Convolutional and Recurrent Deep Neural Networks

Marco Frasca
Università degli Studi di Milano

marco.frasca@unimi.it

DeepLife Course
4EU+

4 March 2024

Deep Learning in Life Sciences

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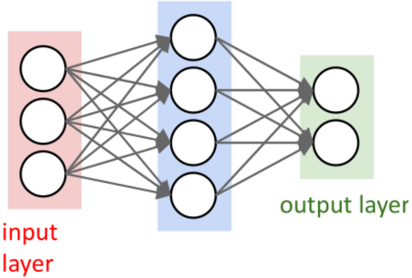
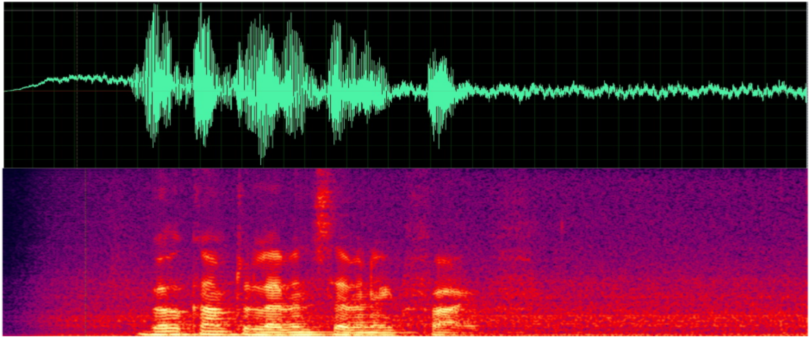
Outline

Recap



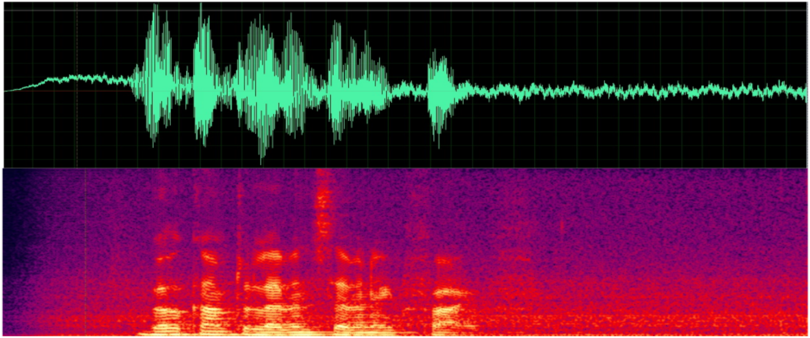
- Multi-layer Perceptron (MLP) is able to detect patterns in input data
- Inputs are numeric vectors
  - E.g. digits, numeric signals etc.

A different problem



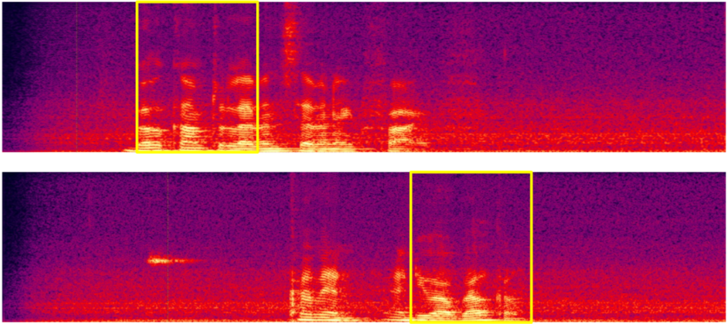
- Given a signal, does it contain a given word? E.g., "welcome"?

