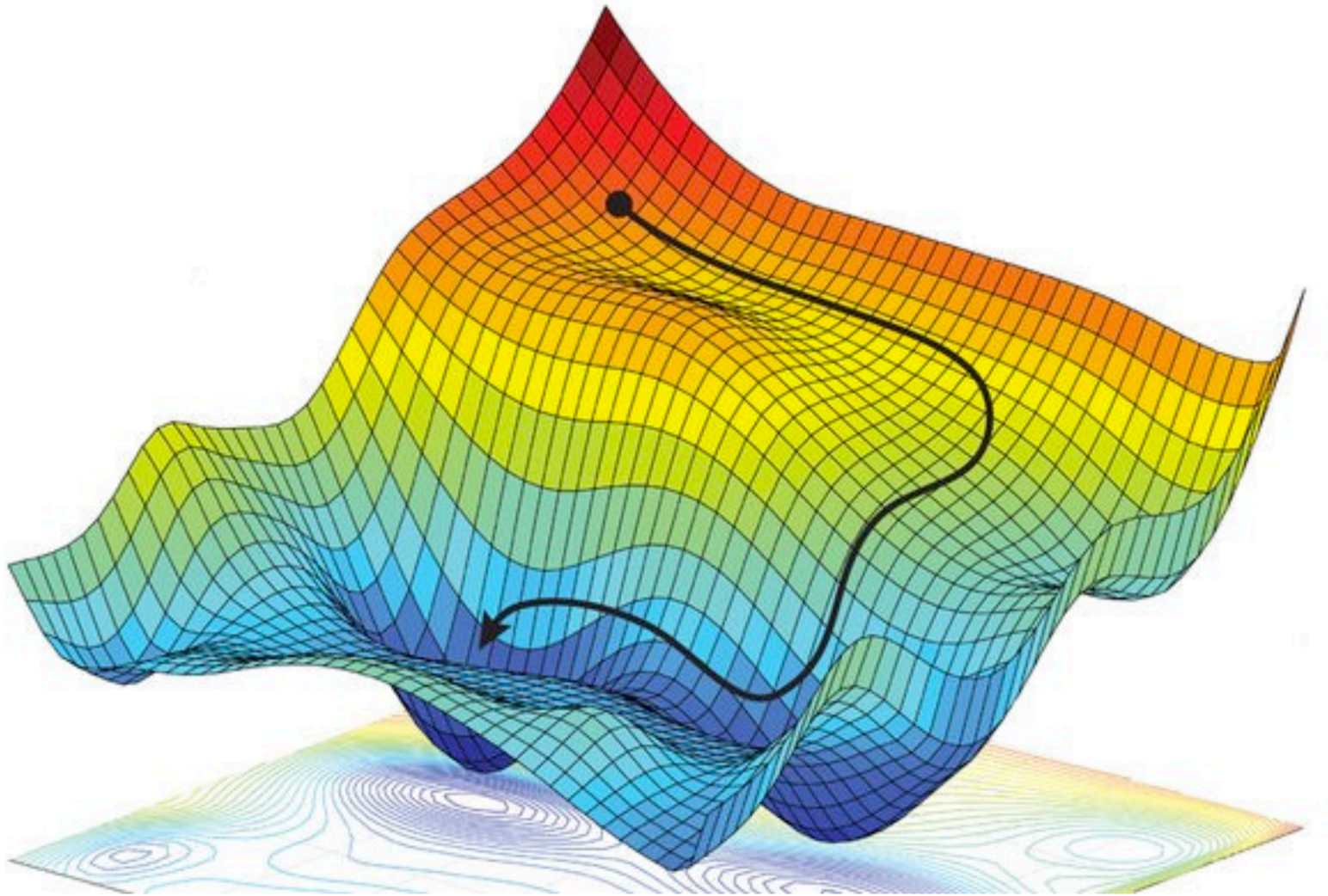
- How we optimize? Gradient descent (or backpropagation)!

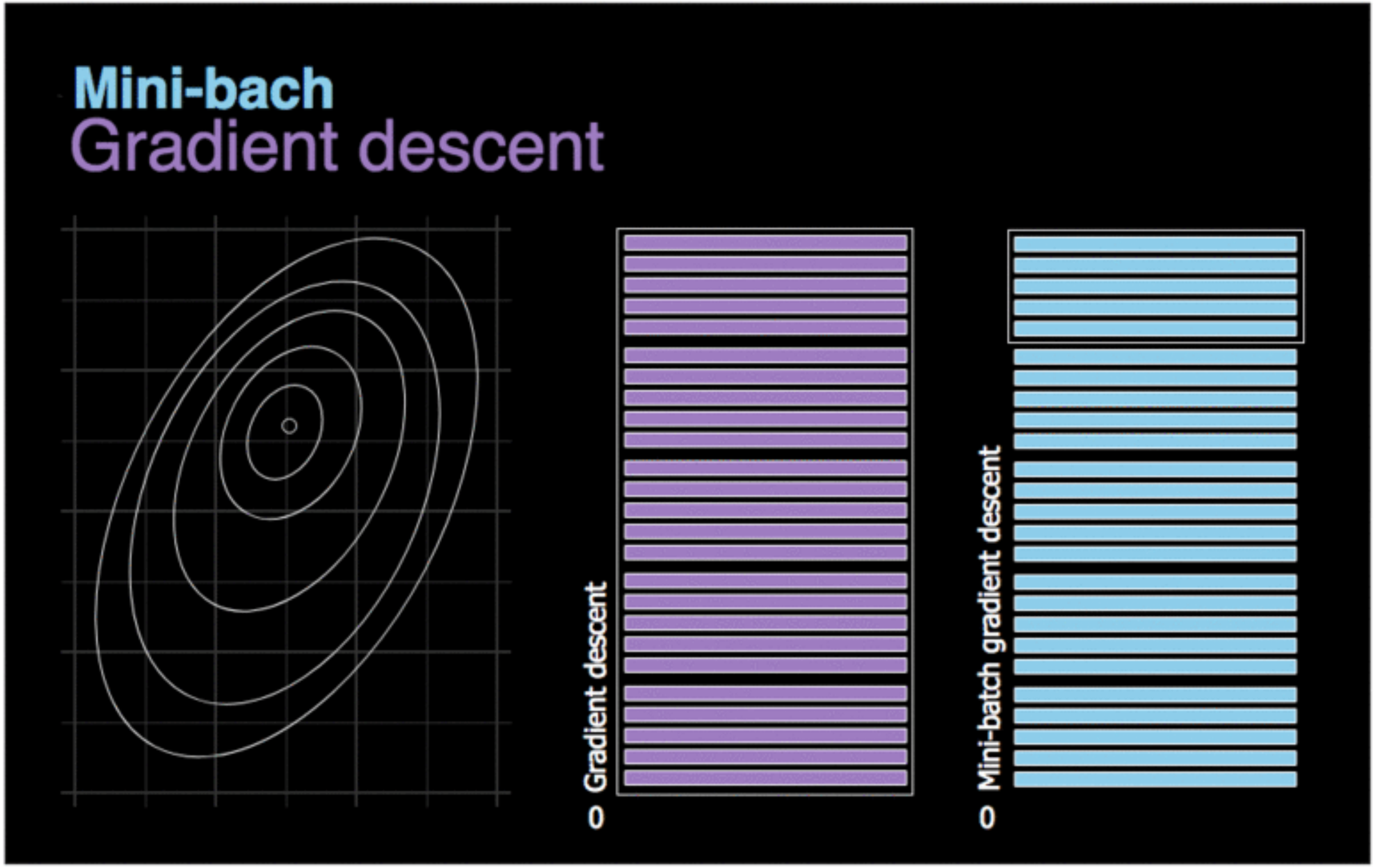
$$\theta_{t+1} = \theta_t - \eta \nabla \mathcal{L}_{i_t}(\theta_t)$$

Underlying principles in ML: Optimization



- In practice, we use variants of GD: Adam, AdaGrad, AdamW, ..

Stochastic gradient descent



Tribute to
Piotr Skalski

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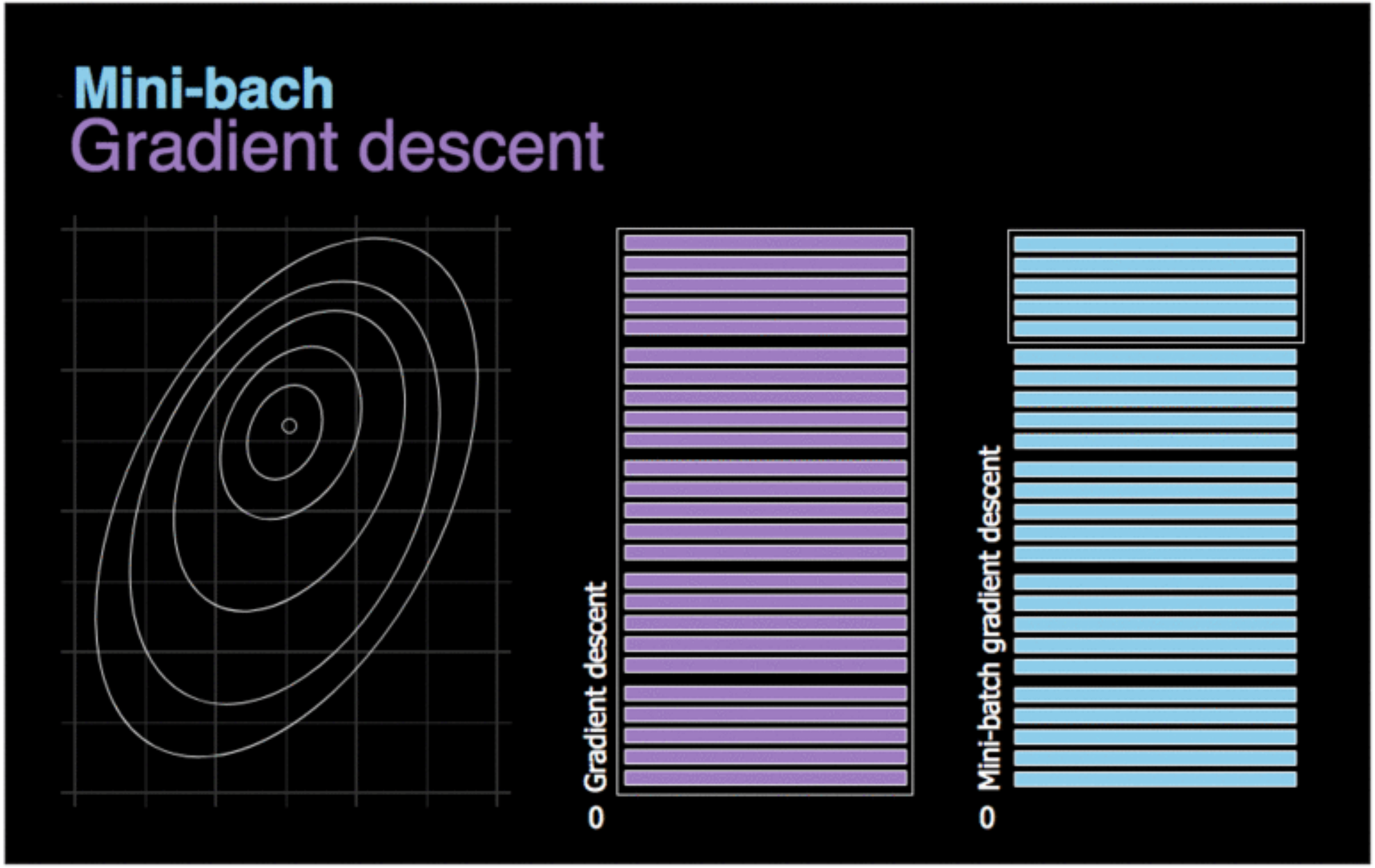

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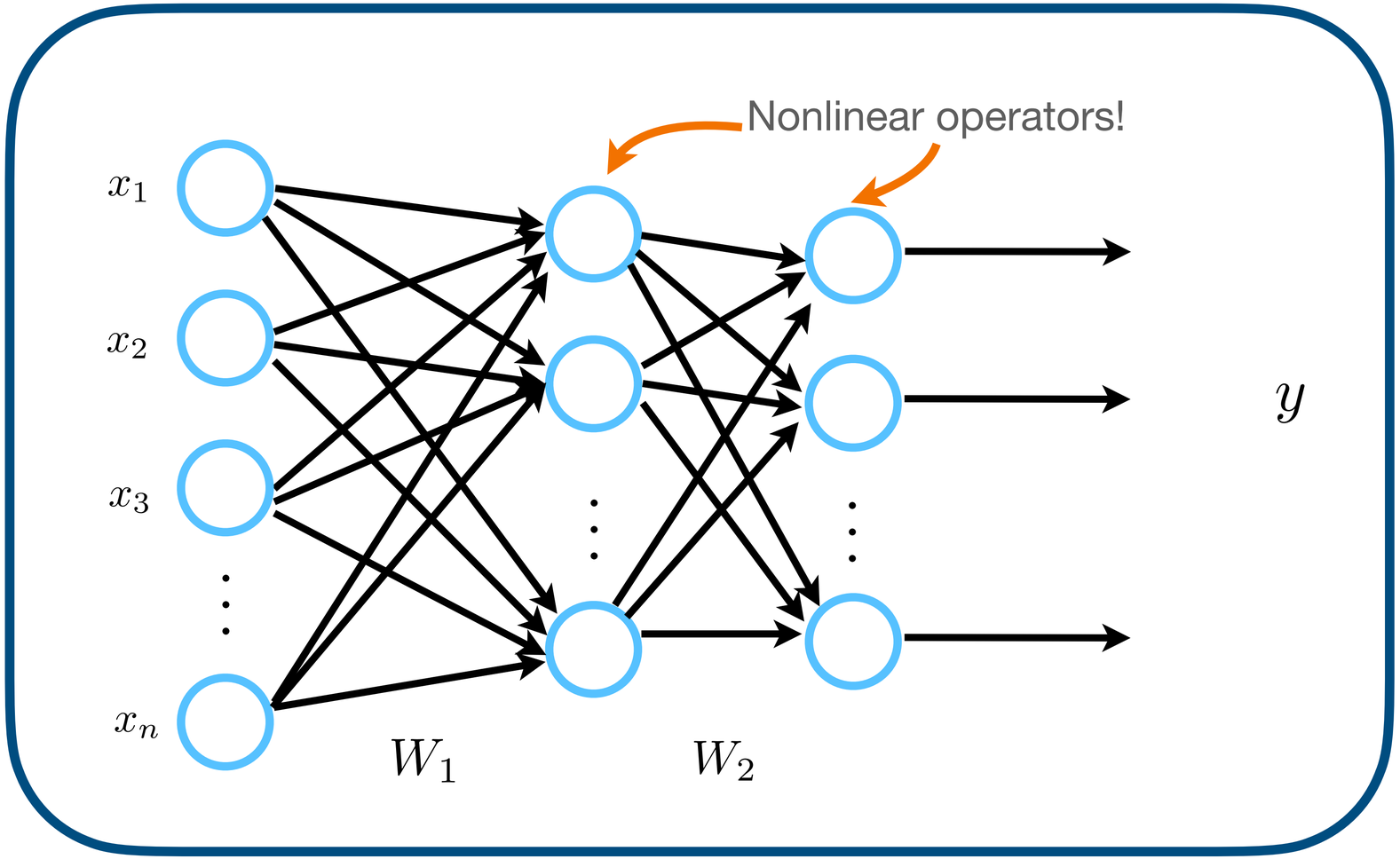
Multi-Layer Perceptrons or MLPs

Feedforward/fully connected neural network



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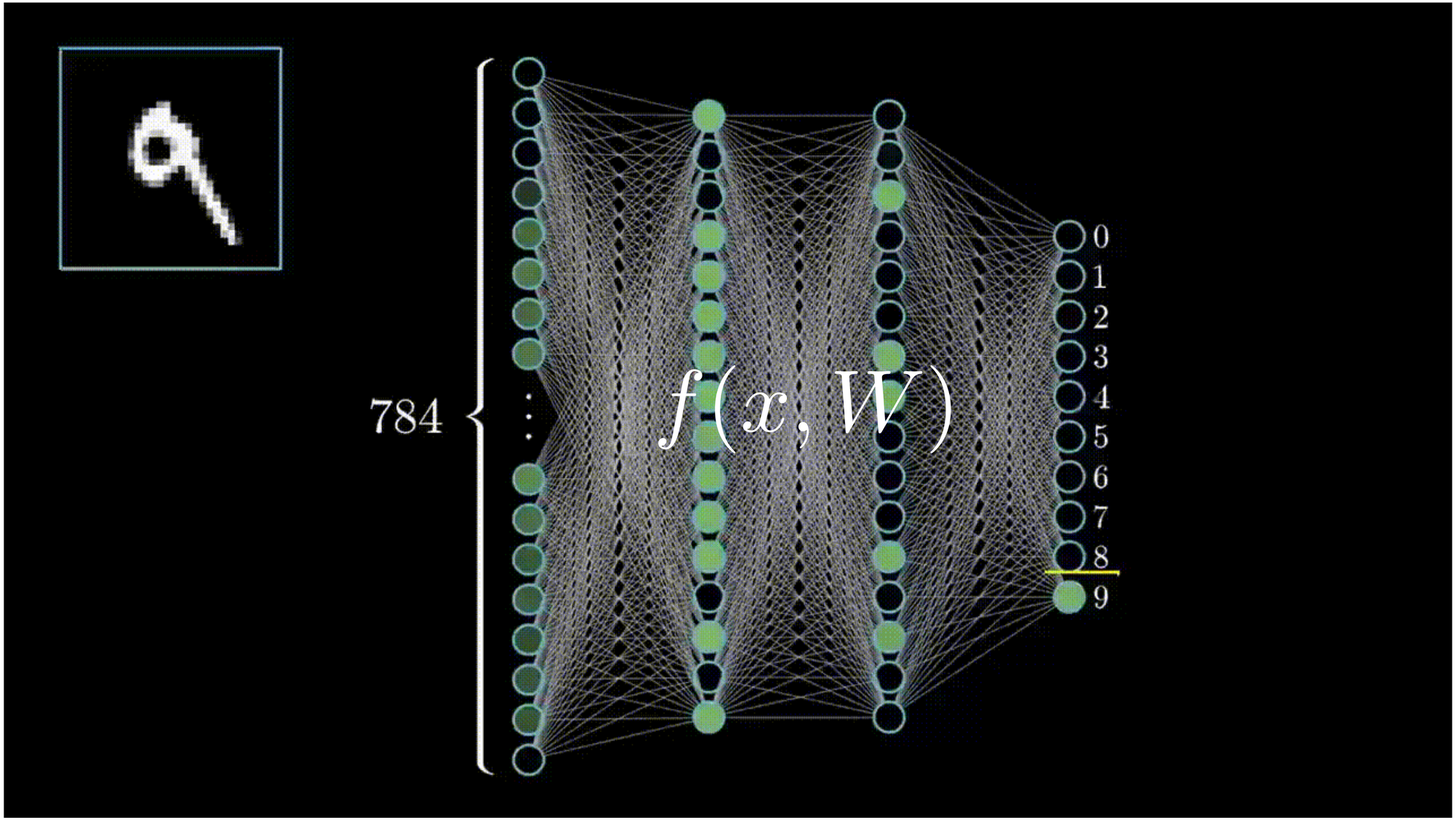

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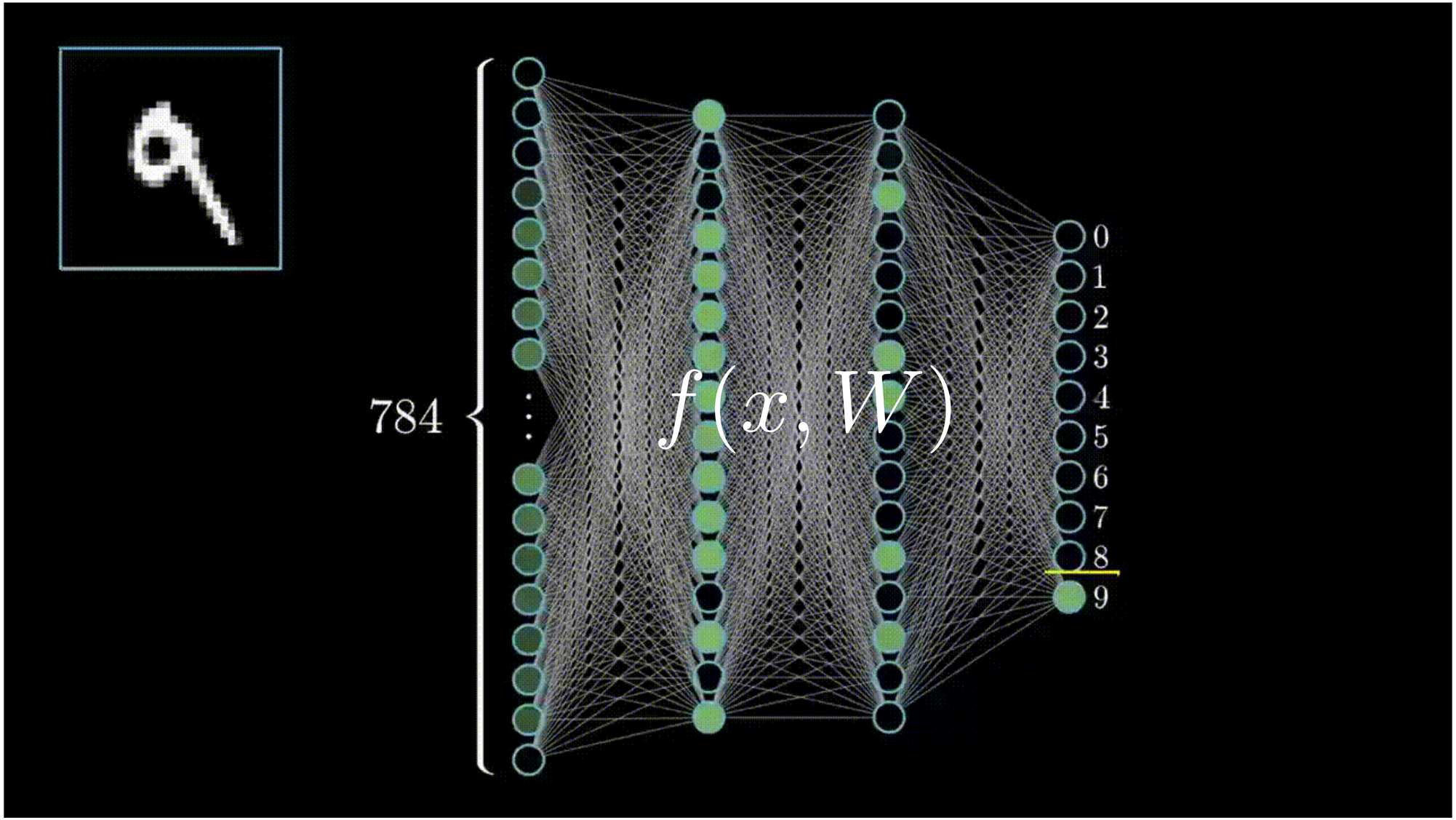

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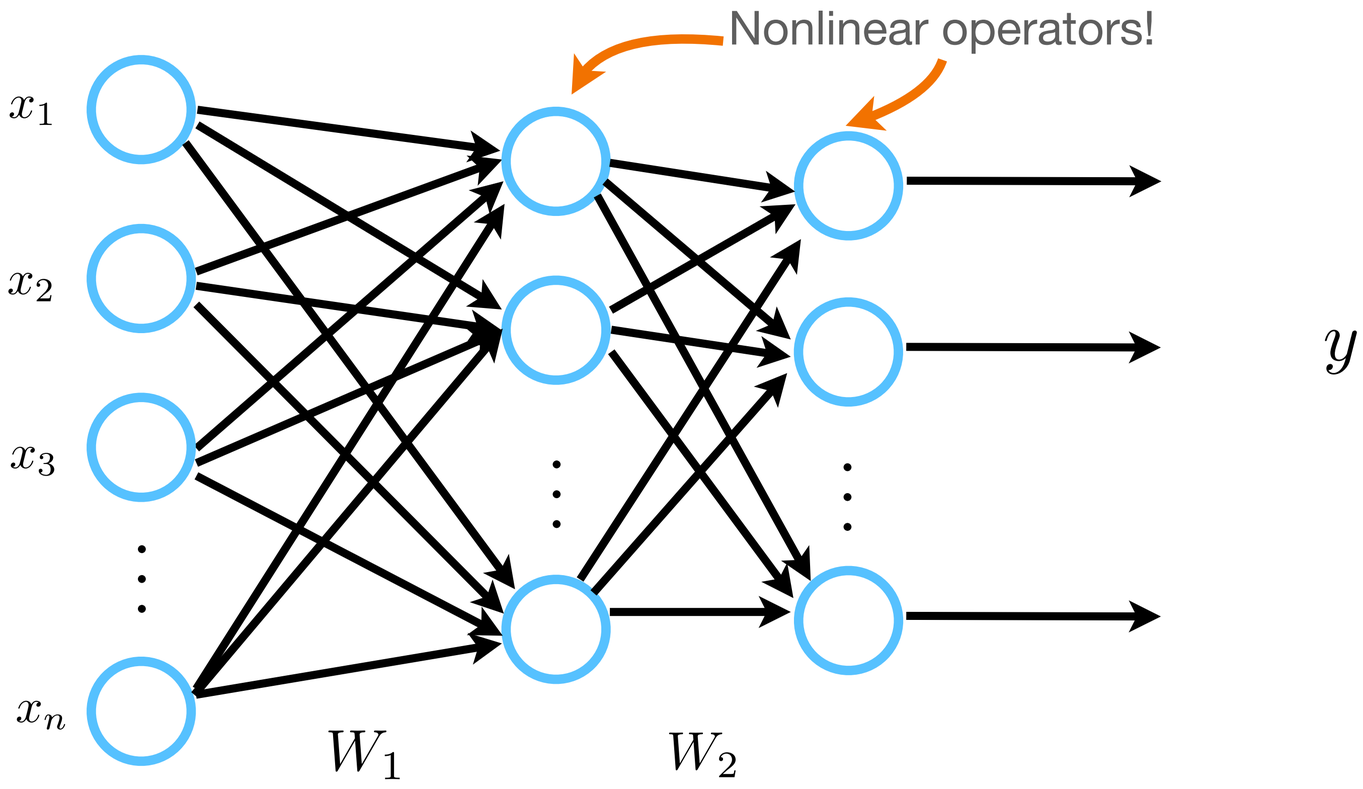

