Convolutional and Recurrent Deep Neural Networks

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DeepLife Course
4EU+

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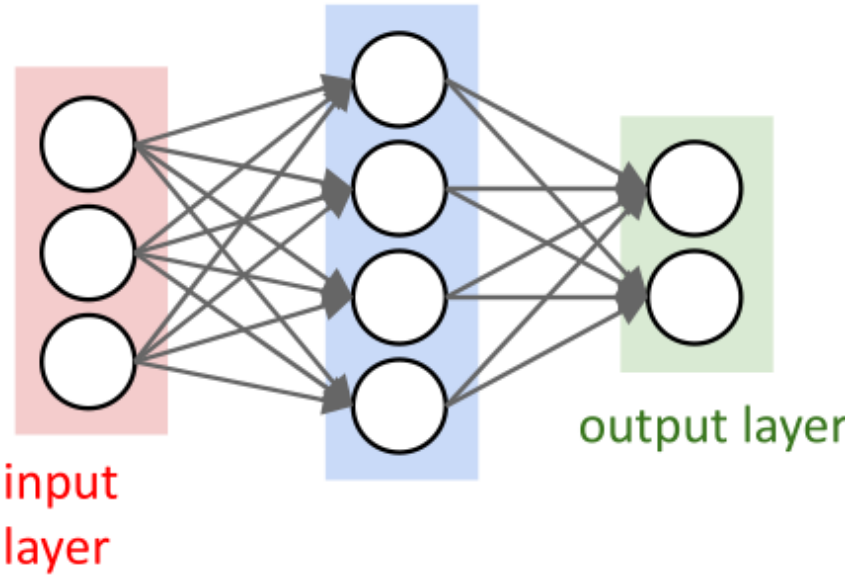
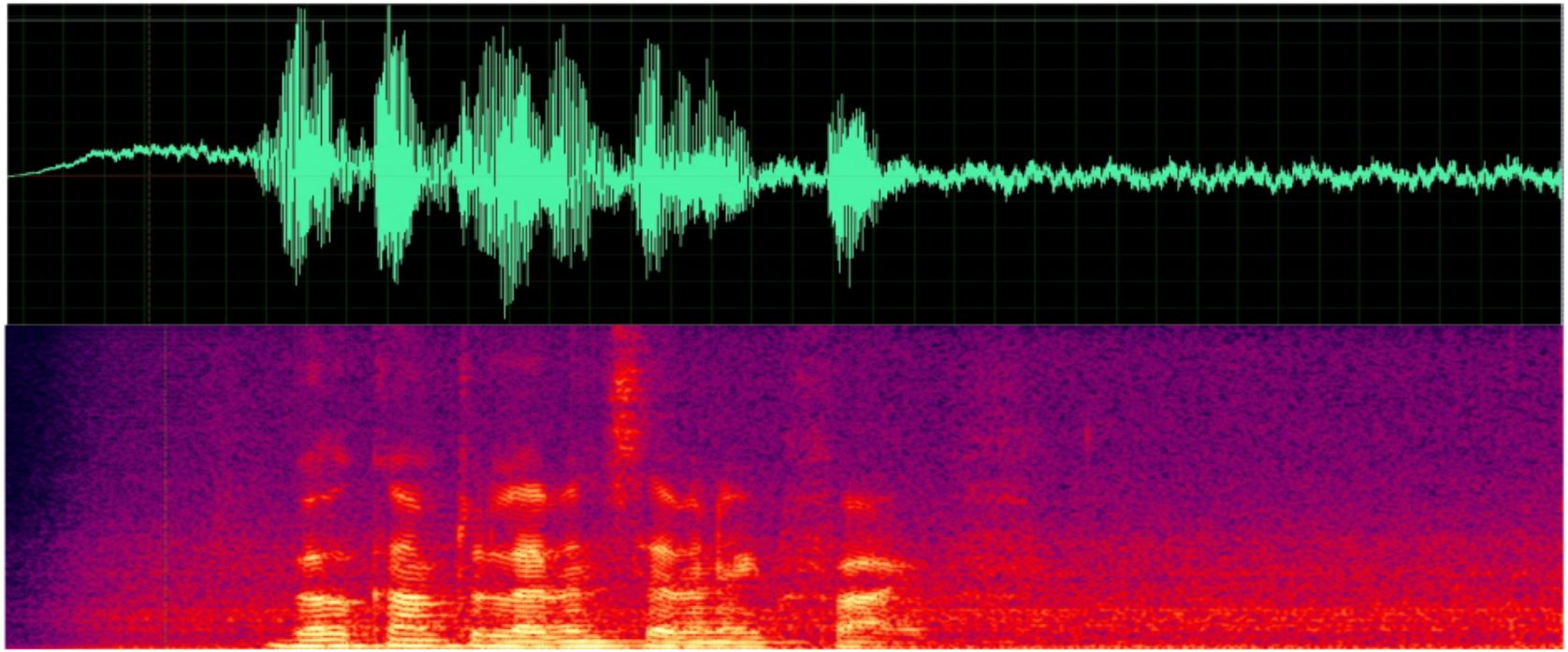
Outline

Recap



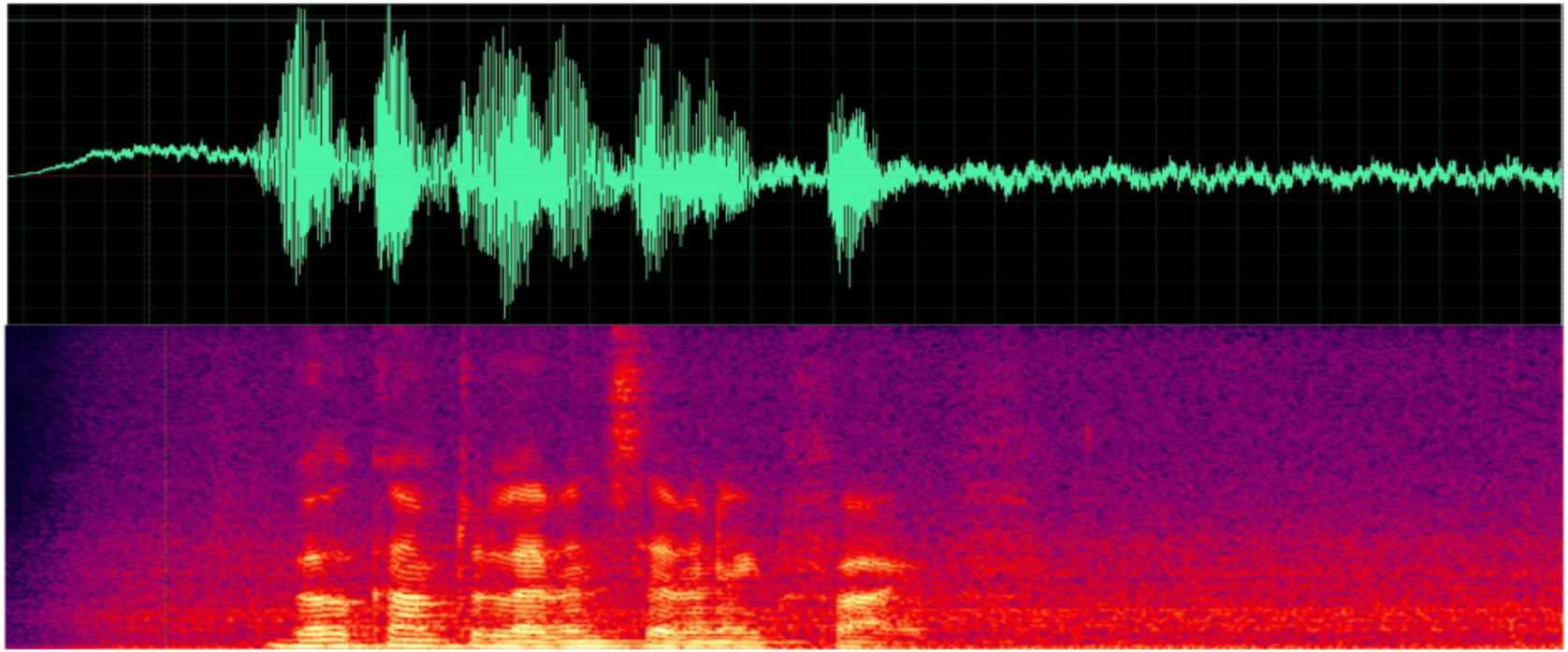
- Multi-layer Perceptron (MLP) is able to detect patterns in input data
- Inputs are numeric vectors
  - E.g. digits, numeric signals etc.

A different problem



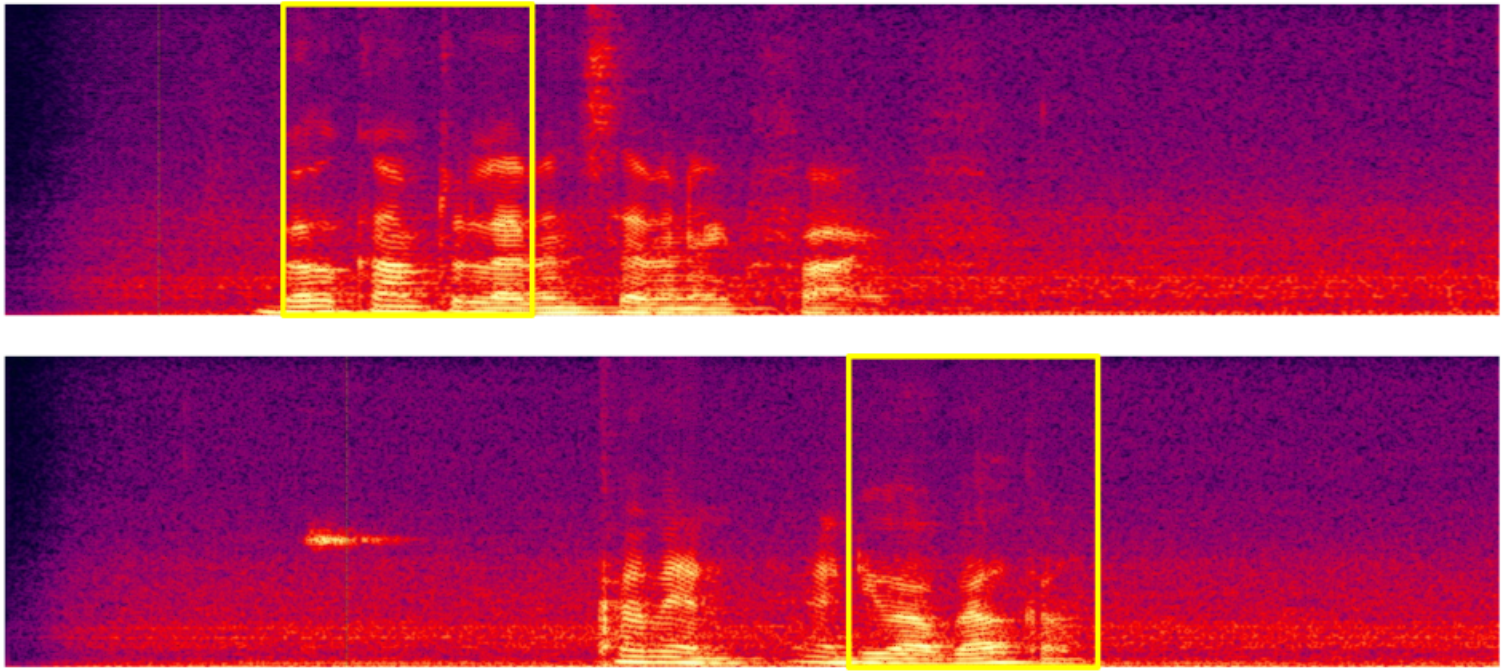
- Given a signal, does it contain a given word? E.g., "welcome"?

A different problem



- Given a signal, does it contain a given word? E.g., "welcome"?
- **Solution 1**: MLP which takes the whole time-frequency signal and output 1 if there is a "welcome" in
- Does it work?

Shift Variance Issue



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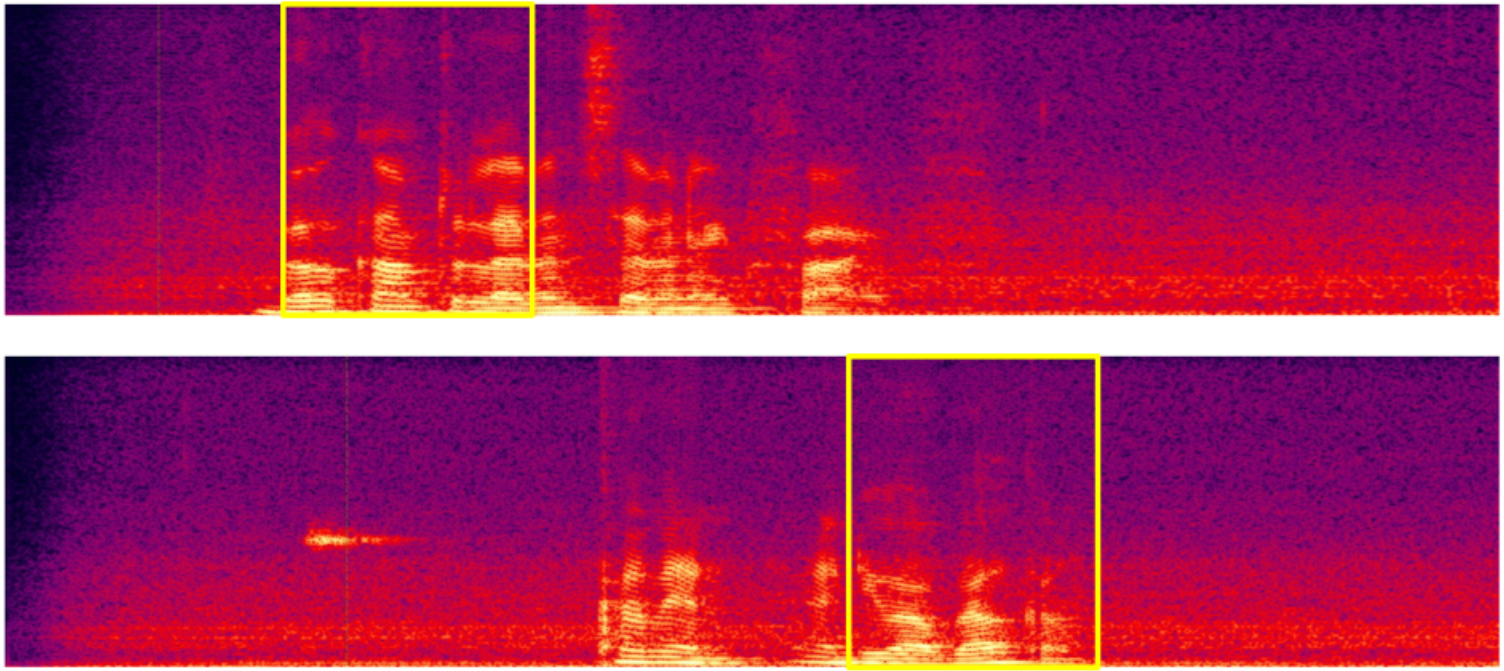

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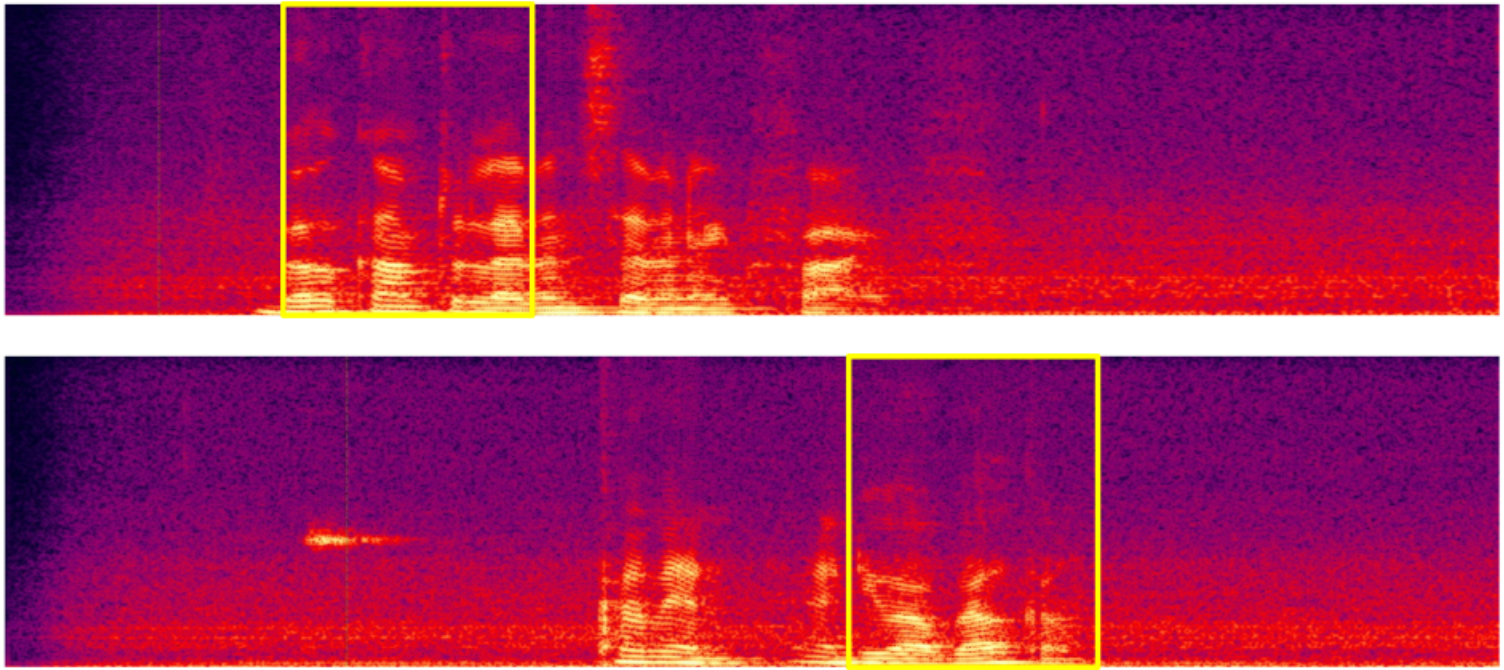
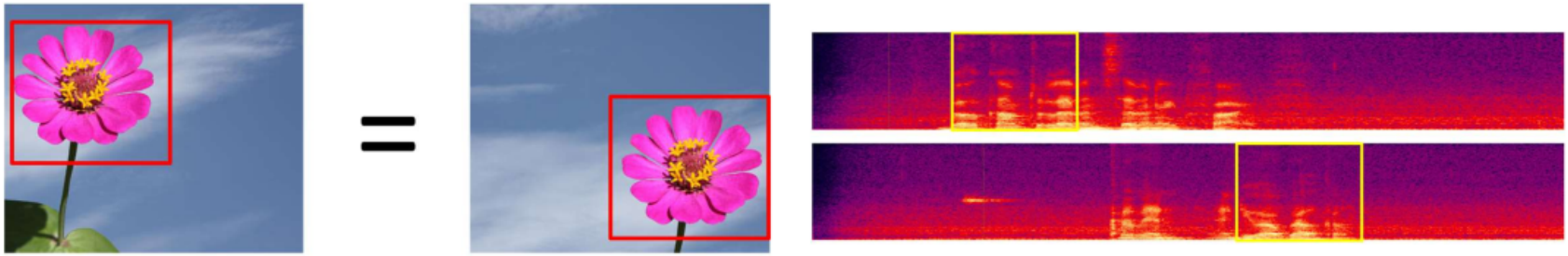


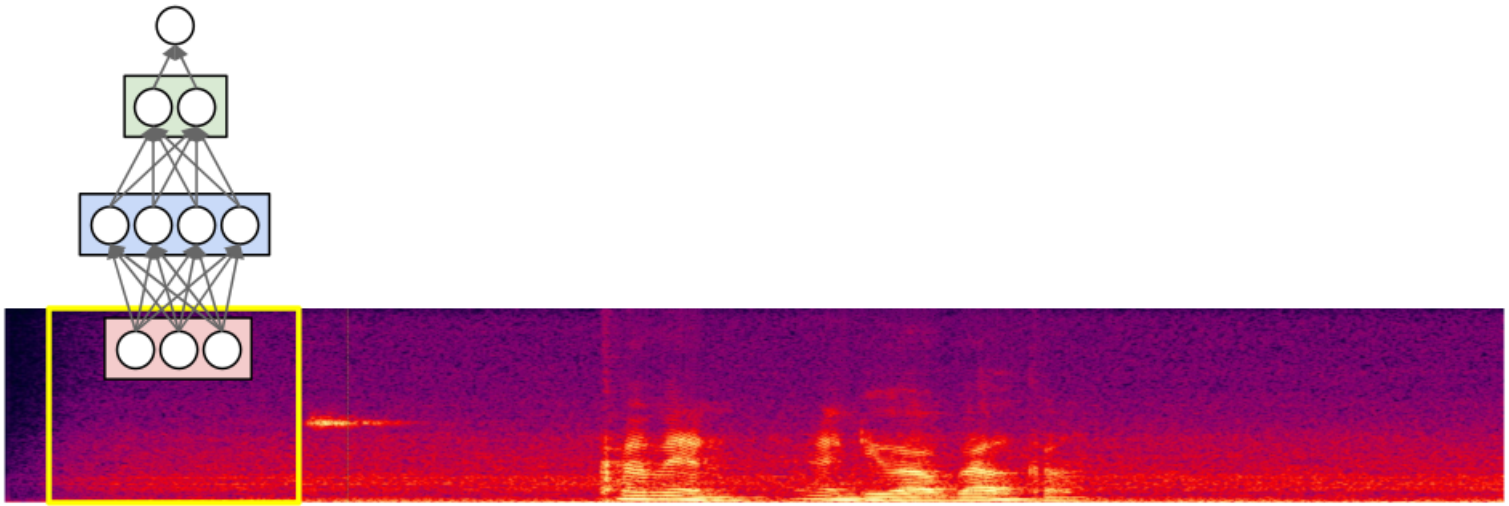
- Shift variance problem: a MLP that finds a "welcome" in the top recording will not find it in the lower one
- Unless trained with both
- This would require a very large network and a large amount of training data to cover every case

Shift Variance Issue



- In many problems the *location* of a pattern is not important
  - Only the presence of the pattern
- Conventional MLPs are sensitive to the location of the pattern
  - Moving it by one component results in an entirely different input that the MLP won't recognize
- Requirement: Network must be *shift invariant*

Possible solution: scan the input



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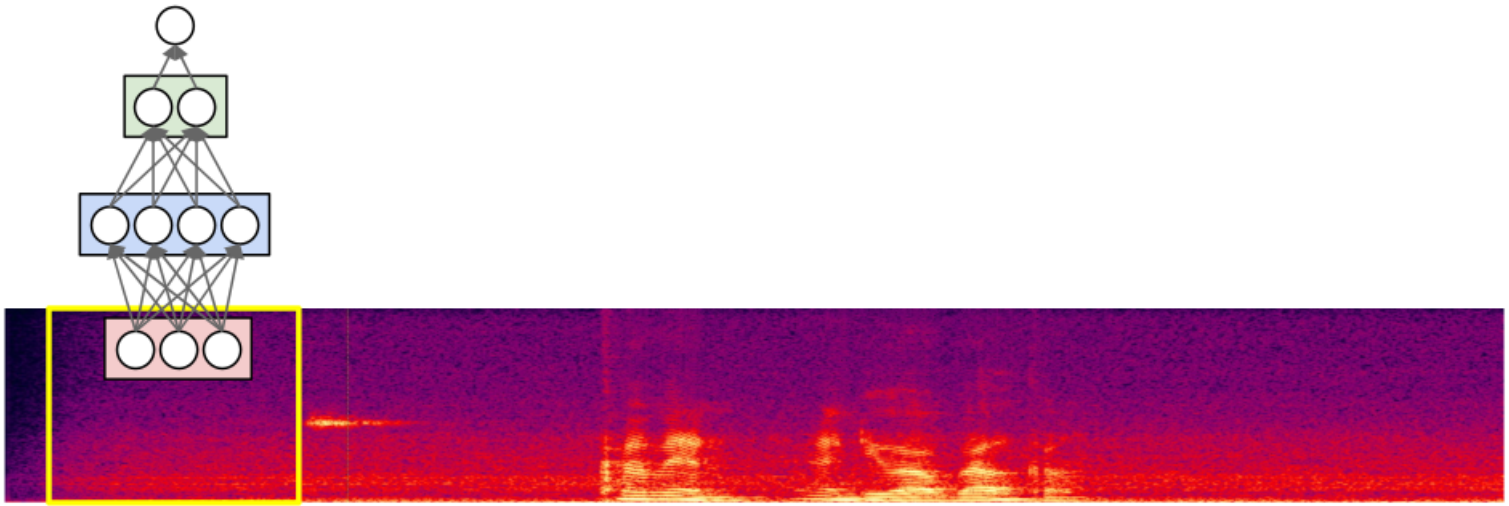