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



- Shift variance problem: a MLP that finds a “welcome” in the top recording will not find it in the lower one

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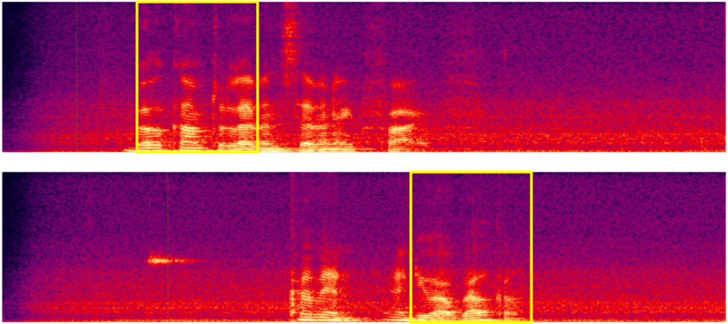

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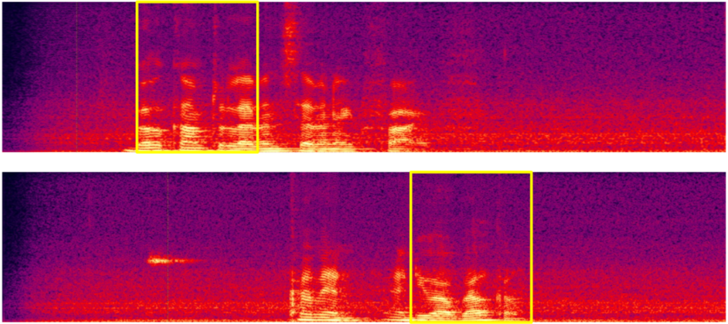
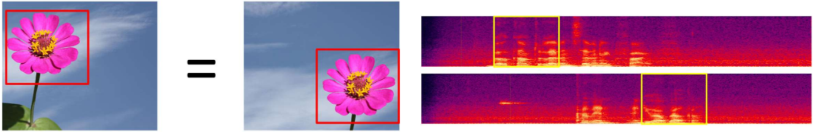


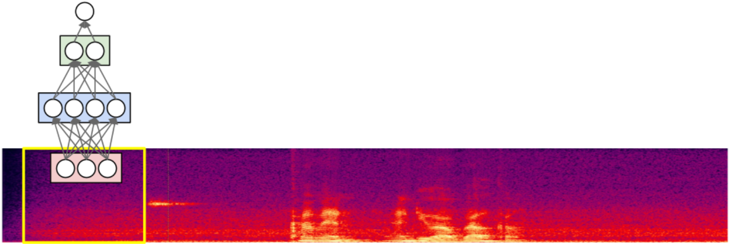
- Shift variance problem: a MLP that finds a “welcome” in the top recording will not find it in the lower one
- Unless trained with both
- This would require a very large network and a large amount of training data to cover every case

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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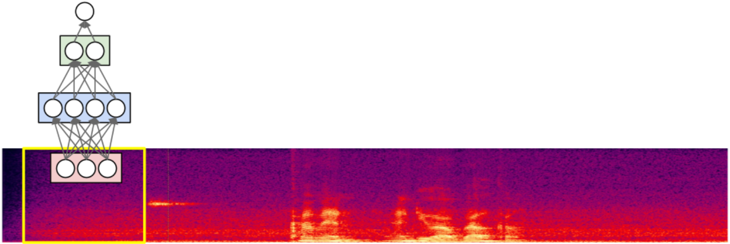

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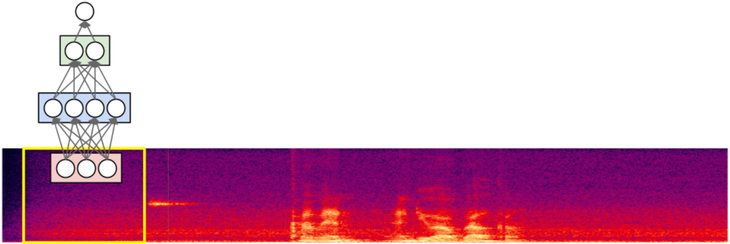

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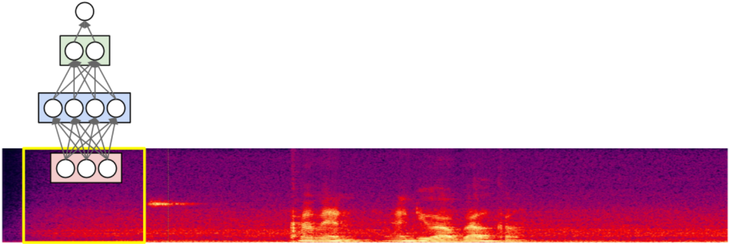