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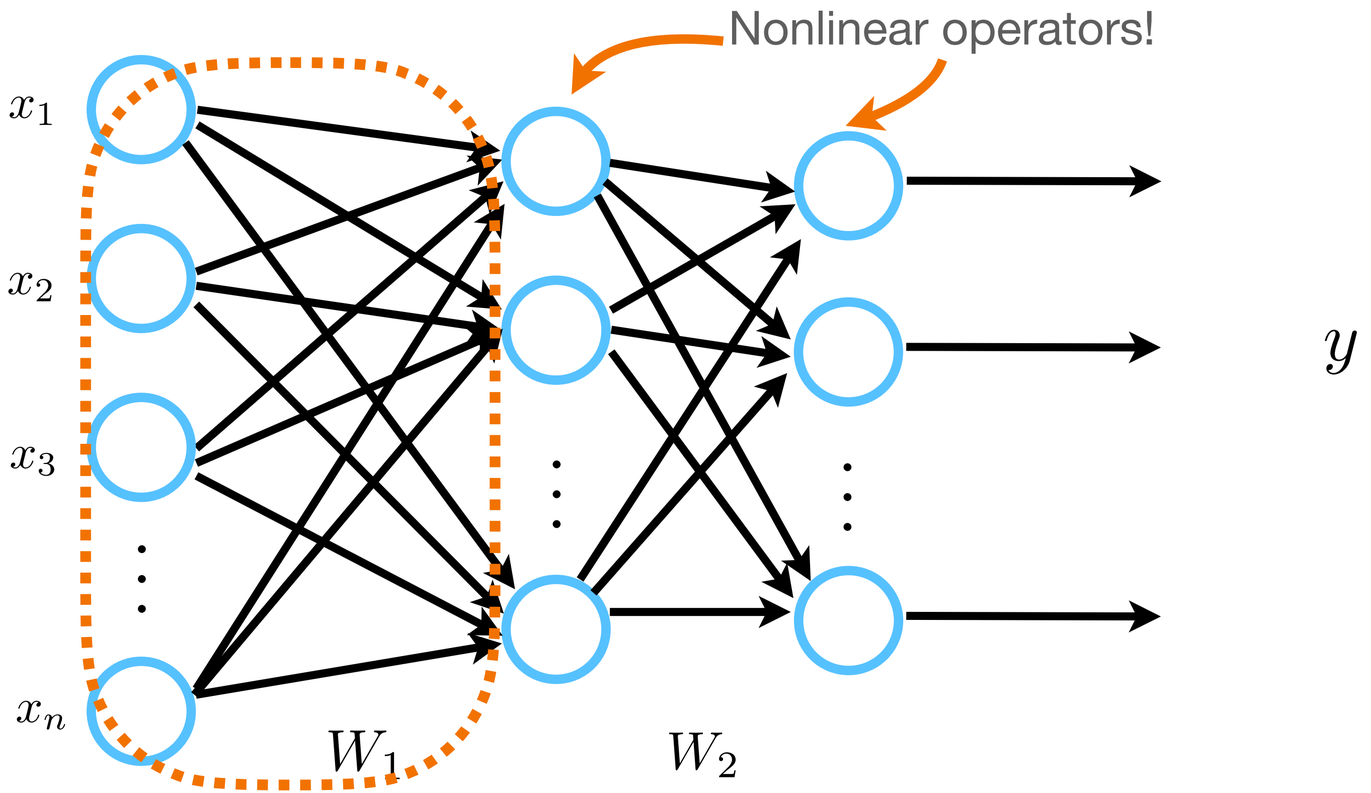

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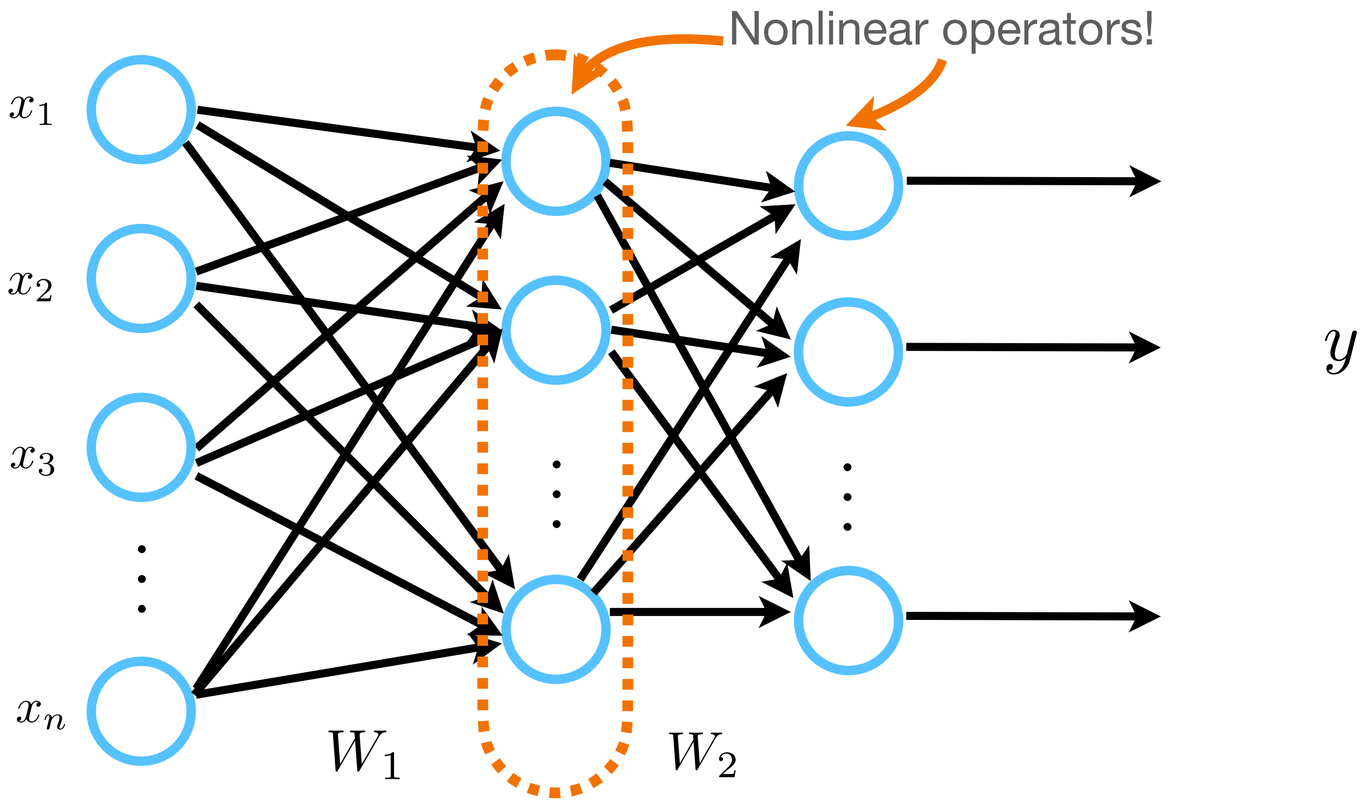

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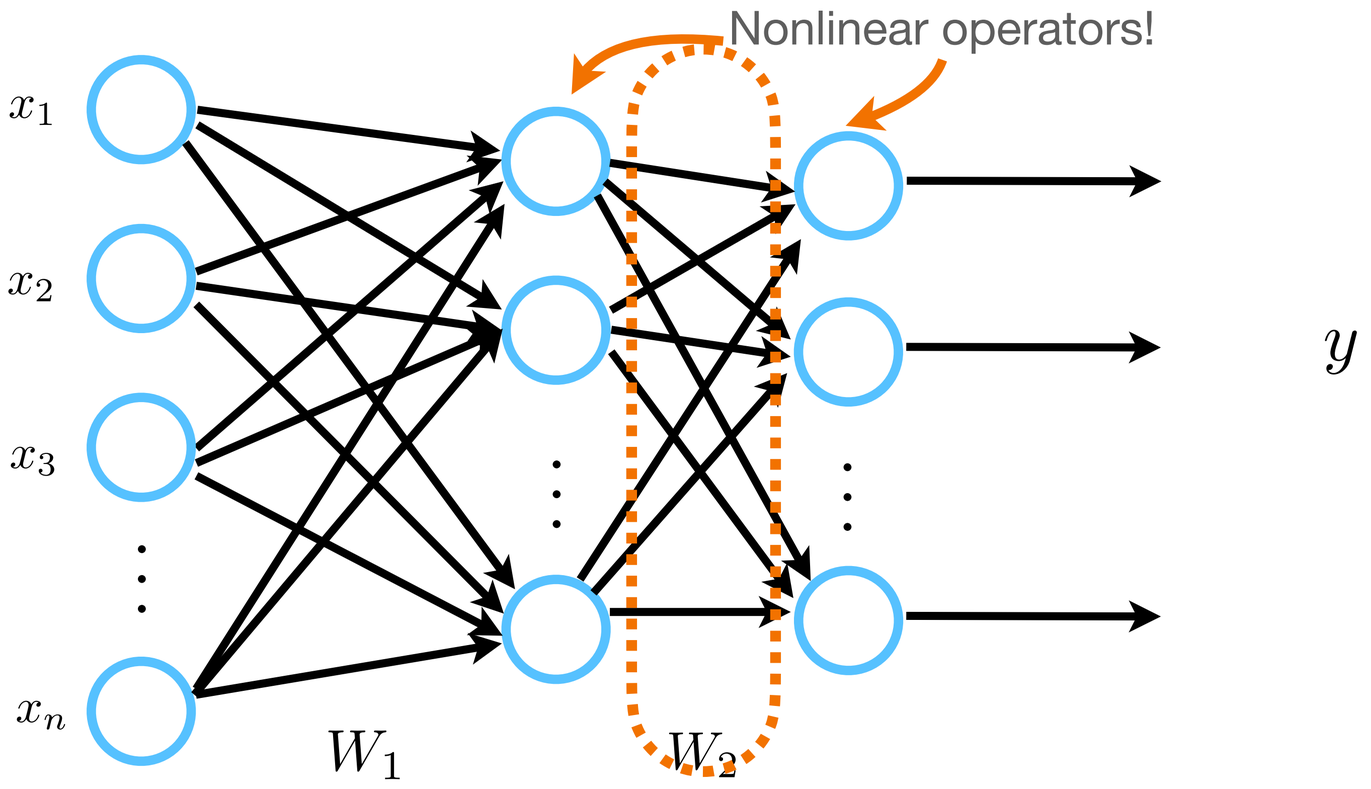

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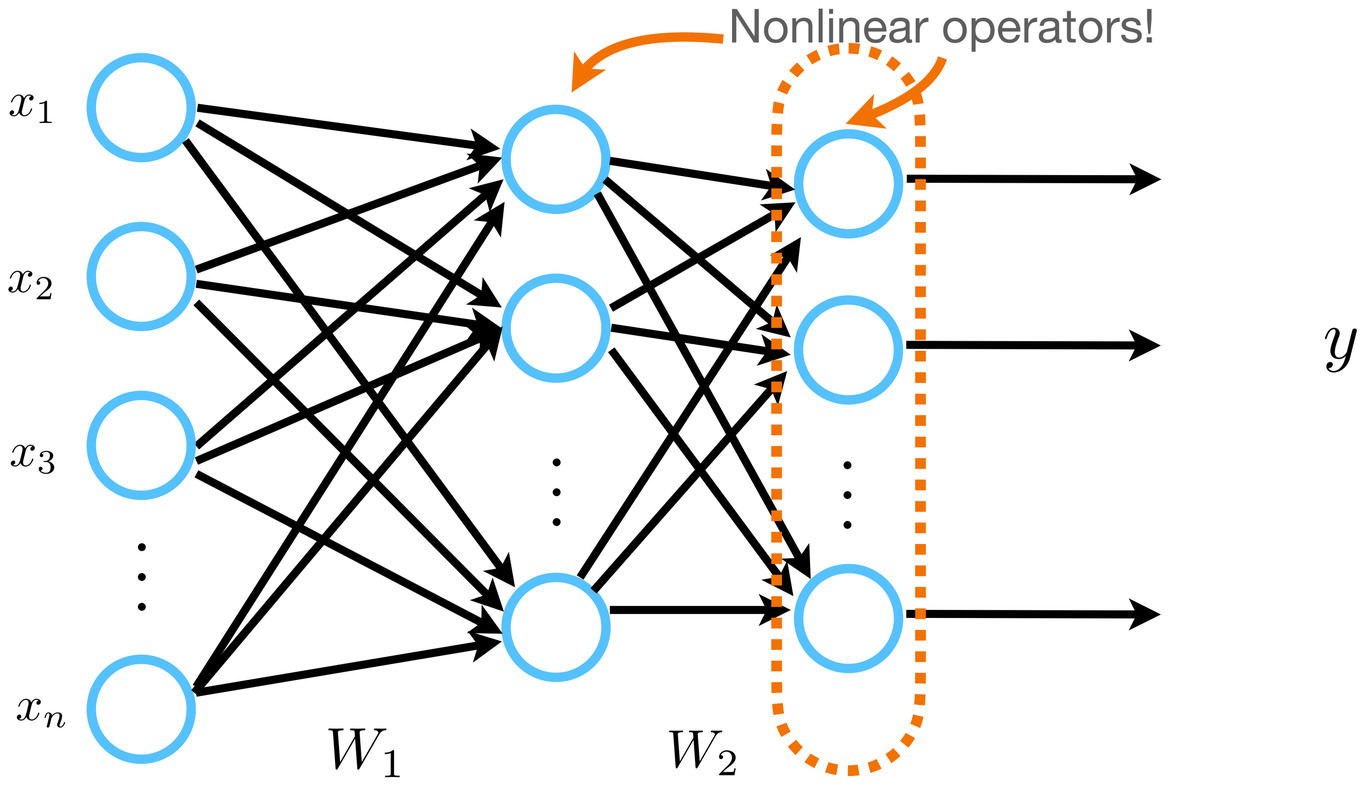

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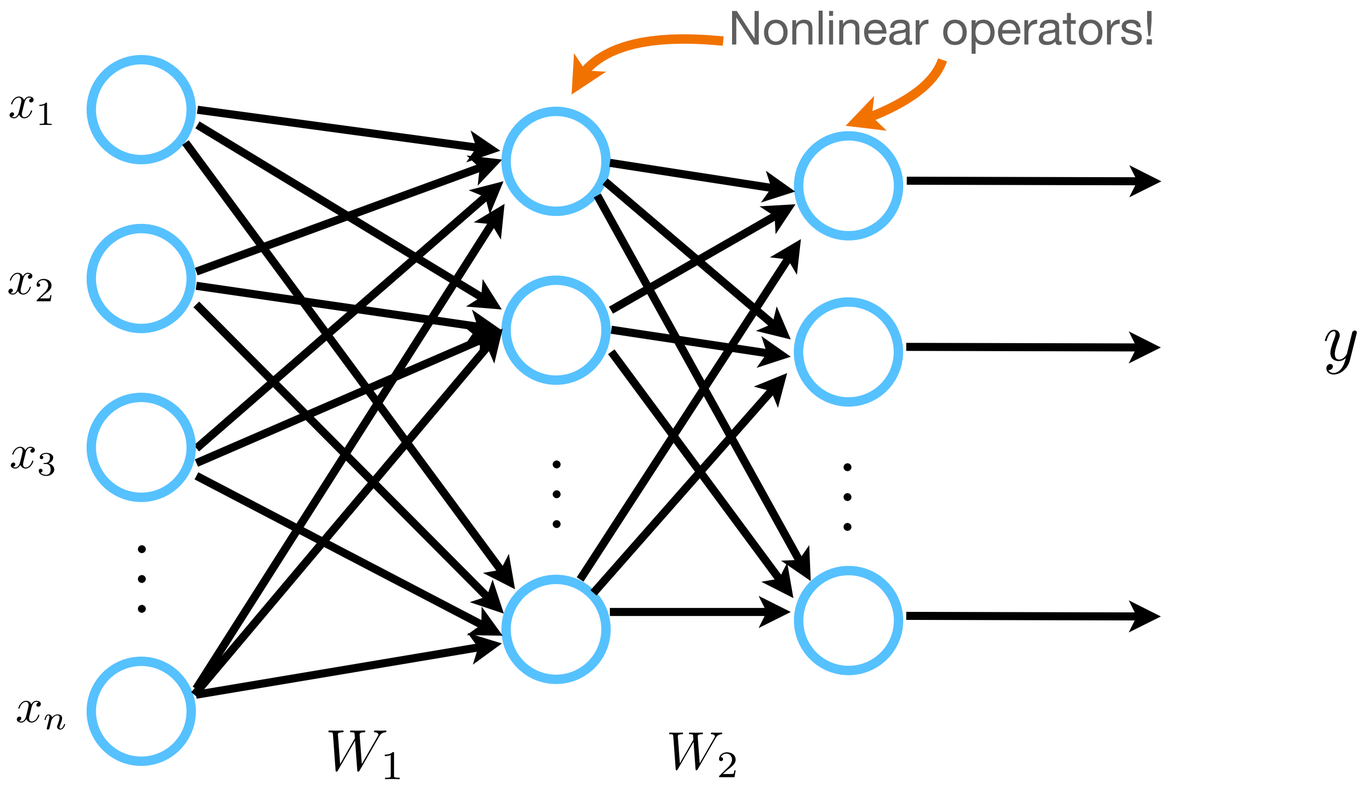

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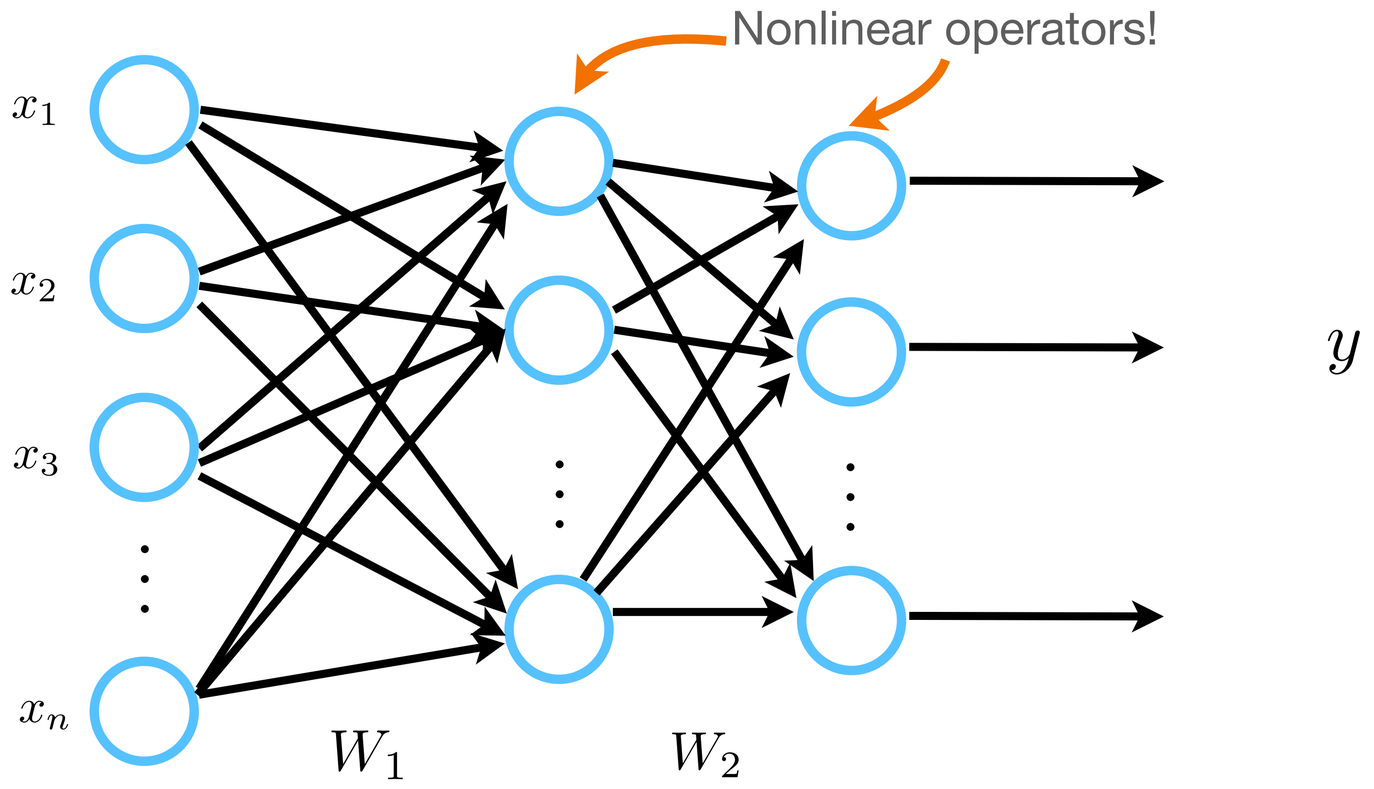
- Boils down to what modules will be used
- Famous architecture due to simplicity and theoretical guarantees

Fully connected neural networks or MLPs

This sequence of operations is also known as the **forward pass on the neural network**

You can think of forward pass as function evaluation



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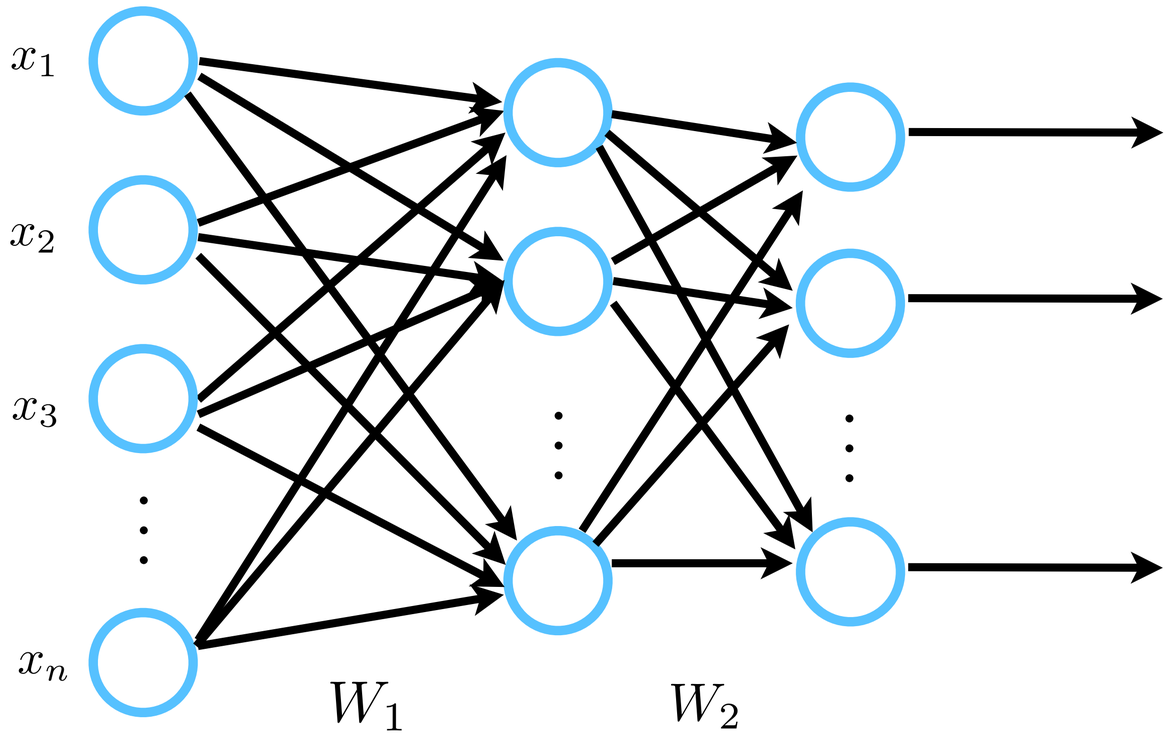
- Deep vs. shallow, wide vs. narrow: Although shallow wide NNs work well in theory, deep nets are more efficient, and generalize better.
- Objective functions: euclidean norm (regression), cross entropy (classification) only input data (autoencoders), min-max (GANs), etc.
  (or type of learning)

What are our options here wrt modules?



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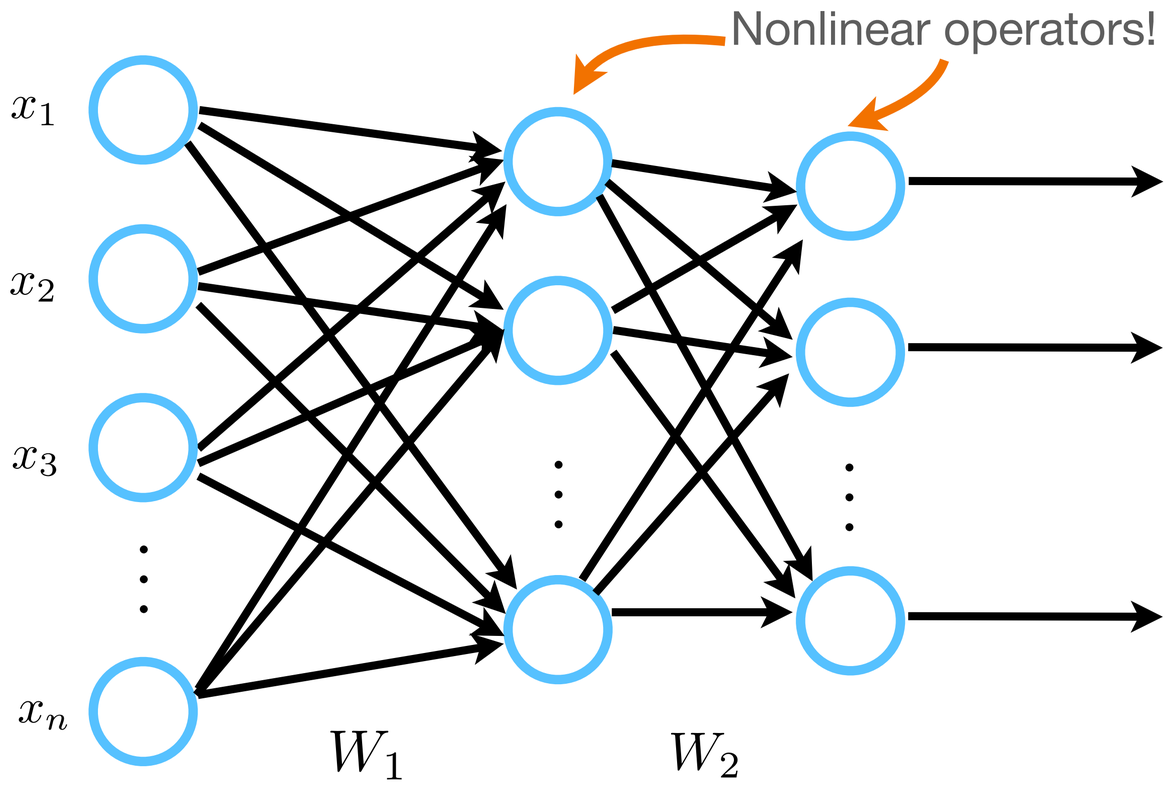

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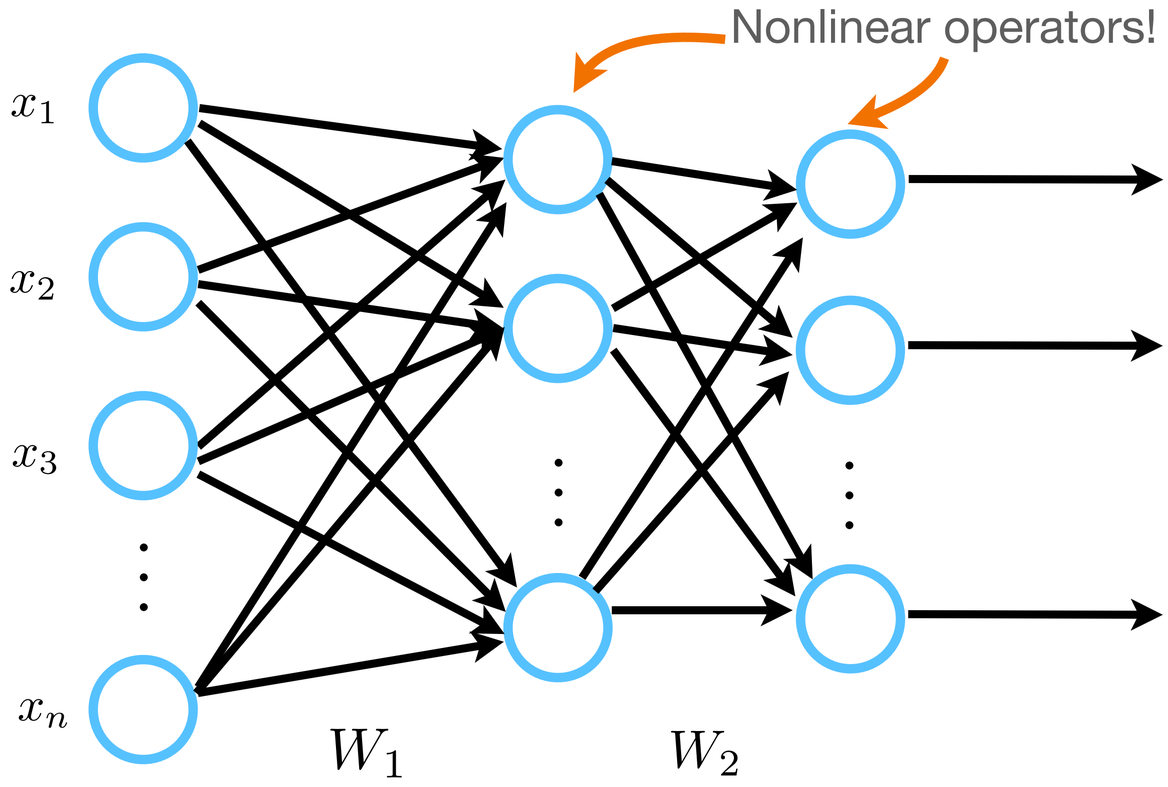