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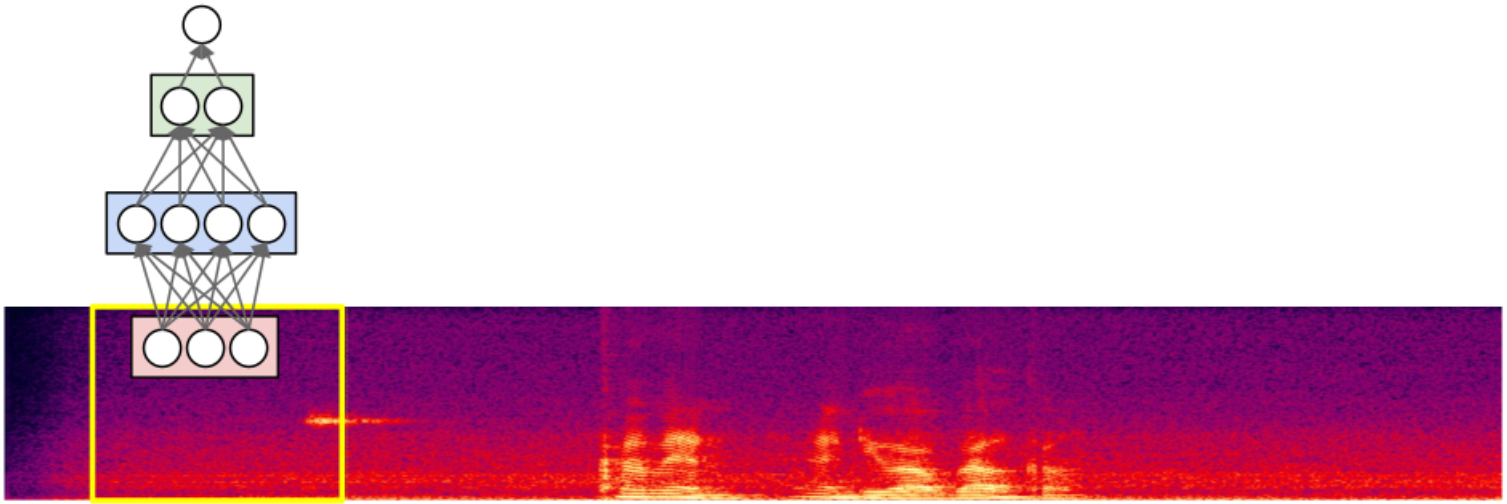

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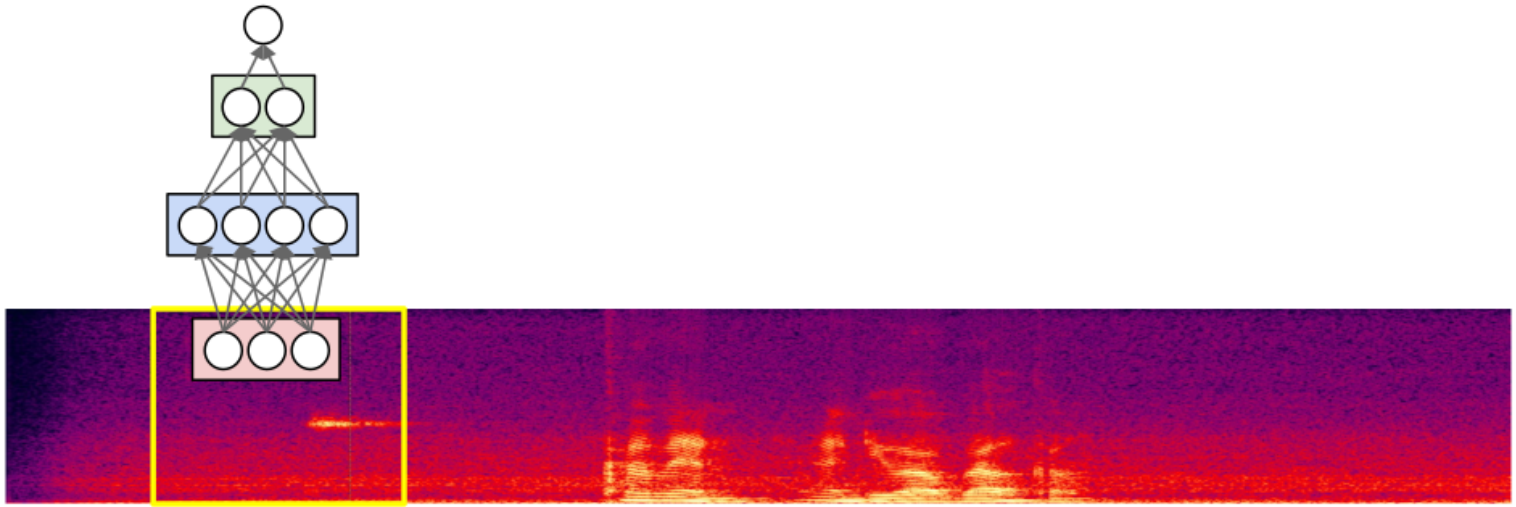

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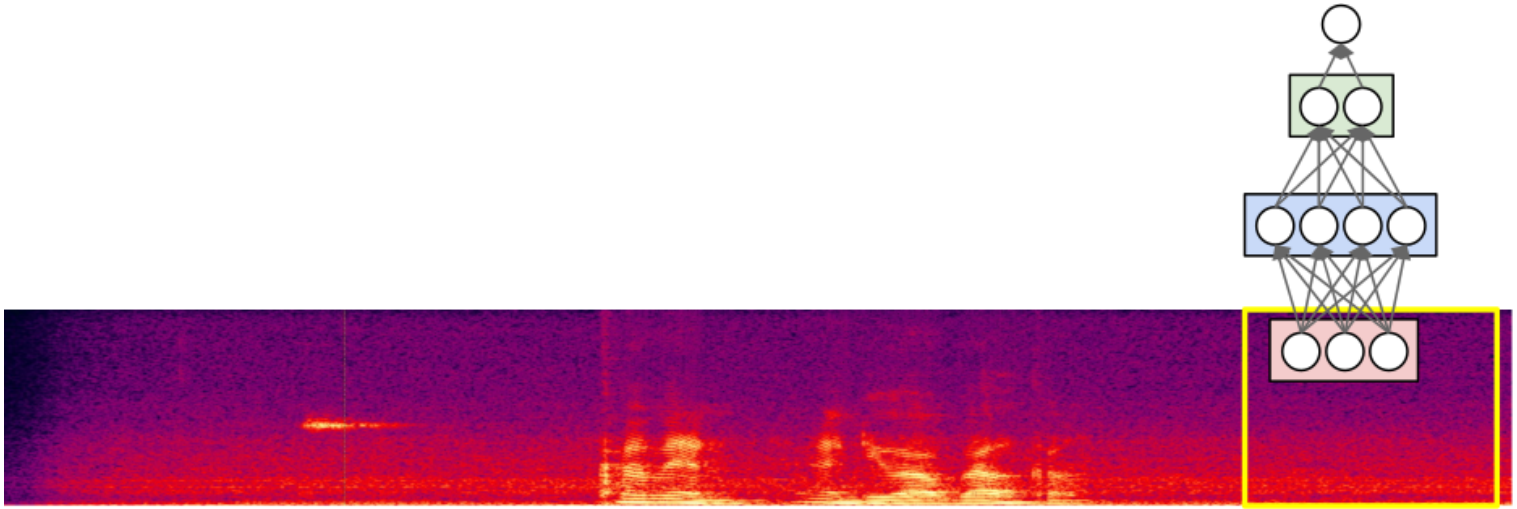

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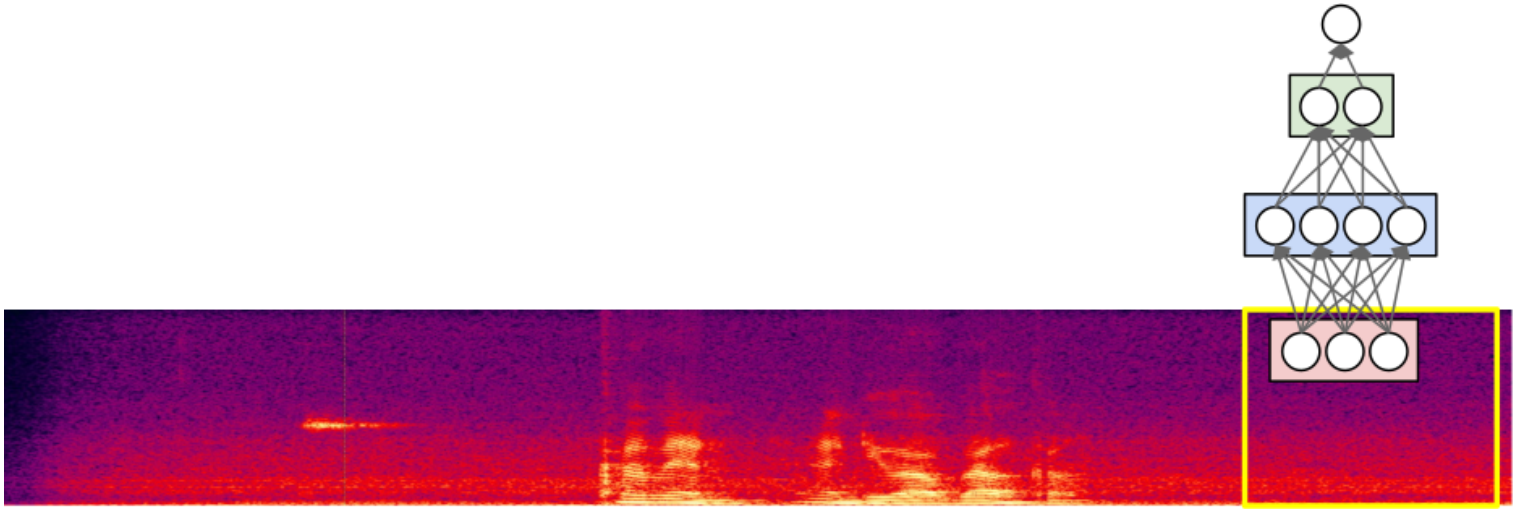

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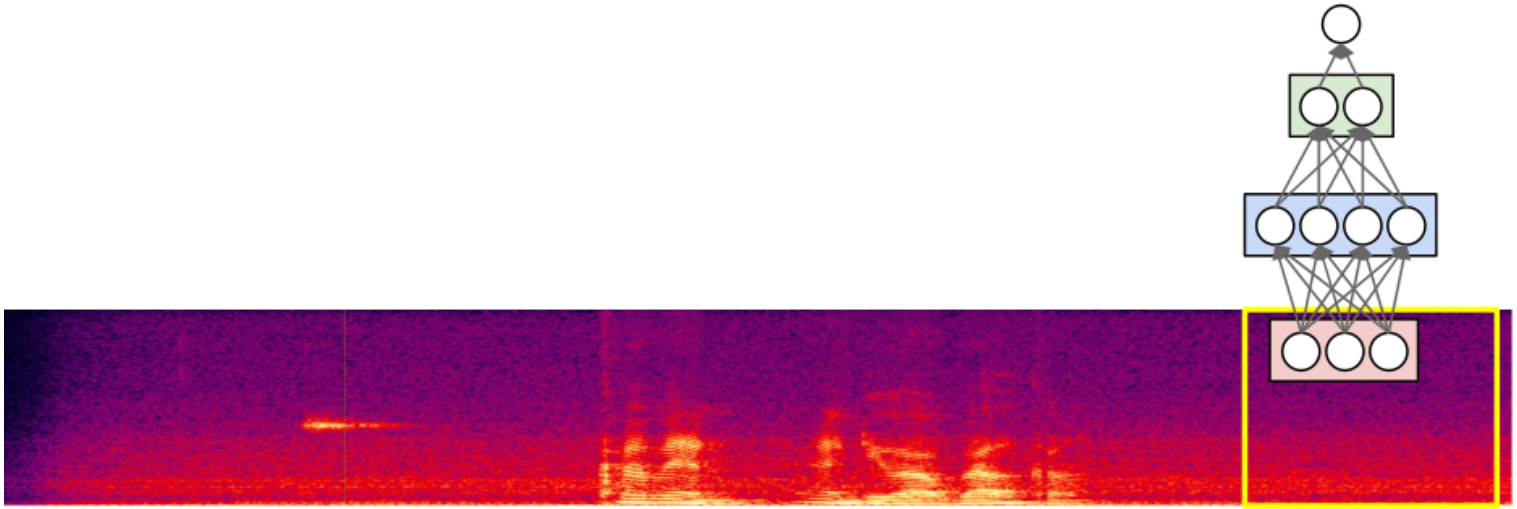

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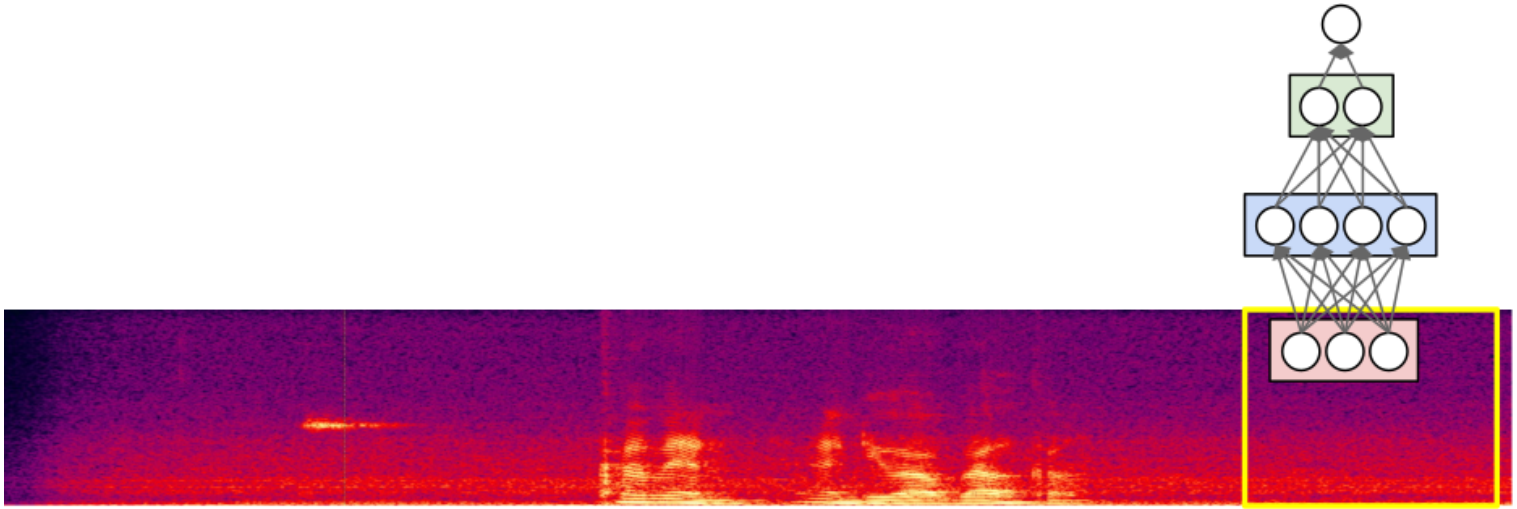

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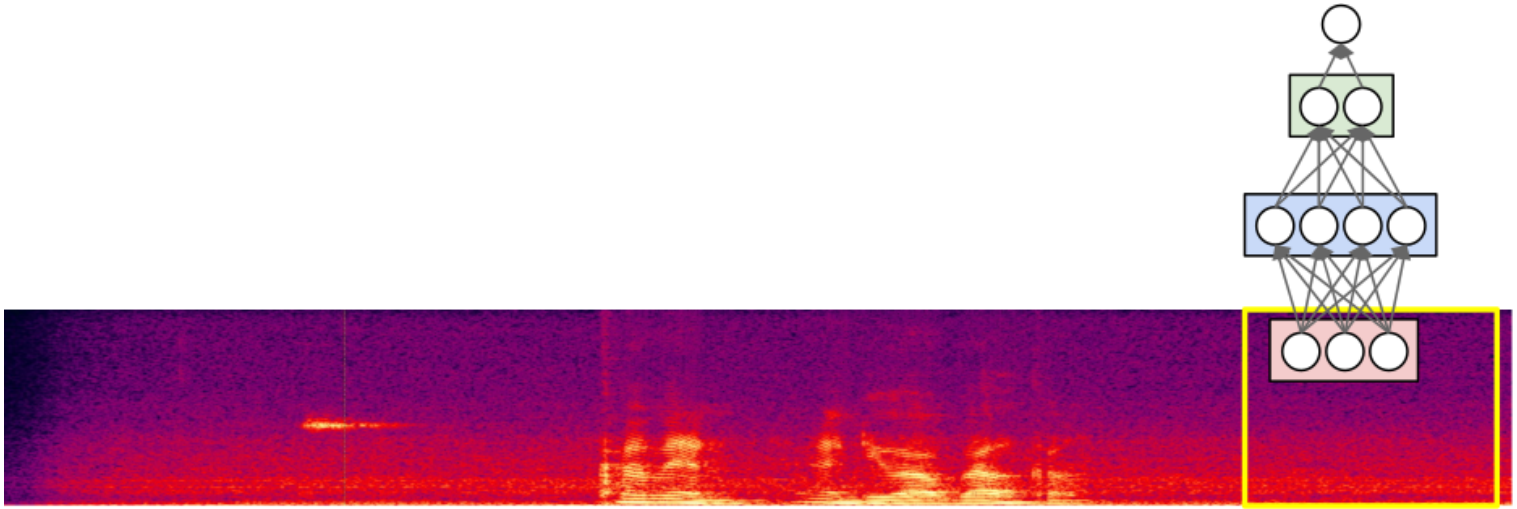

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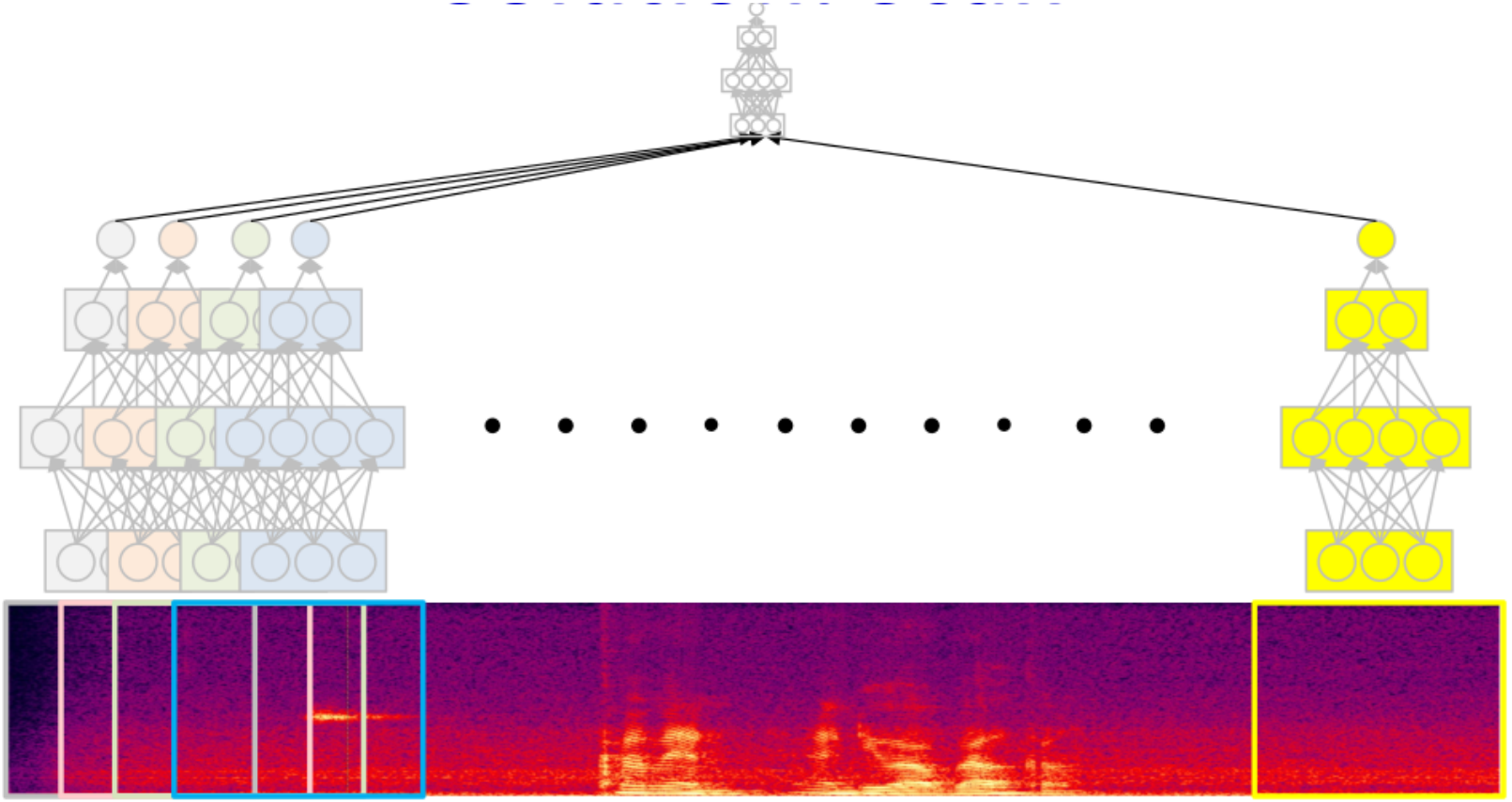
- What to do on each window to take into account even overlapping portions? Operate a convolution on each window!
- This is what a Convolutional Layer does!
- Nice thing: the model scanning each window is the same! The parameters (connection weights) are thereby shared

Deep Learning in Life Sciences

Combining the Windows



"Does welcome occur in this recording?"

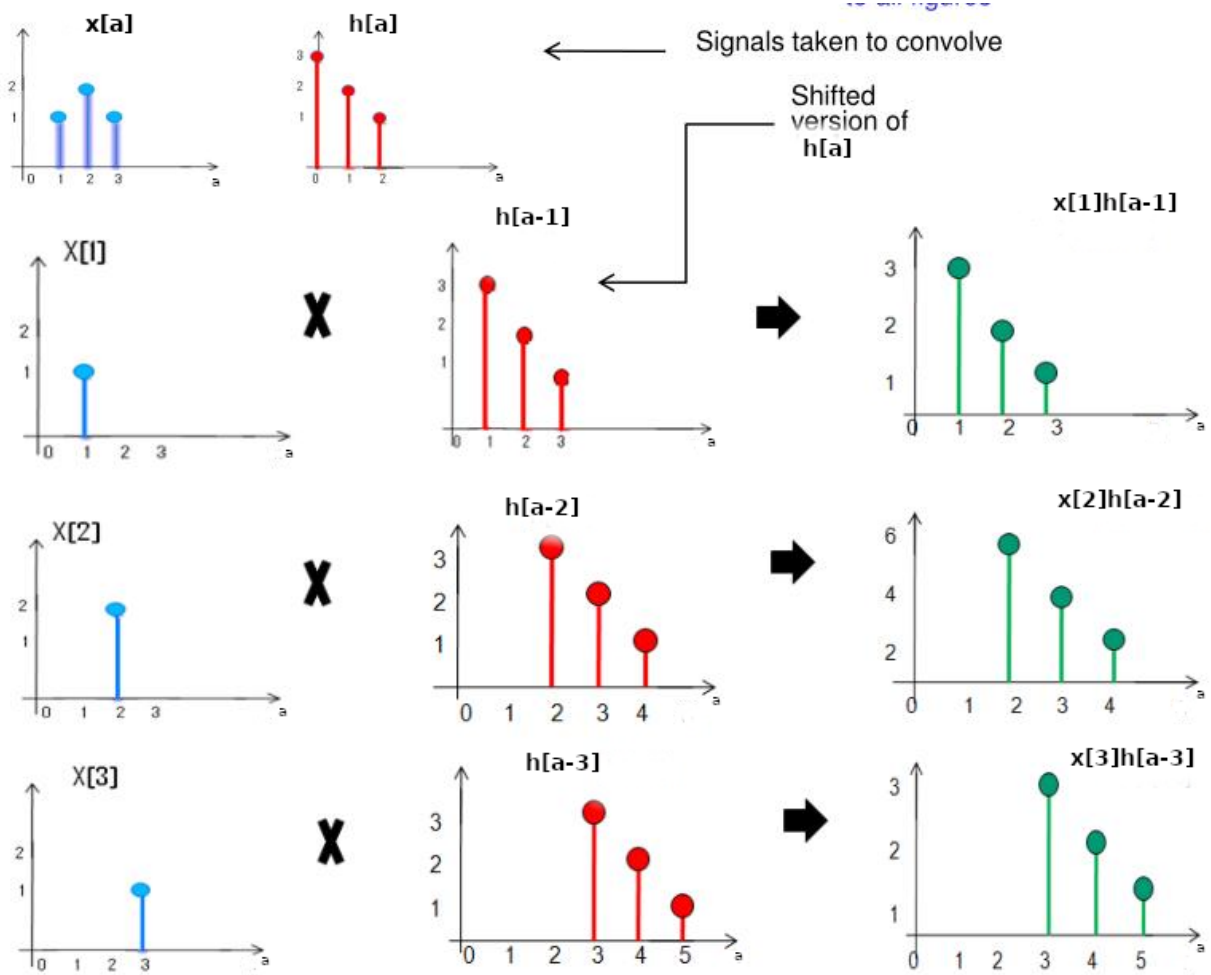
- Maximum of all the outputs (Equivalent of Boolean OR)
- Or a proper softmax/logistic
  - Adjacent windows can combine their evidence
- Or even an MLP

2

Deep Learning in Life Sciences

Outline

Convolution https://www.slideserve.com/sylvie/discrete-convolution-of-two-signals-powerpoint-ppt-presentation