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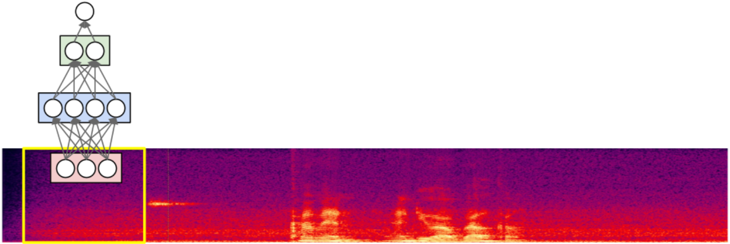

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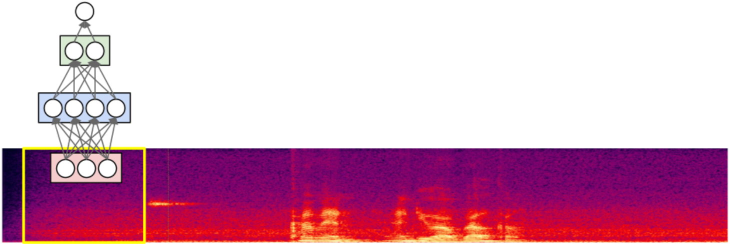

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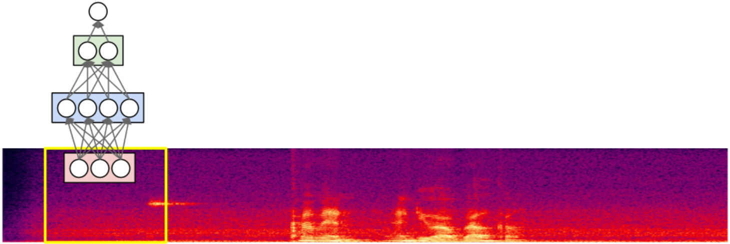

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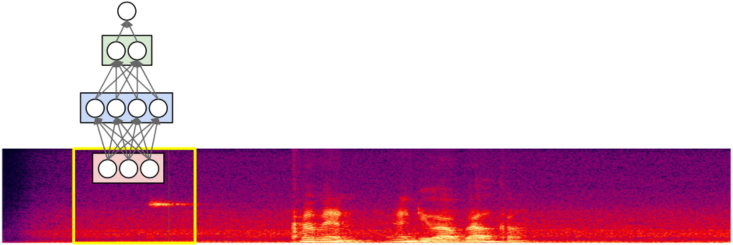

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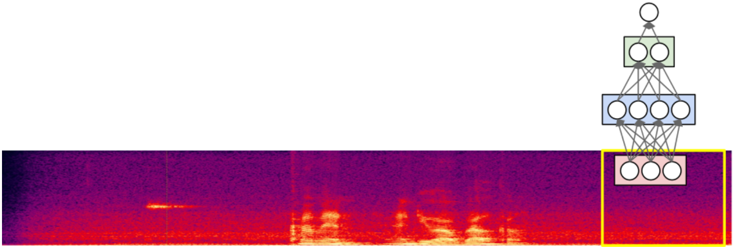

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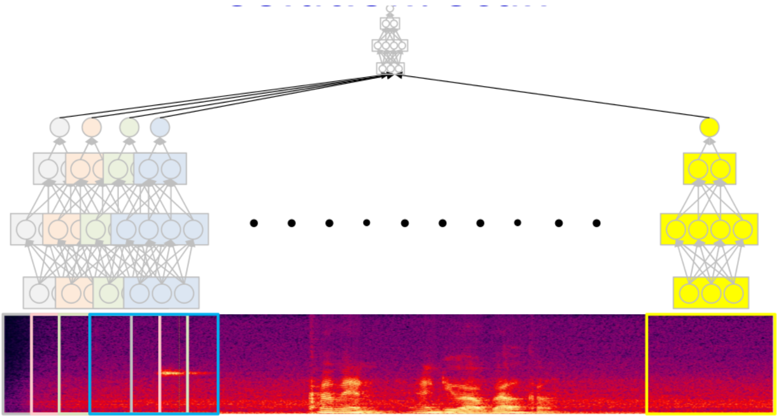
Combining the Windows