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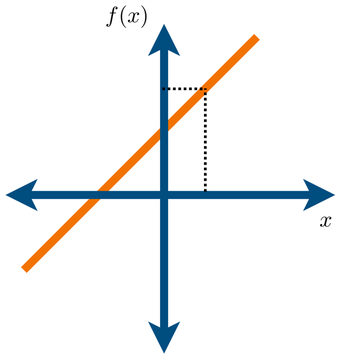

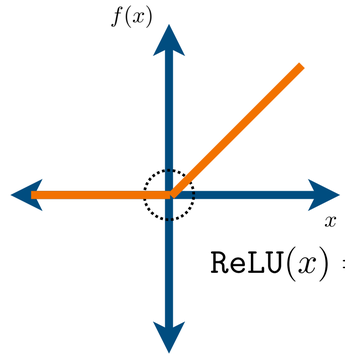

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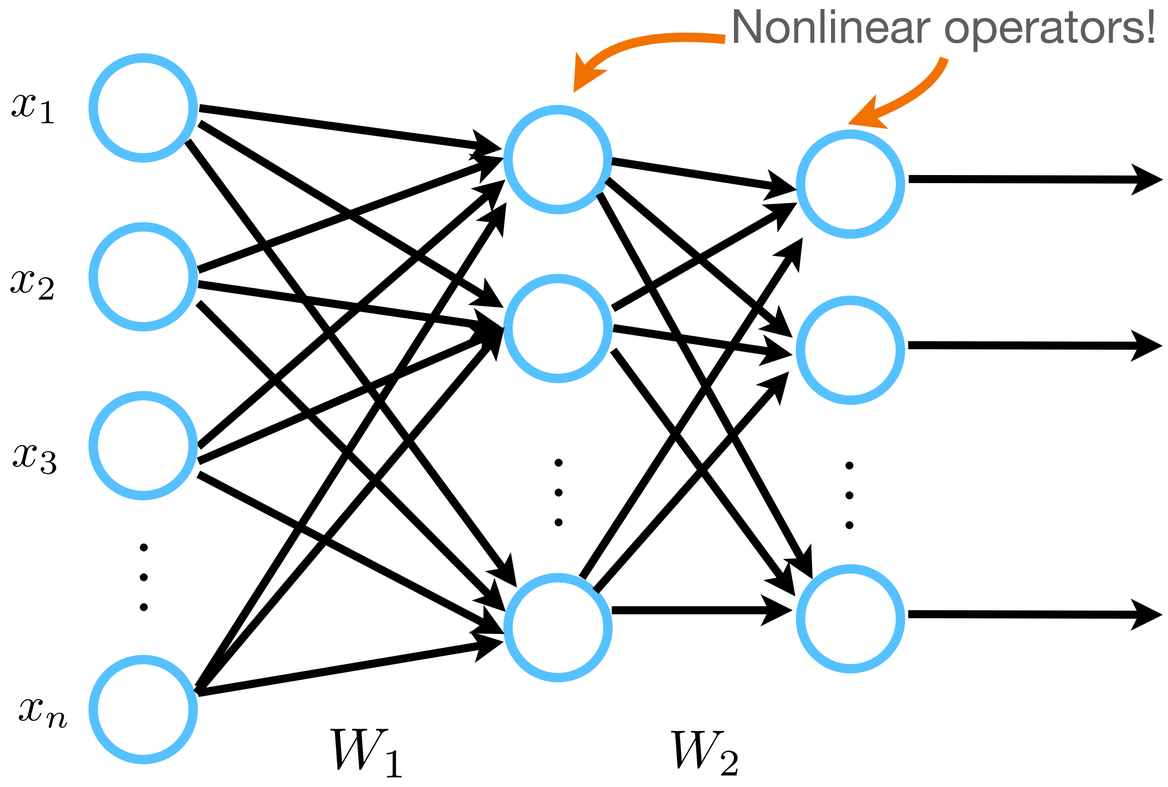

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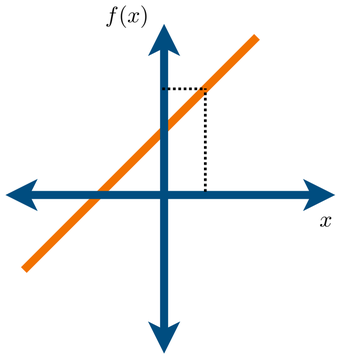

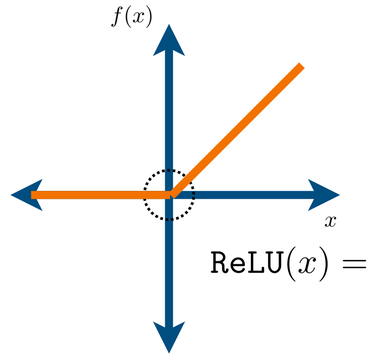

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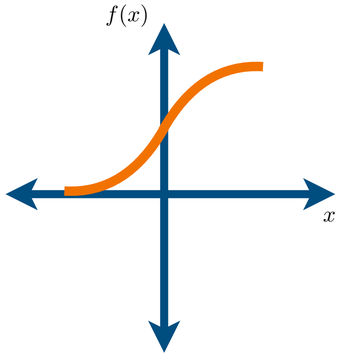
- There is also sigmoid..



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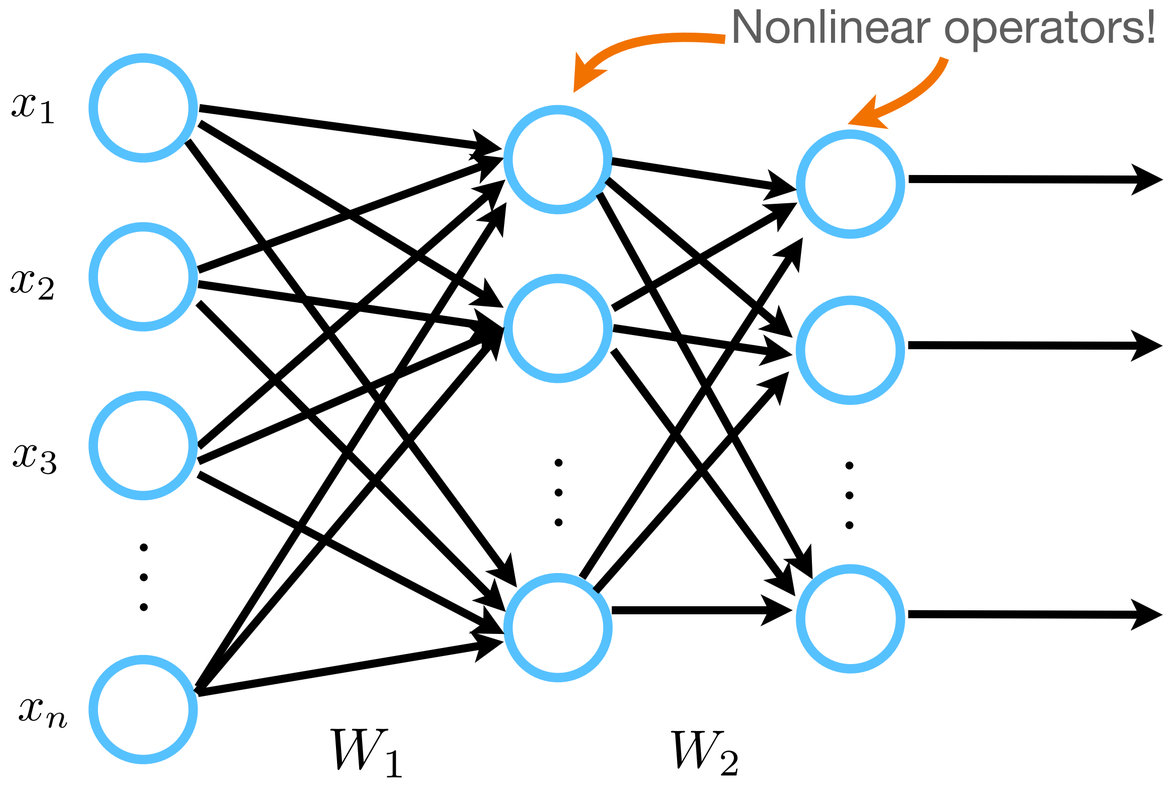

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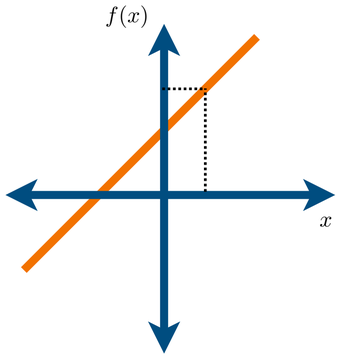
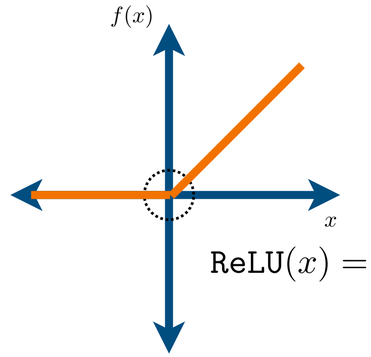
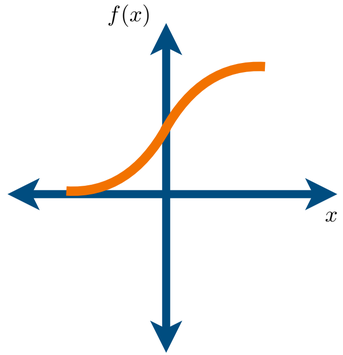
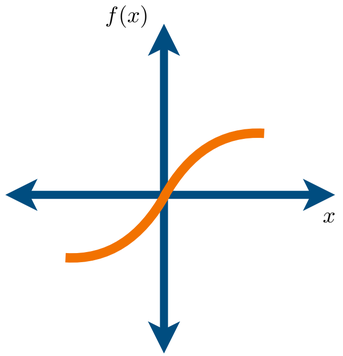




$$\texttt{ReLU}(x) = \begin{cases} x, & x \geq 0 \\ 0, & \text{otherwise} \end{cases}$$

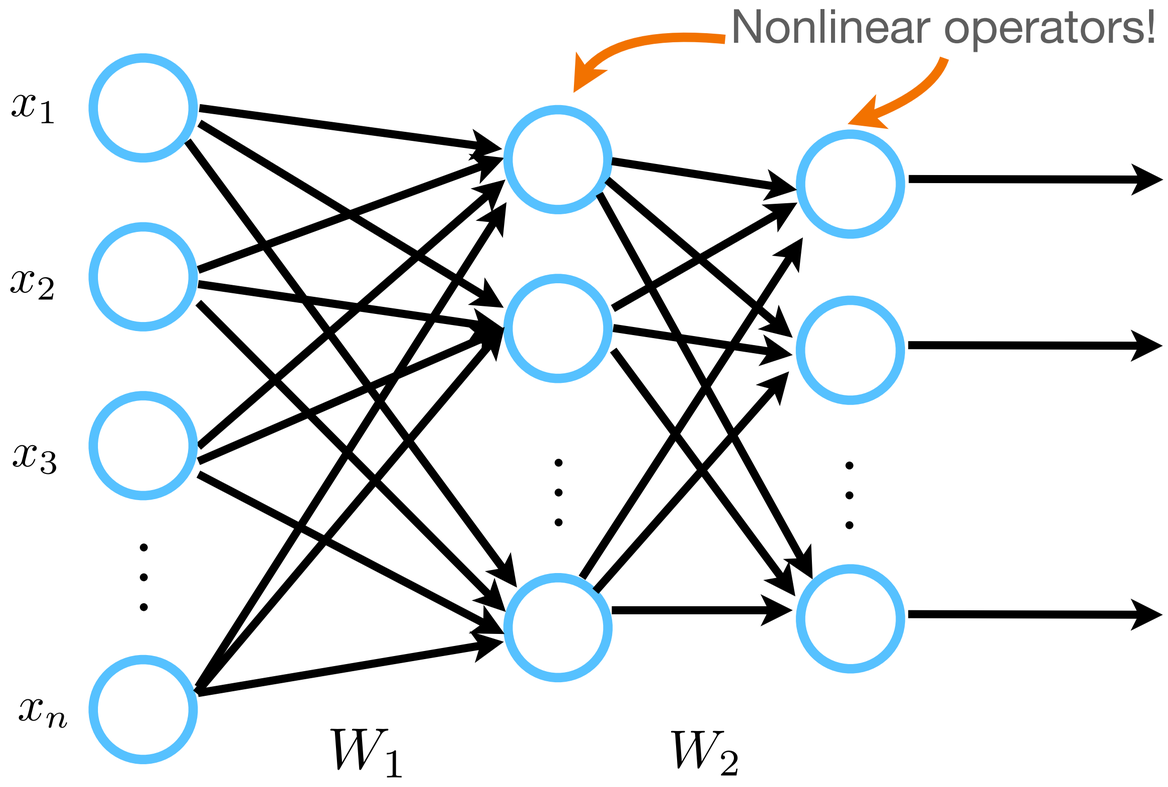
- There is also sigmoid..





- ..and tanh functions.

What are our options here wrt modules?



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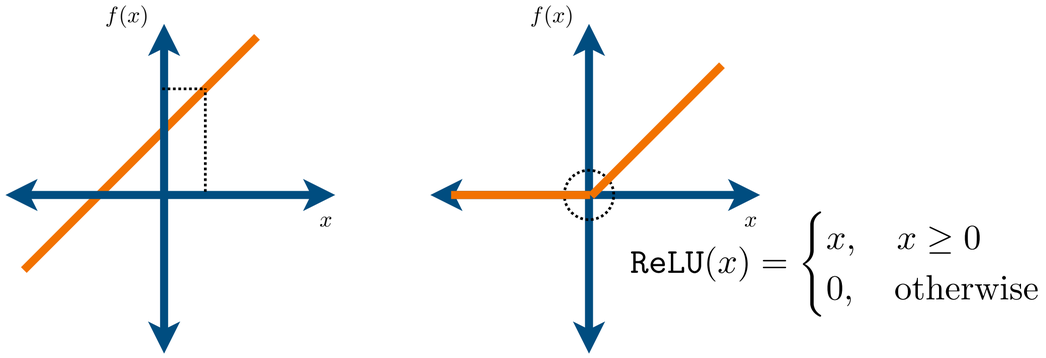

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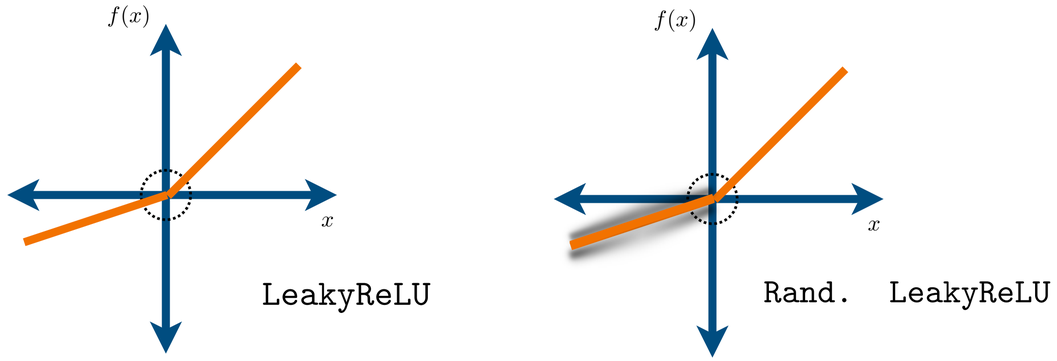

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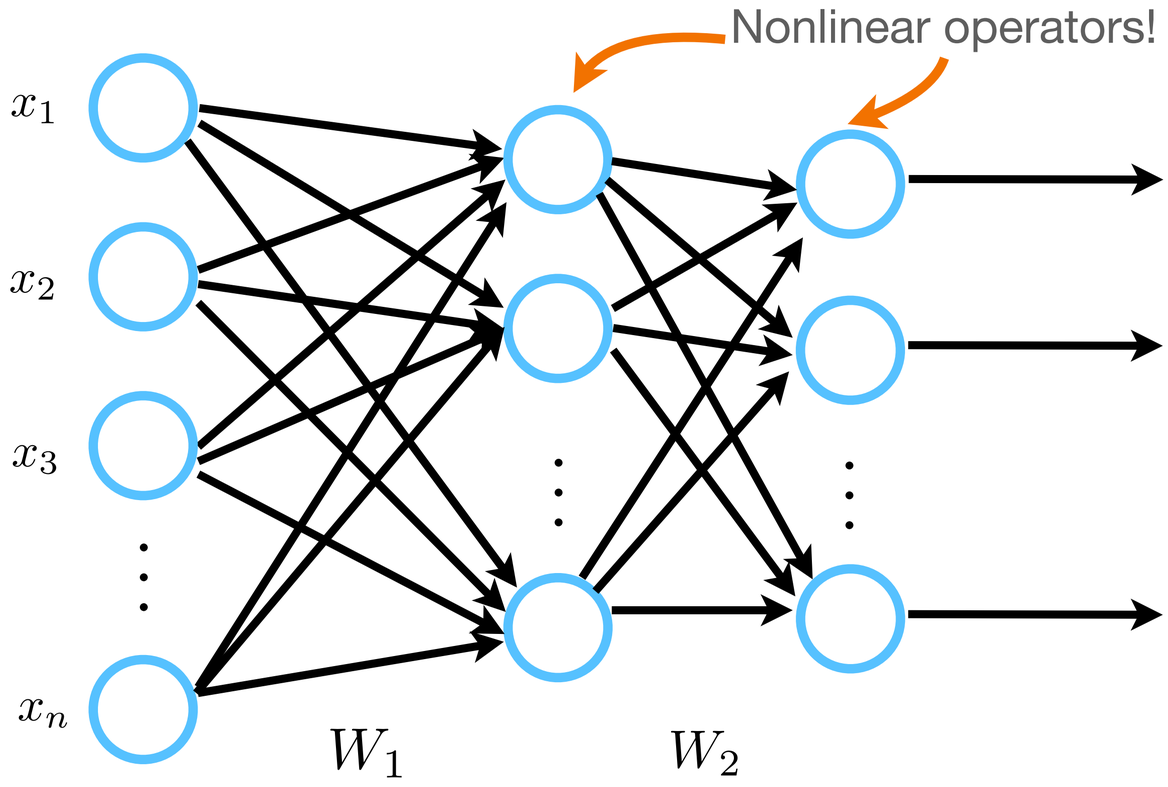

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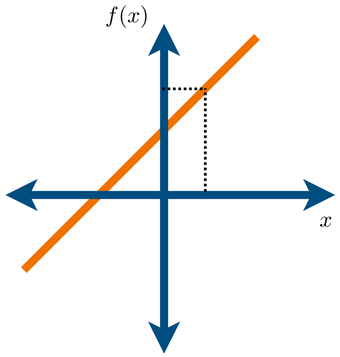

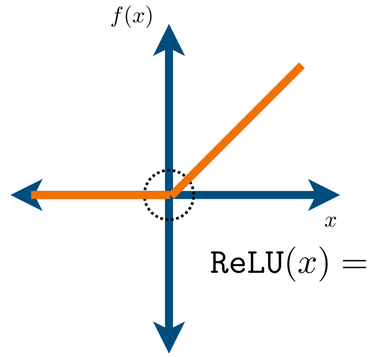

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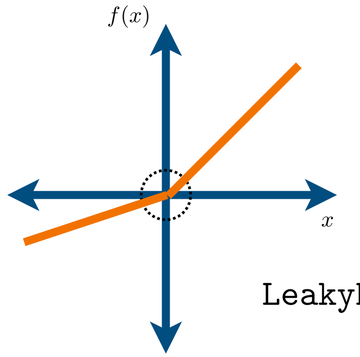
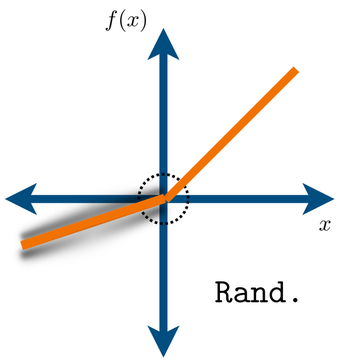


`LeakyReLU`



`Rand.` `LeakyReLU`

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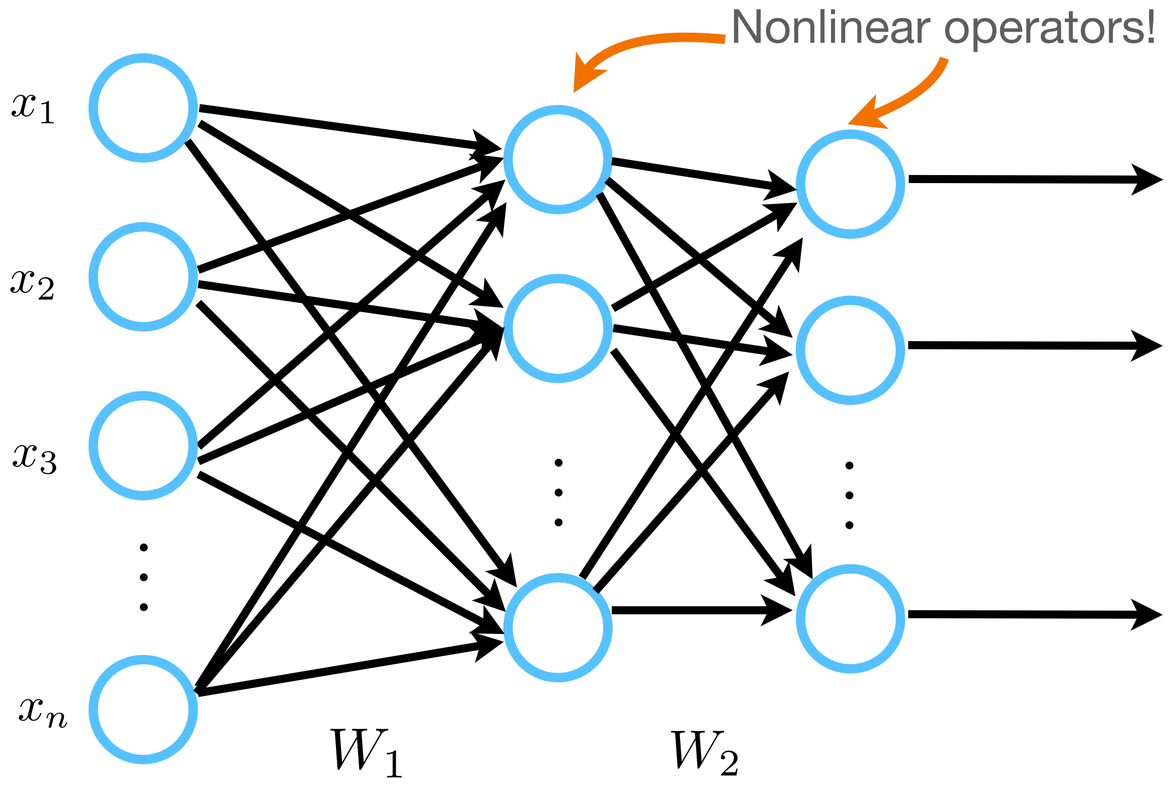

- What are the differences?
  - Some modules have simpler derivates than others (affects optimization)

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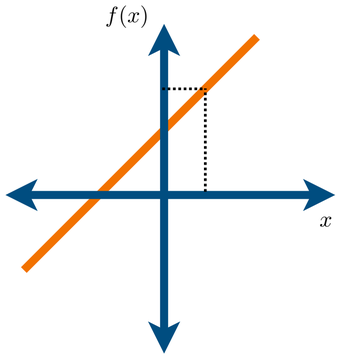

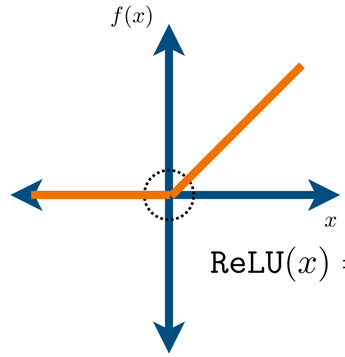

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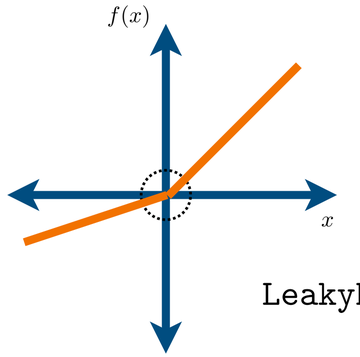

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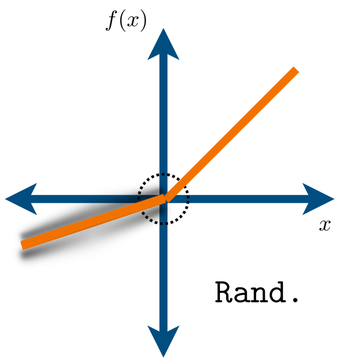

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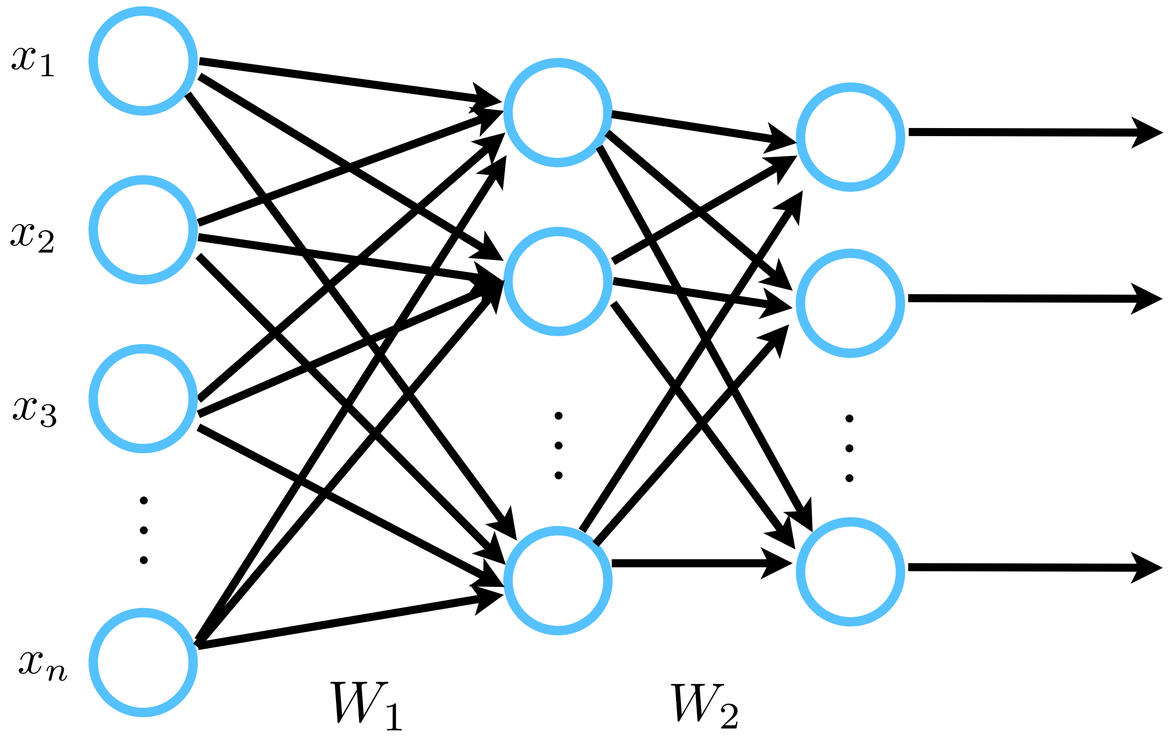