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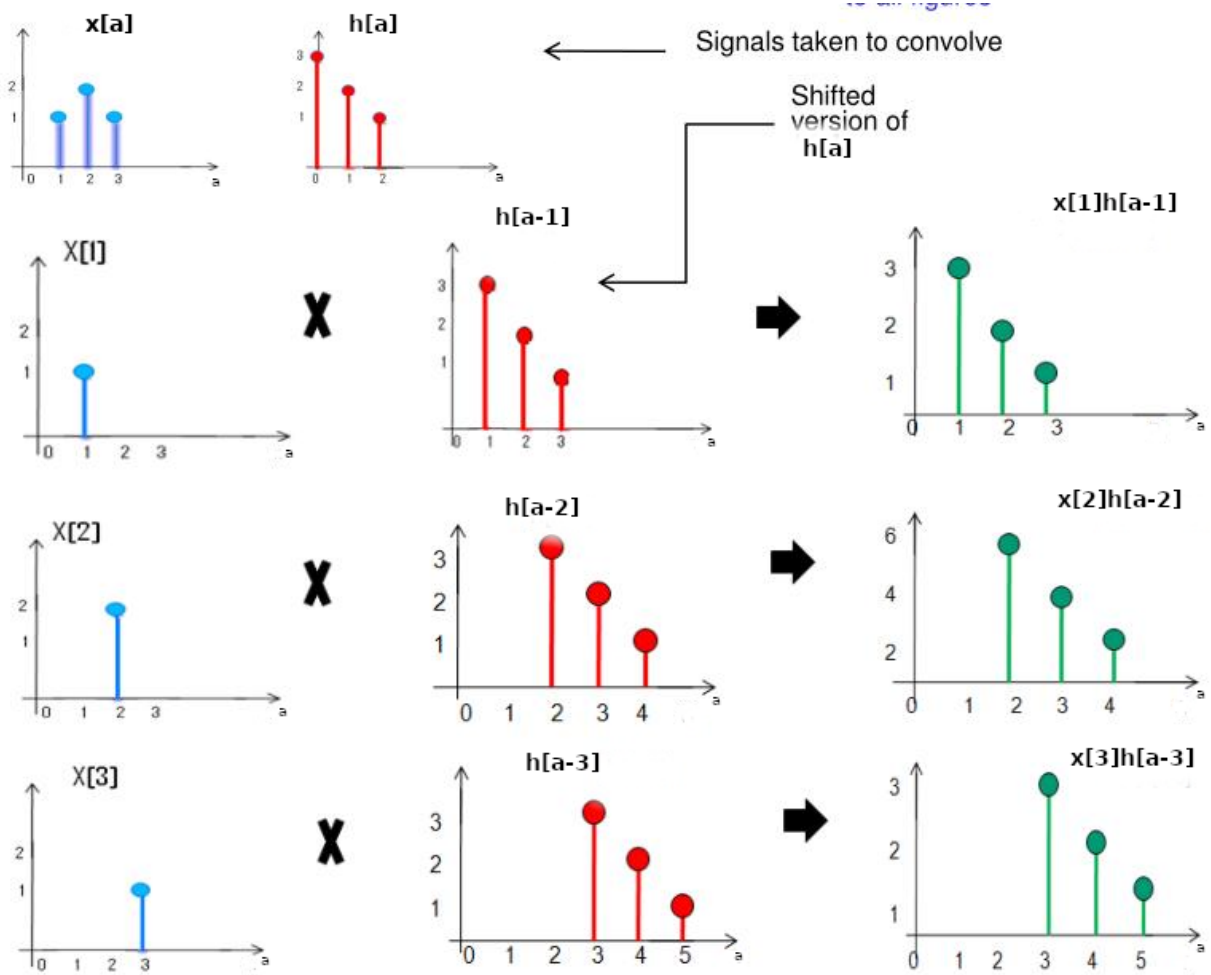

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Deep Learning in Life Sciences

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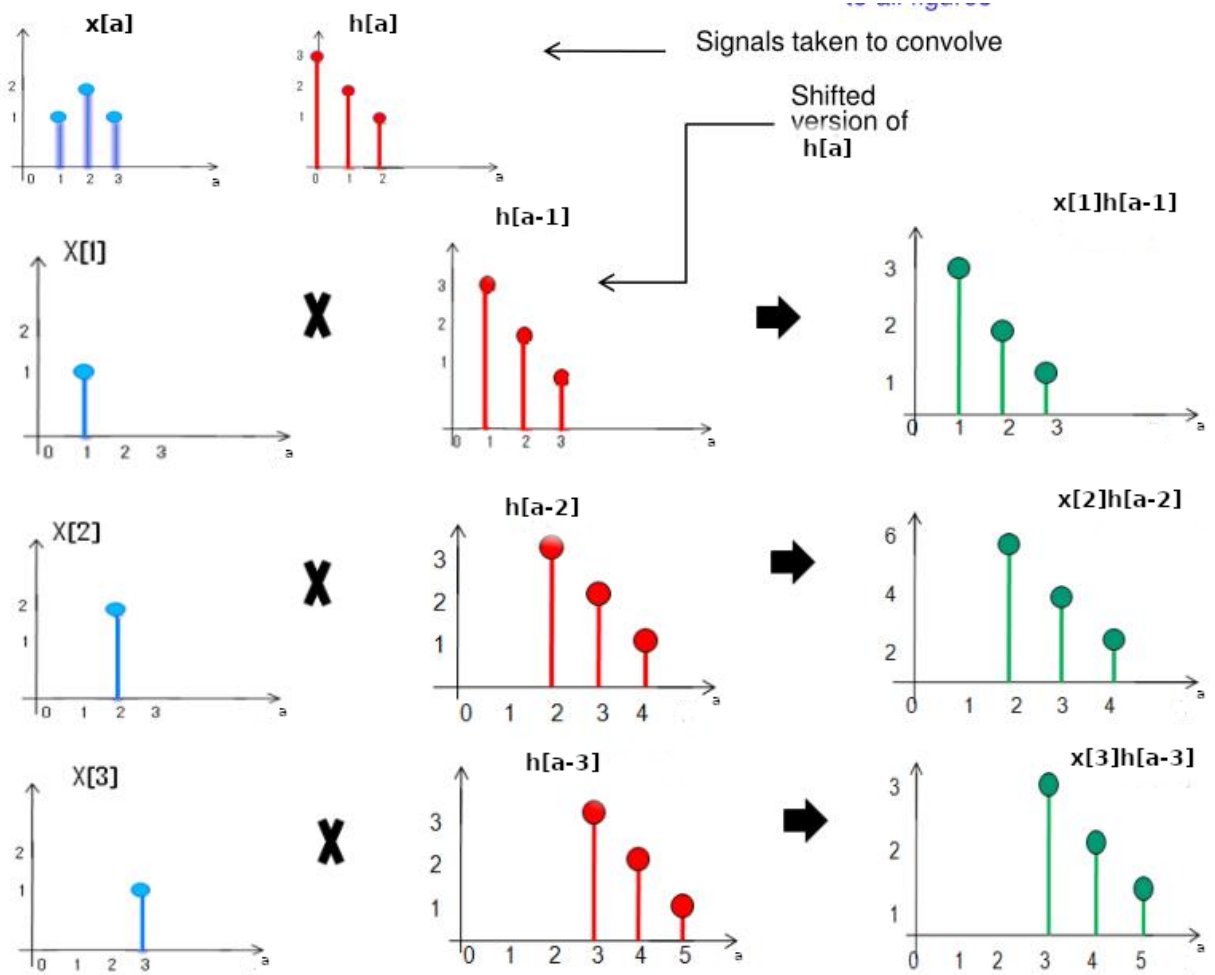

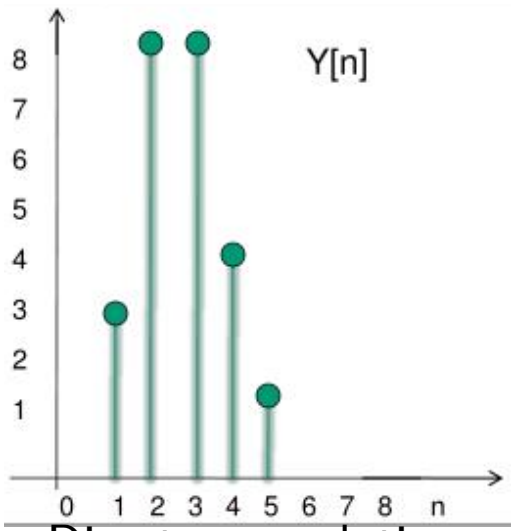

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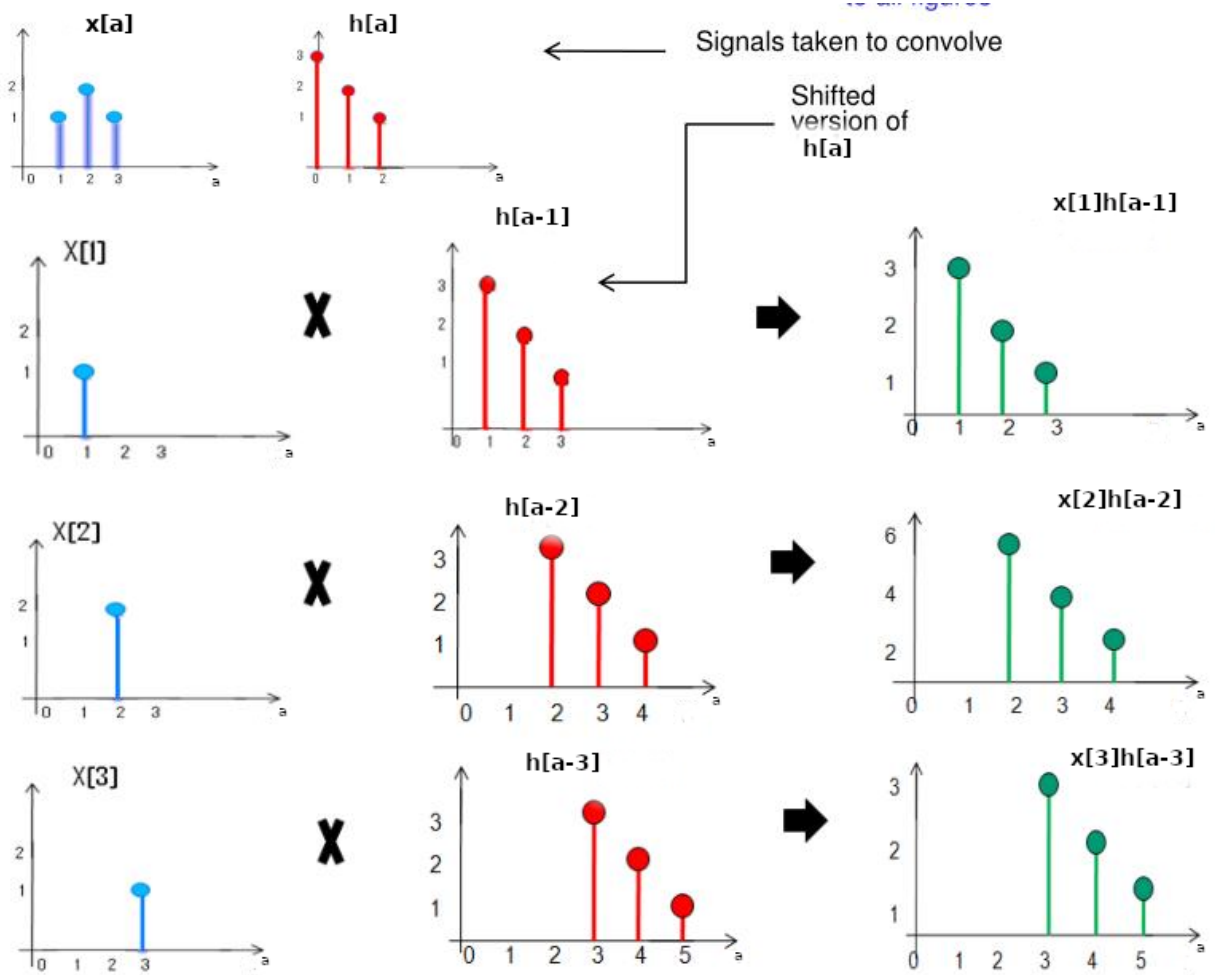

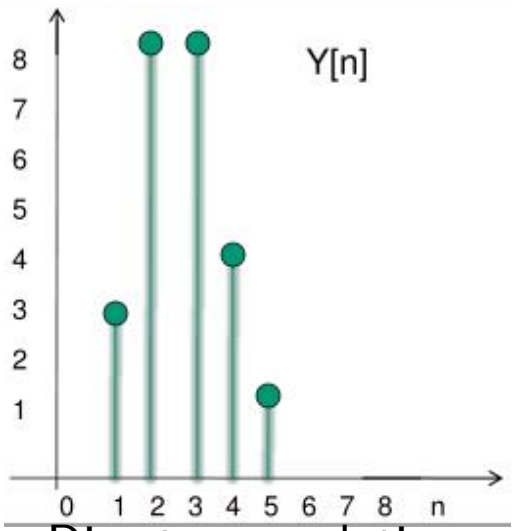

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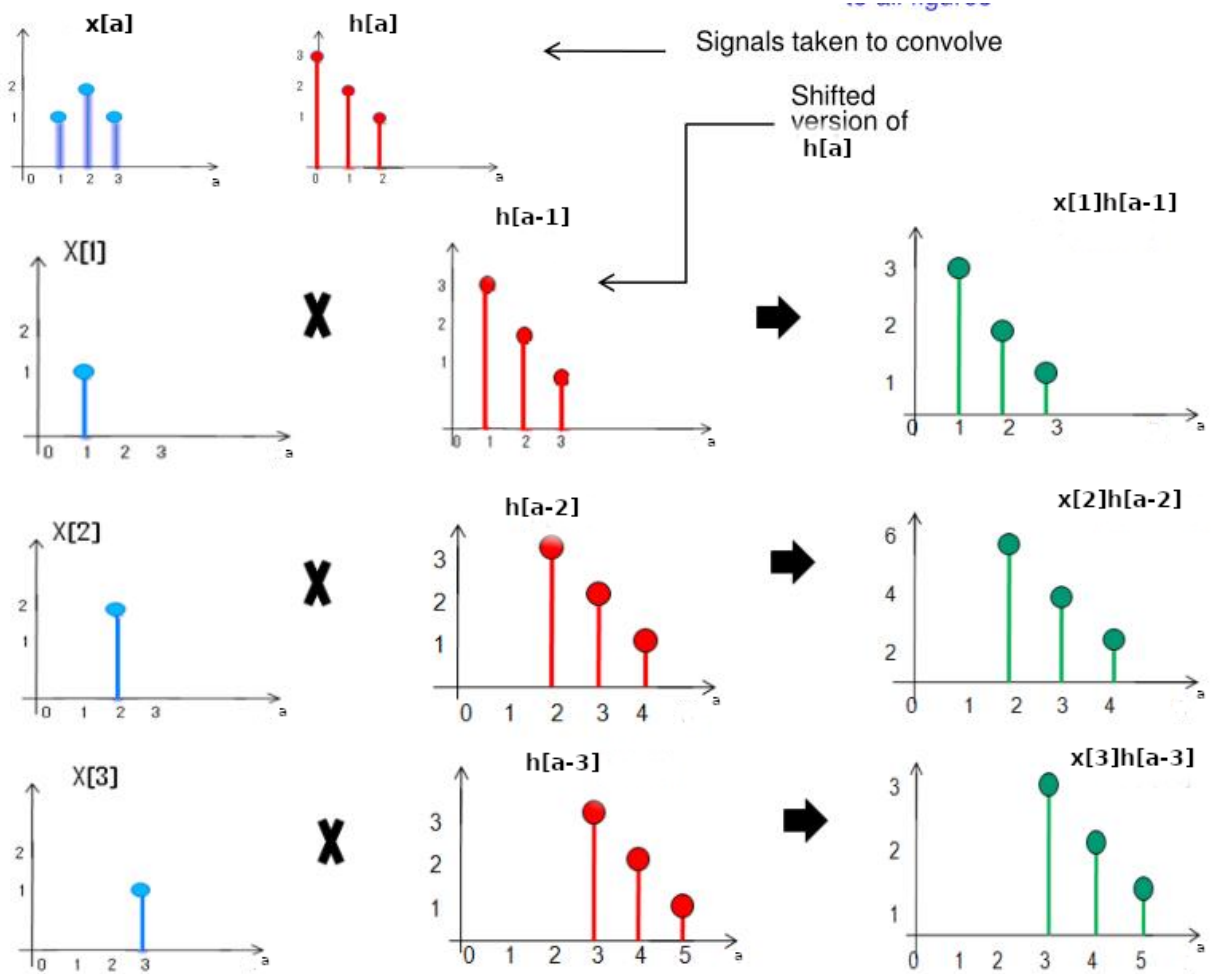

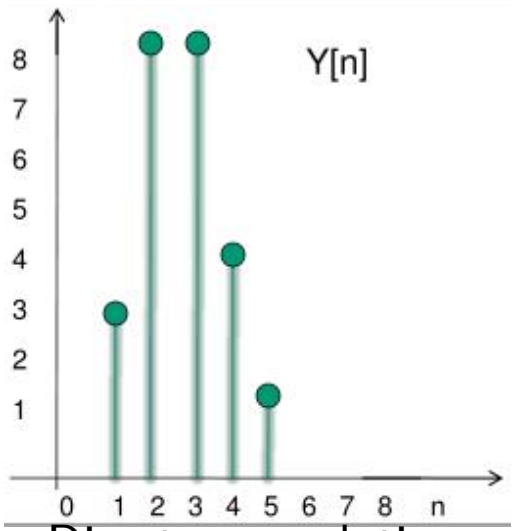

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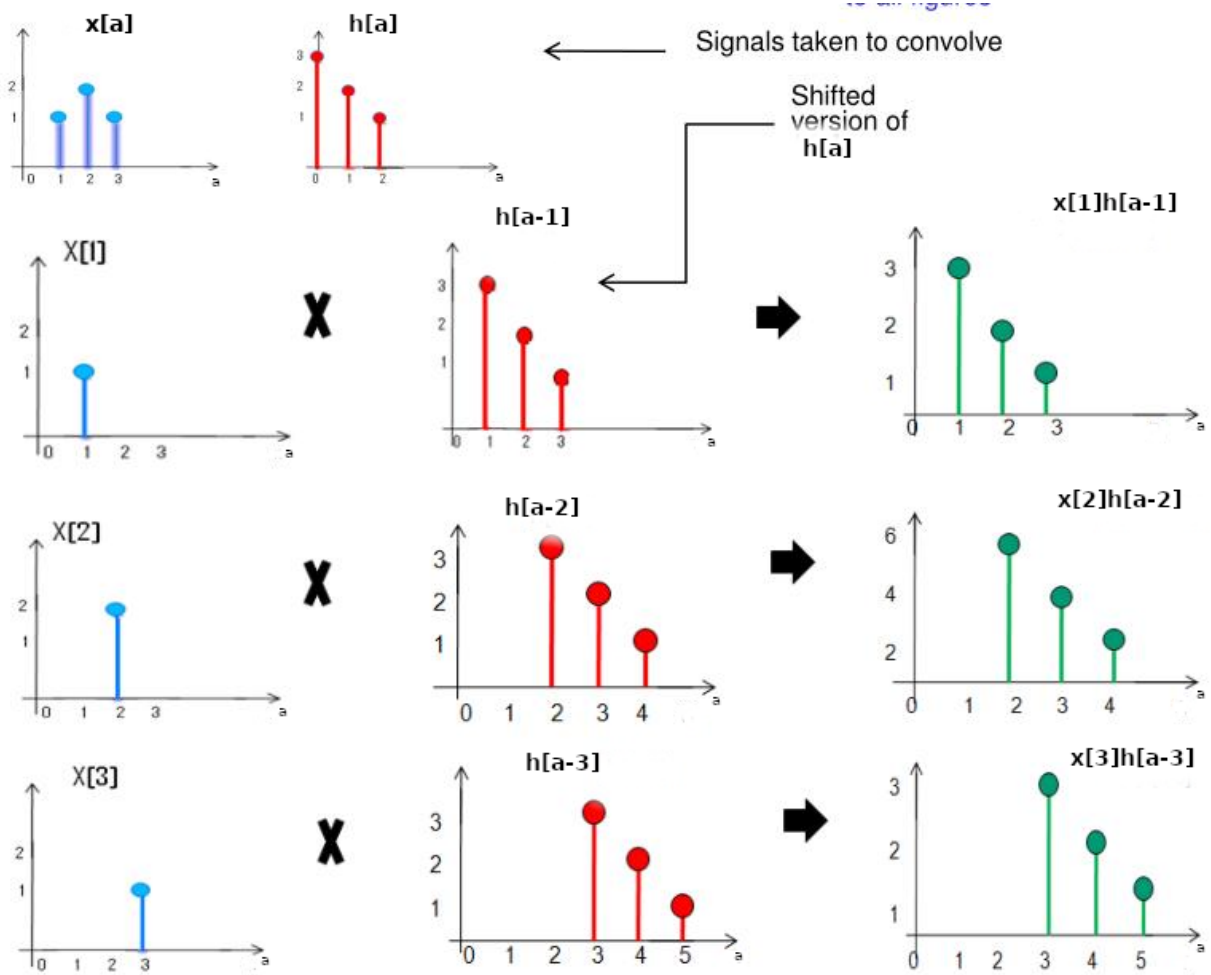

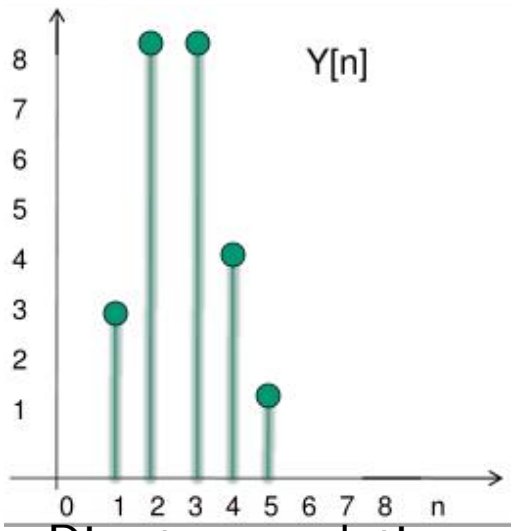

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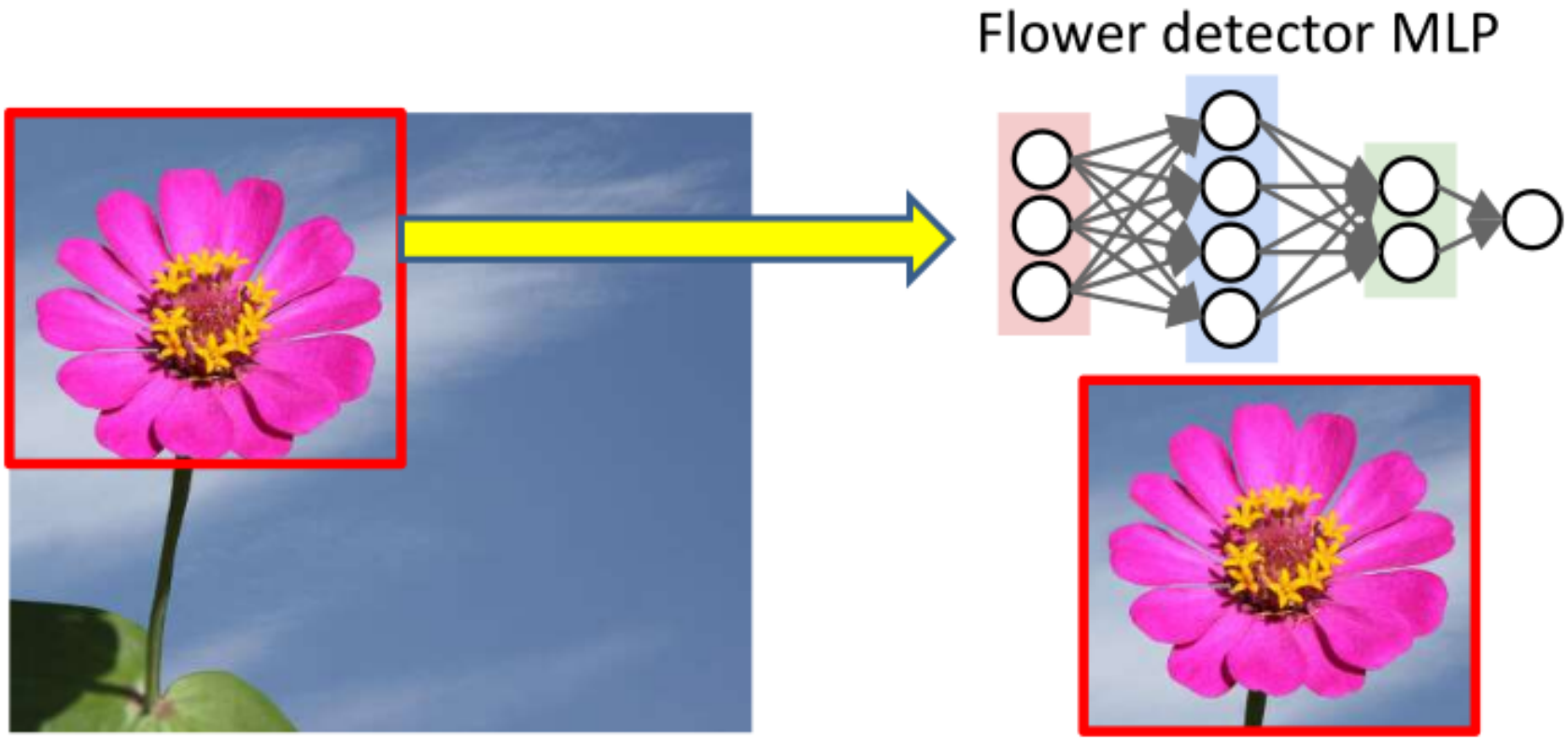
– $Y(2) =$?