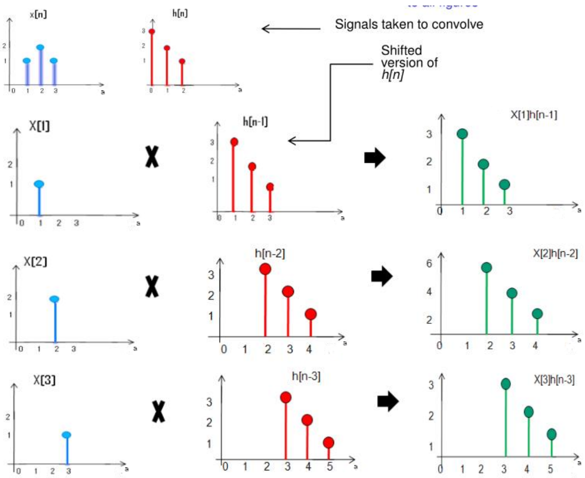
"Does welcome occur in this recording?"

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

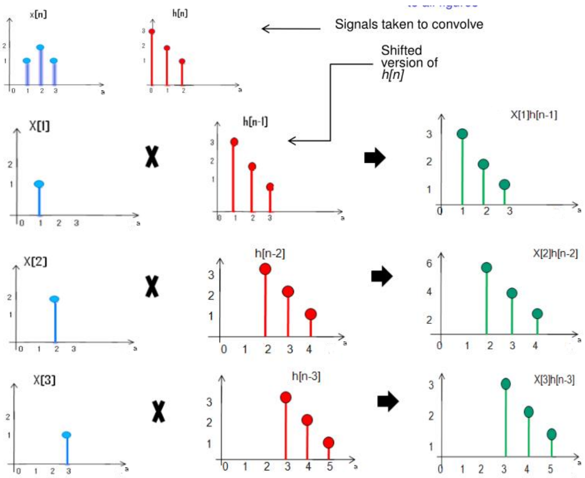
2

Outline

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



- A convolution is a composition of two real-valued functions x and h to get a smoothed version of x



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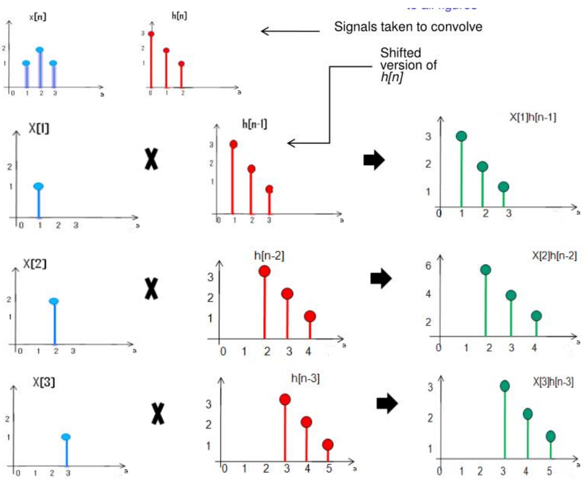

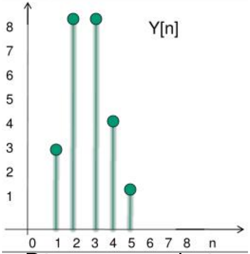

– Dicrete convolution: a new function Y of n

$Y(n) := (x * h)(n) := \sum_{a \in A} x(a)h(n-a)$

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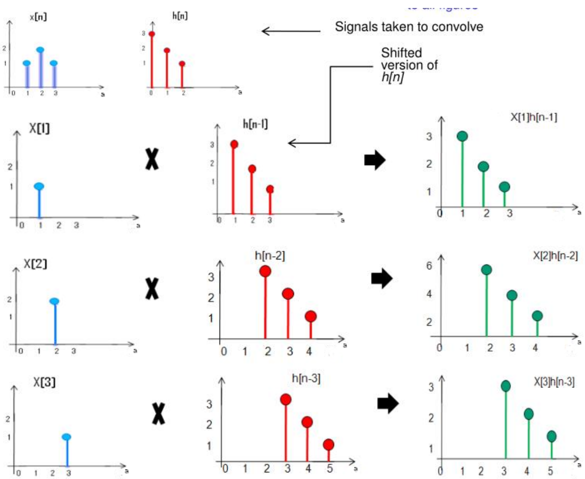