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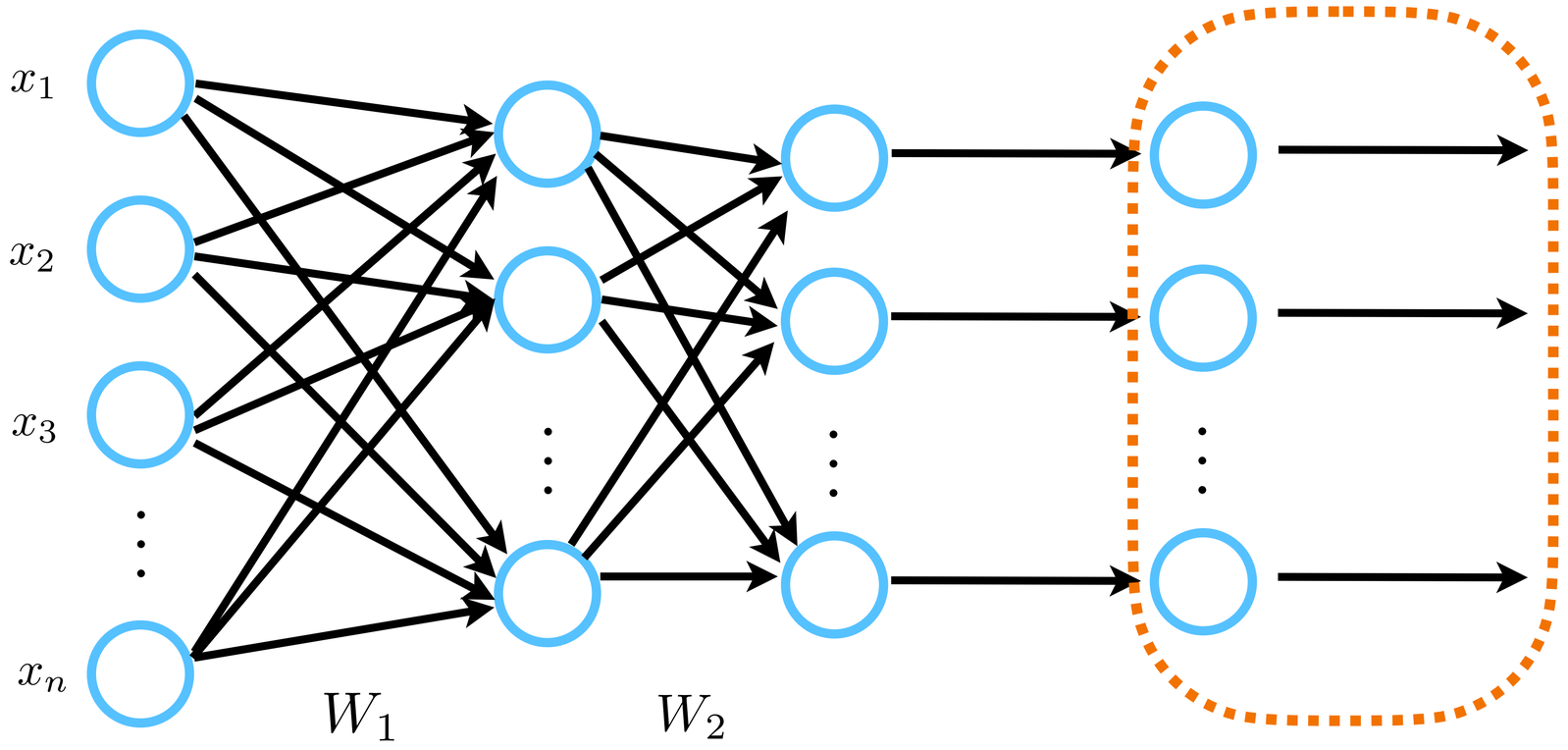

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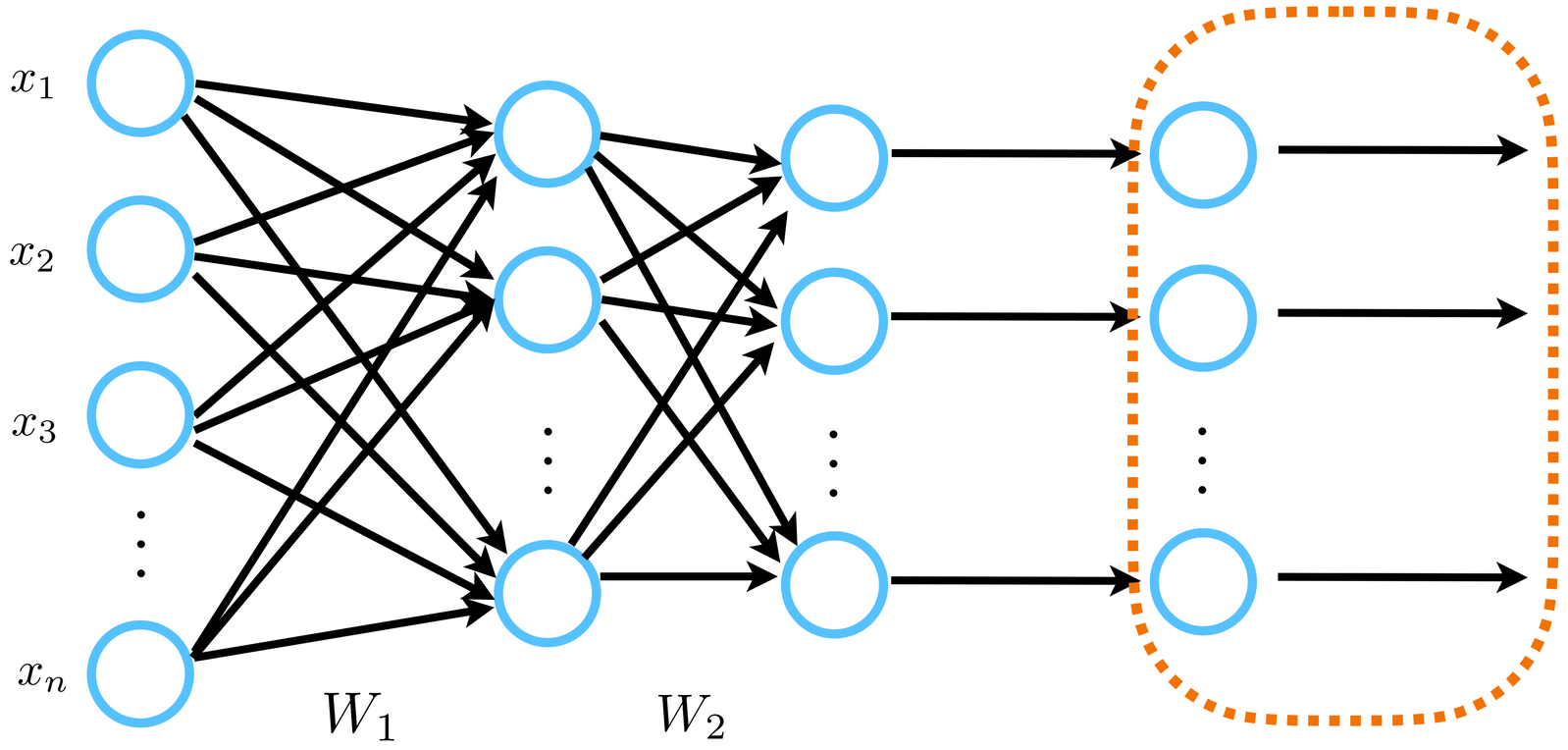

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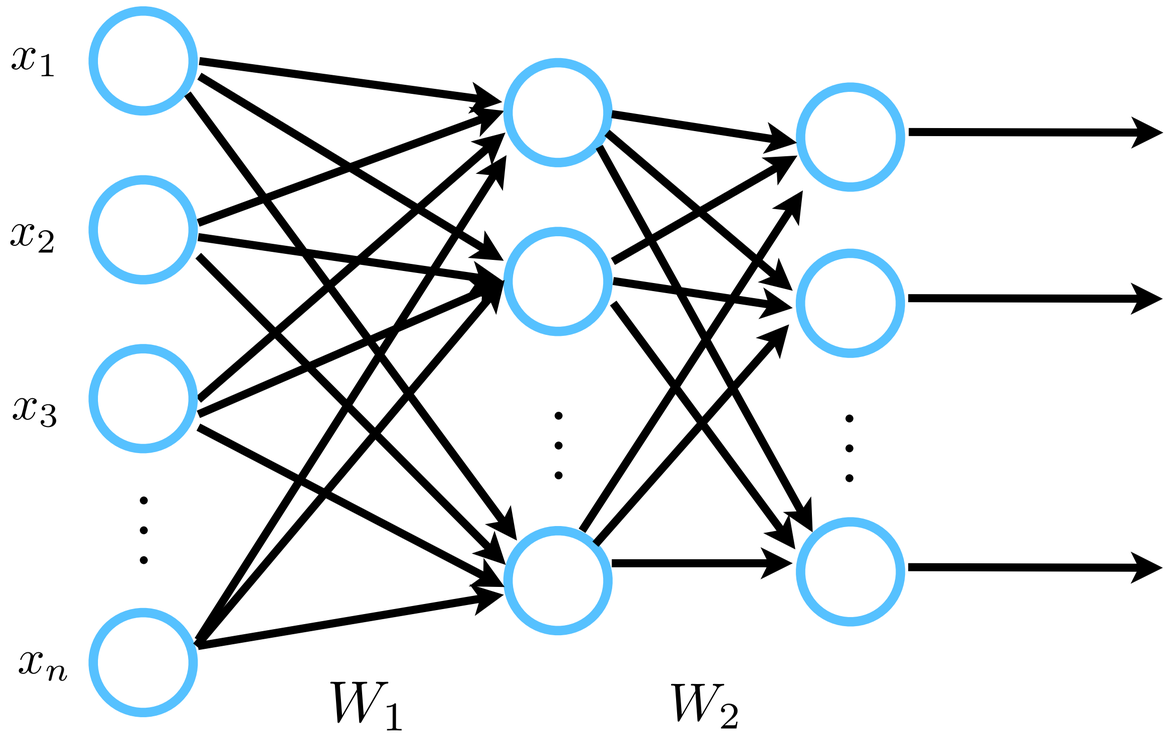
$$\texttt{softmax}(z)_i = \frac{e^{z_i}}{\sum_j e^{z_j}}$$

- Even for this module, there are alternatives: sparsemax, sparse projections onto the simplex, ..
- Out of scope

What are our options here wrt modules?



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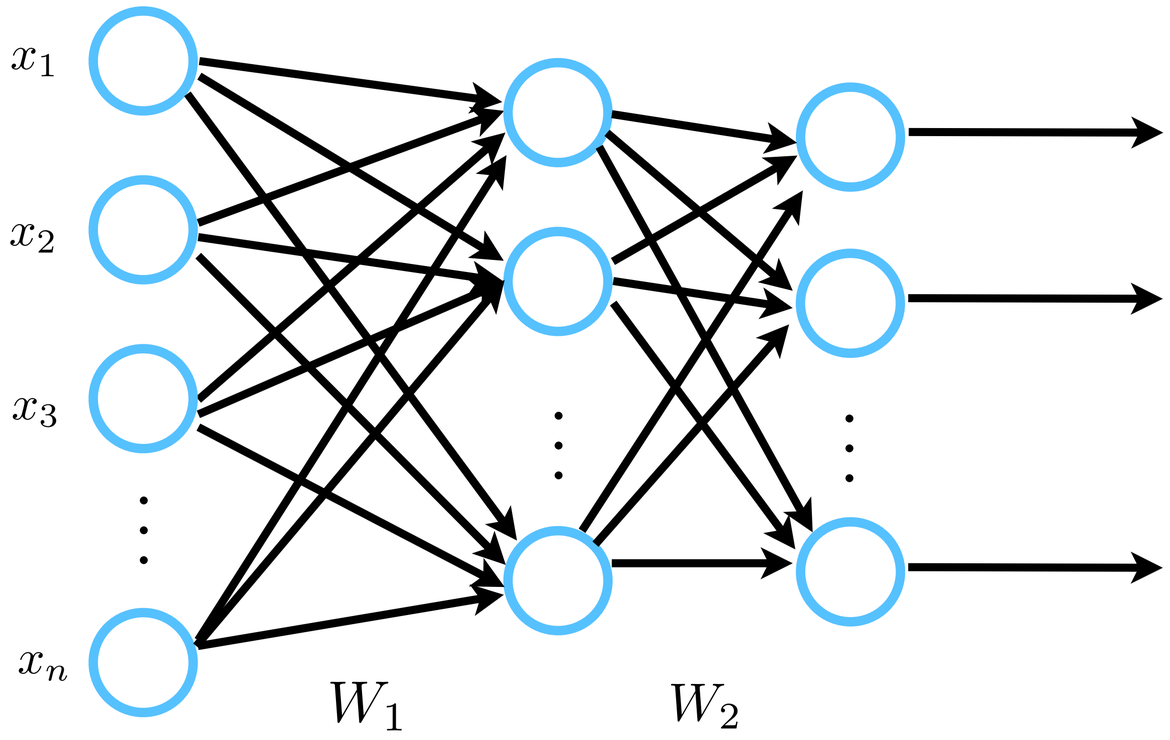

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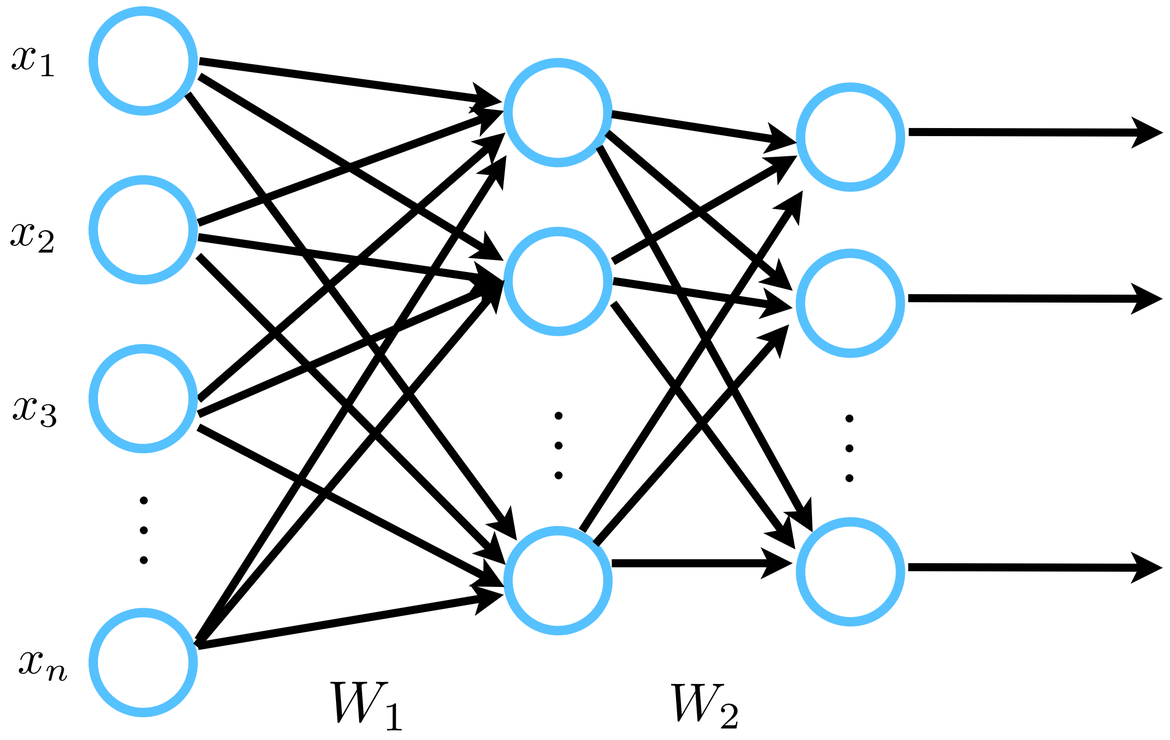

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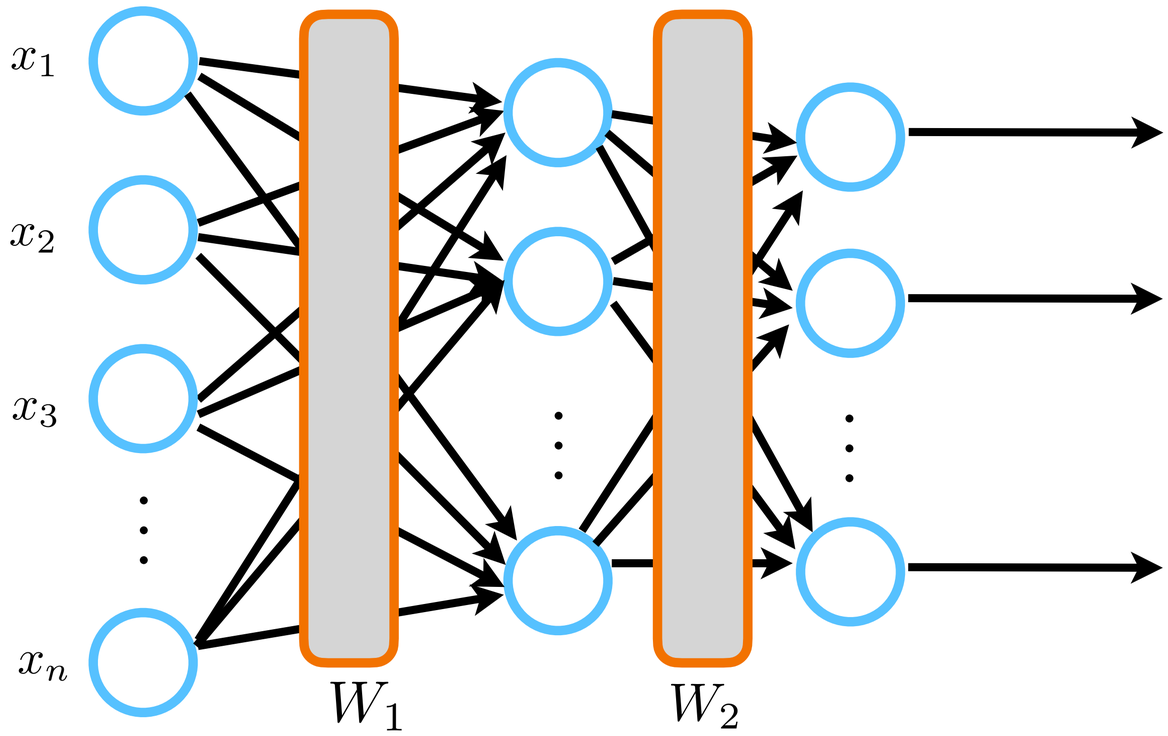

$$\mu_B = \frac{1}{B}\sum_{i=1}^{B} x_i$$

$$\sigma_B = \frac{1}{B}\sum_{i=1}^{} (x_i - \mu_B)^2$$

$$\widehat{x}_i = \frac{x_i - \mu_B}{\sqrt{\sigma_B^2 + \varepsilon}}$$

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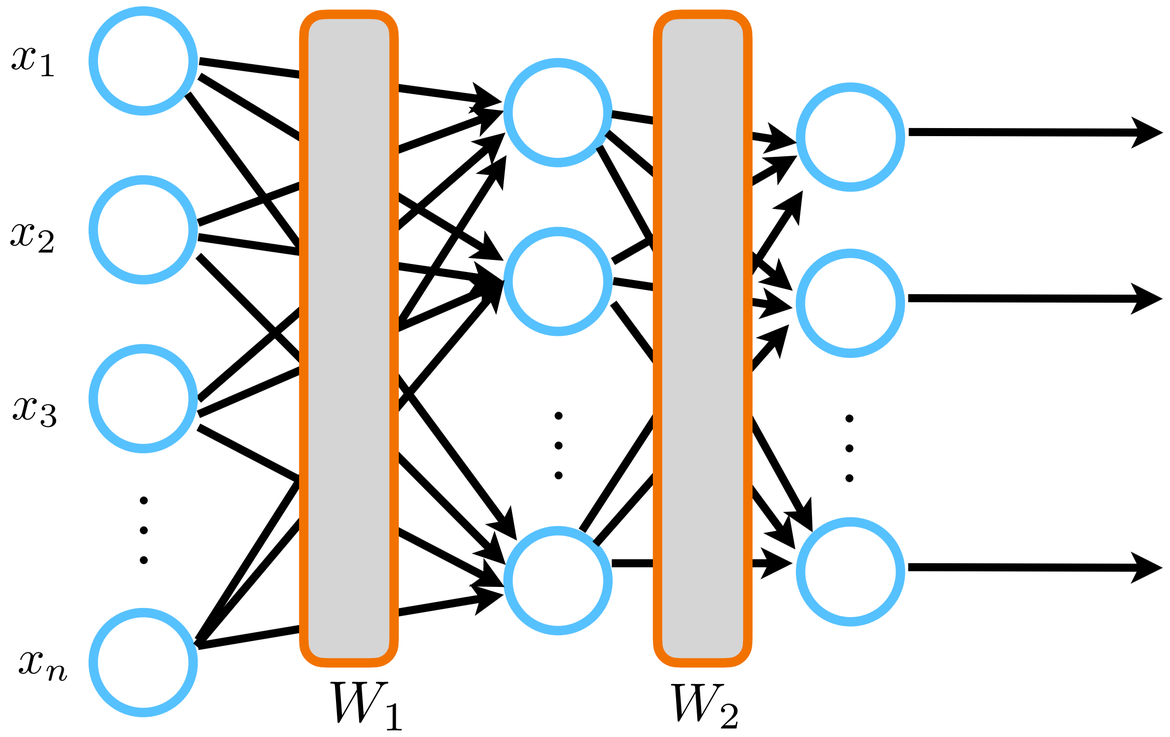

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Both techniques increase significantly the performance of a neural network (e.g., BN allows larger step sizes)

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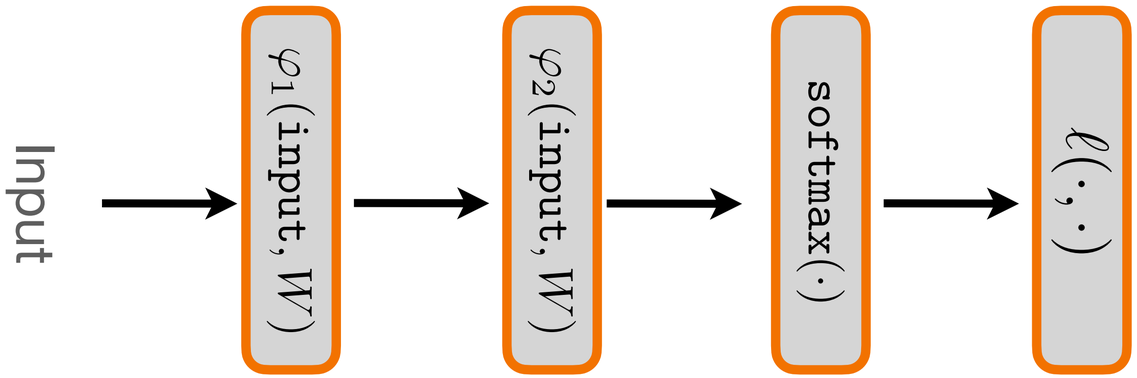
“But how do we train a neural network?”

Motivation: Gradient descent for MLPs

$$\min_{W_i} f(W_1, W_2) := \frac{1}{n} \sum_{i=1}^{n} \ell(\widehat{y}_i,\ y_i) \quad \text{where} \quad \widehat{y}_i = \texttt{softmax}\left(\sigma\left(W_2 \cdot \sigma\left(W_1 \cdot x_i\right)\right)\right)$$

– Using modules:

$\varphi_1(\texttt{input}, W) = \sigma(W_1 \cdot x_i)$
$\varphi_2(\texttt{input}, W) = \sigma(W_2 \cdot \varphi_2(\cdot))$



$$\begin{aligned}
\nabla f_i(x) &= \frac{\partial \ell(y_i, \widehat{y}_i)}{\partial W} \\
&= \frac{\partial \ell(y_i, \widehat{y}_i)}{\partial \texttt{softmax}(\cdot)} \cdot \frac{\partial \texttt{softmax}(\cdot)}{\partial W} \\
&= \frac{\partial \ell(y_i, \widehat{y}_i)}{\partial \texttt{softmax}(\cdot)} \cdot \frac{\partial \texttt{softmax}(\cdot)}{\partial \varphi(\cdot, W_2)} \cdot \frac{\partial \varphi(\cdot, W_2)}{\partial W} \\
&= \dots
\end{aligned}$$

(chain rule of derivatives)

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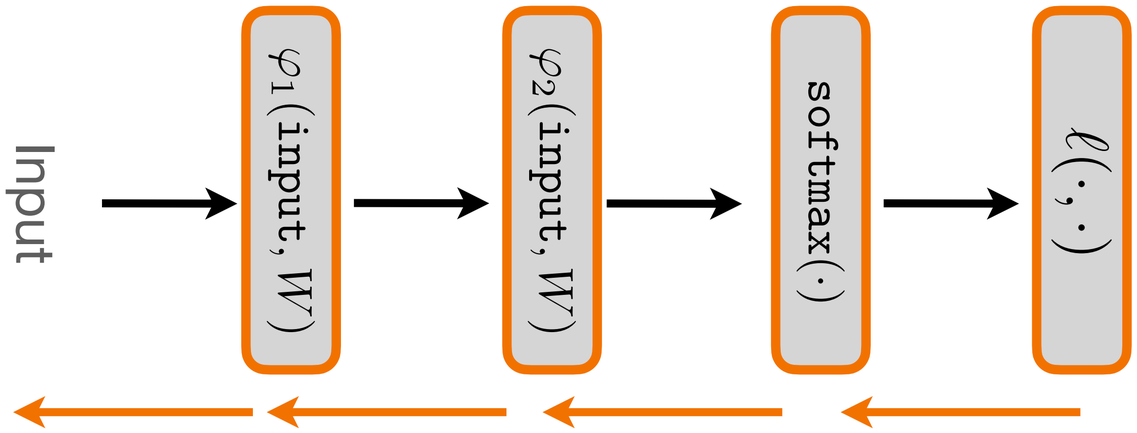

(backward pass on modules!)