Deep Learning in Life Sciences

Convolution in Convolutional layers

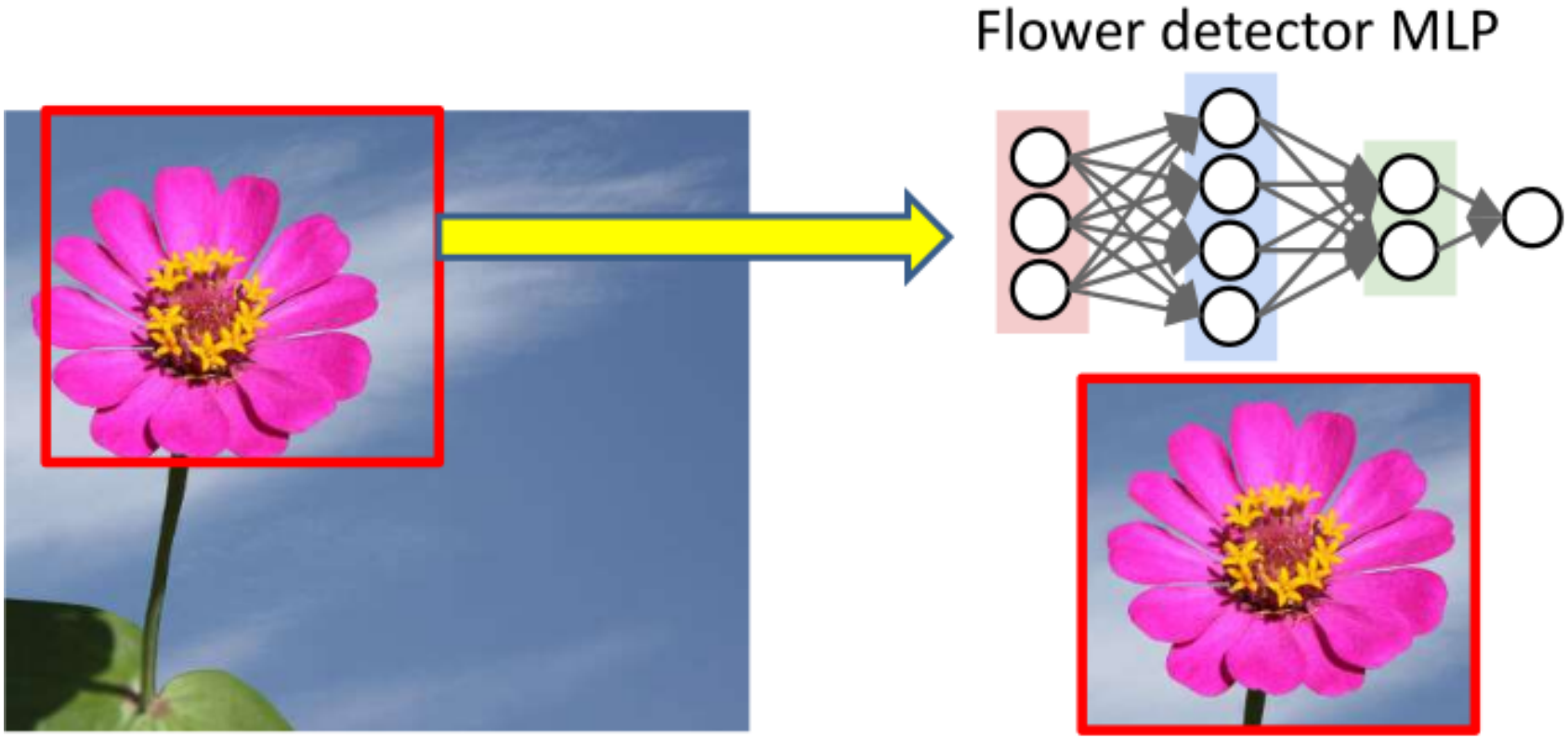
- In the case of a convolutional Neural Nets (CNN), the "scanning MLP" operates a convolution
- The input values in a window are the h values
- The connection weights of the sliding window (to be learned) represent the x values

2D (Discrete) Convolution



For images our window moves in 2 directions!

2D Convolution



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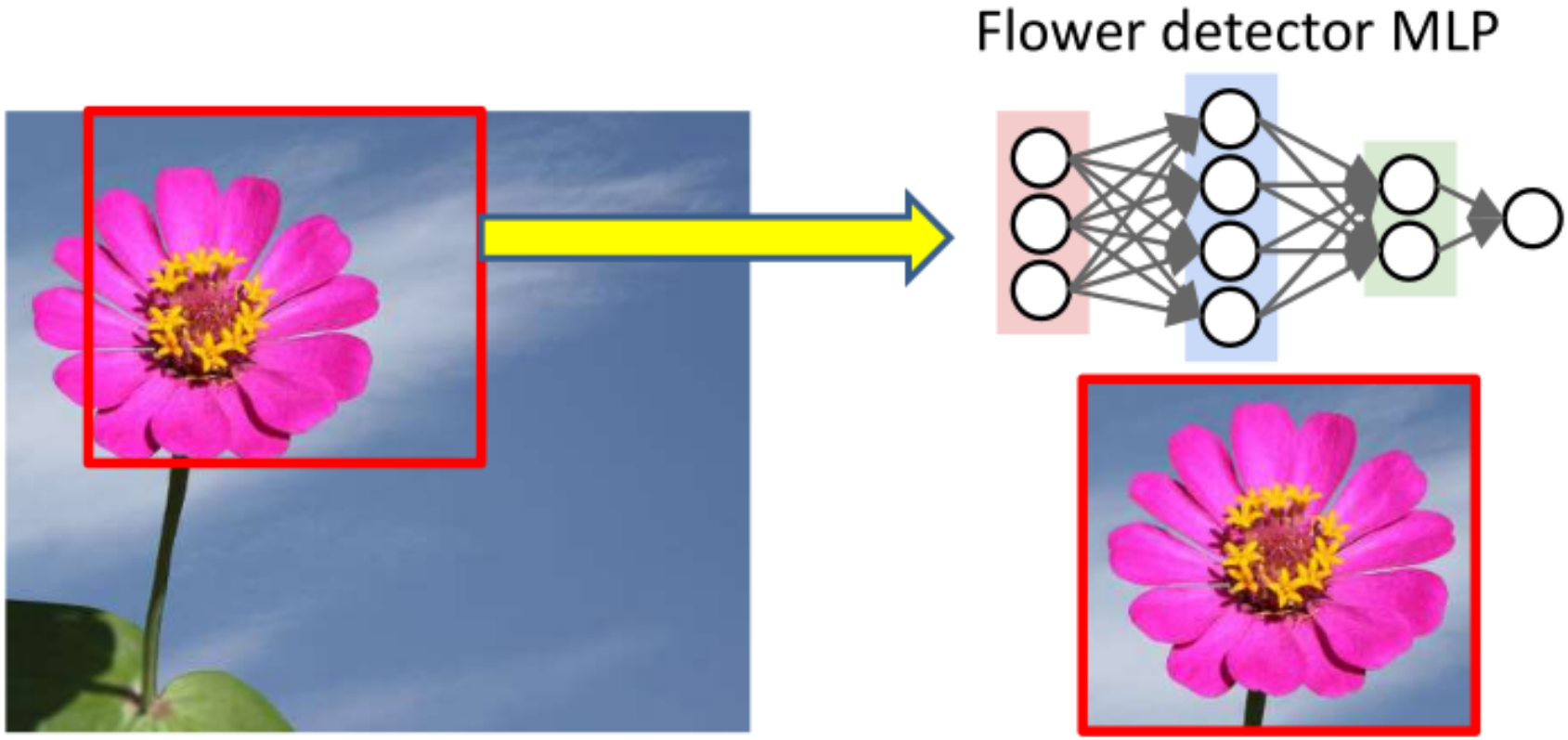

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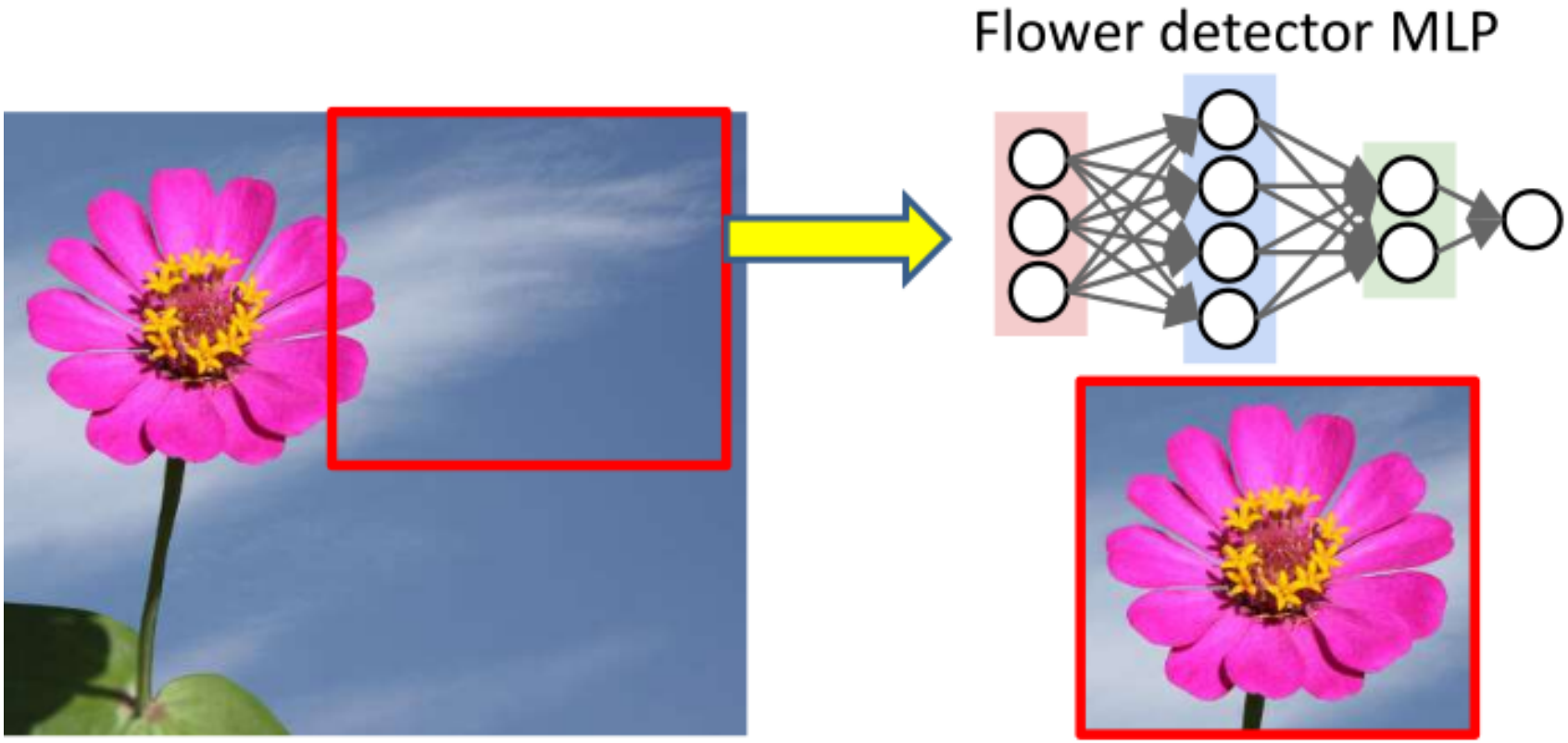

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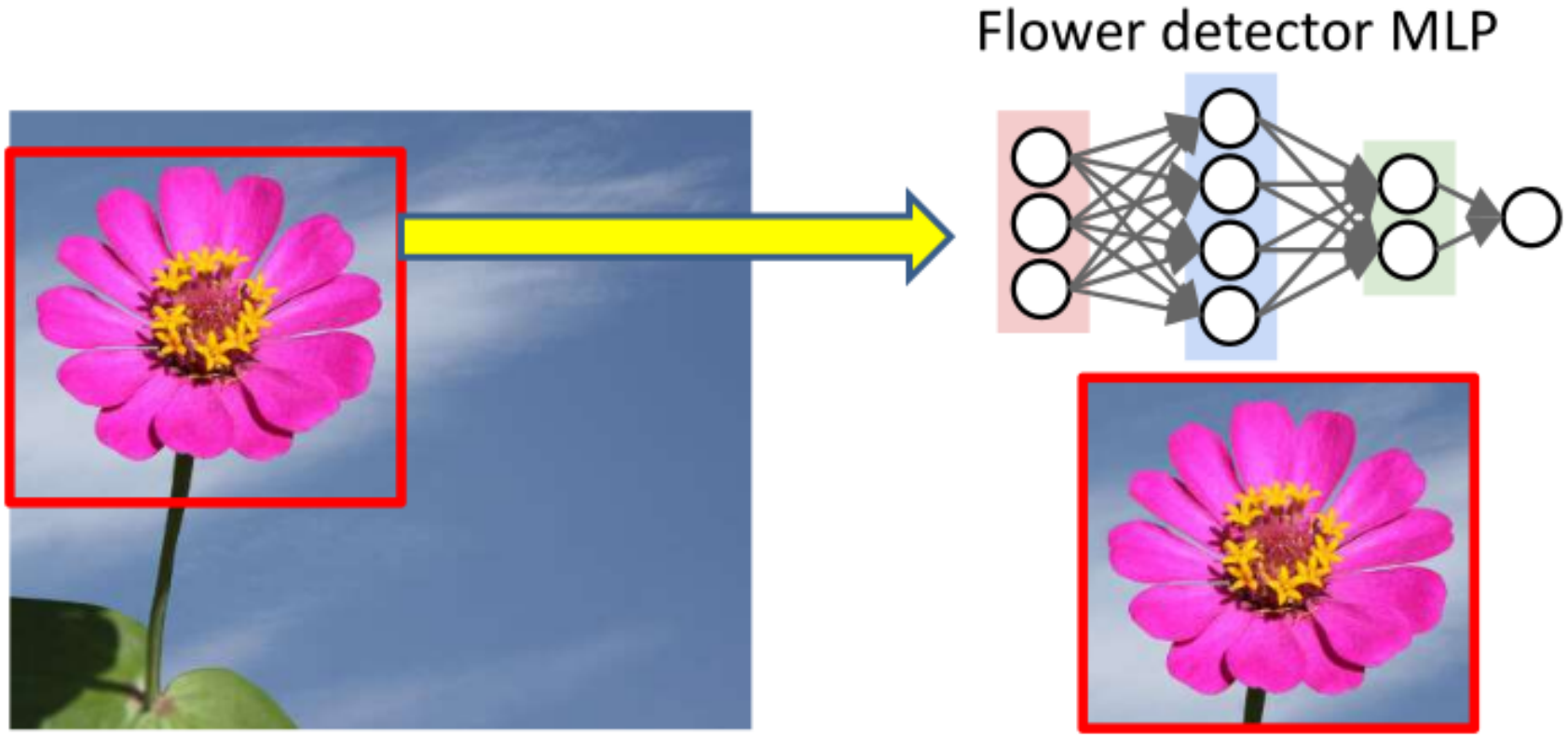

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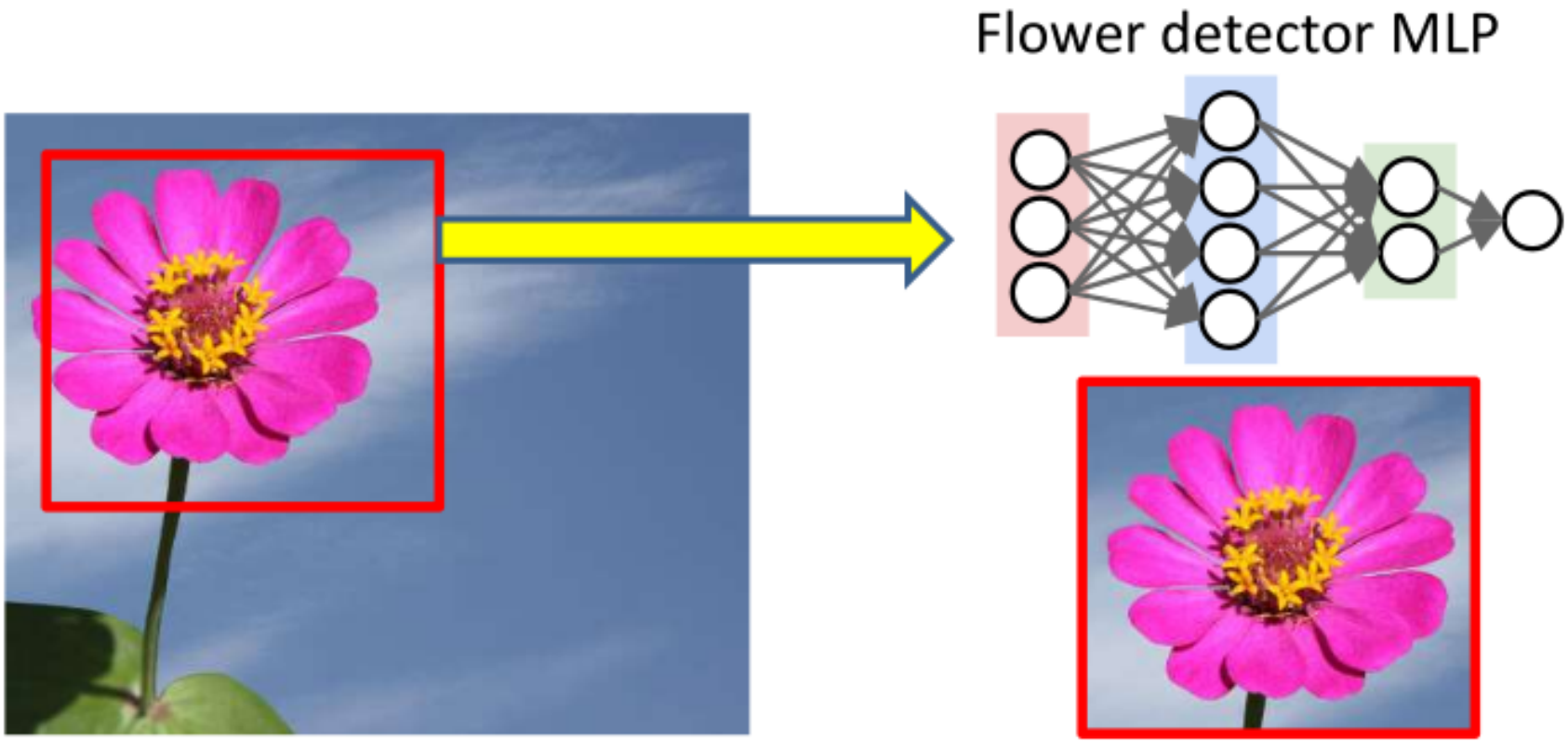

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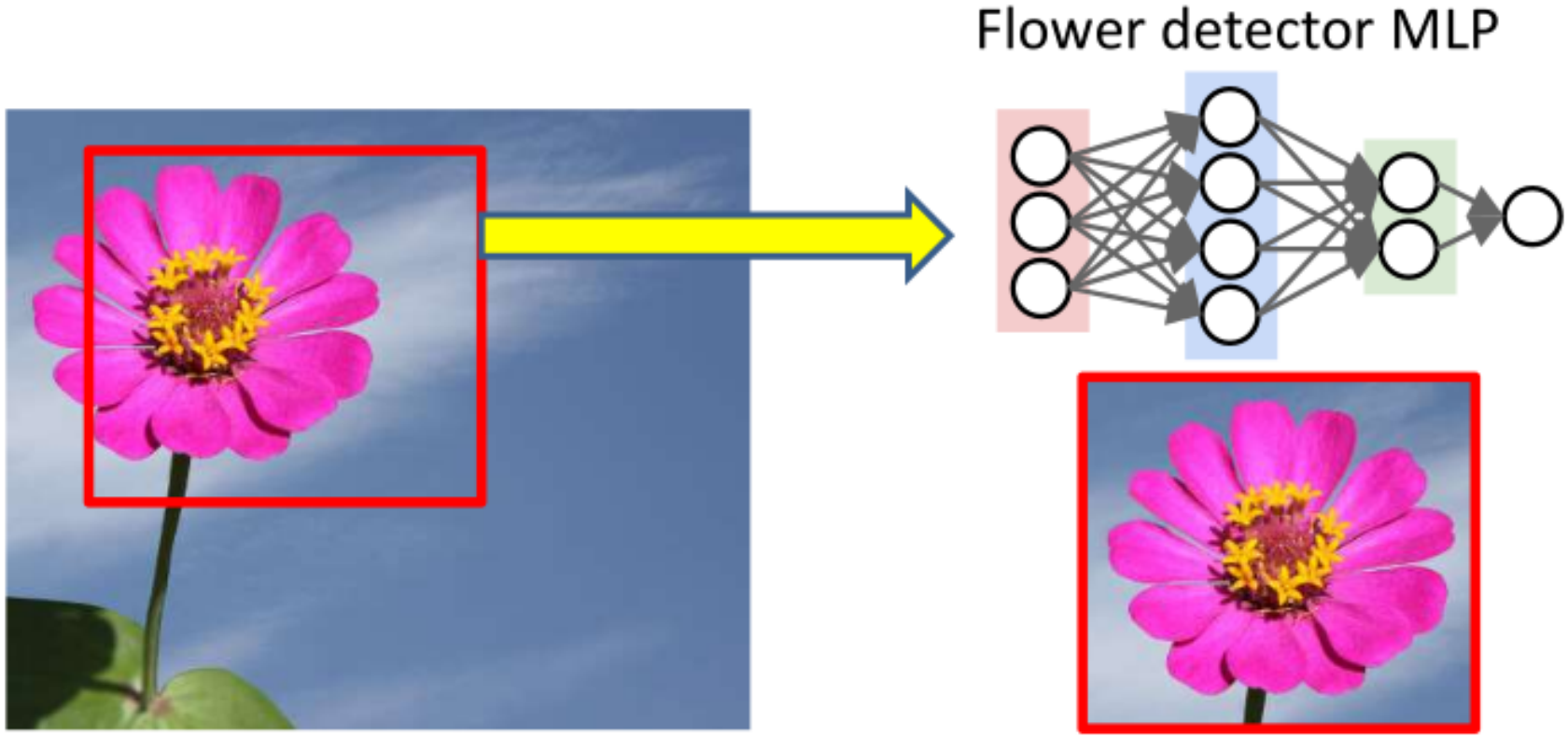

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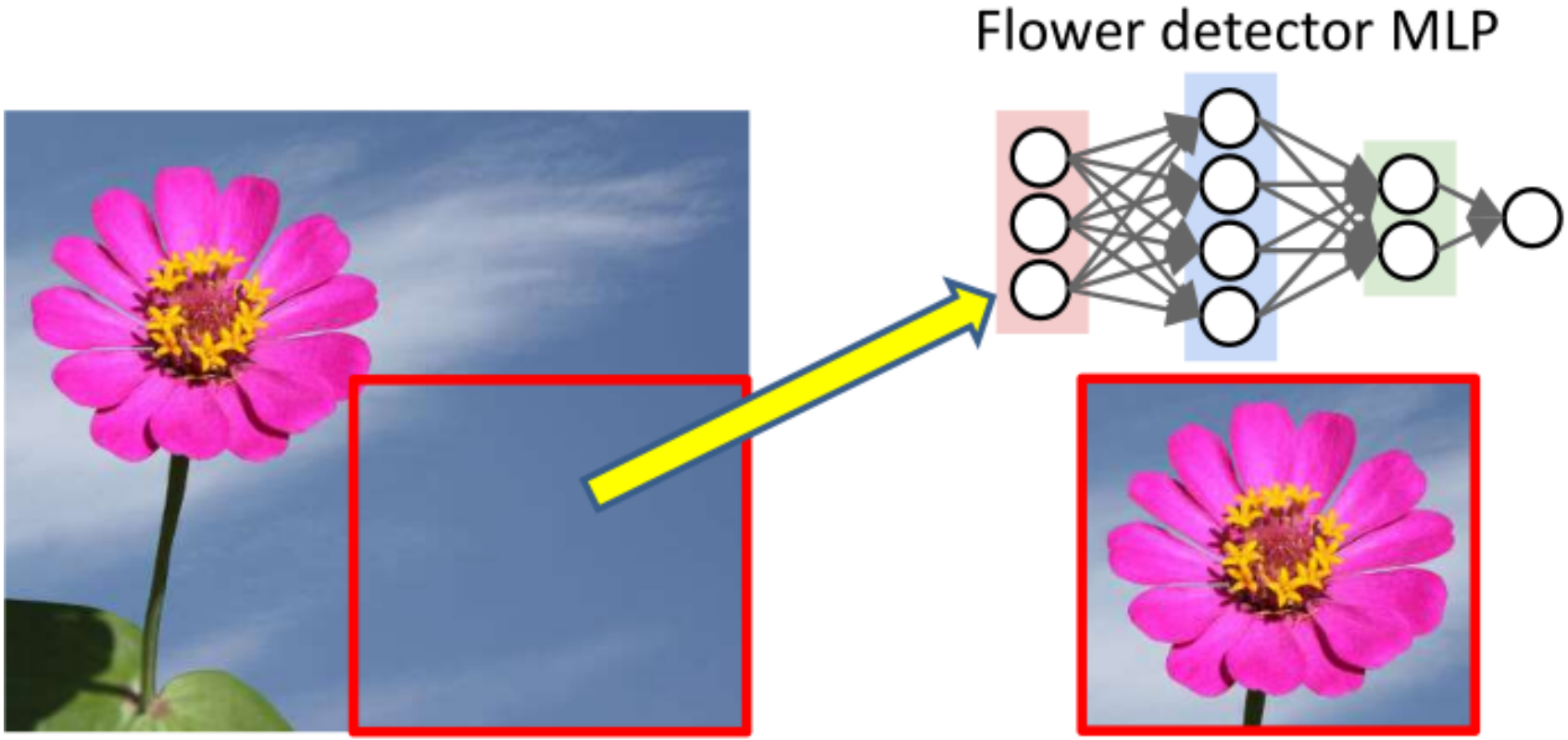

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Shared parameters of a Convolutional Layer

RECAP:

- Backing to the "imaginary" welcome-detector scanning-MLP, it operates the same job in each window

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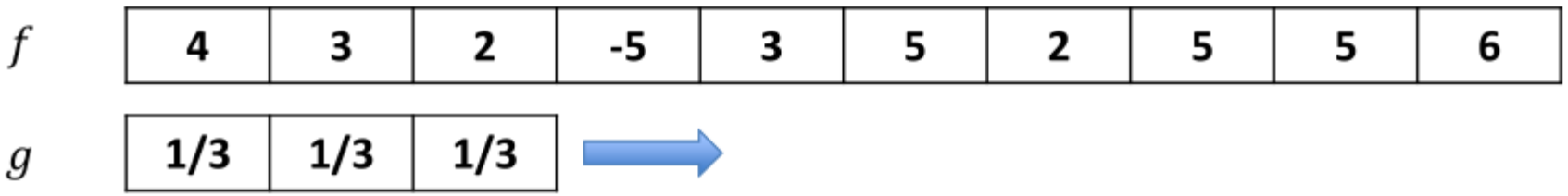
RECAP:

- Backing to the "imaginary" welcome-detector scanning-MLP, it operates the same job in each window
- We can thereby use the same model for all inputs windows!
  - Shared parameters!
- A Convolutional layer has much less parameters than a fully-connected one!