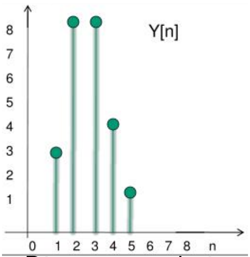

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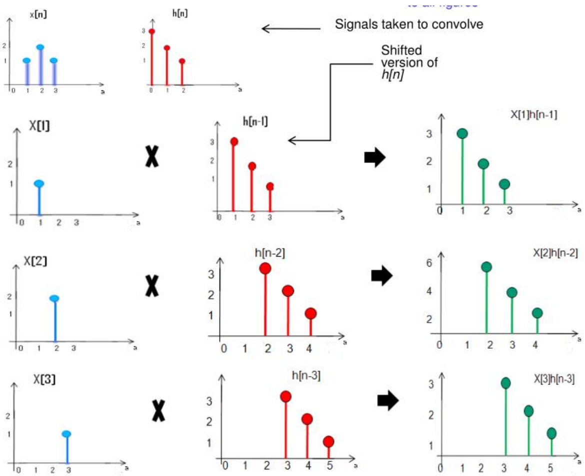

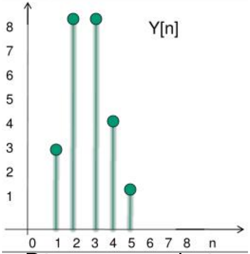

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– $Y(1) = \sum_{a \in A} x(a)h(1-a) = 1 \cdot 3 + 2 \cdot 0 + 1 \cdot 0 = 3$

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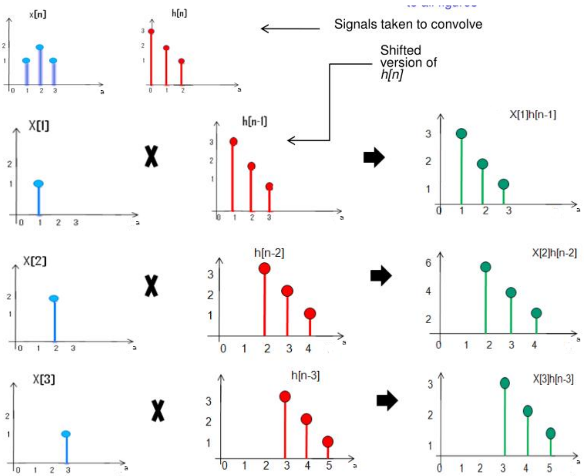

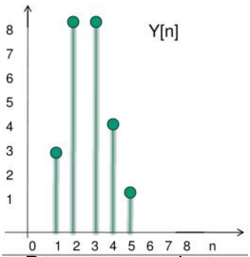

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- In the example $A = \{1, 2, 3\}$
- $Y(1) = \sum_{a \in A} x(a)h(1-a) = 1 \cdot 3 + 2 \cdot 0 + 1 \cdot 0 = 3$
- $Y(2) = ?$

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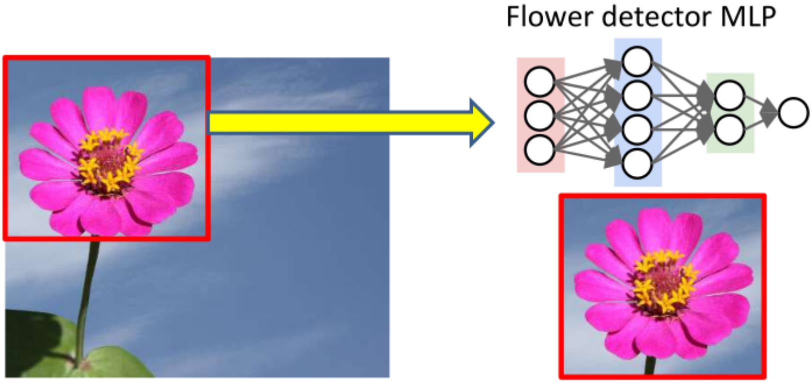
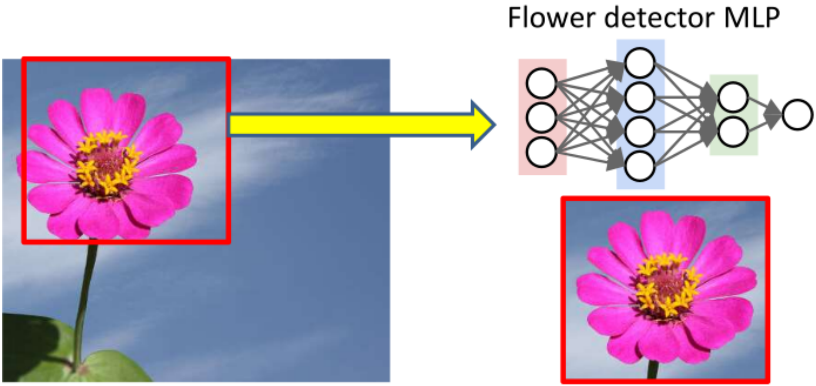
Convolution in Conv layers