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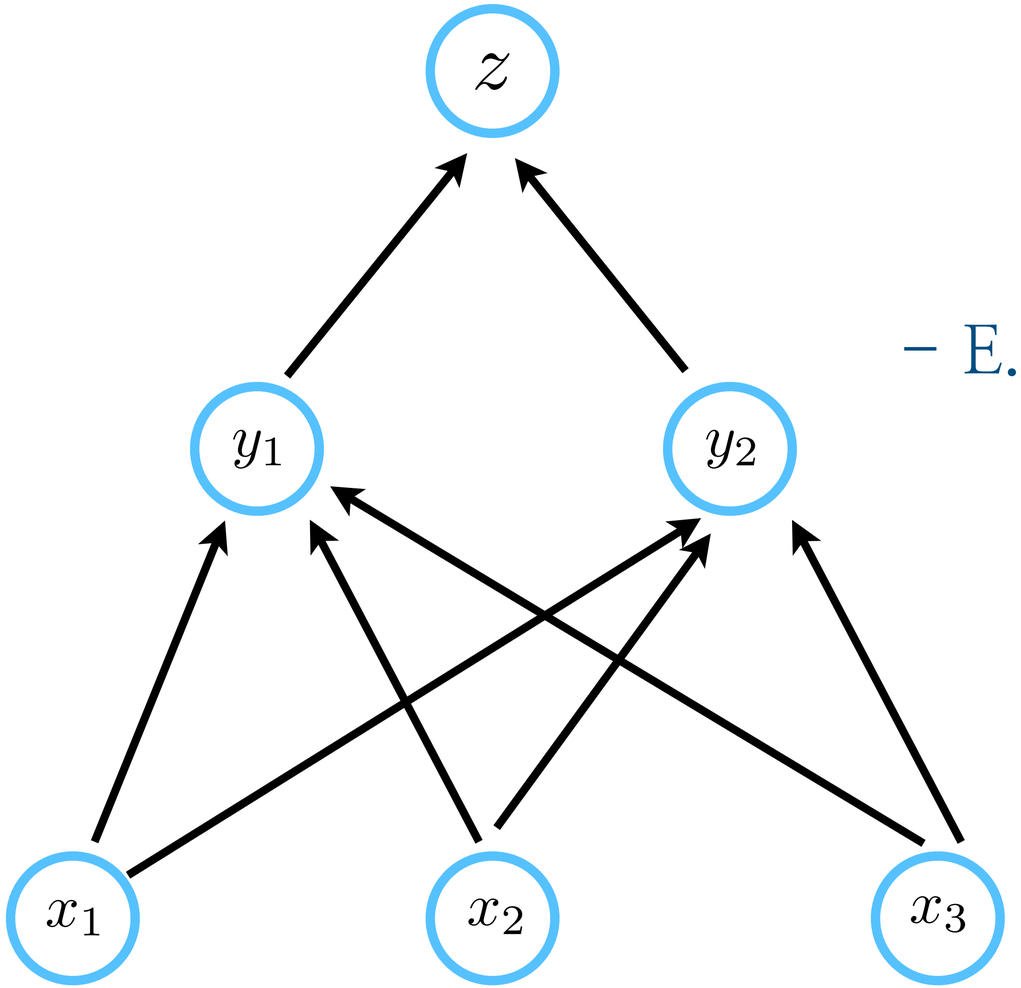

$$\frac{\partial z}{\partial x} = \frac{\partial z}{\partial y} \cdot \frac{\partial y}{\partial x}$$

– E.g.,

$$\frac{\partial z}{\partial x_3} = \frac{\partial z}{\partial y_1} \cdot \frac{\partial y_1}{\partial x_3} + \frac{\partial z}{\partial y_2} \cdot \frac{\partial y_2}{\partial x_3}$$

(Follow all relevant paths)

Backpropagation = Gradient descent

(Just done efficiently on graphs, without redoing calculations)

Overview

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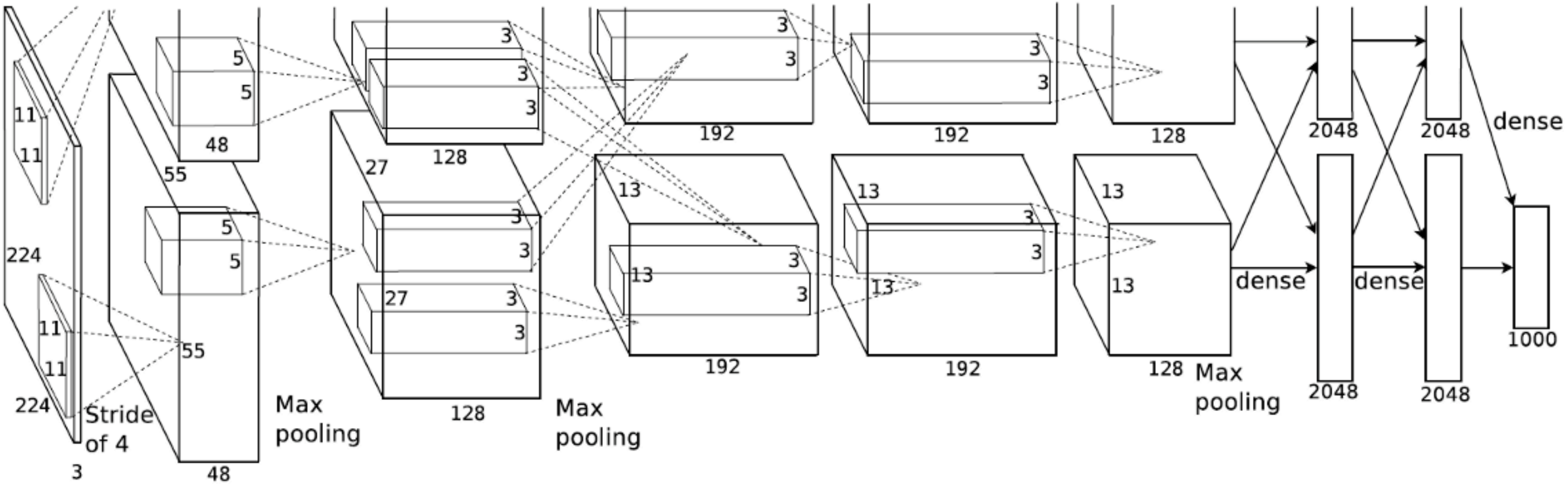

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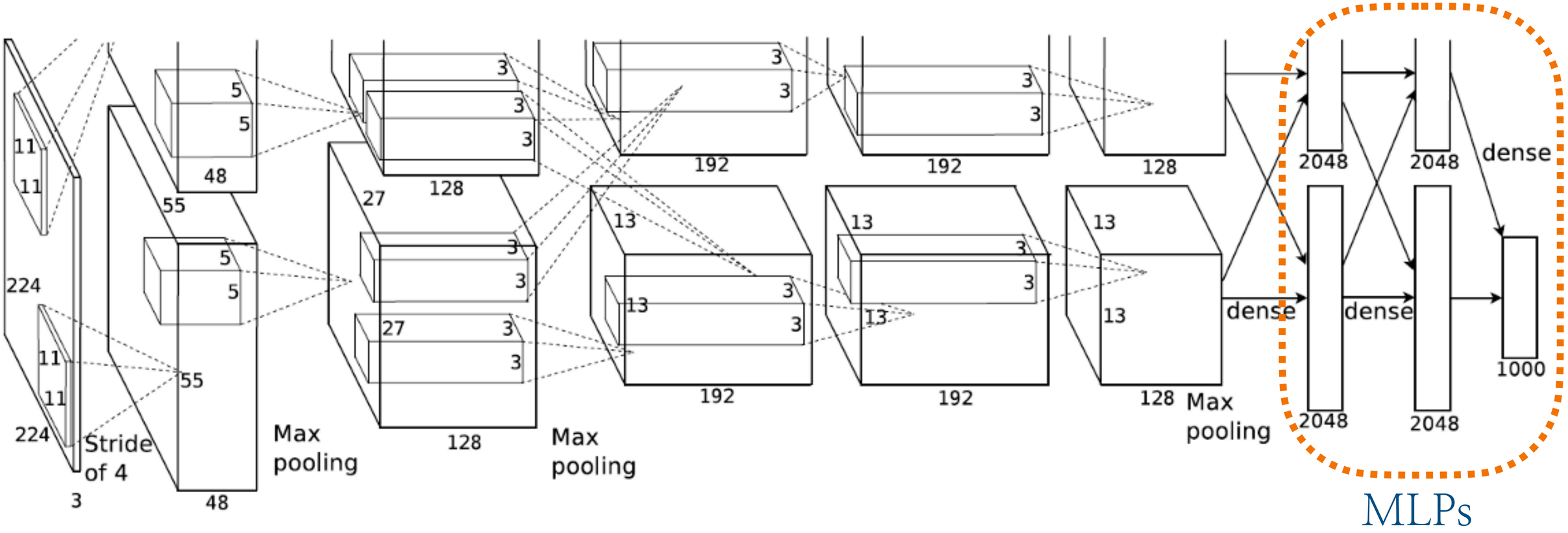

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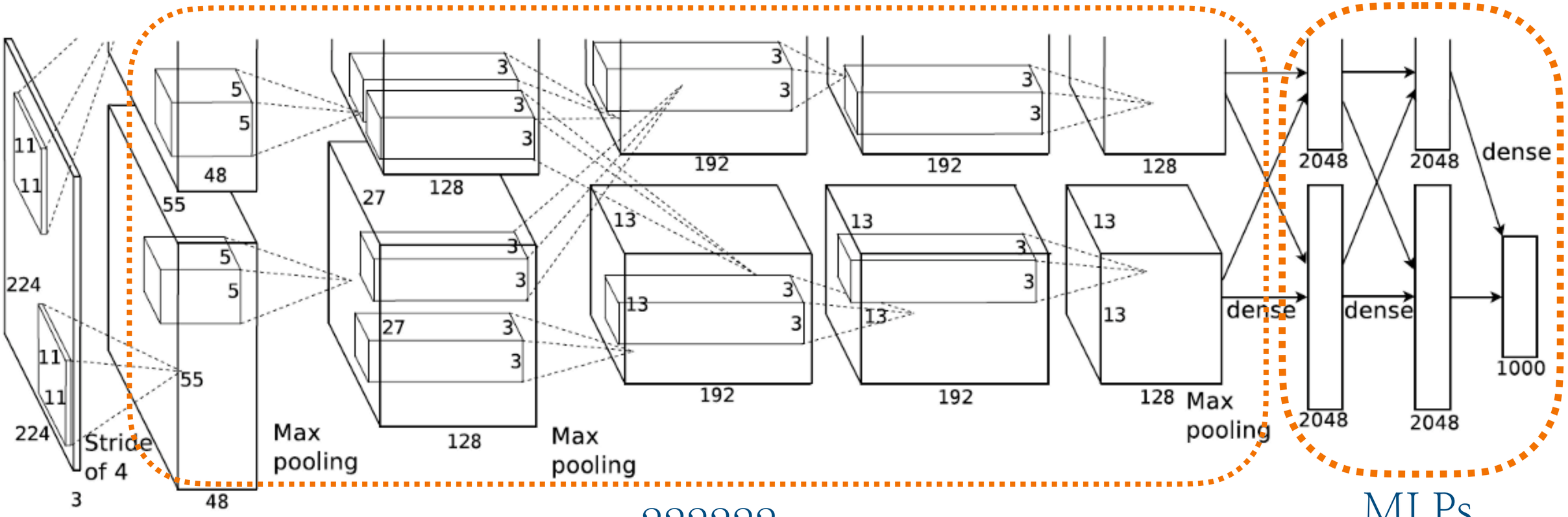

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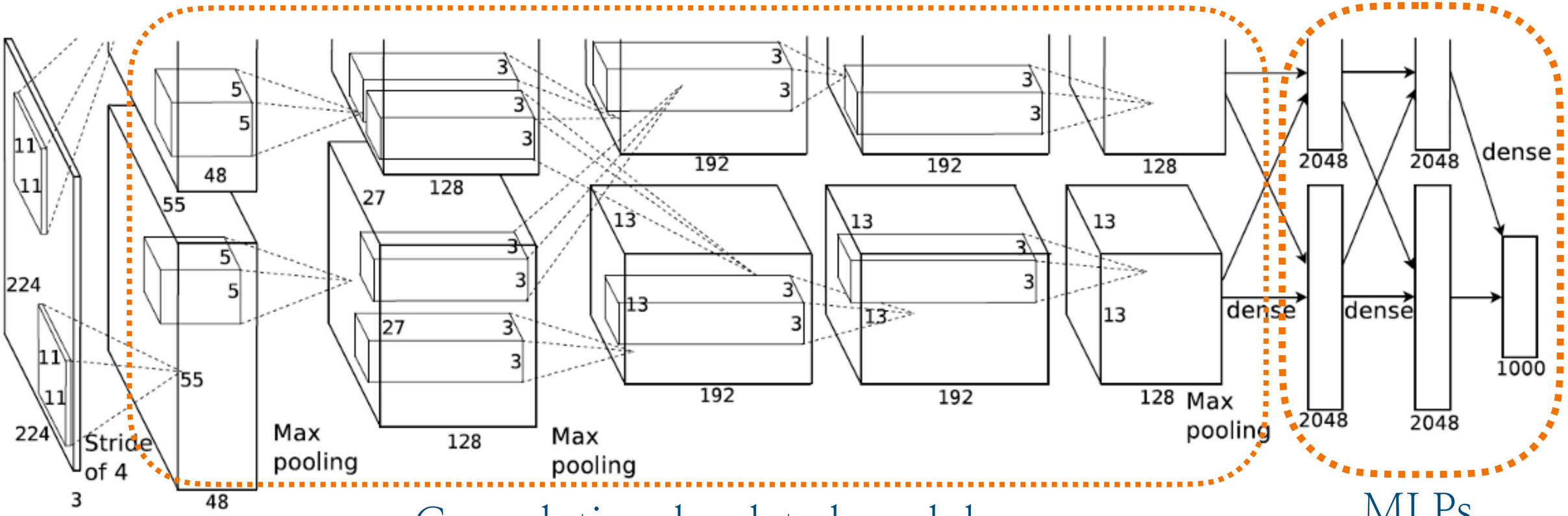

Convolutional-related modules

MLPs

Convolutional neural networks (CNNs)

- Another type of neural networks

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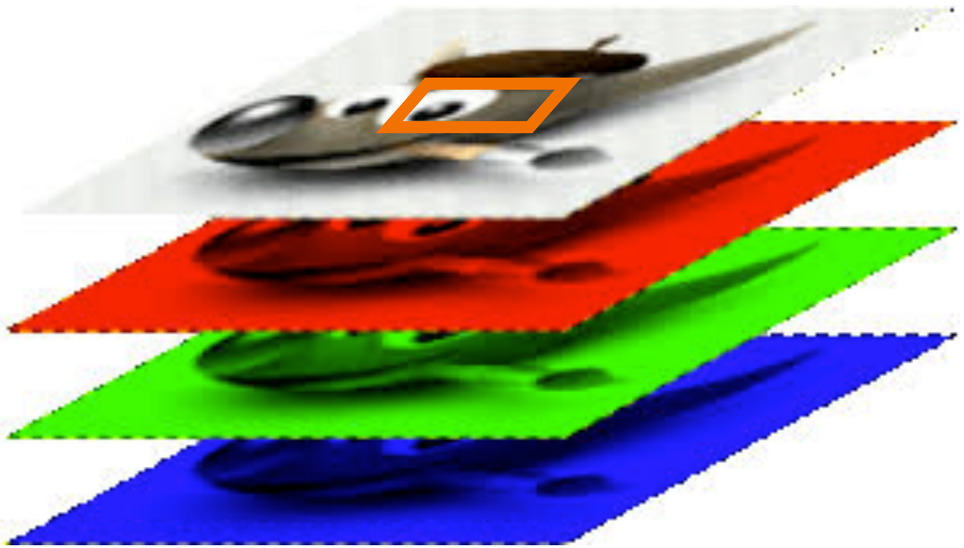
  Convolutions preserve such spatial structure and create relevant features
- Secondary but important module: pooling – robustifies against local variances

Images and their spatial properties



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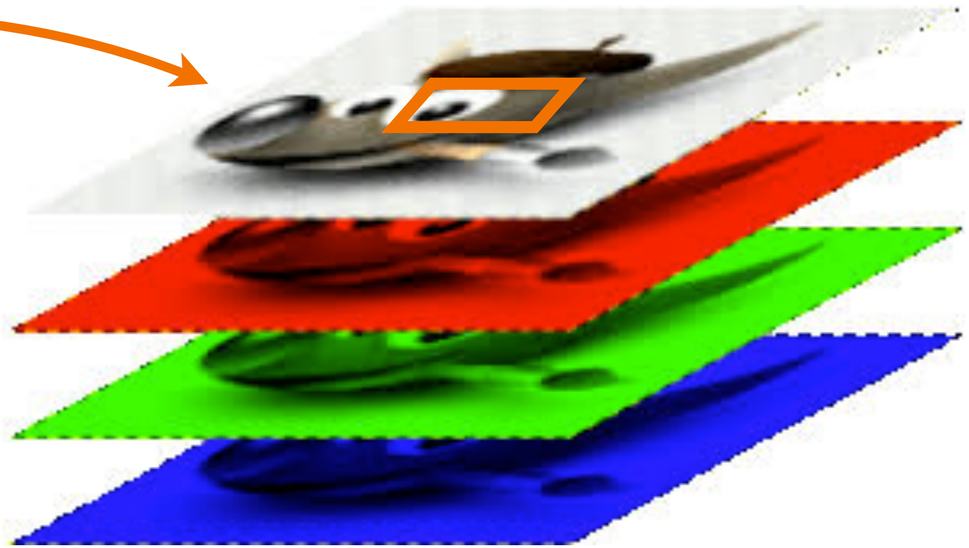
Original image



Images and their spatial properties

Original image

Decomposition
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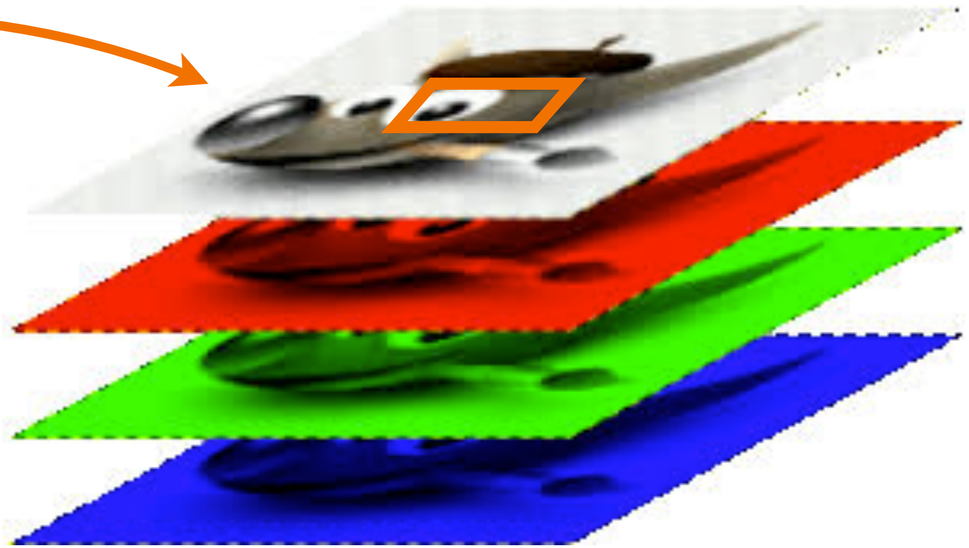

Images and their spatial properties

Neighboring pixels
are locally correlated

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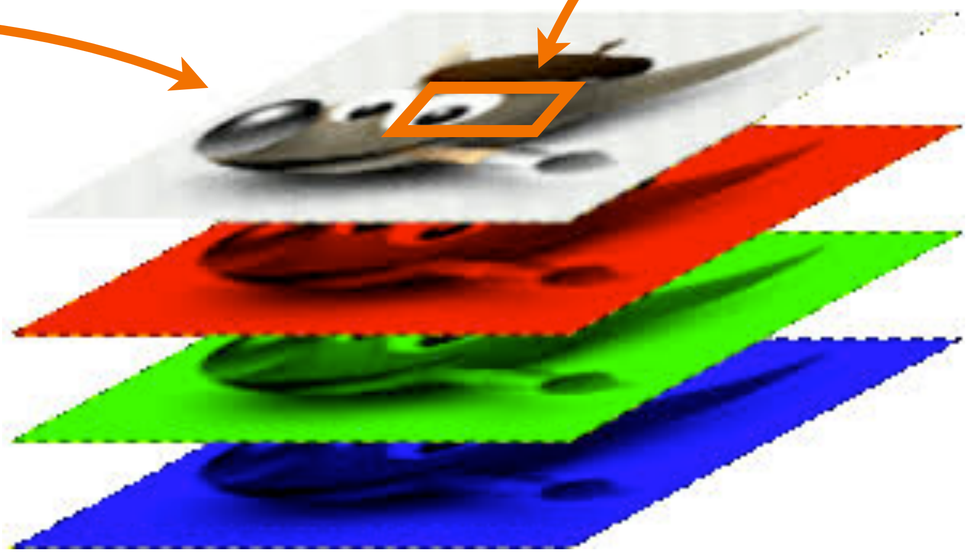

Filters/Kernels

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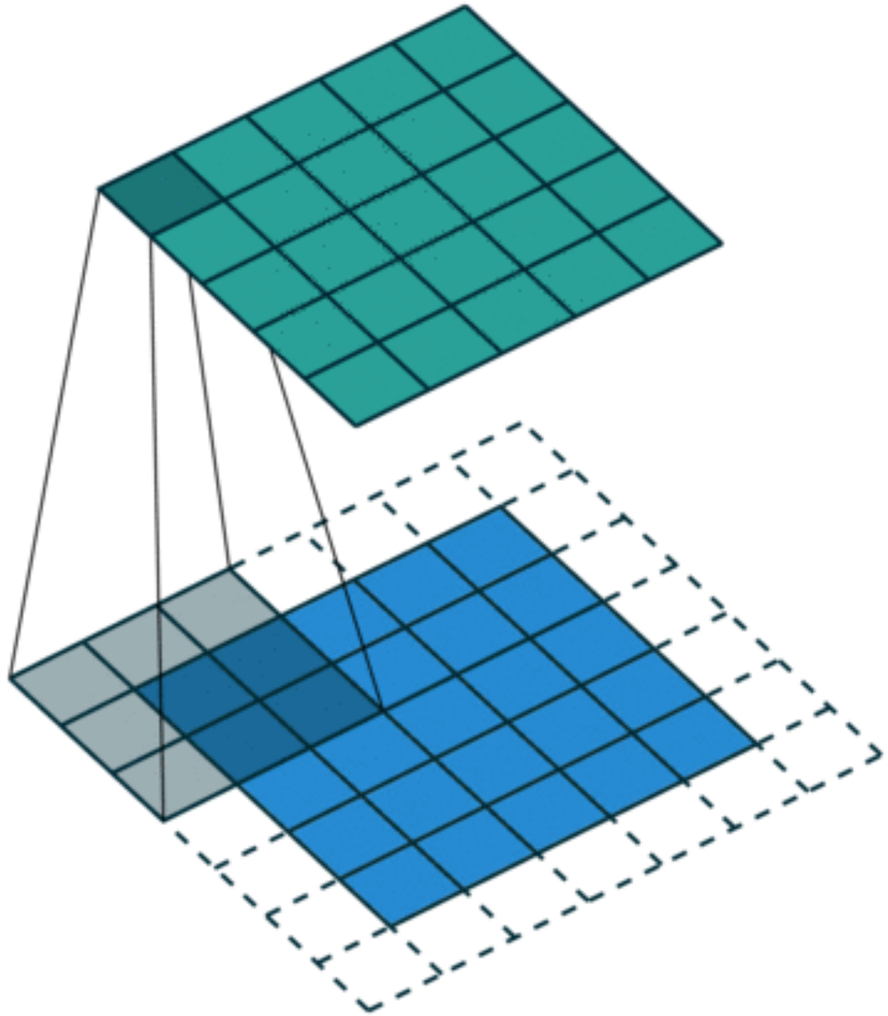

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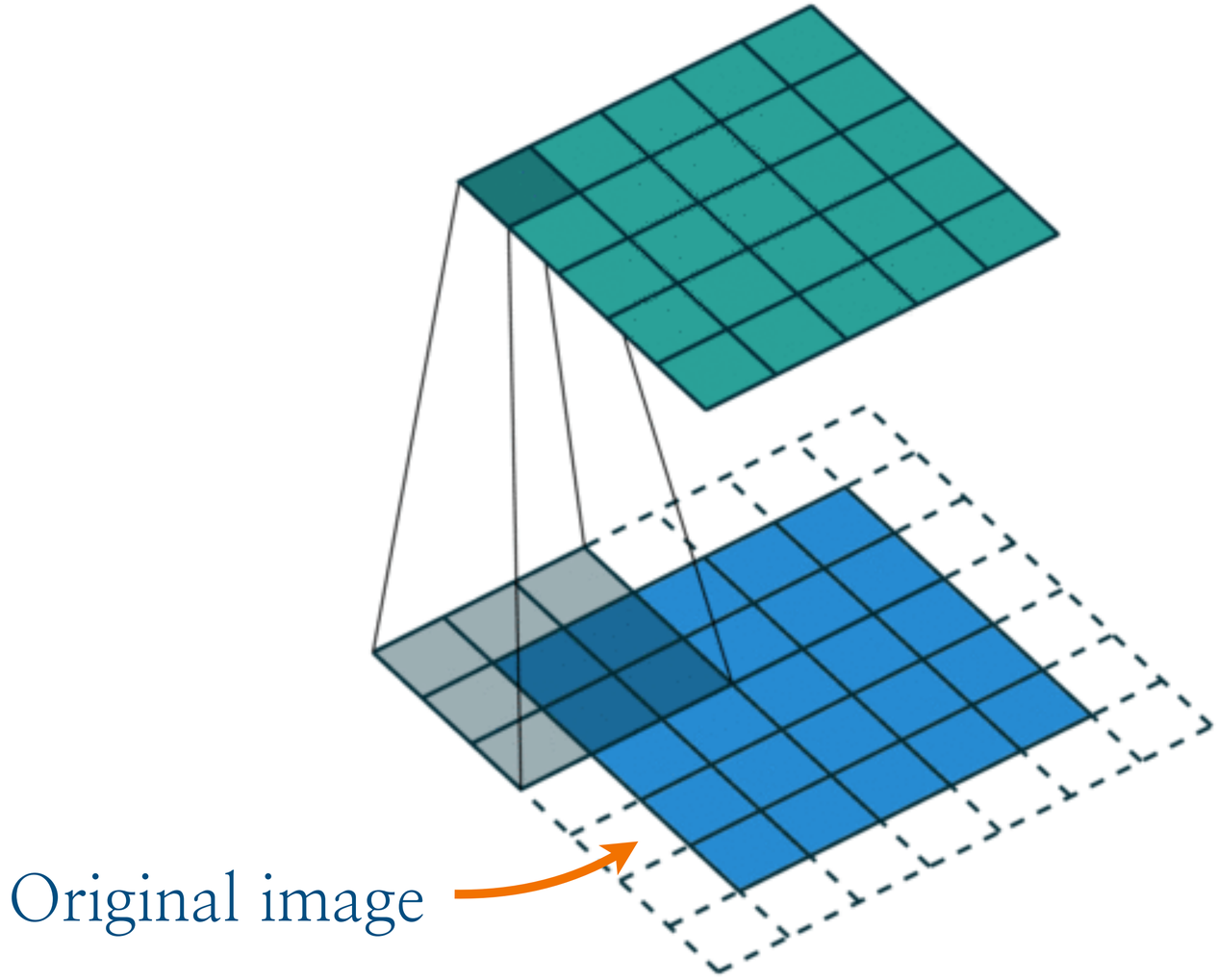