Discrete Convolution: 1D case

In a convolutional layer, with little abuse of terminology, x (g in the figure) is often referred to as a "filter", or a "kernel" or a "filter kernel"



'Slide' **filter kernel** from left to right; at each position, compute a single value in the output data

Which value this operation outputs?

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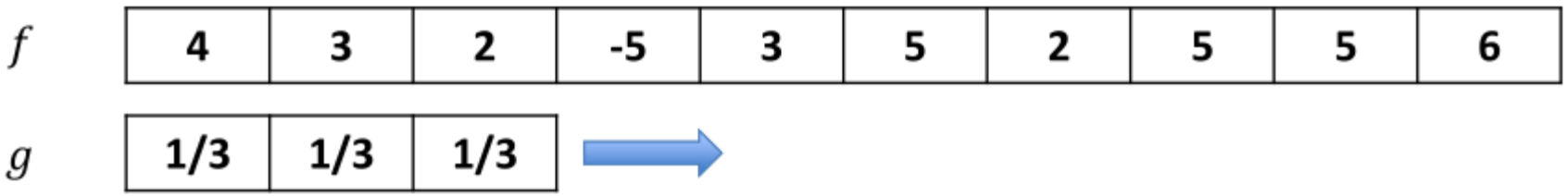
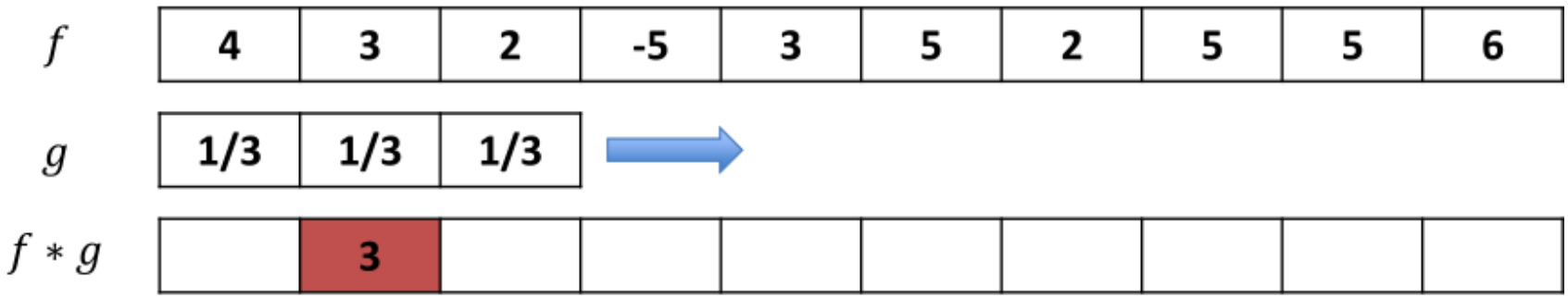


'Slide' **filter kernel** from left to right; at each position, compute a single value in the output data

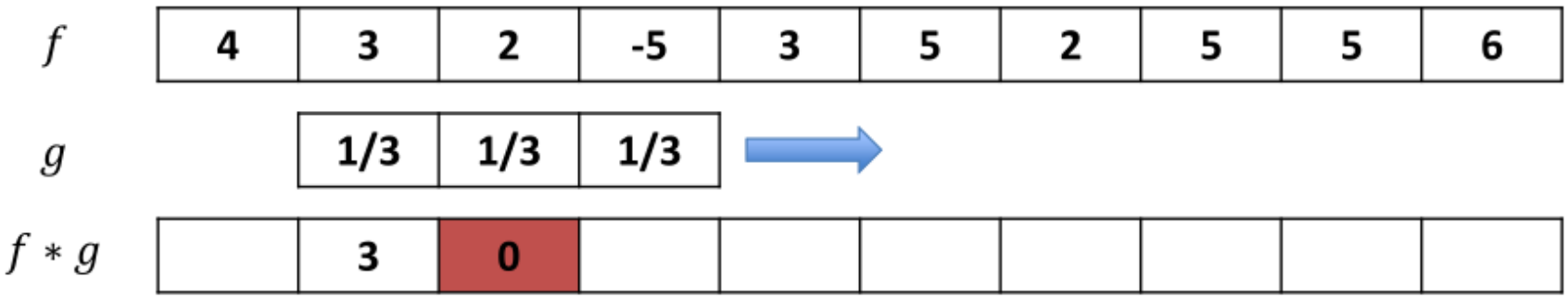
Which value this operation outputs? Exactly the result of the convolution with the input!

Discrete Convolution: 1D case



$$4 \cdot \frac{1}{3} + 3 \cdot \frac{1}{3} + 2 \cdot \frac{1}{3} = 3$$

Discrete Convolution: 1D case



$$3 \cdot \frac{1}{3} + 2 \cdot \frac{1}{3} + (-5) \cdot \frac{1}{3} = 0$$

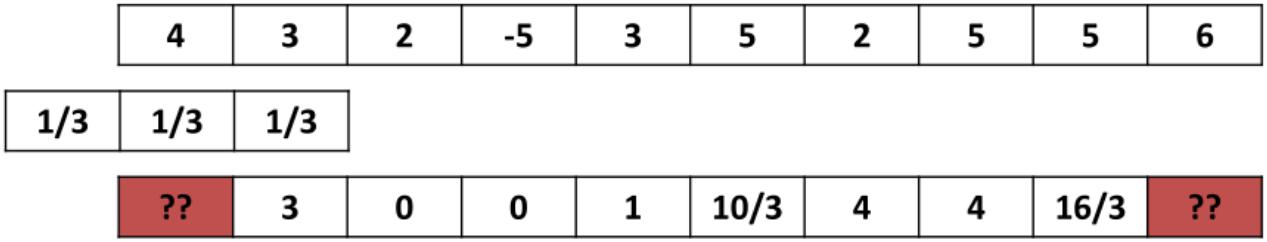
Discrete Convolution: 1D case

f	4	3	2	-5	3	5	2	5	5	6
g								1/3	1/3	1/3
$f * g$		3	0	0	1	10/3	4	4	16/3	

$$5 \cdot \frac{1}{3} + 5 \cdot \frac{1}{3} + 6 \cdot \frac{1}{3} = \frac{16}{3}$$

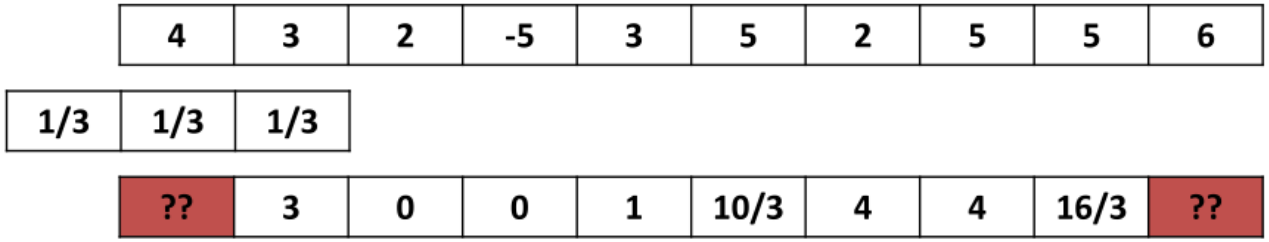
The step used to slide the window is called a STRIDE

Discrete Convolution: 1D case



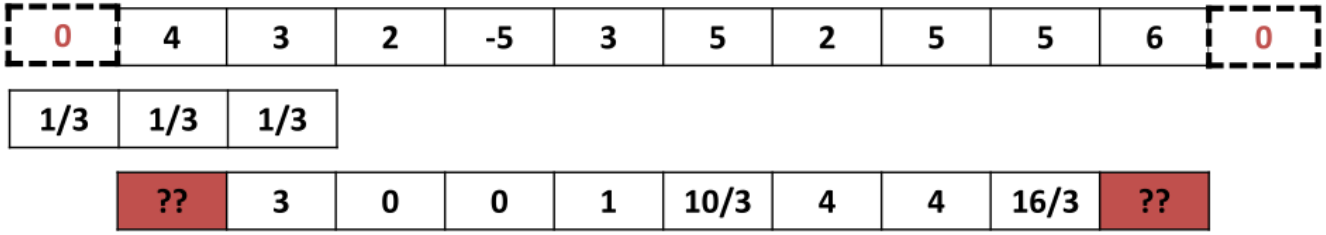
What to do at boundaries?

Discrete Convolution: 1D case



What to do at boundaries?

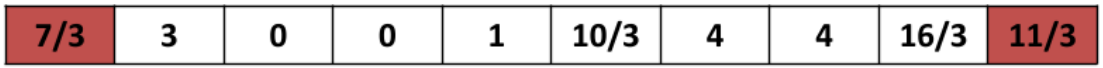
Possible Solution: 0-Padding



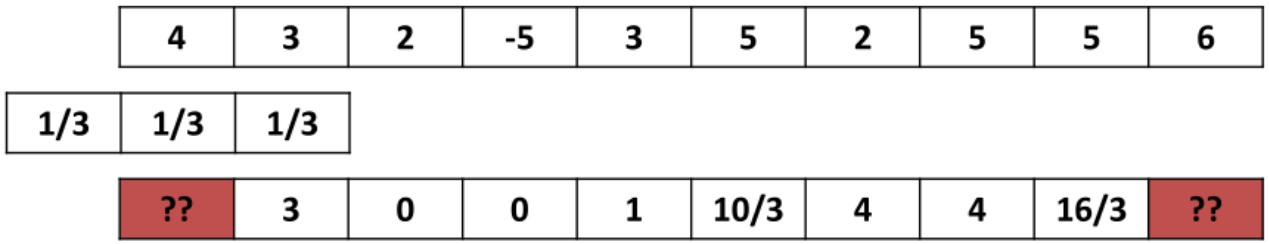
$$0 \cdot \frac{1}{3} + 4 \cdot \frac{1}{3} + 3 \cdot \frac{1}{3} = \frac{7}{3}$$

What to do at boundaries?

- Pad (often 0's)



Discrete Convolution: 1D case



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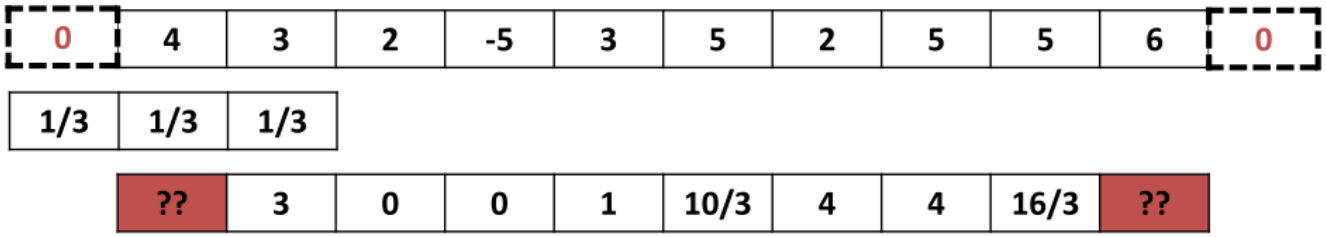

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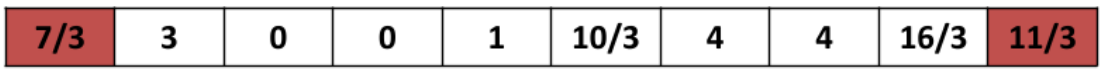
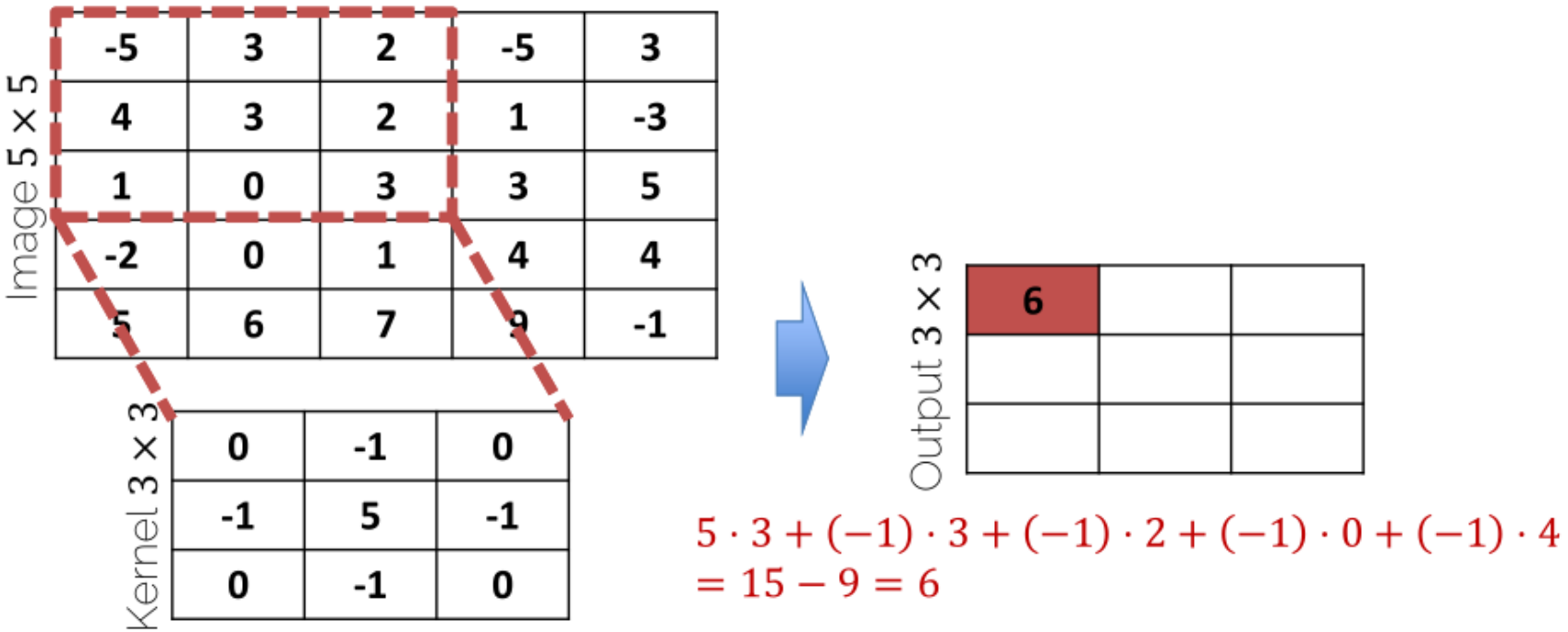


Padding allows the output channel to keep the size of the input

Deep Learning in Life Sciences

Discrete Convolution: 2D case

– In 2D the sliding window moves in two directions
– The stride can be different in the two directions



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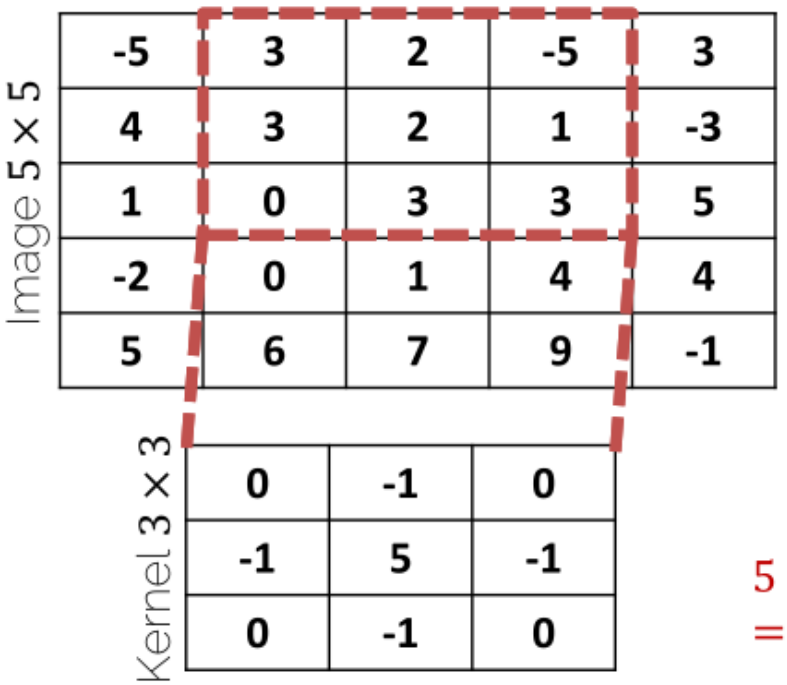
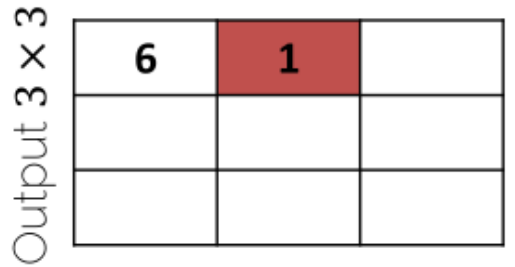
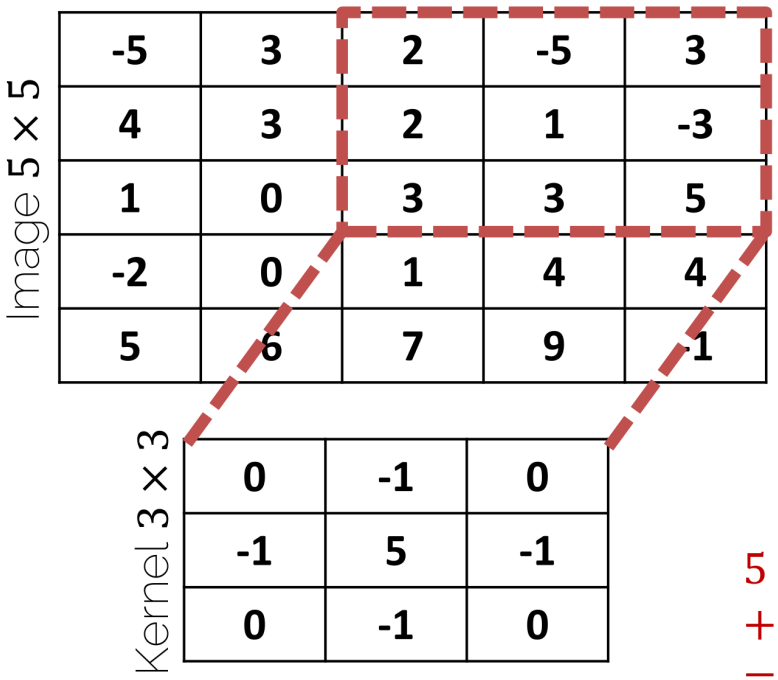
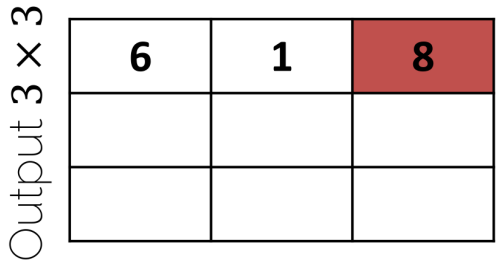




$$5 \cdot 2 + (-1) \cdot 2 + (-1) \cdot 1 + (-1) \cdot 3 + (-1) \cdot 3 = 10 - 9 = 1$$

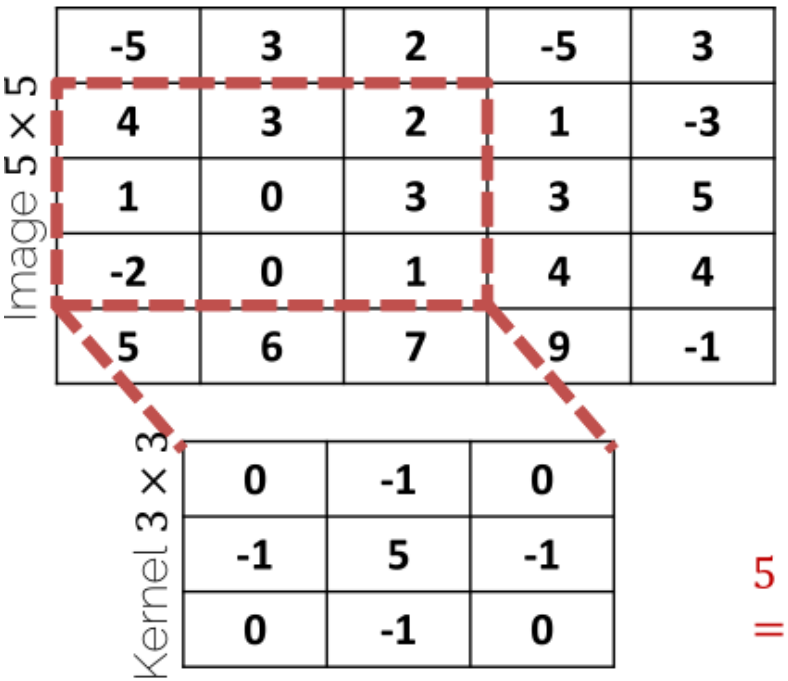
Discrete Convolution: 2D case

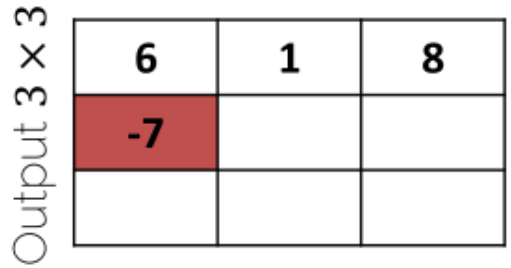




$$5 \cdot 1 + (-1) \cdot (-5) + (-1) \cdot (-3) + (-1) \cdot 3 + (-1) \cdot 2 = 5 + 3 = 8$$

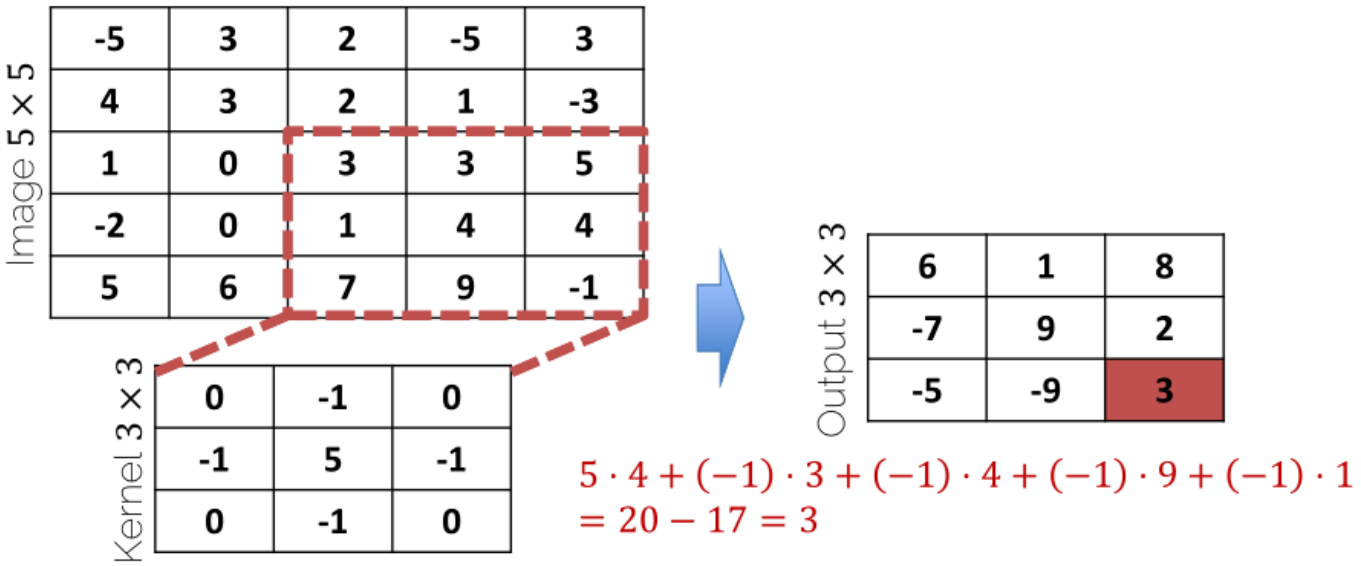
Discrete Convolution: 2D case





$$5 \cdot 0 + (-1) \cdot 3 + (-1) \cdot 0 + (-1) \cdot 1 + (-1) \cdot 3 = 0 - 7 = -7$$

Discrete Convolution: 2D case



- the kernel size in the example is 3×3 or simply 3 by shortening

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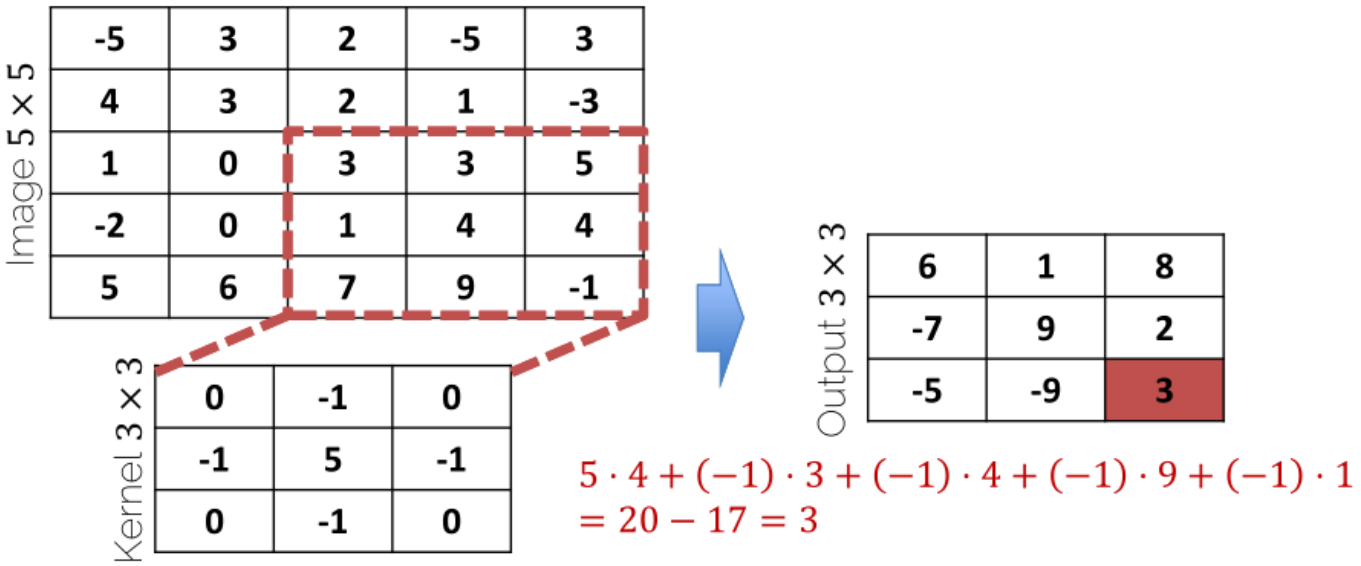

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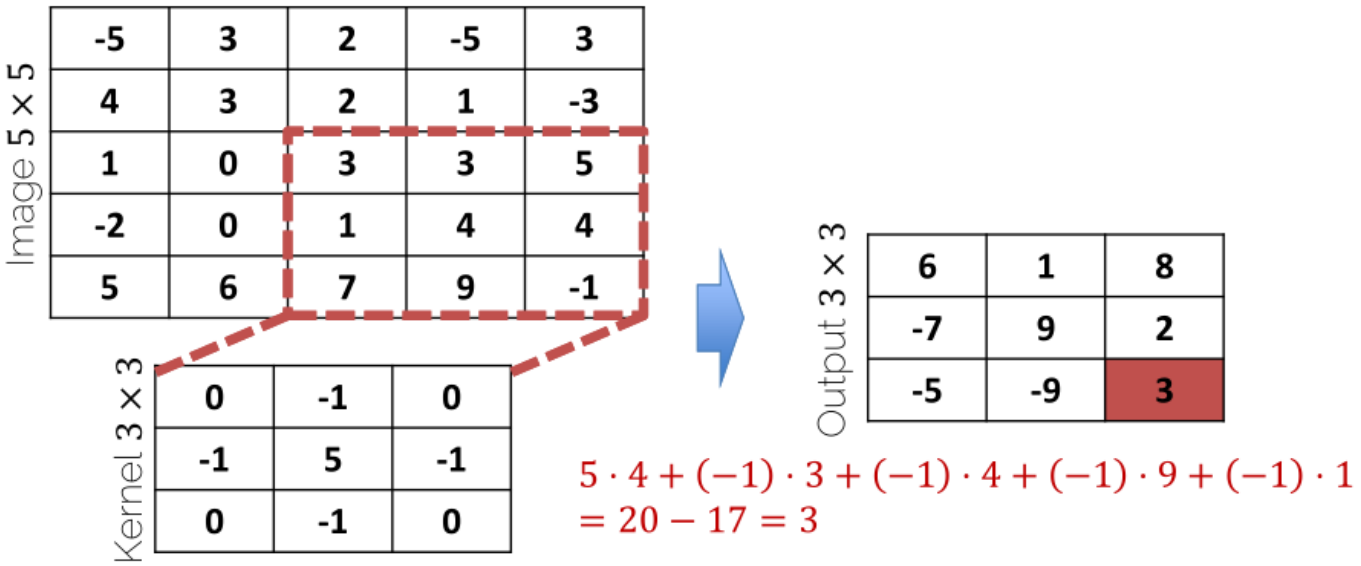

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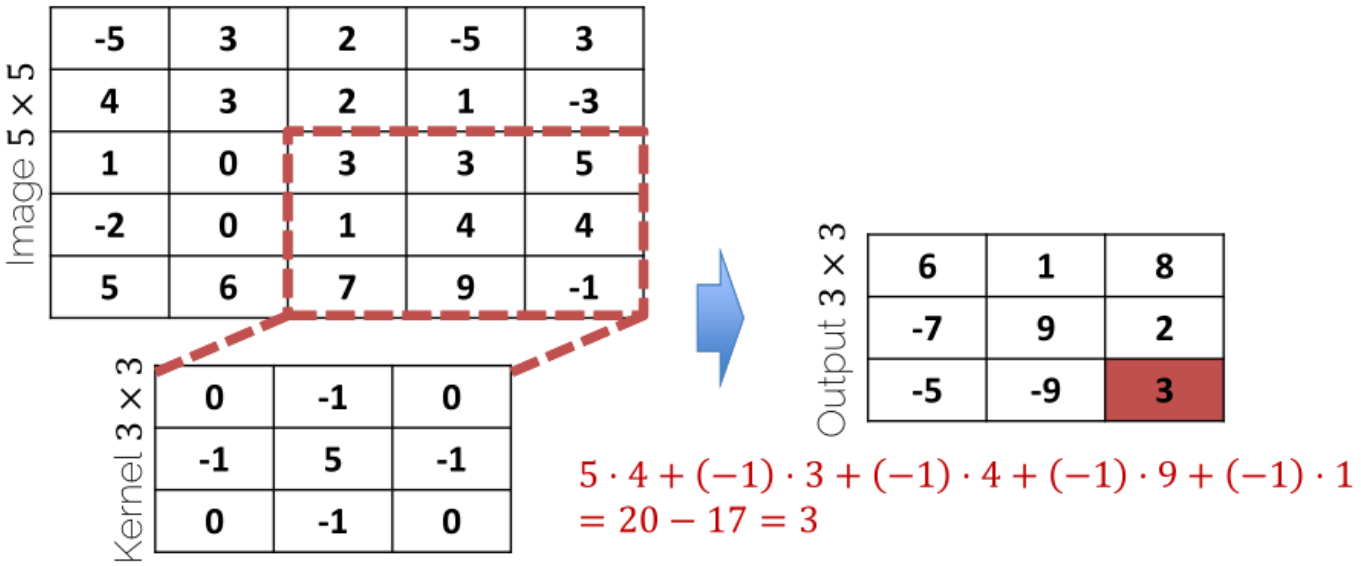
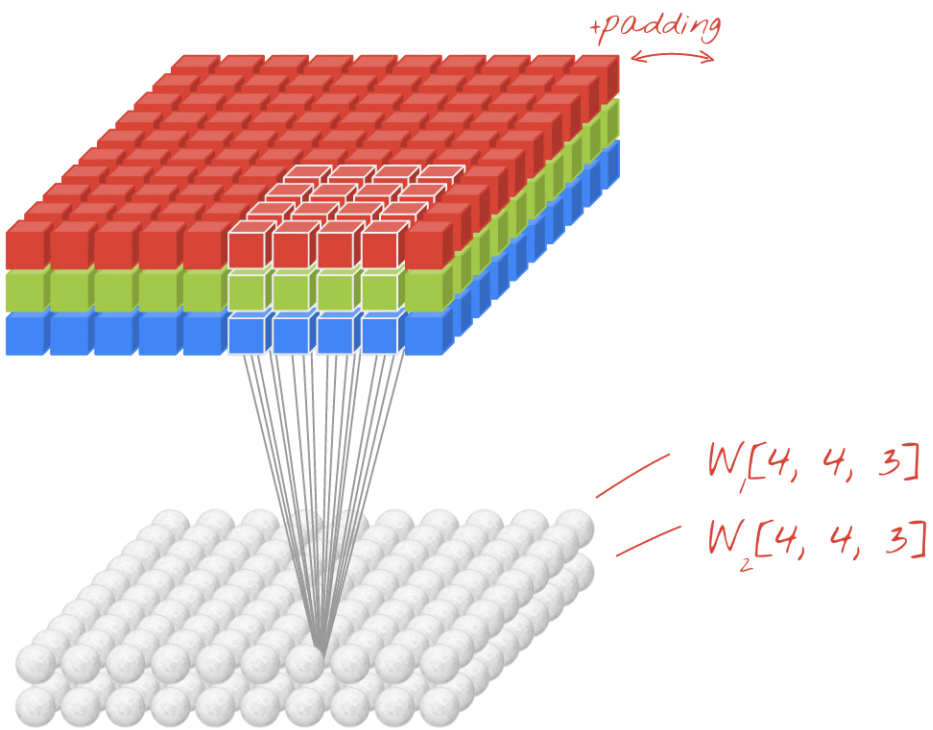


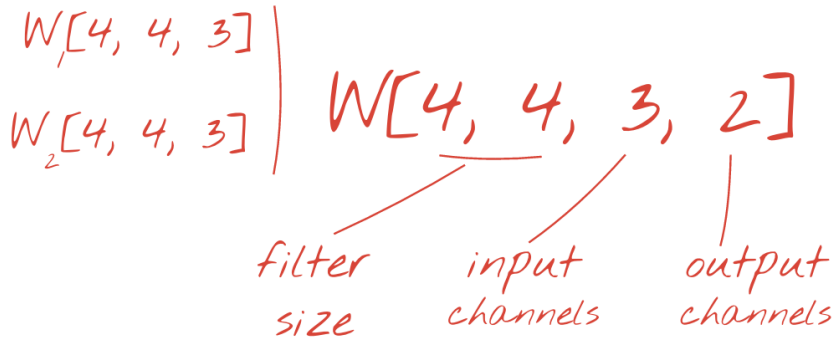
- the kernel size in the example is 3×3 or simply 3 by shortening
- The output is also known as a feature map
- The feature map size is 3×3 as well in this example
- Even in this case we could 0-pad the input grid for the feature map to have the same size of the input

Deep Learning in Life Sciences

Convolution: 3D case



Source: https://stats.stackexchange.com/questions/240926/how-are-convolutional-layers-connected-in-theano



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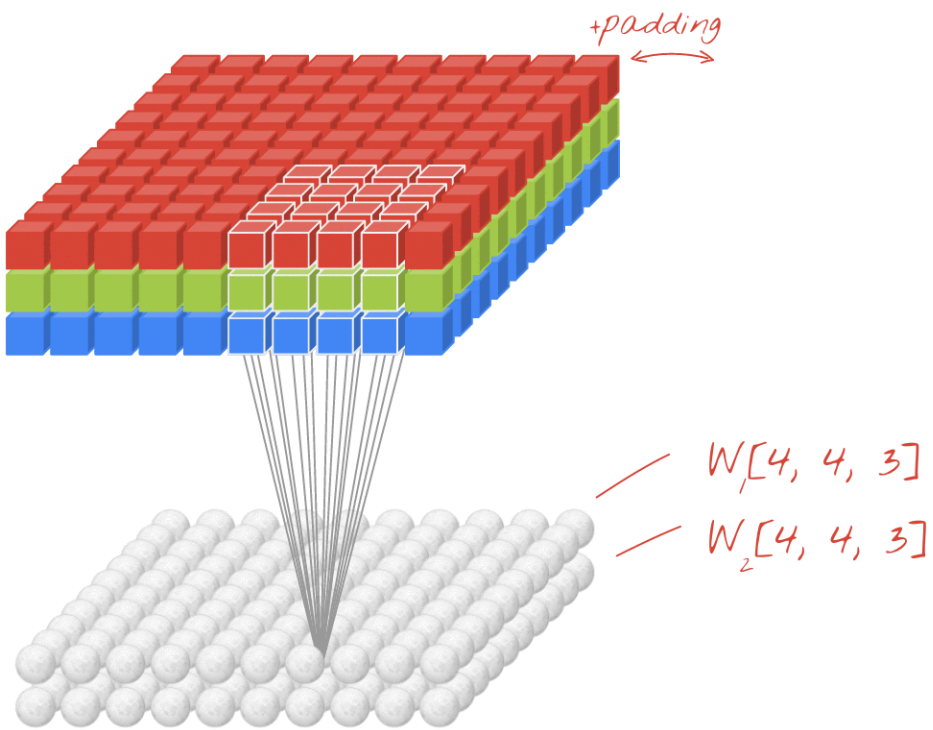

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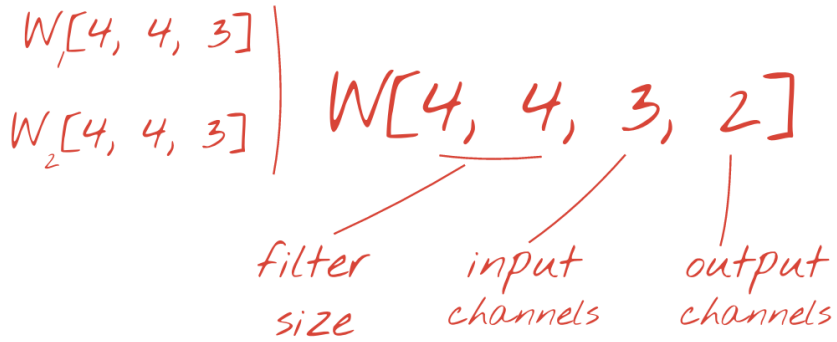

- In 1D,2D, or 3D cases, the number of filters used is the number of output channels (regardless of the number of input maps!)
- Each feature map produced by a filter is an output channel

Convolutional Layer

- Suppose we use a 2D filter of size k. How many parameters?

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  - In this case, the feature map (output) has a depth N
  - In other words, each filter produces an output channel, which are stacked atop each other

Outline

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Nothing prevent us to use more convolutional layers in sequence!

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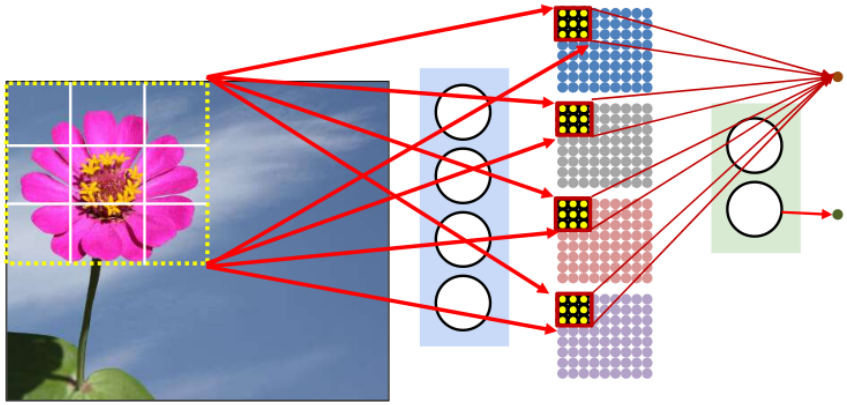

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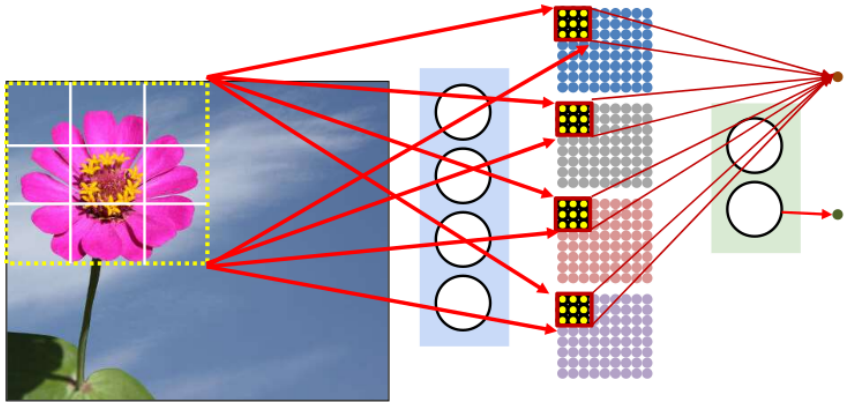

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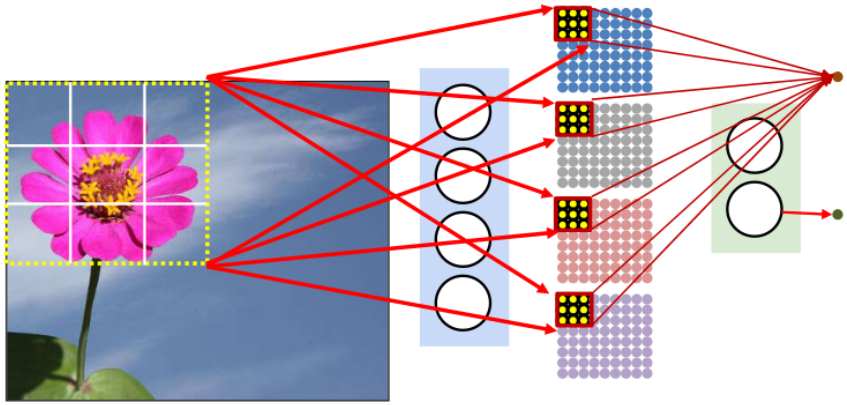

- Each neuron in the second convolutional layer is performing the equivalent of a convolution of a 9×9 filter!
- Total parameters per filter: 9 in the first layer, and 9 in the second layer. 18 vs 81!!

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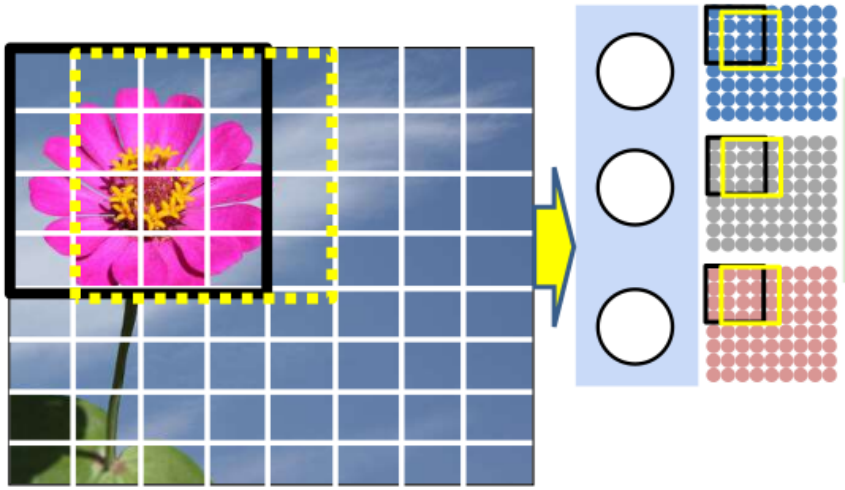
  3. Fewer computations (we ca resuse computations in overlapping windows)

Advantage of Distributed Convolution

Overlapping windows in the second conv layer share most computations: computed at the first conv layer!! (small squares in the pic)



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- Pay attention to use valid convolution: Shrink the feature map, but can loose information at borders!
- Its usage depends on the semantic of the input!

Outline

Pooling

- Pooling neurons replace the weighted sum of the inputs with a pooling function $f(x_1, \ldots, x_k) = pool(x_1, \ldots, x_k)$
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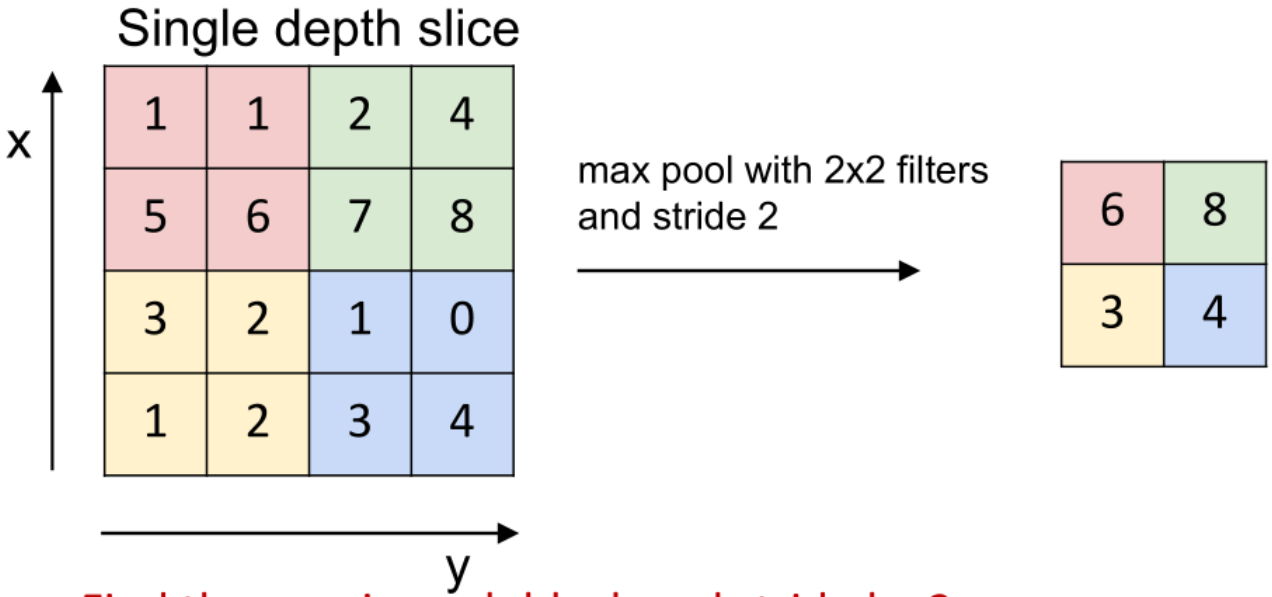
For these reasons pooling layers usually follow convolutional layers

Max/Mean Pooling

Source:https://www.geeksforgeeks.org/introduction-convolution-neural-network/



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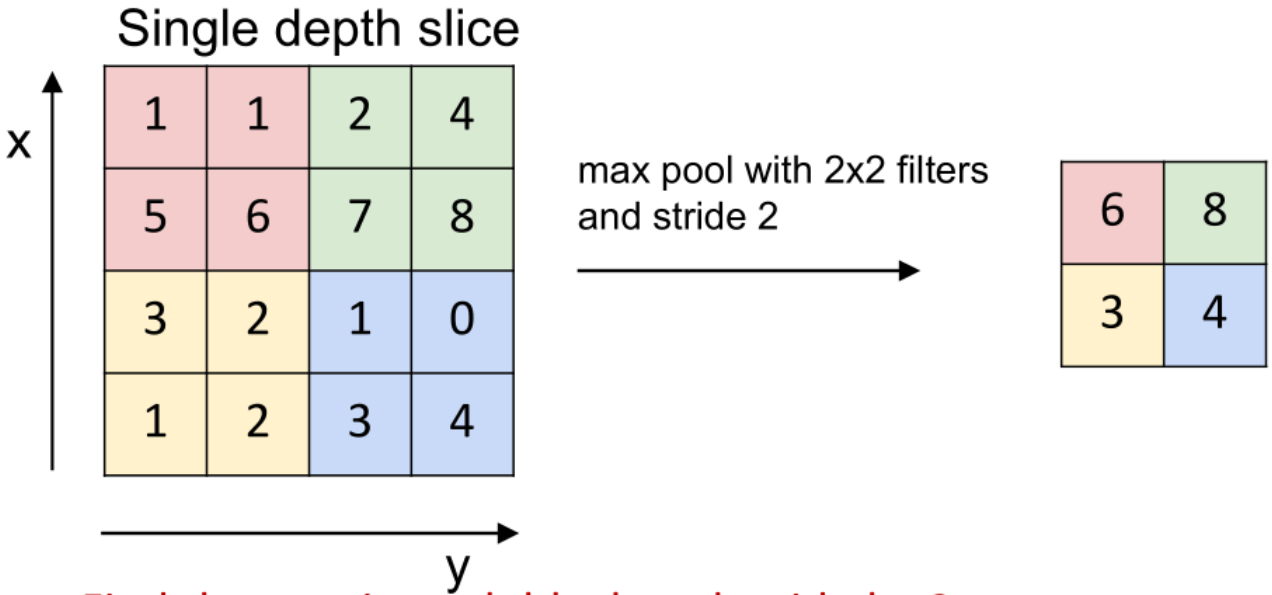