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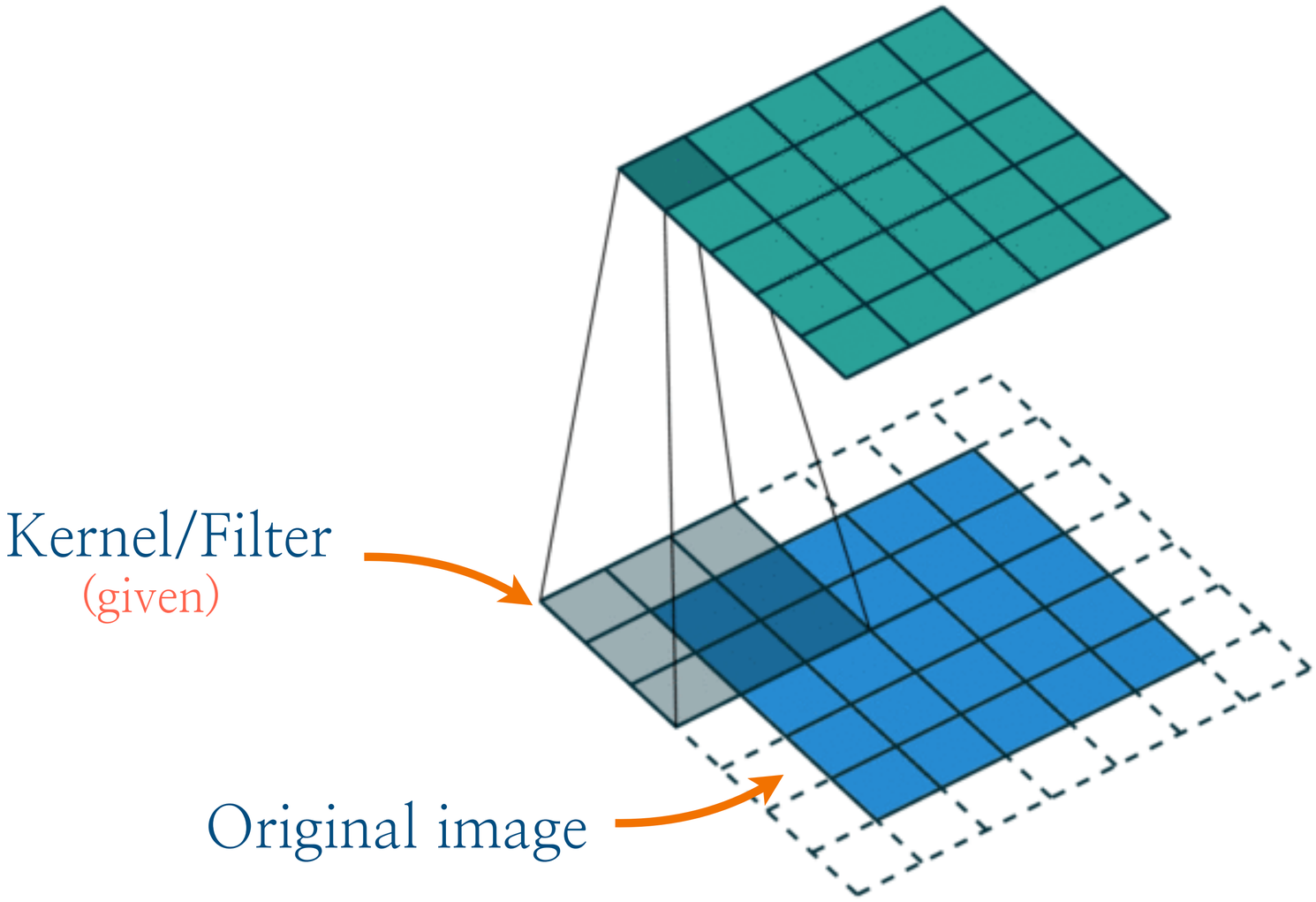

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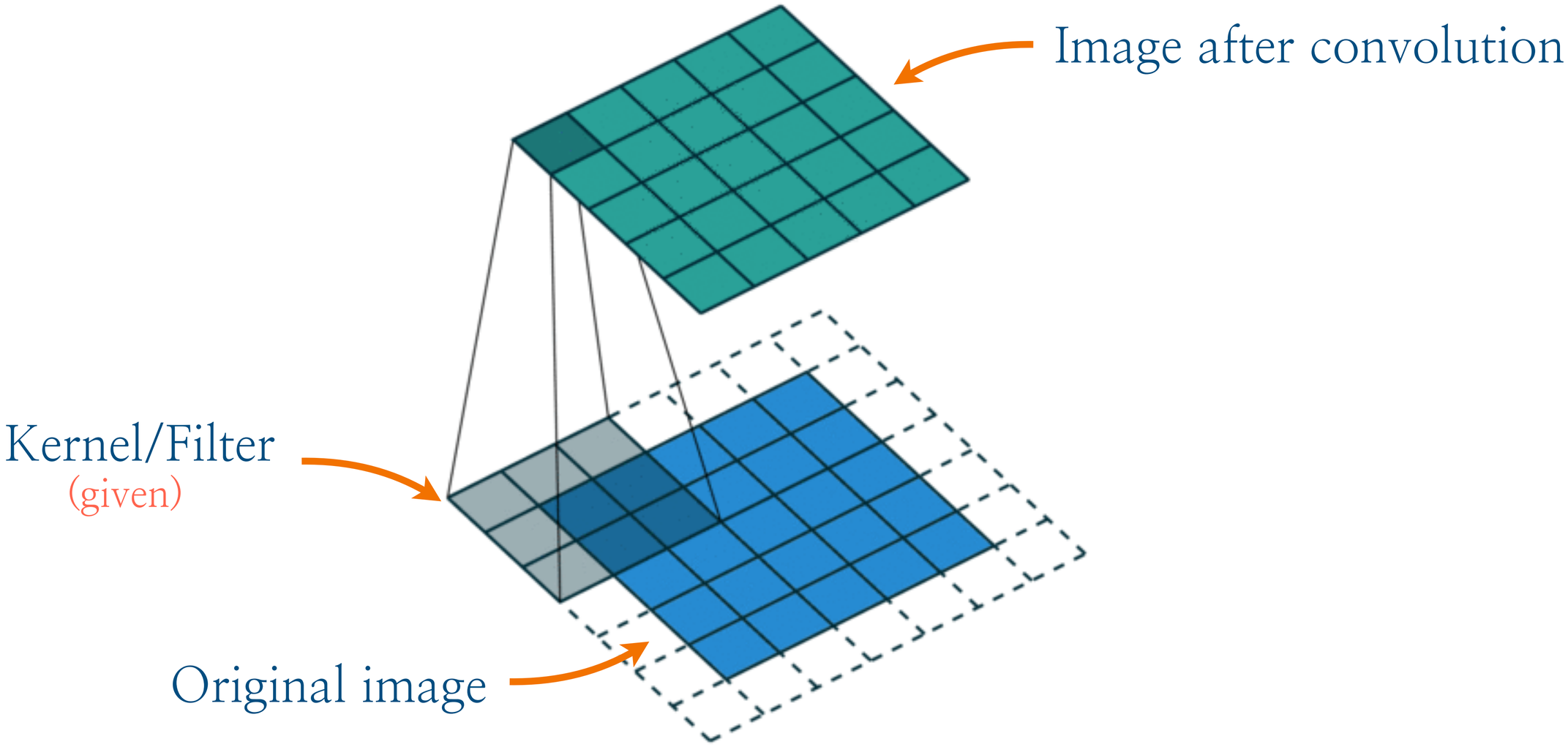
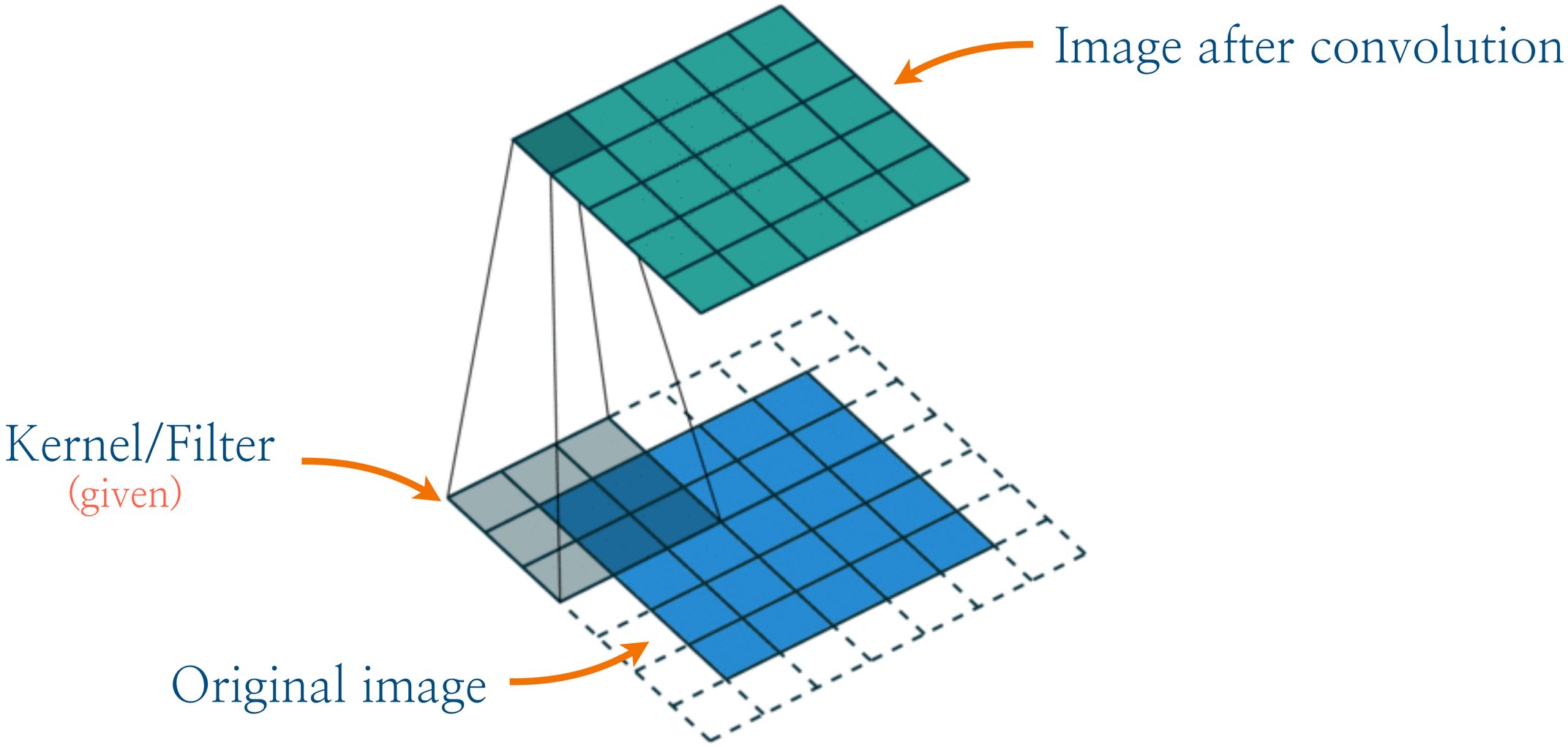


Convolution operation: Basic operation



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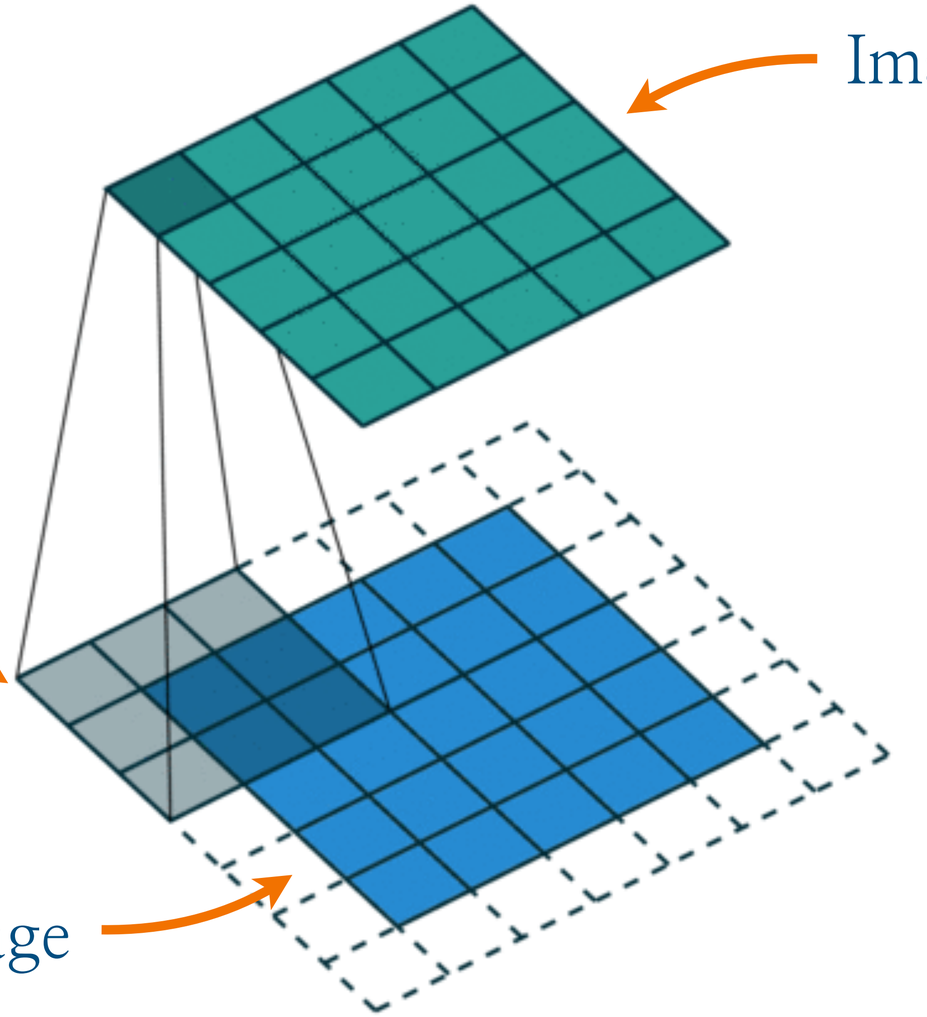
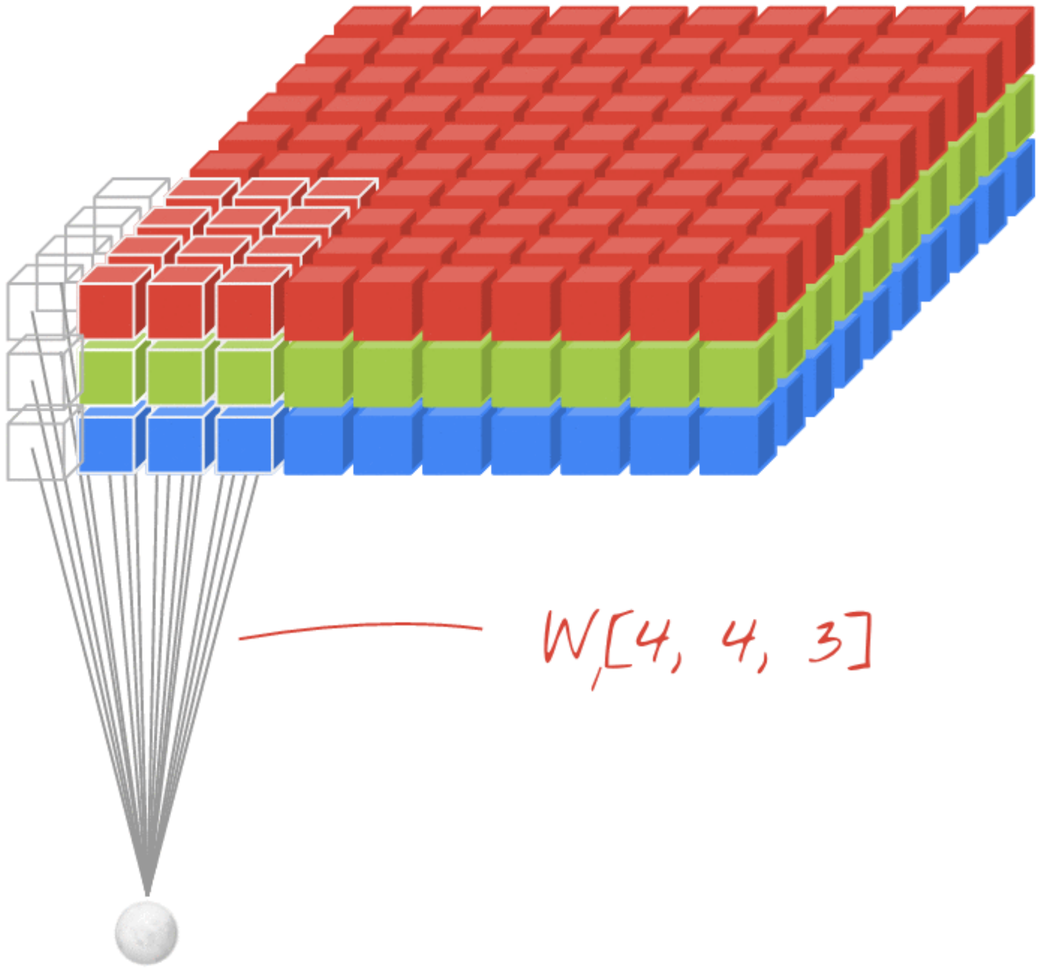


Input				Kernel			Output	
0	1	2	*	0	1	=	19	25
3	4	5		2	3		37	43
6	7	8						

Convolution operation: Channels and multiple filters



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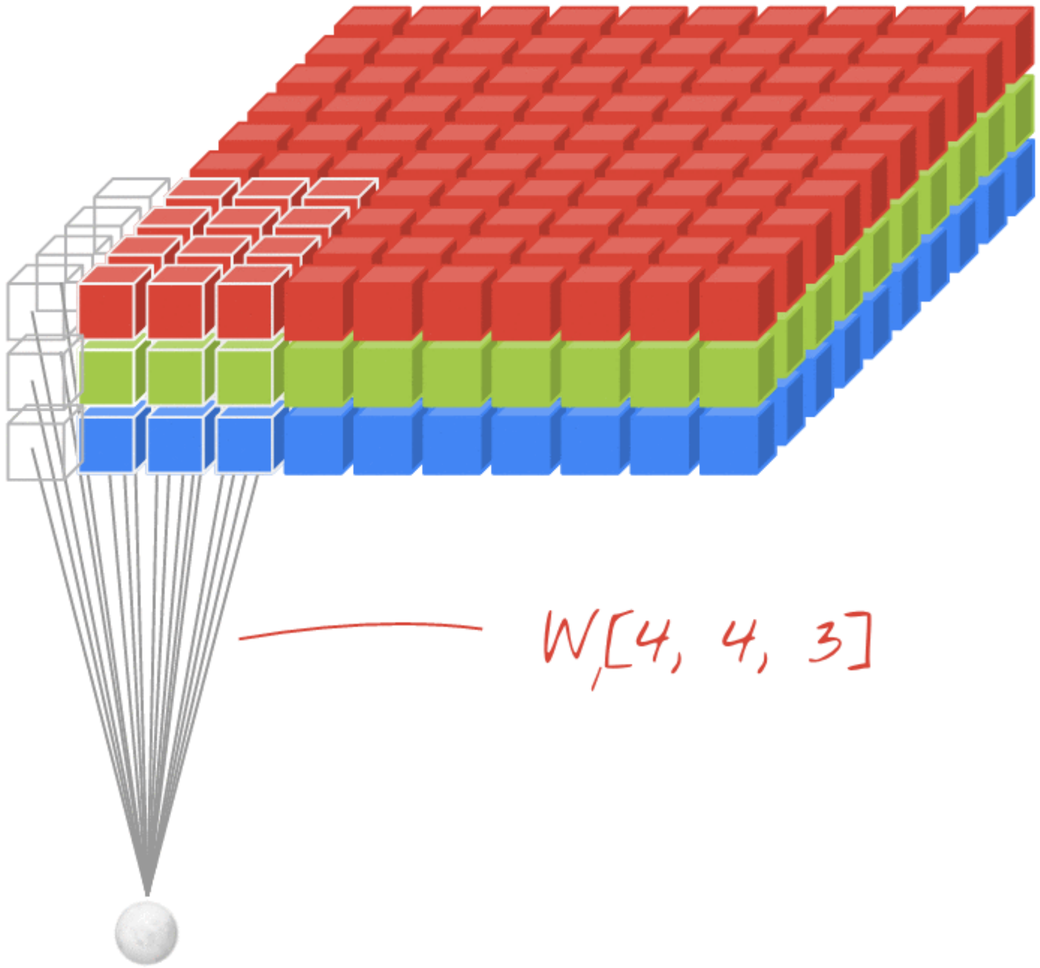

Convolution operation

- Fairly old concept of extracting information from images
- Example: Sobel filters

Horizontal

$$\begin{bmatrix} +1 & 0 & -1 \\ +2 & 0 & -2 \\ +1 & 0 & -1 \end{bmatrix}$$

Vertical

$$\begin{bmatrix} +1 & +2 & +1 \\ 0 & 0 & 0 \\ -1 & -2 & -1 \end{bmatrix}$$

- Applying Sobel kernels on original image = edge detection

Convolution operation

"Handcrafted filters/kernels"
(Sobel, Gaussian, smoothness, Gabor, etc.)

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Are they optimal for all computer vision applications?

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Learnable kernels

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.. we try to learn one:

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..based on our application.

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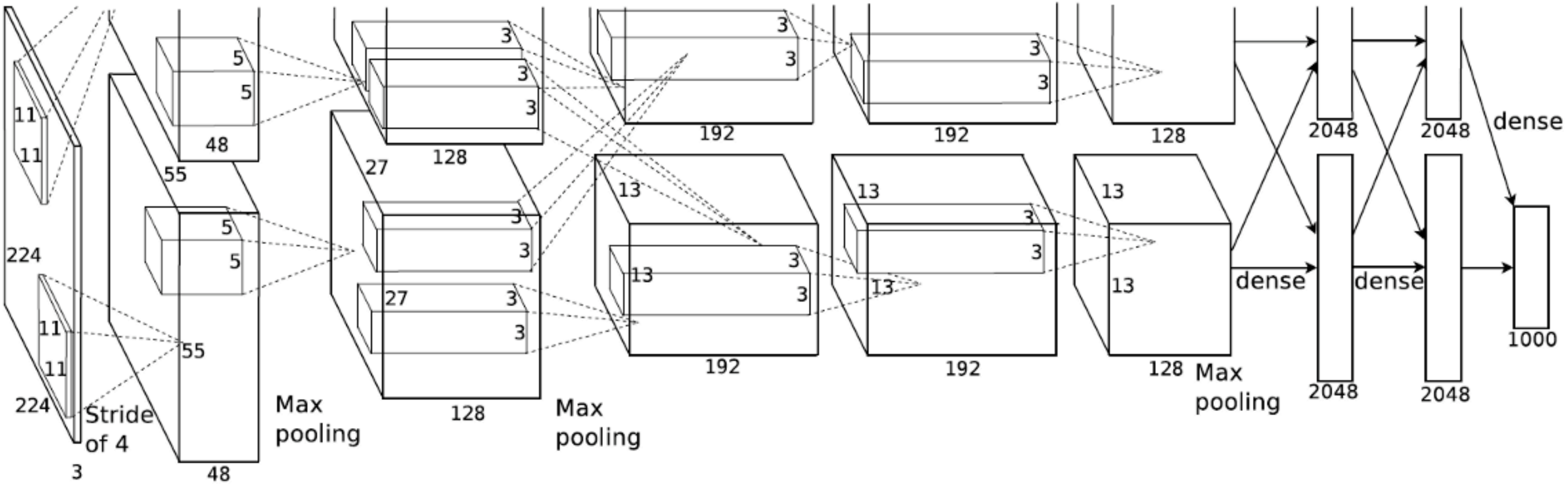
..based on our application.

- Convolution modules are fully differentiable!
- Good practices: Stride 1, 3x3 or 5x5 kernels work well

AlexNet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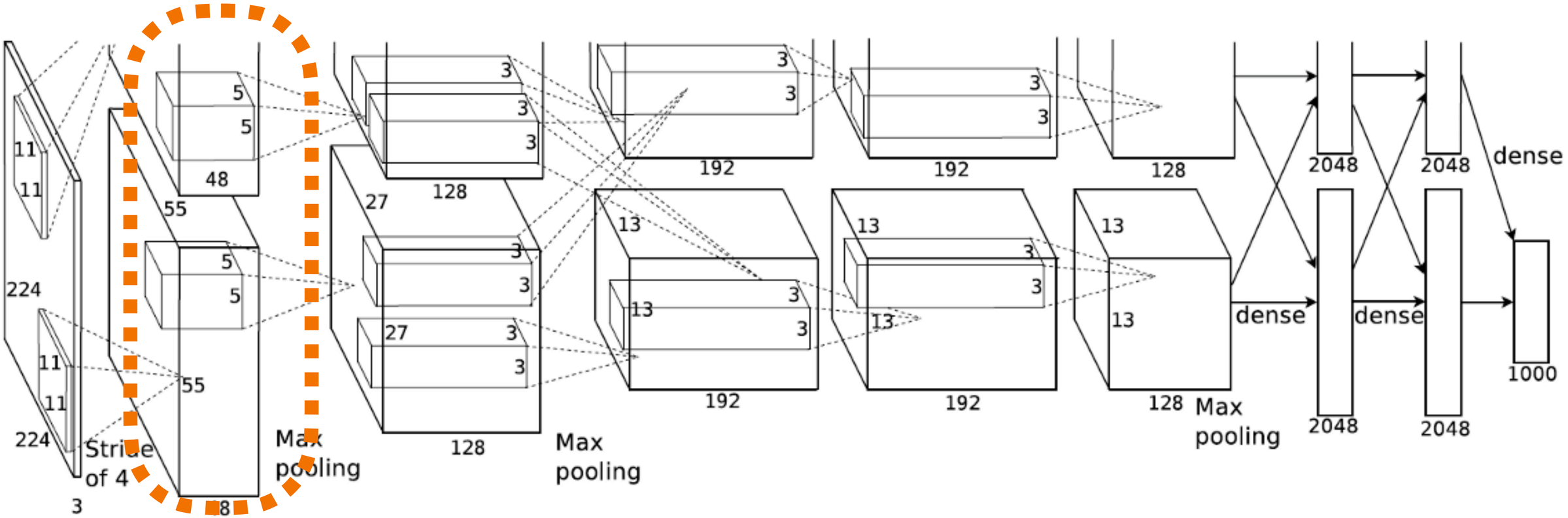
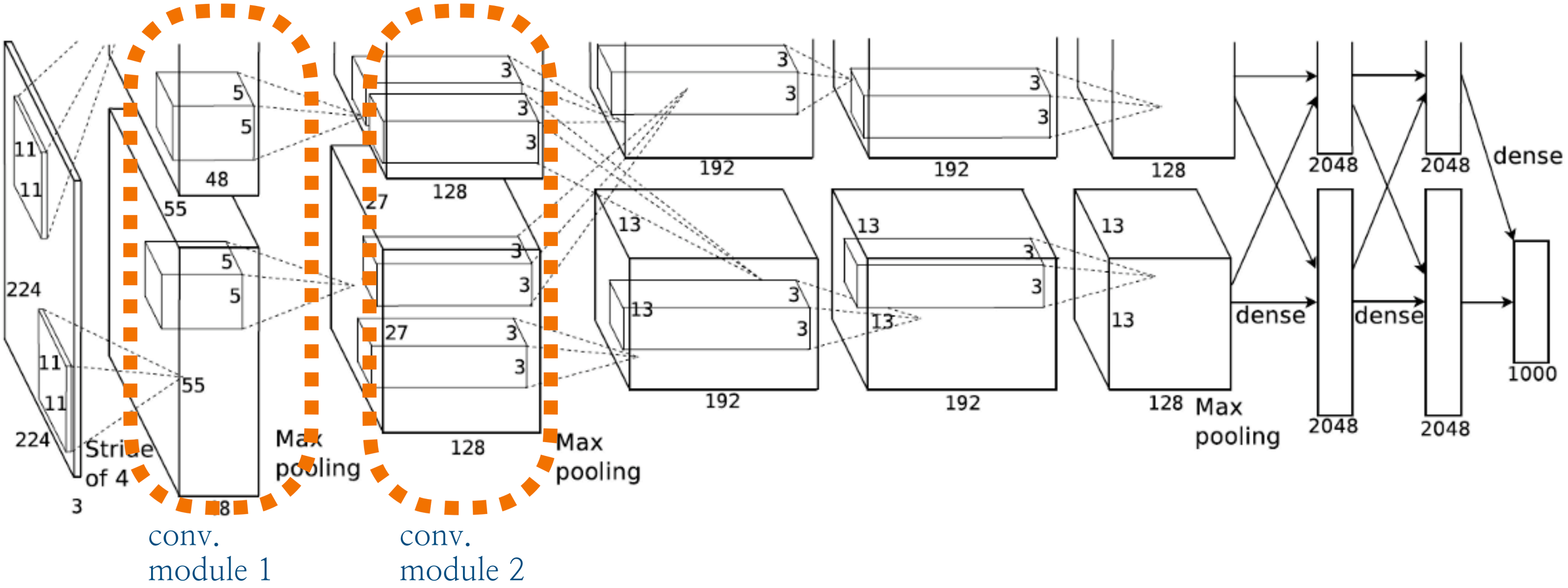
AlexNet



conv. module 1

AlexNet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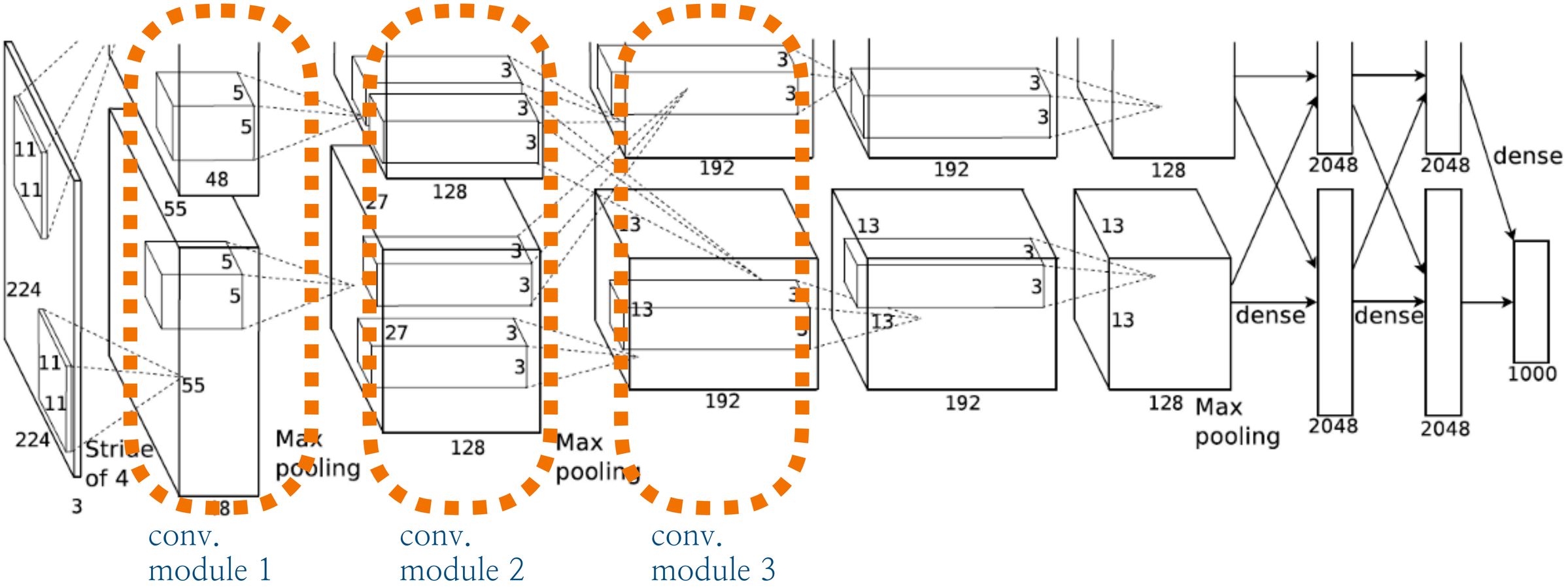
conv. module 1
conv. module 2