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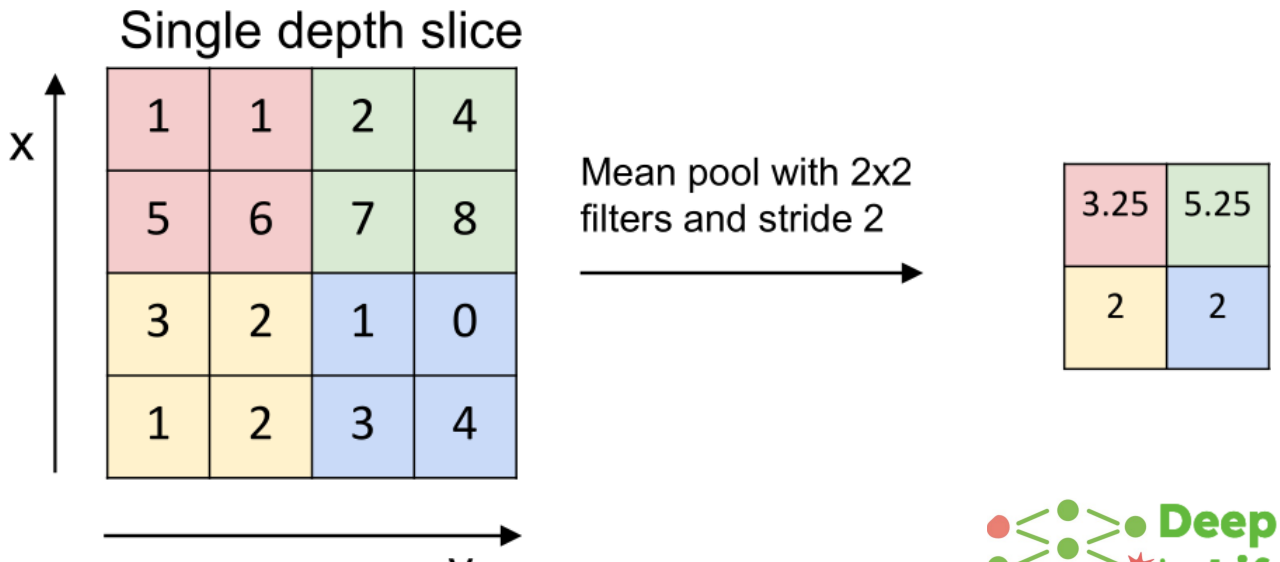

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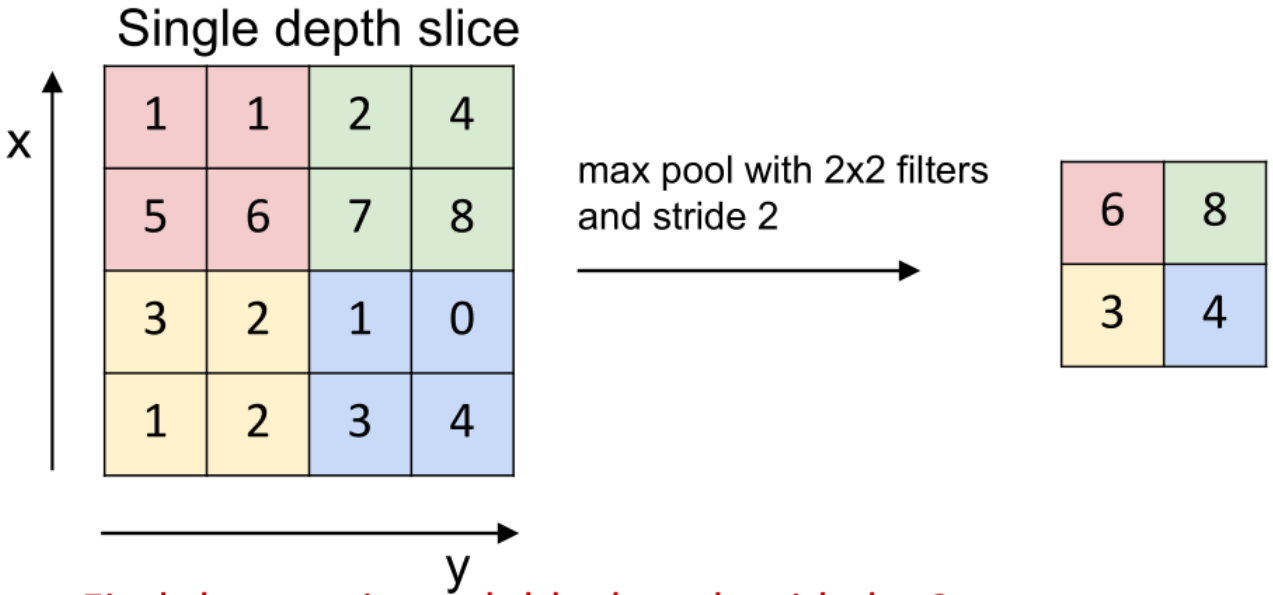
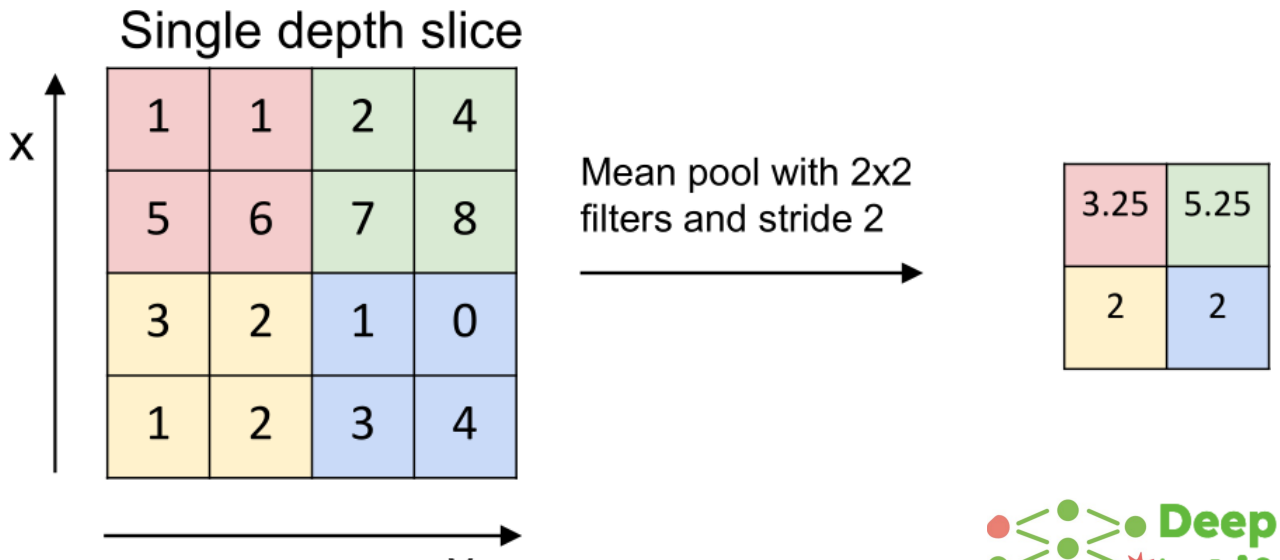


- Find the max in each block and stride by 2



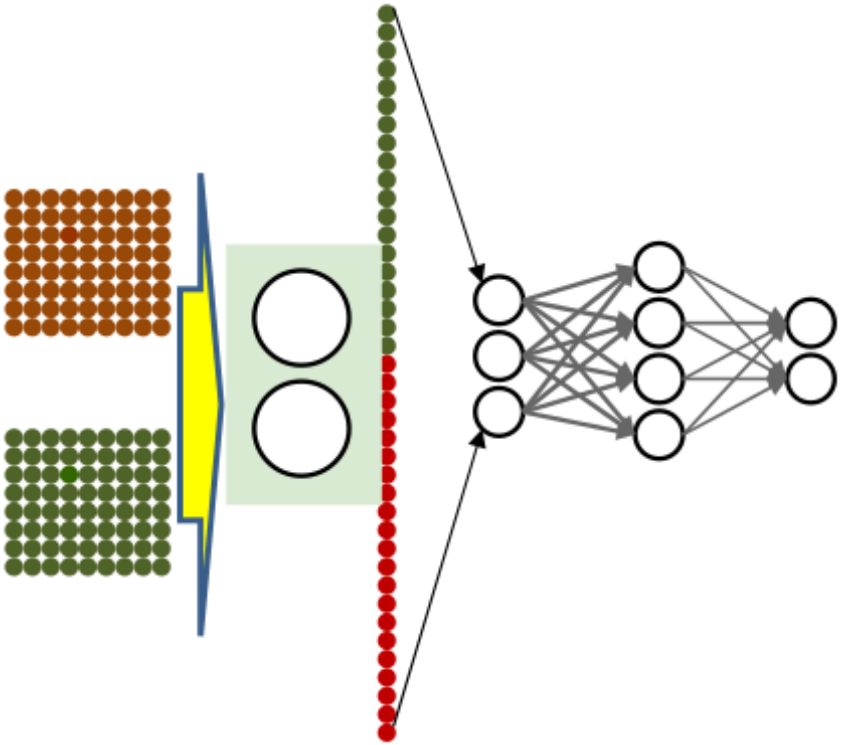
An $N \times N$ picture compressed by a $F \times F$ pooling filter extent with stride S results in an output map of size

$$\left\lceil \frac{(N-F)}{S} \right\rceil + 1$$

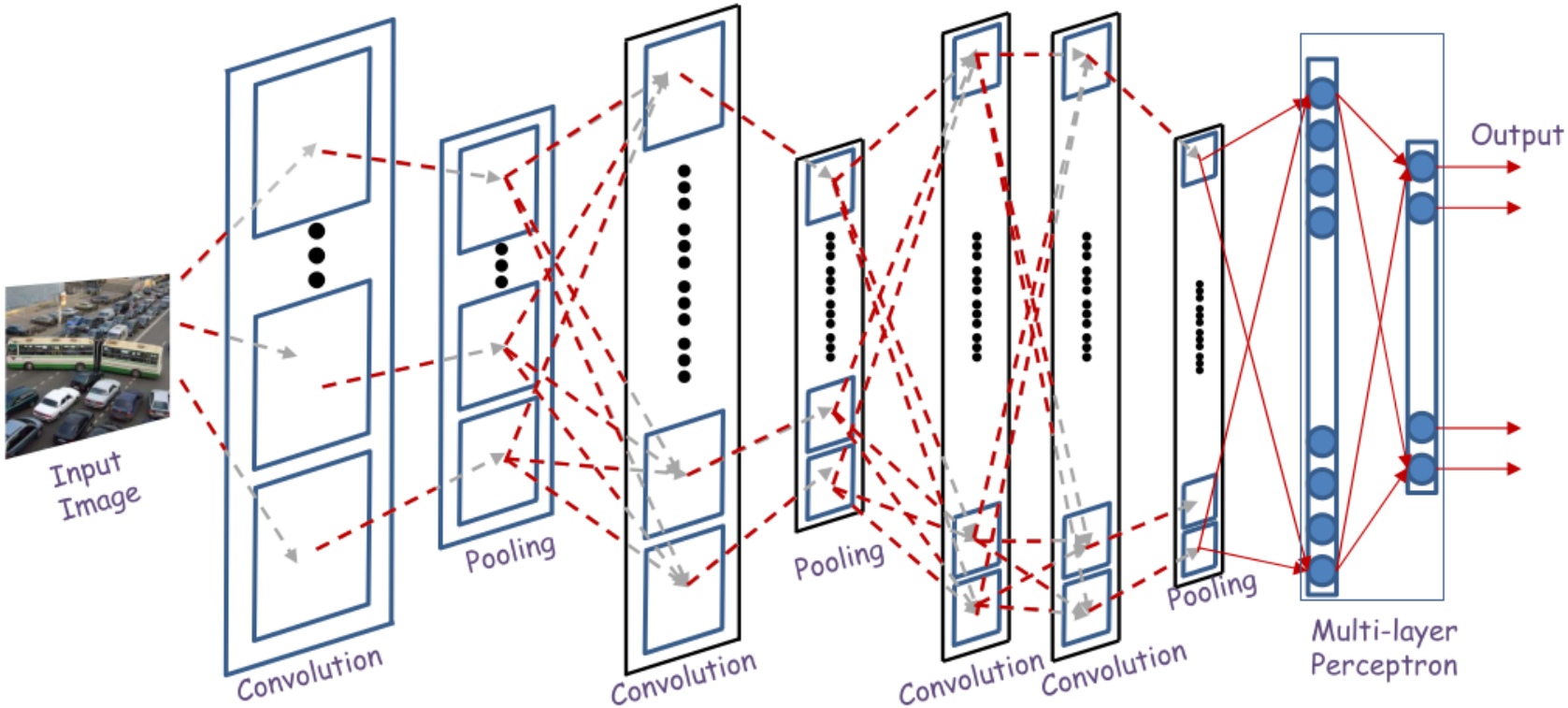
– Typically do not zero pad

Terminology

- The operation of vectorizing the output of a convolutional layer (e.g., to feed the next MLP) is called Flattening



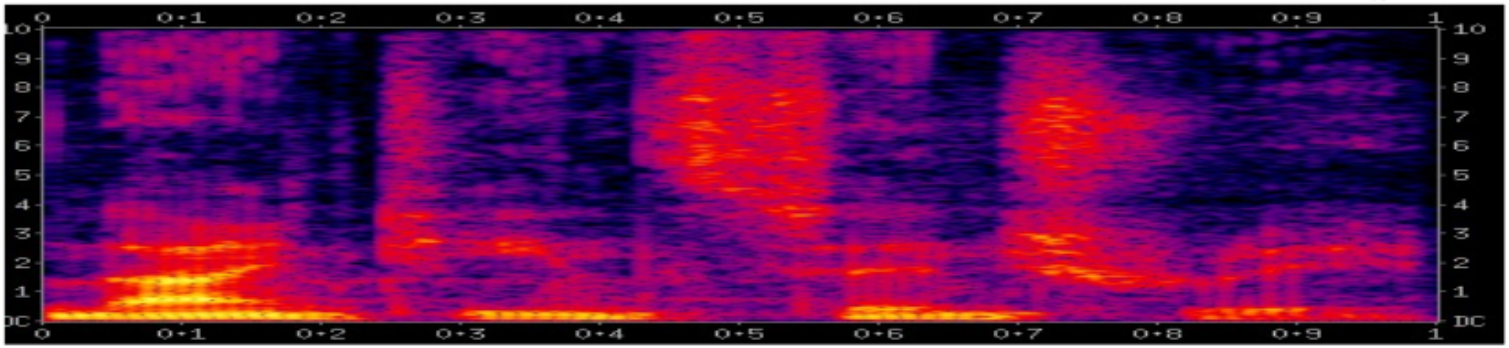
Typical CNN


Input Image
Convolution
Pooling
Convolution
Pooling
Convolution
Convolution
Pooling
Multi-layer Perceptron
Output

Outline

A problem variant

What did they say?



- Speech Recognition
  - Analyze a series of spectral vectors, determine what was said
- Note: Inputs are sequences of vectors. Output is a classification result

A problem variant 2

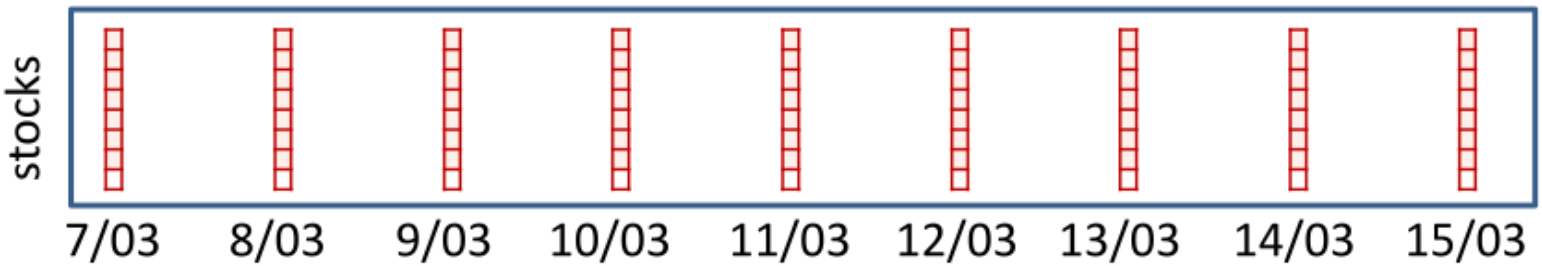
What are they talking about?

The Steelers, meanwhile, continue to struggle to make stops on defense. They've allowed, on average, 30 points a game, and have shown no signs of improving anytime soon.

- Text analysis
  - E.g. analyze document, identify topic
    - Input series of words, output classification output
  - E.g. read English, output French
    - Input series of words, output series of words

A problem variant 3

Should we invest?



Note: Inputs are sequences of vectors. Output may be scalar or vector

- Should I invest, vs. should I not invest in X?
- Decision must be taken considering how things have fared over time

Past/time dependency problems

- In all the considered problems, the output depends not just on the current input, but also on the past
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  - Need to consider a sequence of inputs (scalar or vectors)
- Must produce one or more outputs that take into account prensent and past

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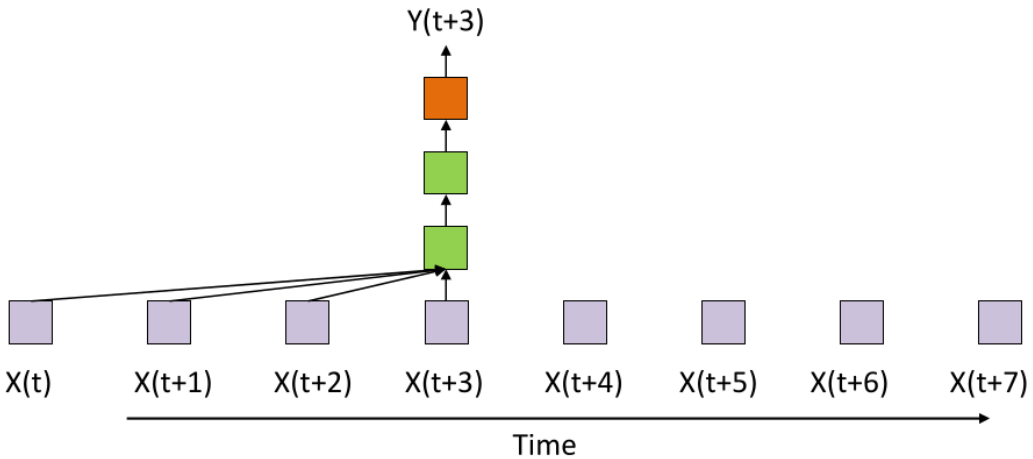
- Longer historic tends however tend to affect us less than more recent events...
- **Possibility**: The idea of "memory" could be cast into the inputs
- Problem: Increasing much the input "history" can make the network too complex



A CNN looking at the last few past temporal steps

Deep Learning in Life Sciences

Infinite dependency

A further problem: what if we need to consider longer (potentially infinite) dependencies?

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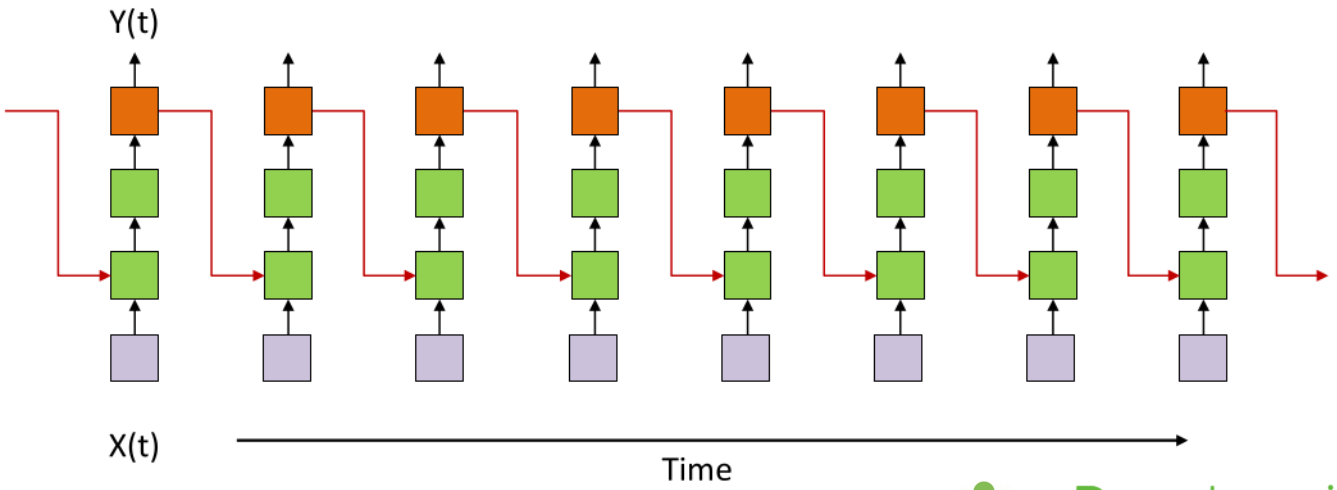
$$Y(t) = f(X(t), Y(t-1))$$

- $Y(0)$ produces $Y(1)$, which produces $Y(2)$ ... till potentially $Y(\infty)$. If we unroll it, we have something like:



Deep Learning in Life Sciences

Going beyond: the state-space model

A state-space model use state variables to describe a system

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$$h(t) = f(X(t), h(t\text{-}1))$$
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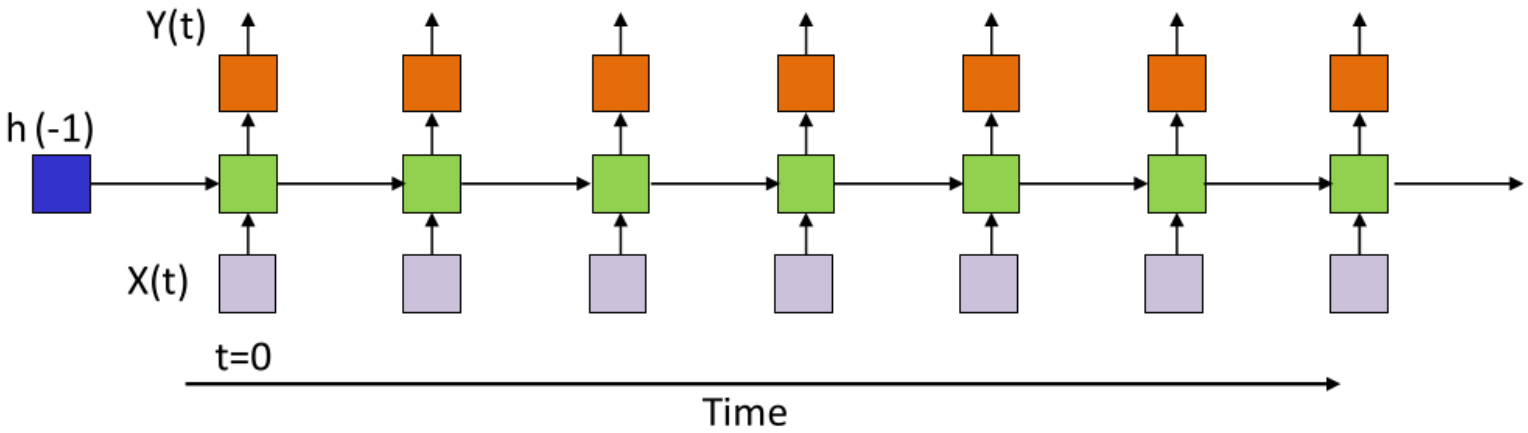
This is a fully recurrent neural network! Or simply a recurrent neural network (RNN)

Recurrent Neural Networks



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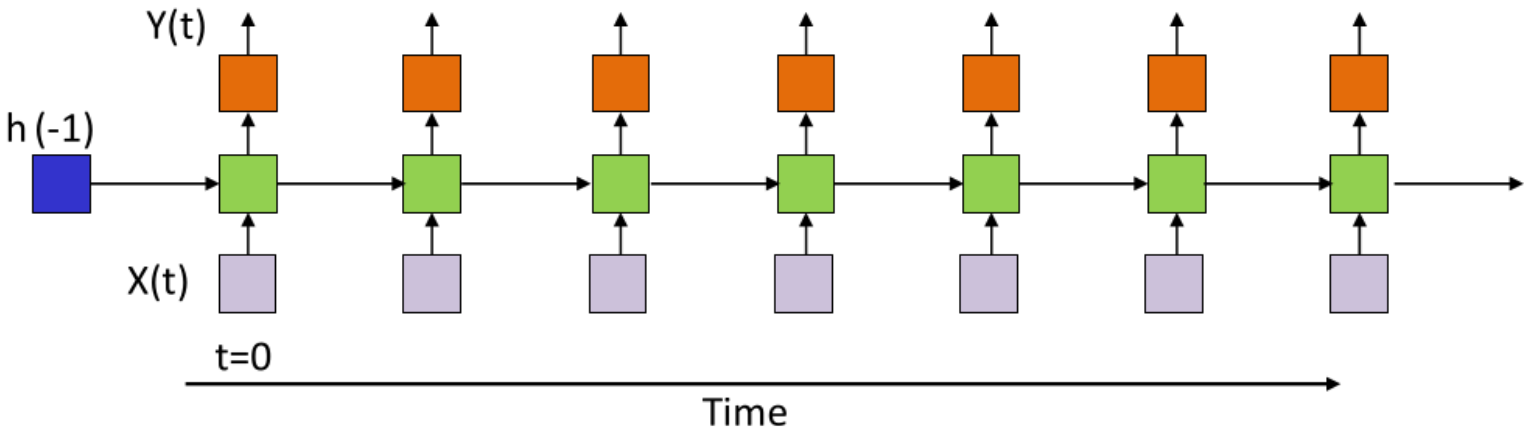