AlexNet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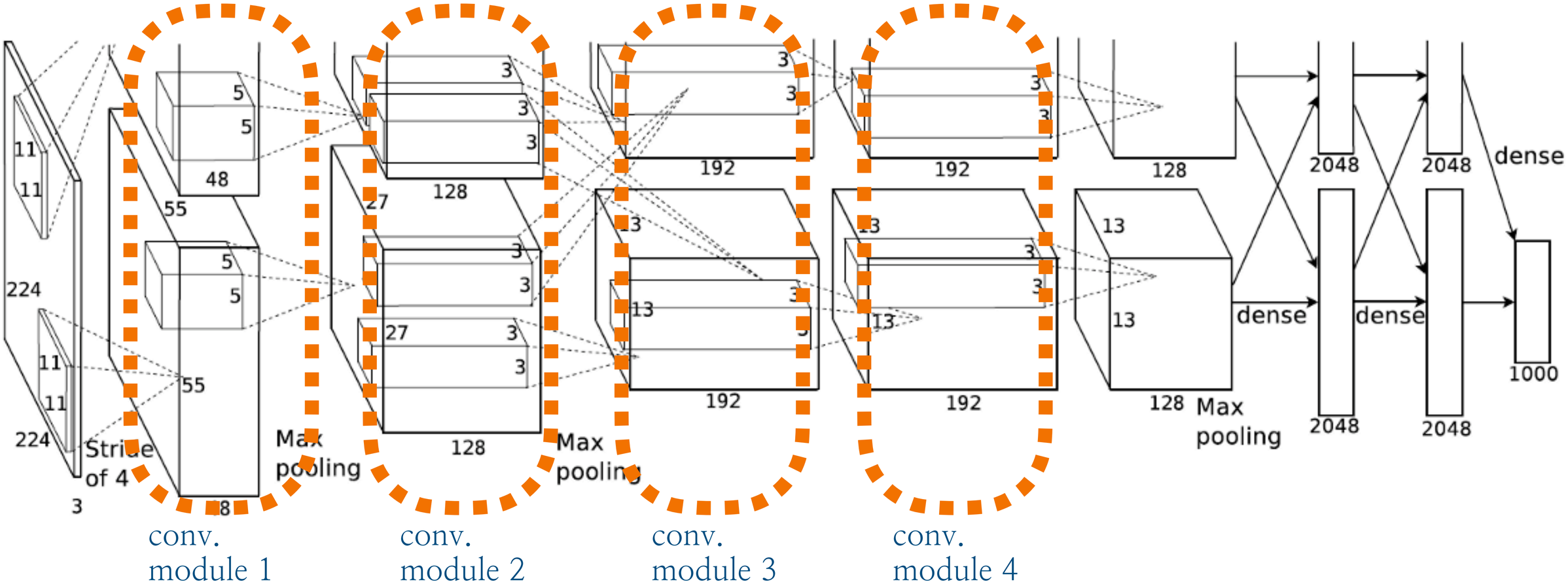
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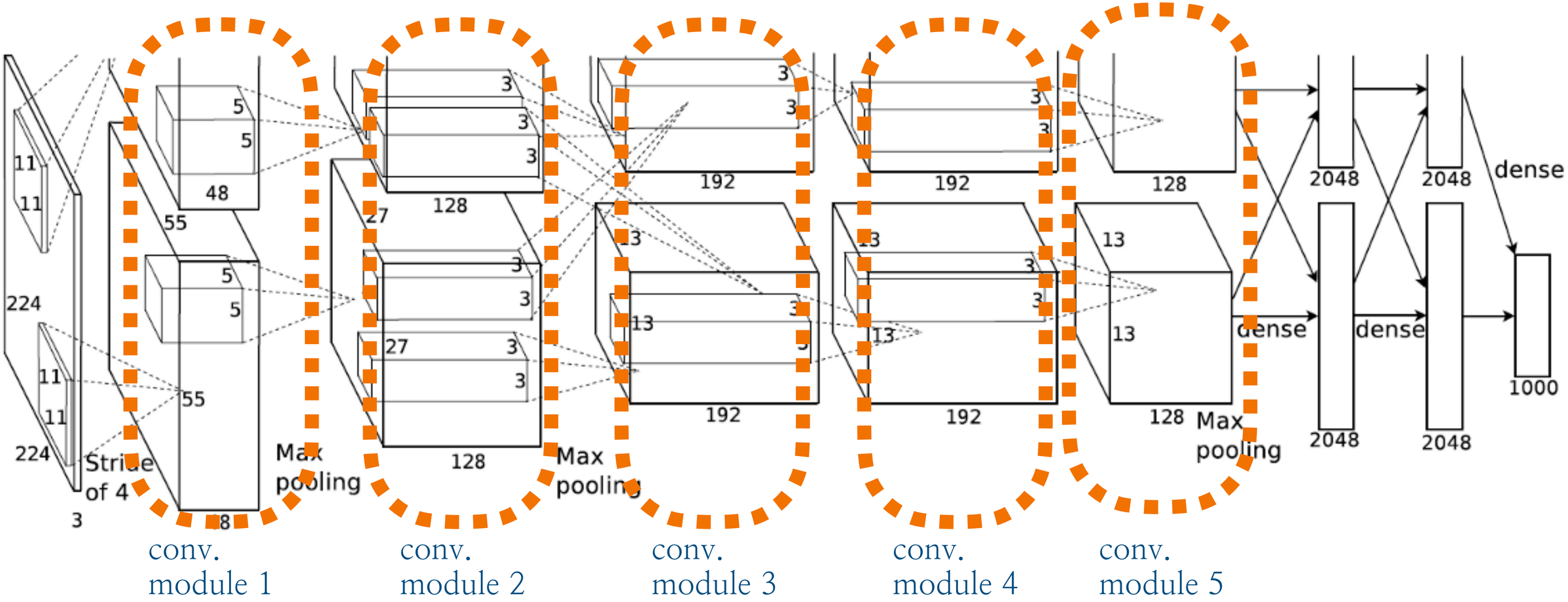
AlexNet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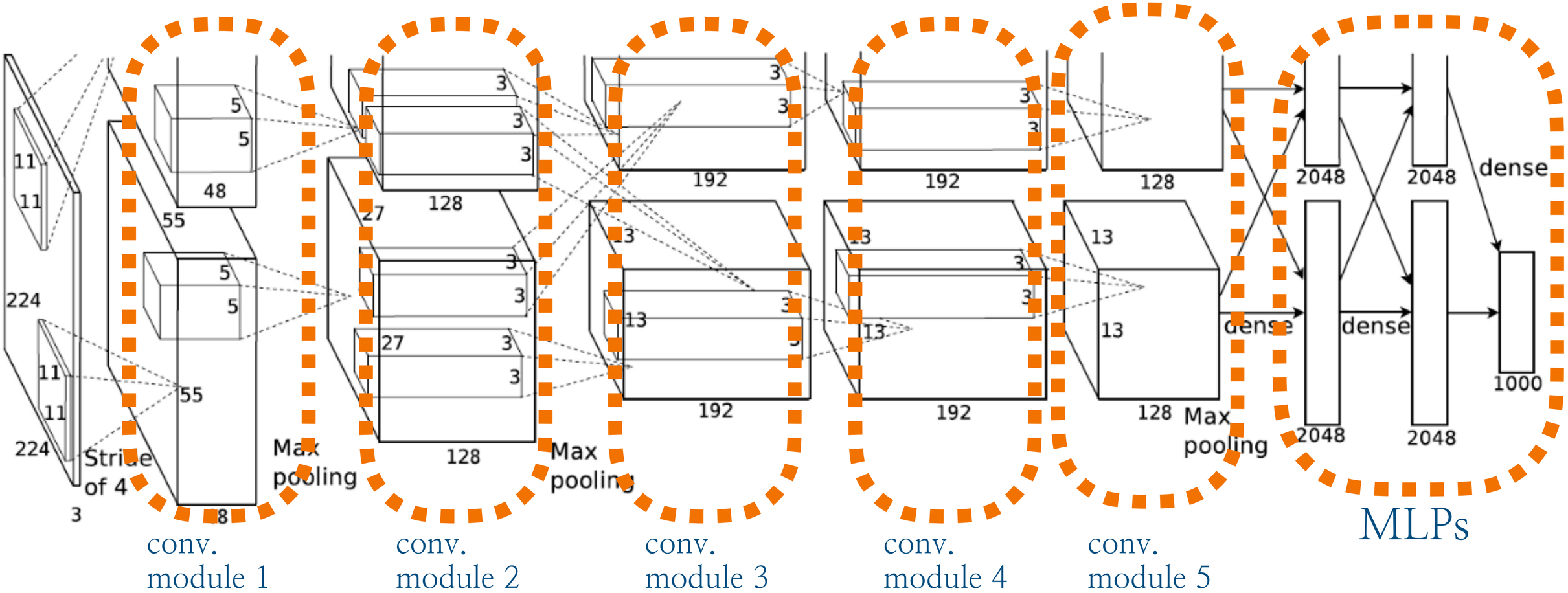
AlexNet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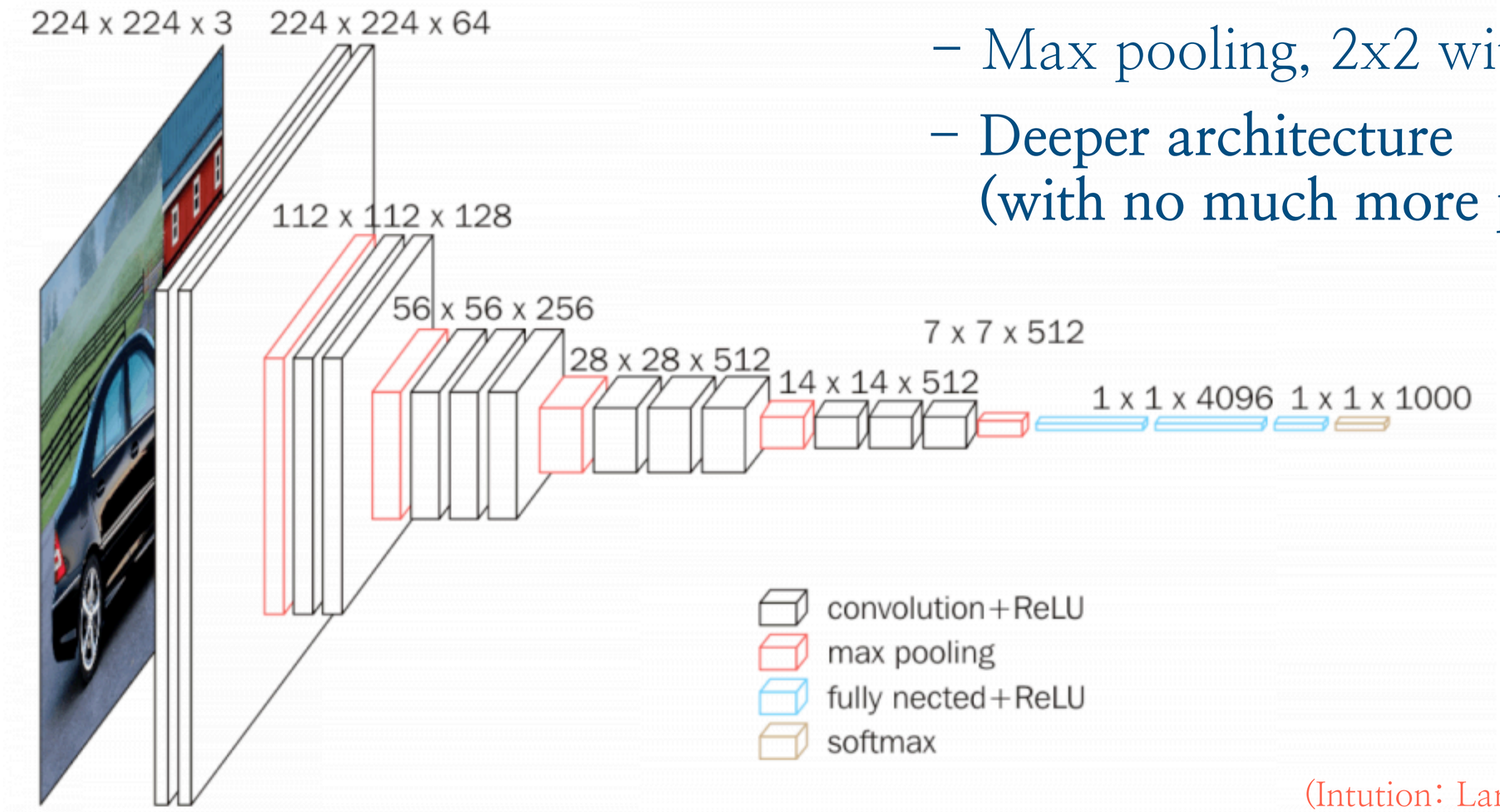
MLPs

VGG architecture

VGG16

- Only 3x3 filters, Stride of 1
- Max pooling, 2x2 with stride of 2
- Deeper architecture
  (with no much more parameters)

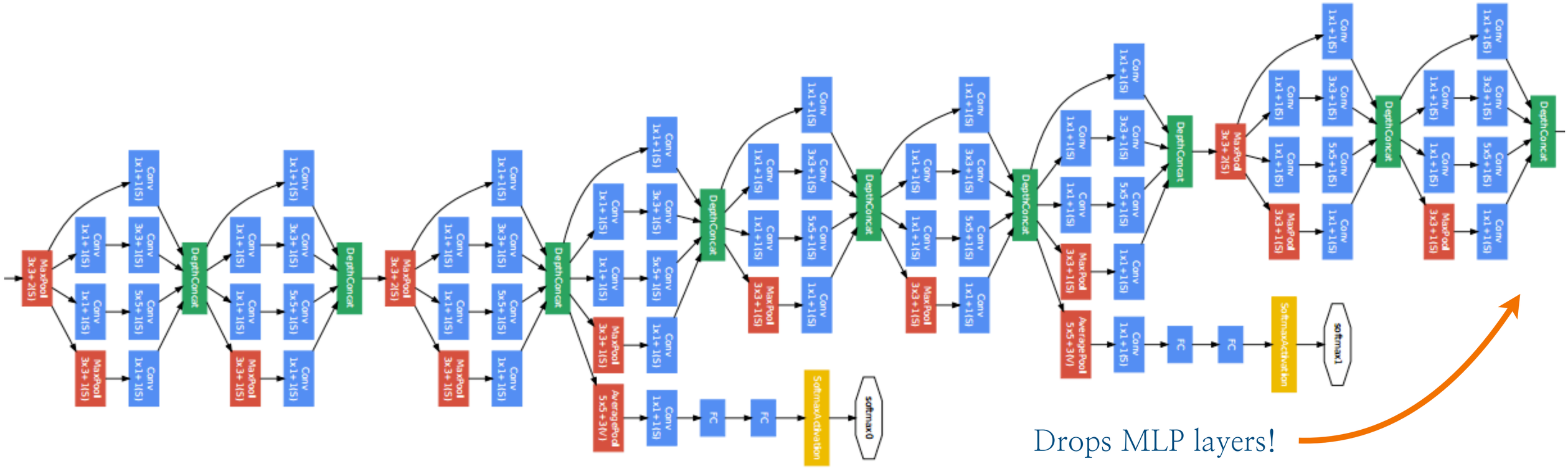


(Intution: Large filters = deep stack of smaller filters: this provides more "power")

Inception

Google's CV architecture

- ImageNet: 93.3% accuracy – compare with 81.8% AlexNet



Residual Networks (ResNets)

- Architecture that allows truly deep networks via skip connections

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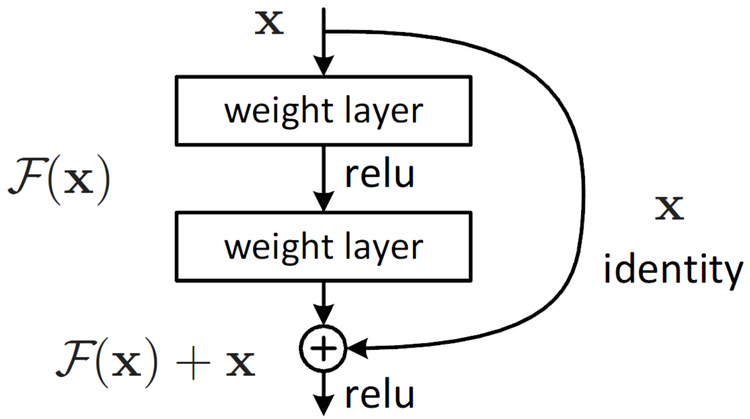

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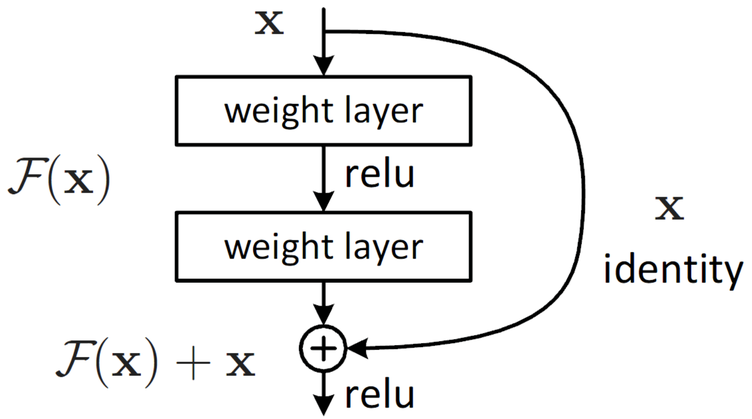

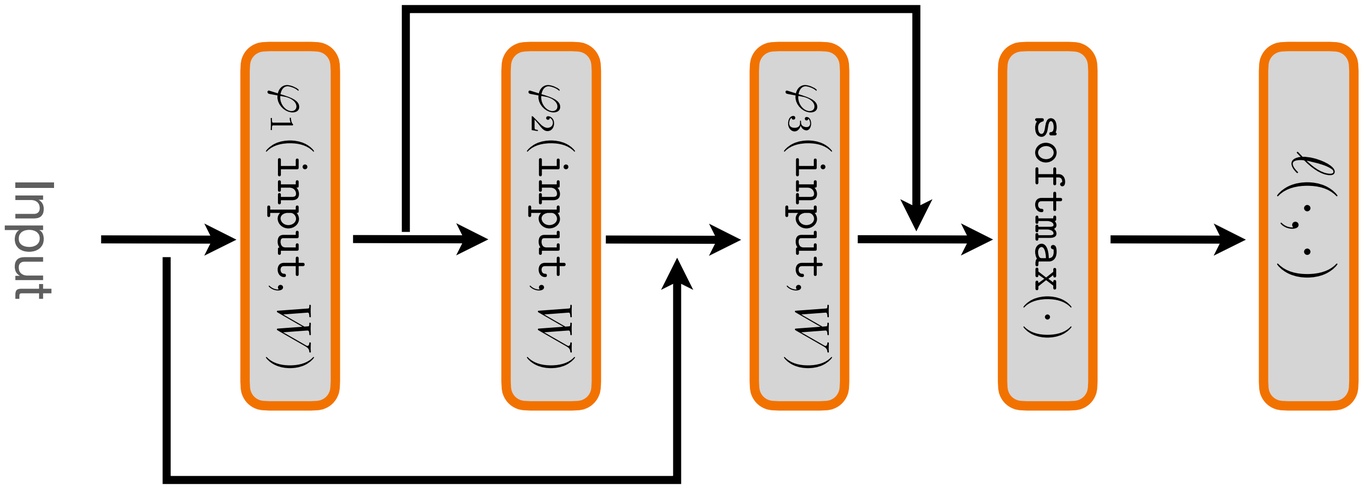

Residual Networks (ResNets)

- Remarks
  - ImageNet accuracy: 96.4%!
  - Winning architecture in many other applications (default module/ strategy in many current architectures)

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- Remarks
  - ImageNet accuracy: 96.4%!
  - Winning architecture in many other applications (default module/ strategy in many current architectures)
    - Nowadays, not exactly an architecture, but a module you can use in your neural networks
    - Several extensions (e.g., ResNext, HighwayNet, DenseNet)

Overview

- Introduction to ML/AI
- Introduction to neural networks
- Feedforward / Fully-connected neural networks or MLPs
- Convolutional neural networks (CNNs)
- Some trends in deep learning

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Transformers everywhere

The notion of self-attention

- Consider Sequence-to-Sequence (seq2seq) models
  (Machine translation, text summarization, image captioning..)

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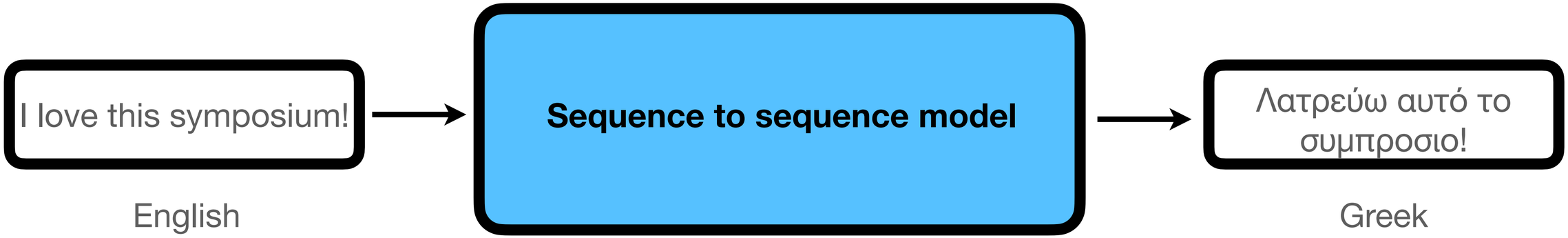

The notion of self-attention

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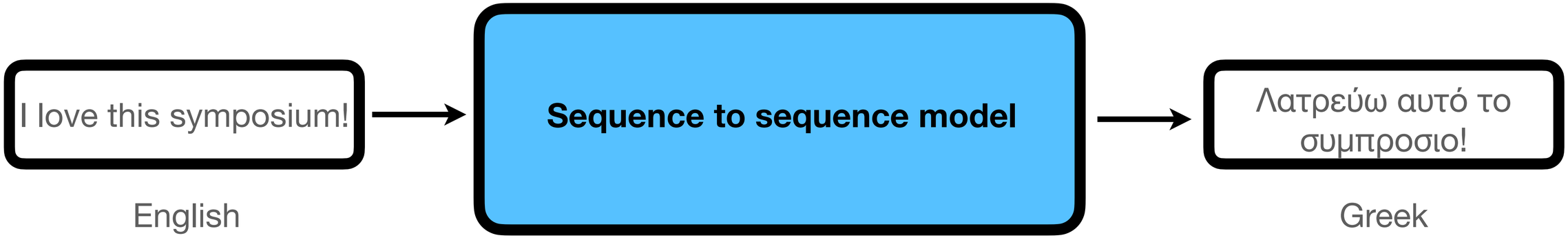
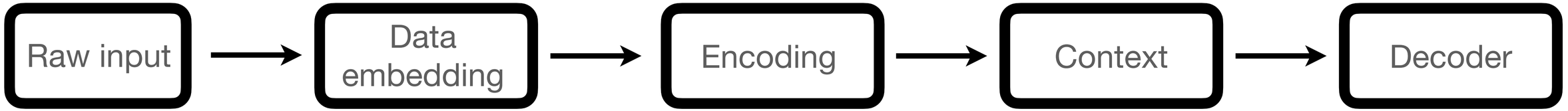


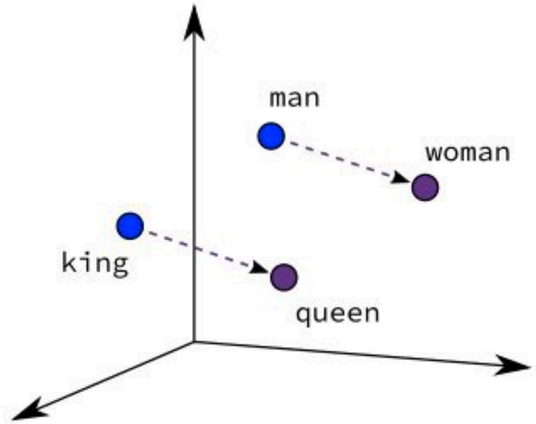
- What happens under the "hood":



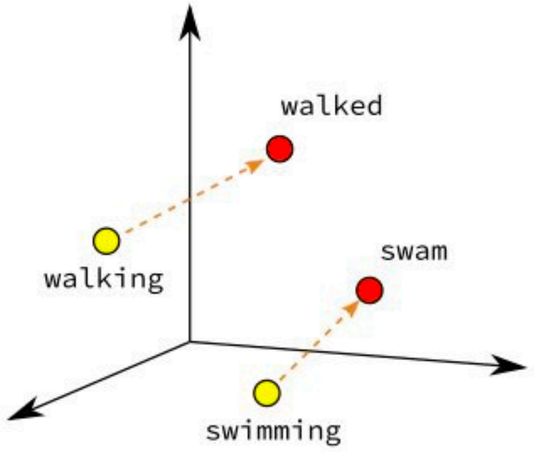
Data representation and word embeddings

Data representation and word embeddings

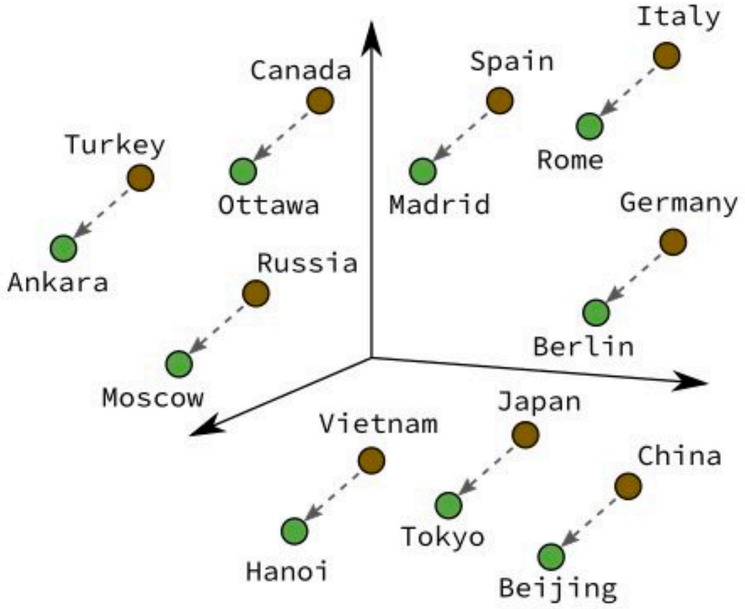
- Mechanisms that turn raw text pieces (words, sentences, etc) into vectors



Male-Female



Verb Tense



Country-Capital

Tribute to
Google Developers

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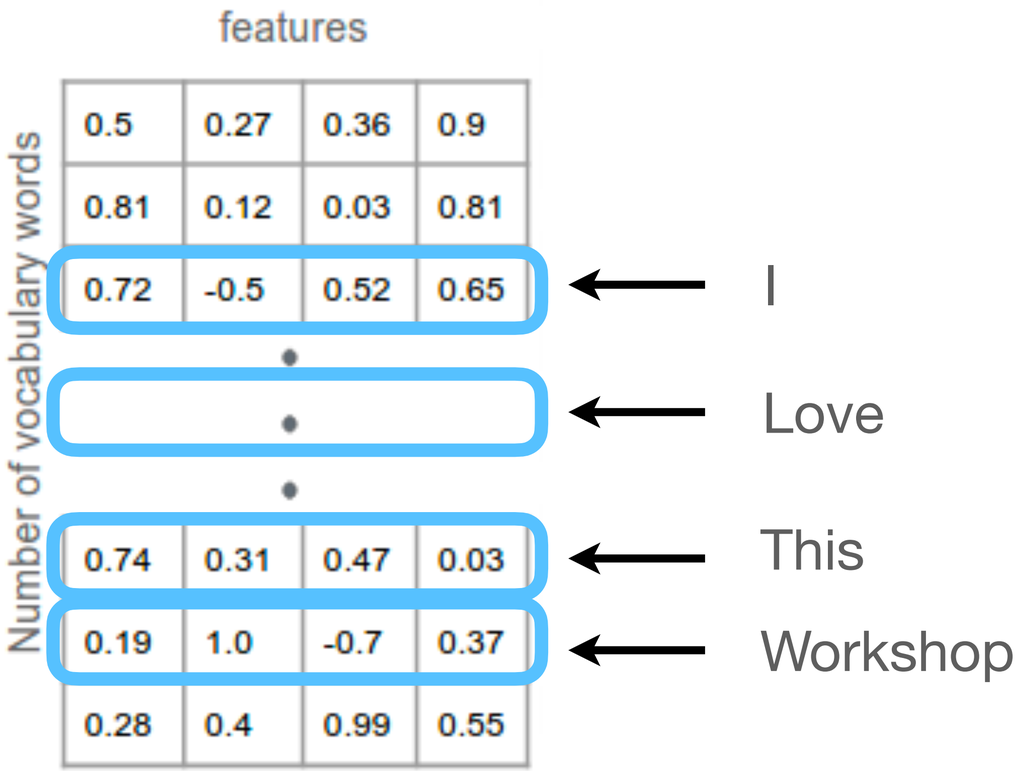
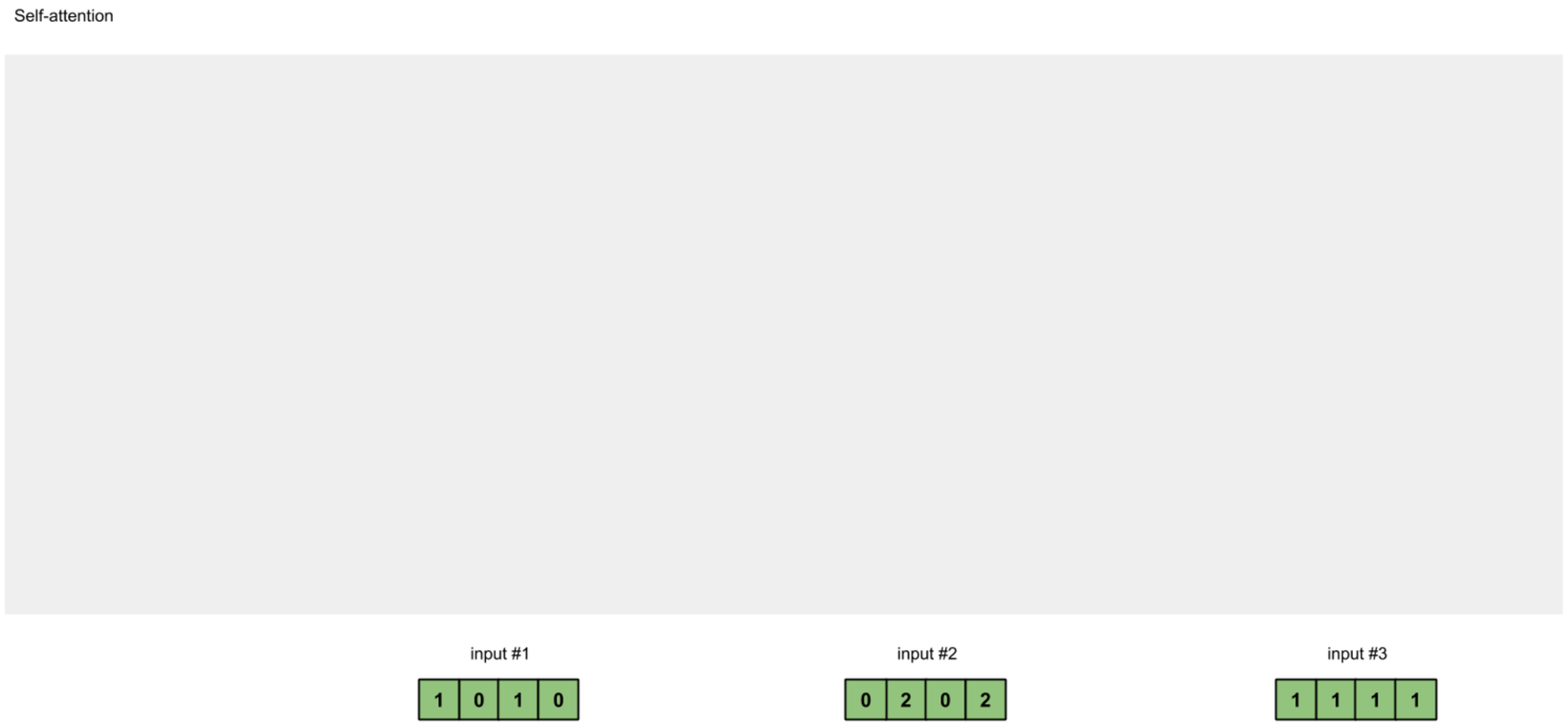


What is self-attention?



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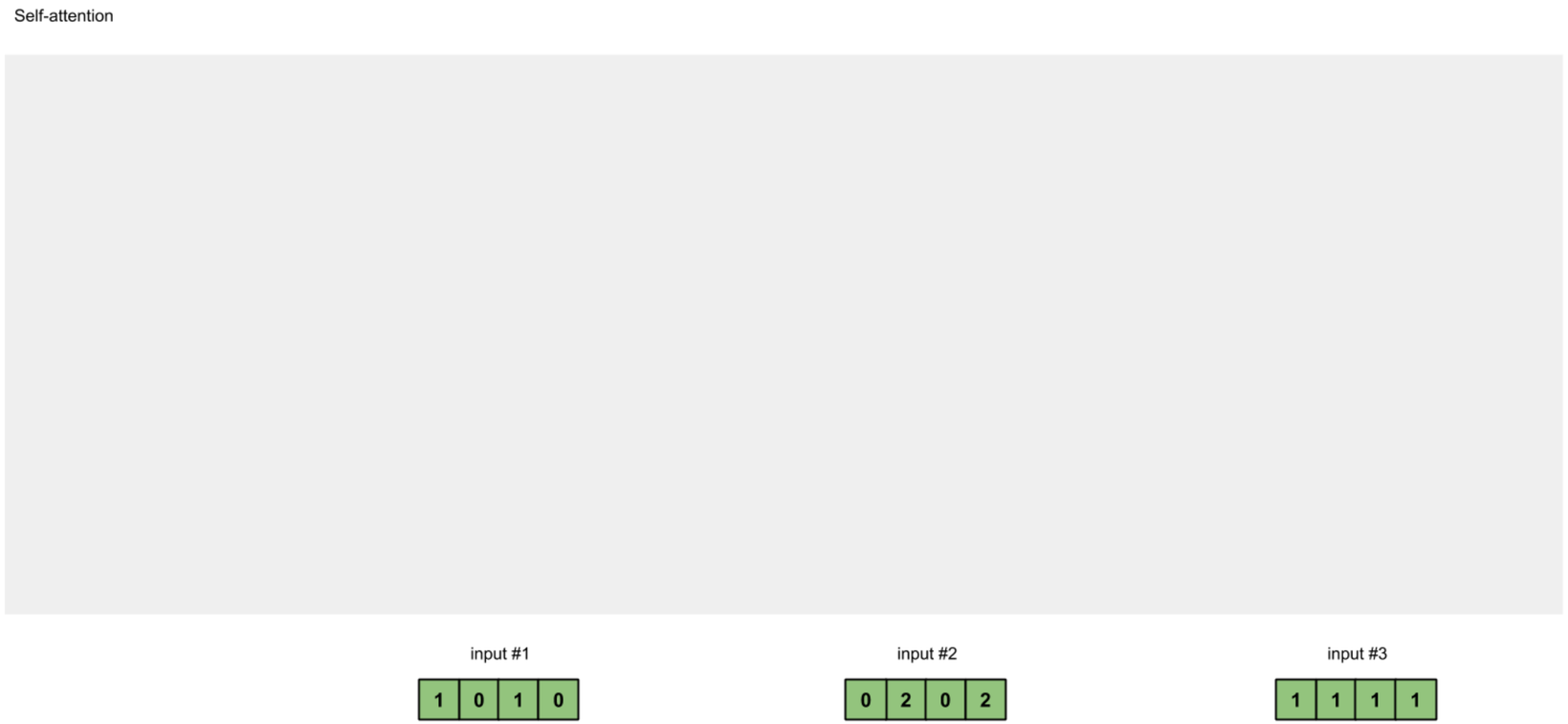

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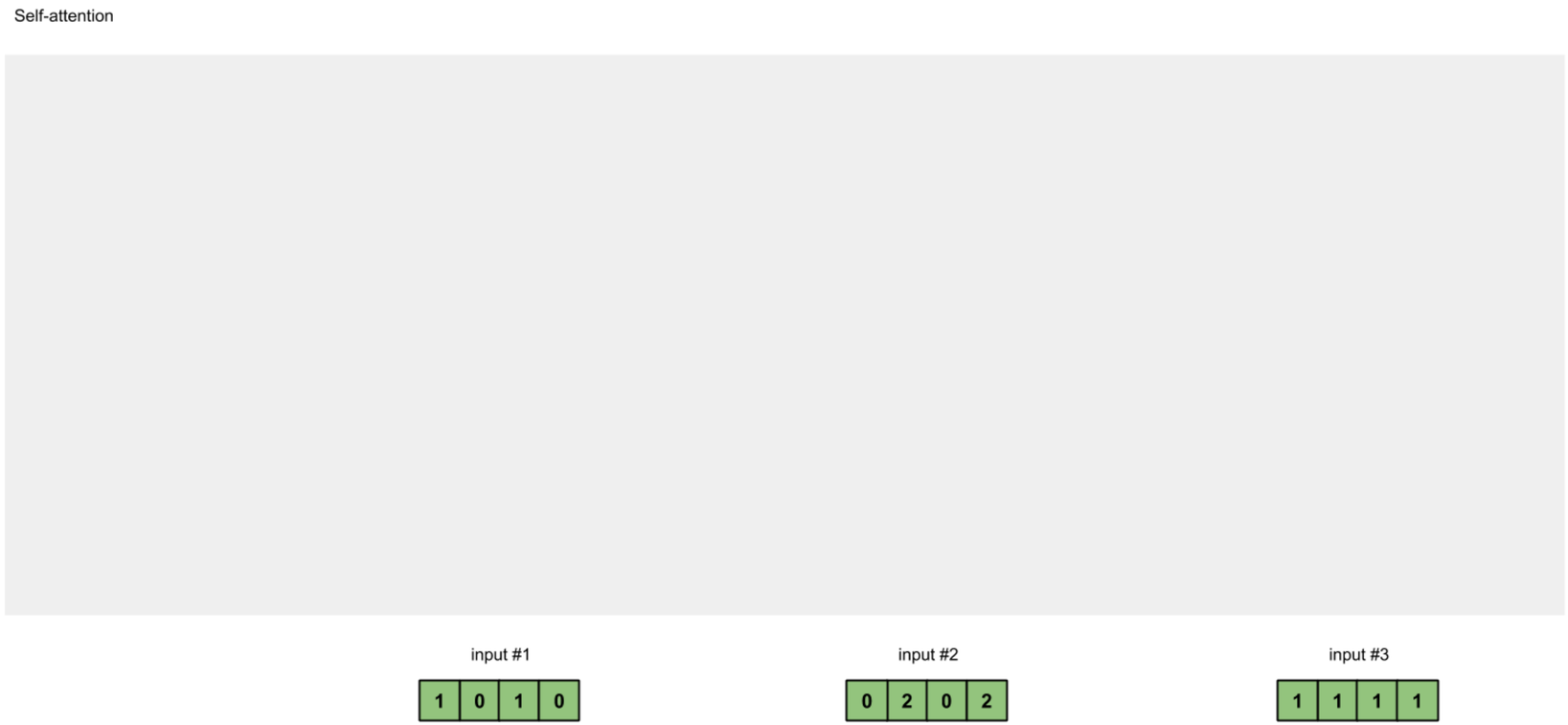
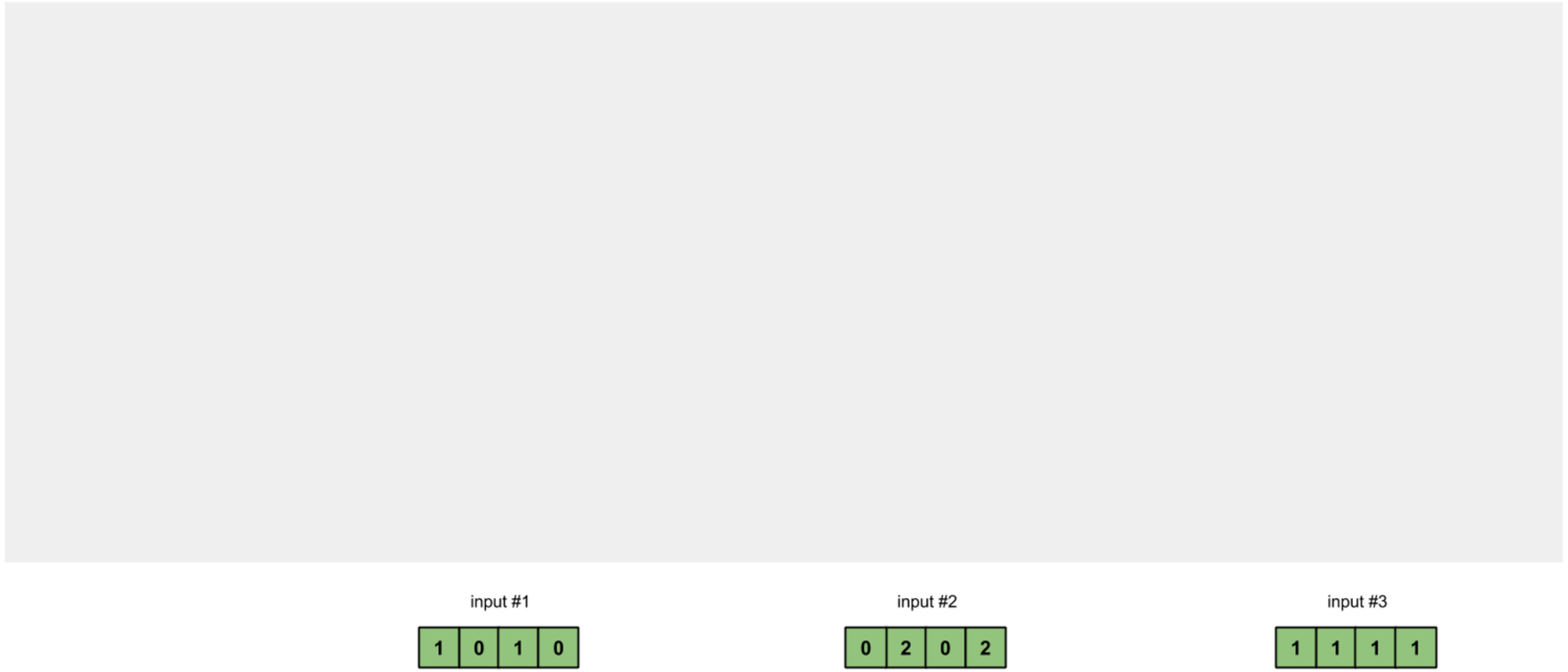
  i.e., the input is a long streak of words, and we compute correlations among ther



What is self-attention?

- Self-attention breaks the sequential nature of some NNs:
  i.e., the input is a long streak of words, and we compute correlations among ther
- Self-attention simultaneously compare each part of the input
  with other parts of the input



Transformers = multiple self-attention + FC layers

- Work by Google on 2017

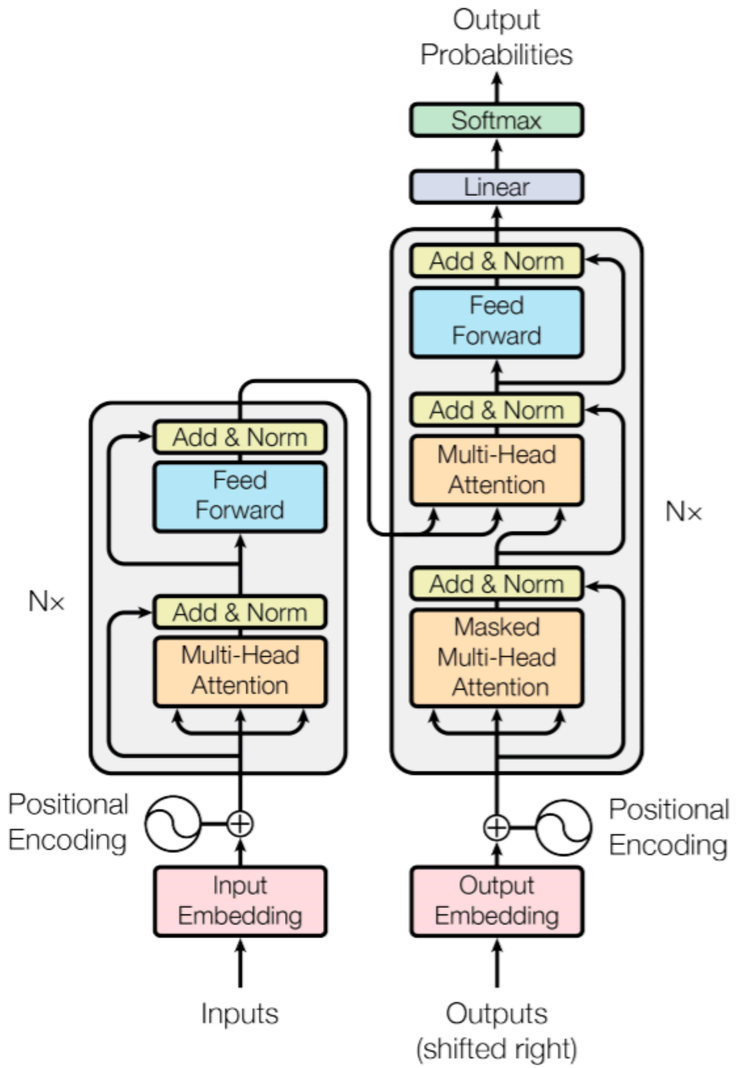


Figure 1: The Transformer - model architecture.

Transformers = multiple self-attention + FC layers

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  document summarization
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  bio sequence analysis
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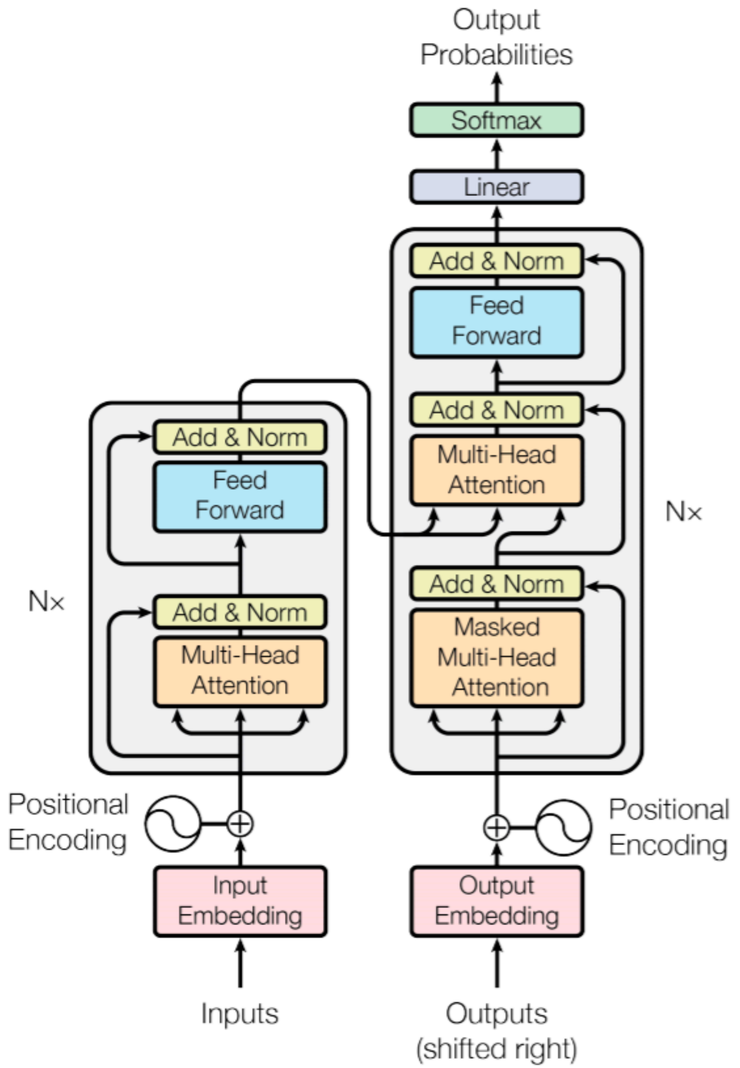

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- Applications: machine translation
  document summarization
  document generation
  bio sequence analysis
  video understanding
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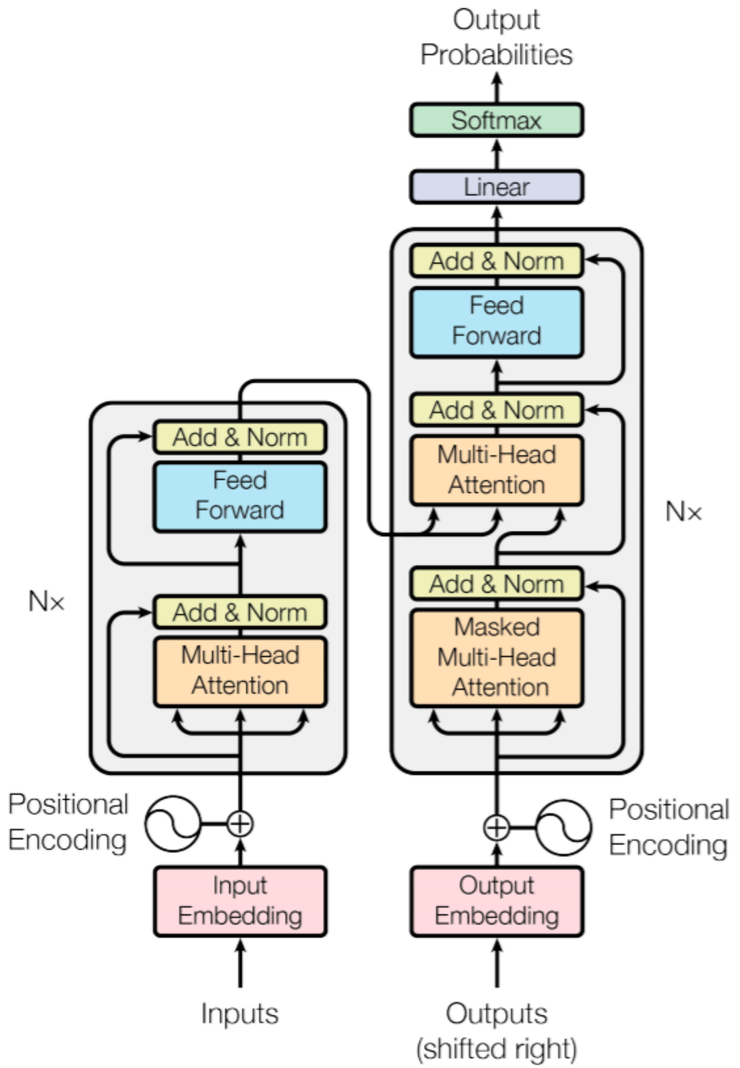
- Known large architectures: GPT-2 (1.5b)
  GPT-3 (175b)
  Wu Dao (1.75tr)
- Large models have raised many environmental questions



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