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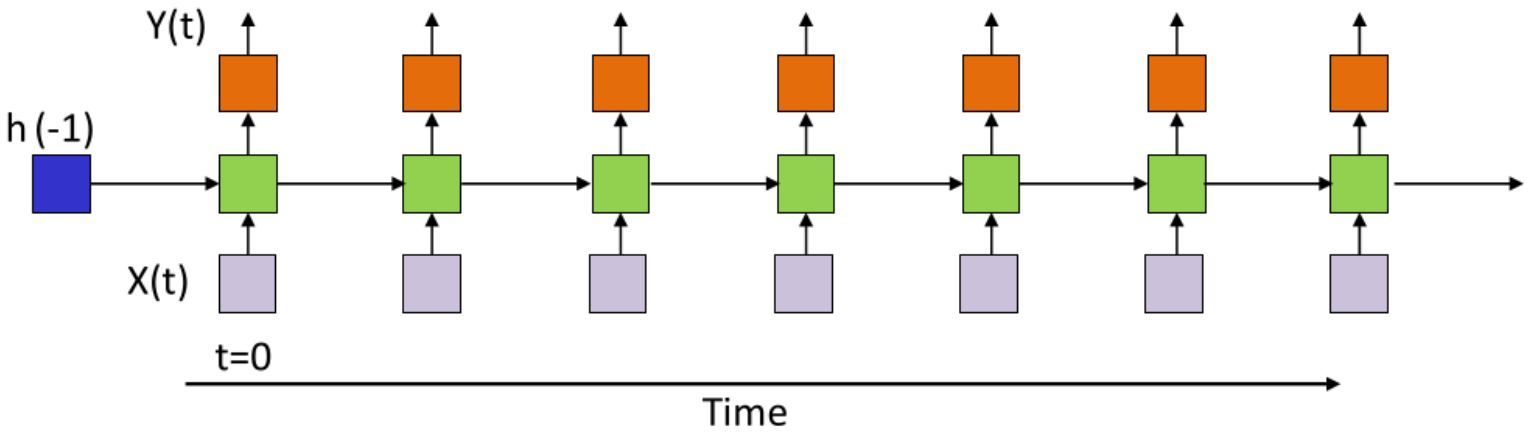

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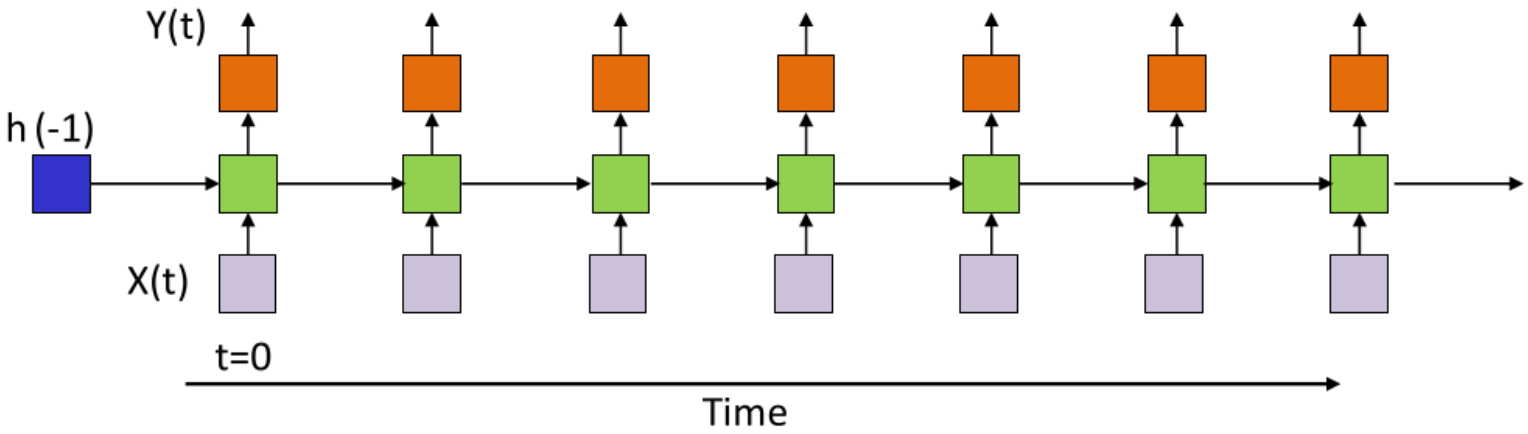

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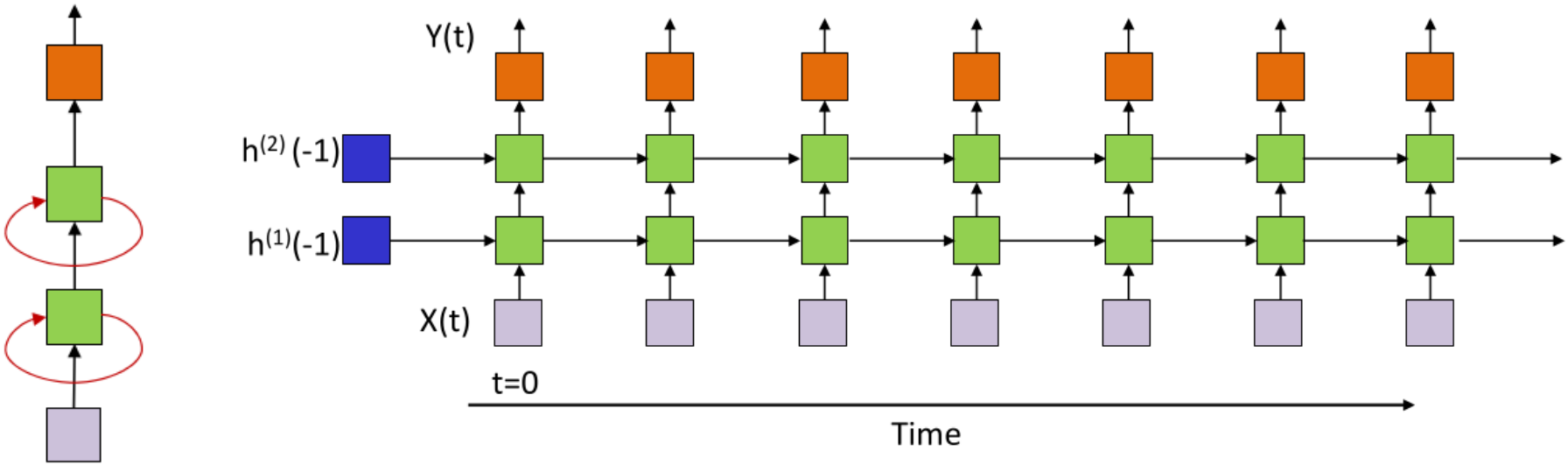
- We can add multiple recurrent layers

Recurrent Neural Networks

Rolled view



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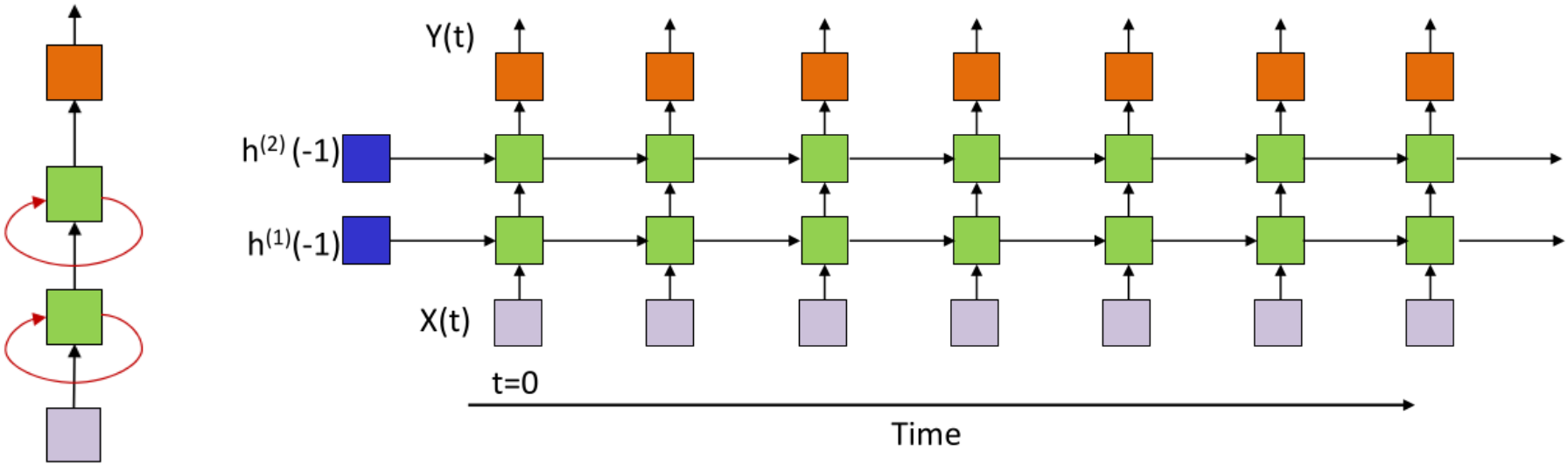
Rolled view



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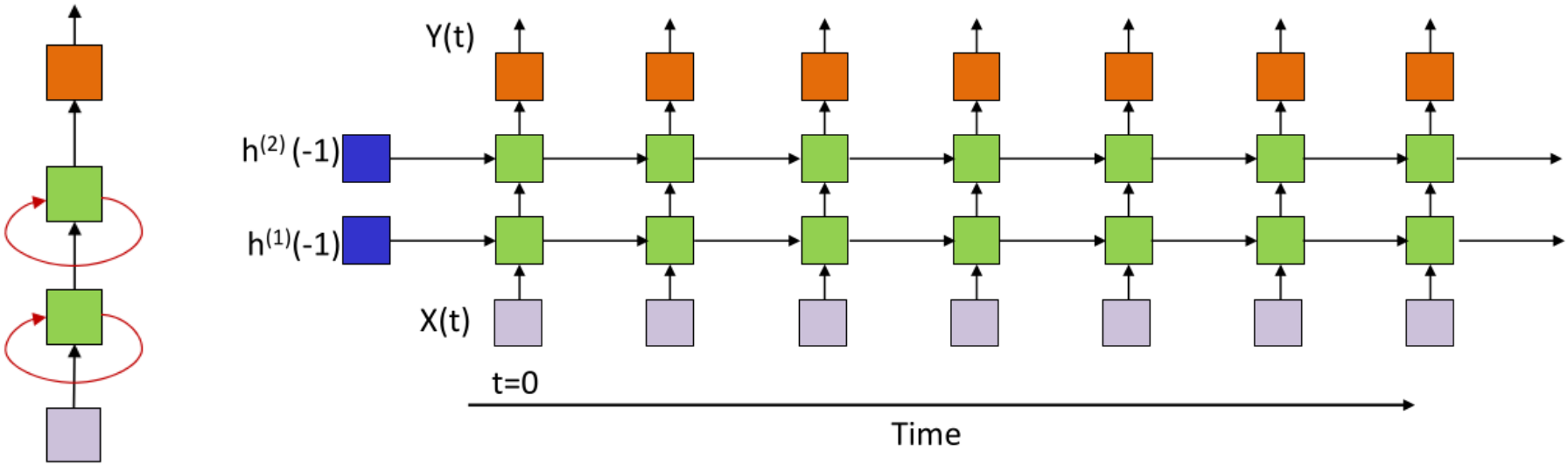

- Loops imply recurrence/memory
- The "unrolled" computation is just a giant shared-parameter neural network
- All columns are identical and share parameters

Deep Learning in Life Sciences

Training RNNs

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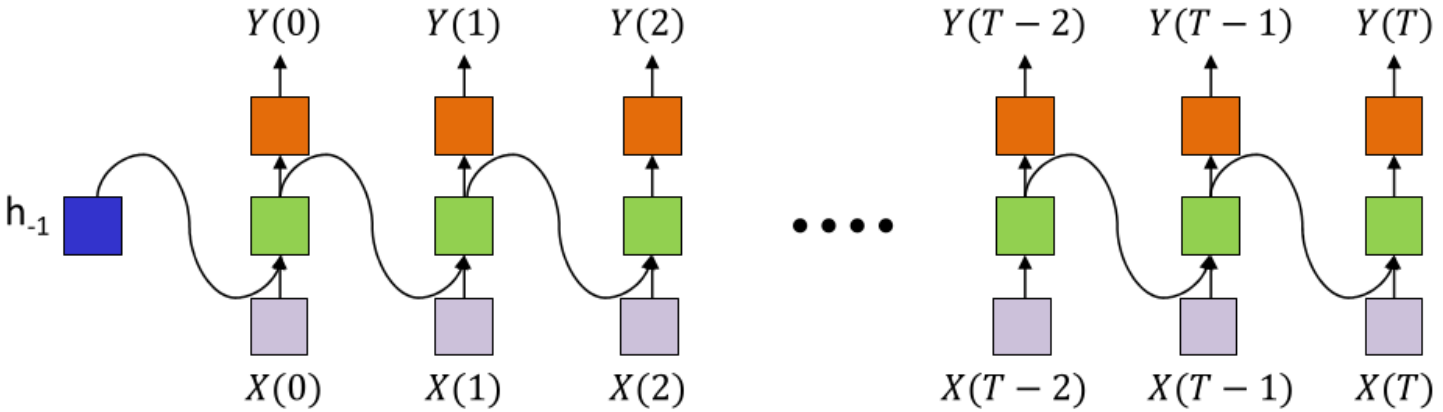
- But we need to account now that the inputs (and the outputs) are through time
- Back Propagation Through Time (BPTT) !

Back Propagation Through Time - main cases



- In general, we have a sequence of $T+1$ inputs $\boldsymbol{X}(0), \ldots, \boldsymbol{X}(T)$
  - and their corresponding outputs $\boldsymbol{Y}(0), \ldots, \boldsymbol{Y}(T)$
  - in a general fashion, they can be vectors

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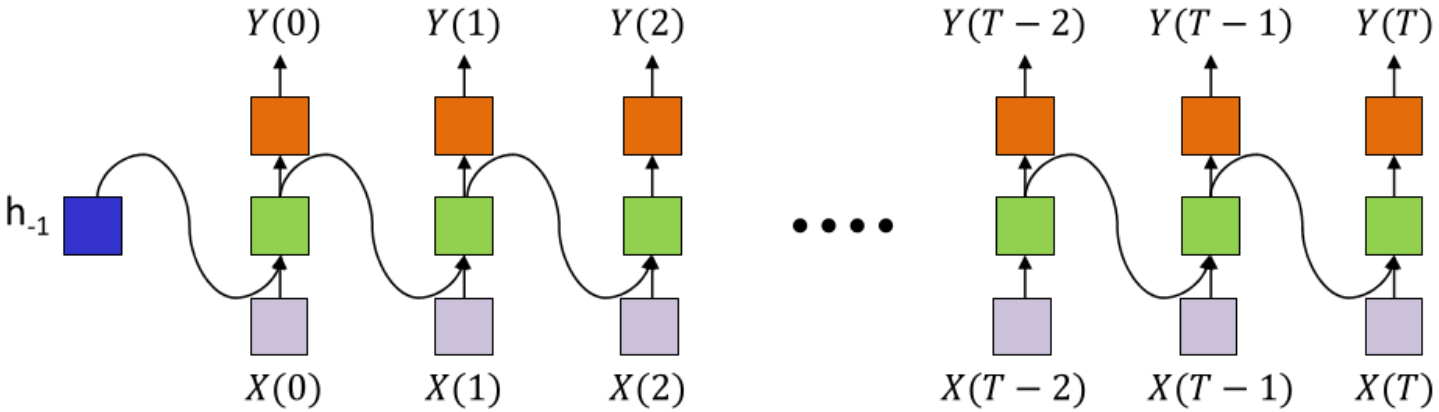

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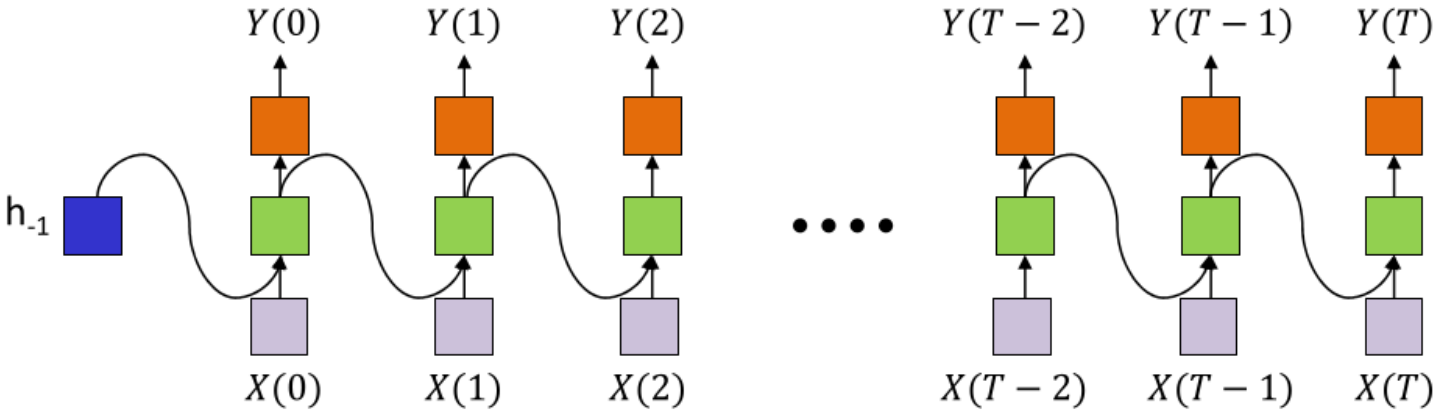

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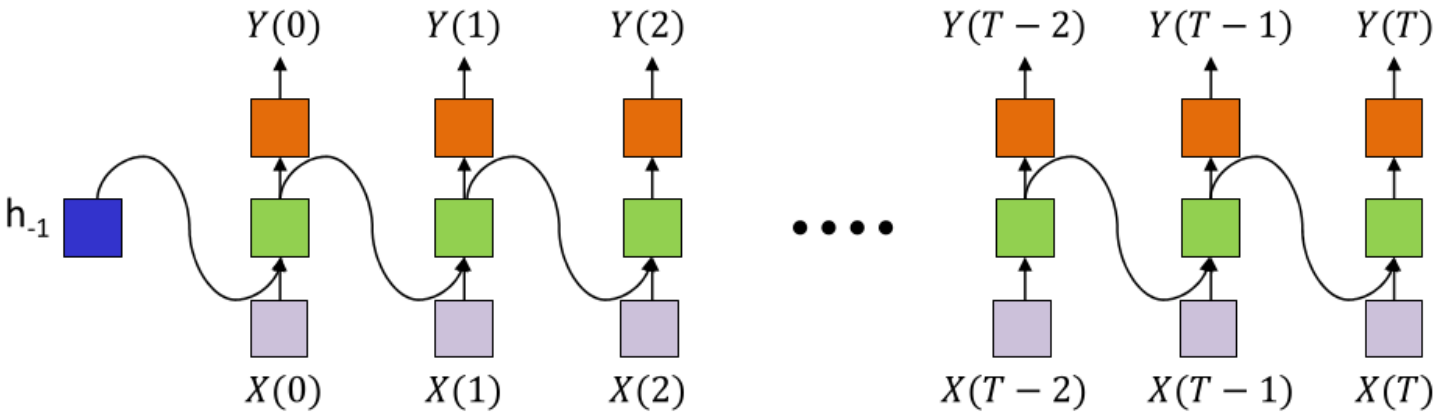

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  - In principle, this is not just the sum of the errors at individual times

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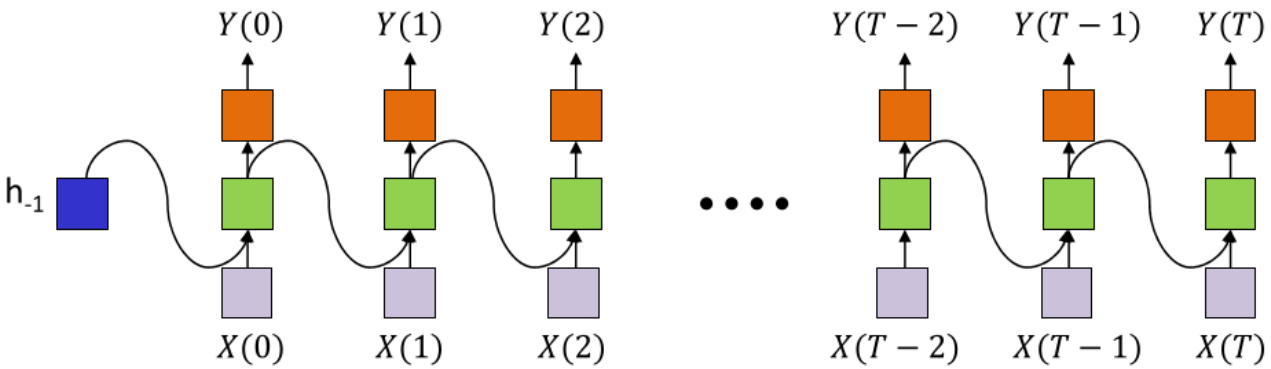

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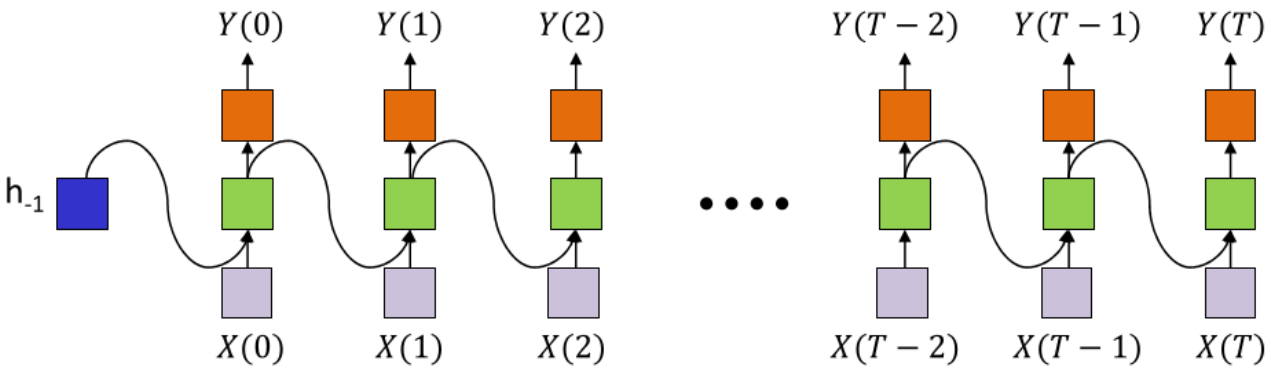

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The long-term dependency problem

- Even for RNN we have the vanishing/exploding gradient problem
- Mainly if we need to store long temporal dependencies

PATTERN1 [.....] PATTERN 2

Jane had a quick lunch in the bistro. Then *she*..

Any other pattern of any length can happen between pattern 1 and pattern 2

– RNN will "forget" pattern 1 if intermediate stuff is too long

– "Jane" → the next pronoun referring to her will be "she"

Must know to "remember" for extended periods of time and "recall" when necessary

– Need an alternate way to "remember" stuff

Deep Learning in Life Sciences

Possible solutions

- Long Short-Term Memory (LSTM) [Hochreiter et al. (1997)]
- Gated Recurrent Unit (GRU)[Cho et al. (2014)]
- More details in the lab session! Next Thursday for UNIMI

CREDITS

Content is inspired and taken from:

- Introduction to Deep Learning, https://deeplearning.cs.cmu.edu/F22/index.html
- Ian Goodfellow and Yoshua Bengio and Aaron Courville, *Deep Learning*, MIT Press, 2016. Chapter 9. http://www.deeplearningbook.org
- Introduction to Deep Learning (I2DL) https://www.3dunderstanding.org/i2dl-w22/, Lecture 11.
- Introduction to Deep Learning, https://deeplearning.cs.cmu.edu/F22/index.html, lectures 13, 14.
- Ian Goodfellow and Yoshua Bengio and Aaron Courville, *Deep Learning*, MIT Press, 2016. Chapter 12. http://www.deeplearningbook.org
- http://colah.github.io/posts/2015-08-Understanding-LSTMs

REFERENCES

Hochreiter, S., and Schmidhuber, Jurgen. (1997). Long short-term memory. Neural Computation, 9(8), 1735–1780.

Cho, K., van Merrienboer, B., et al. (2014). "Learning Phrase Representations using RNN Encoder-Decoder for Statistical Machine Translation". arXiv:1406.1078.

Deep Learning in Life Sciences