- 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!



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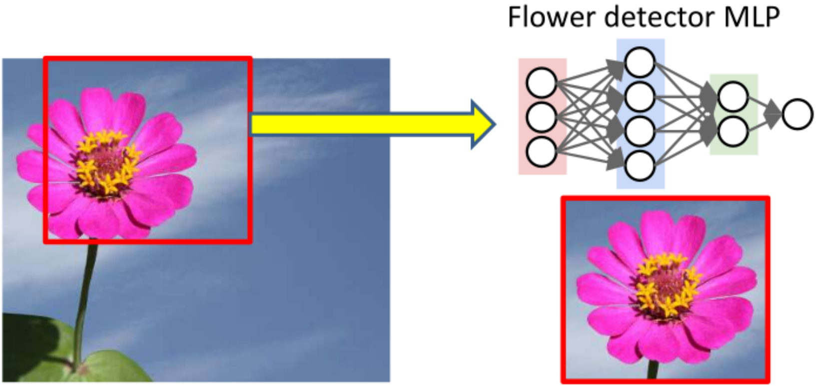

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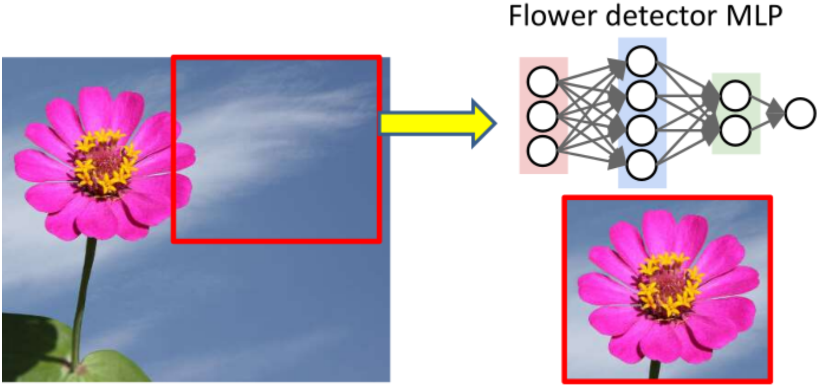

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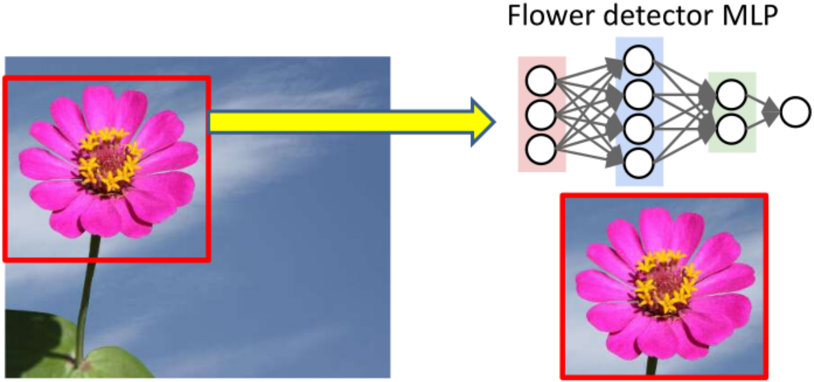

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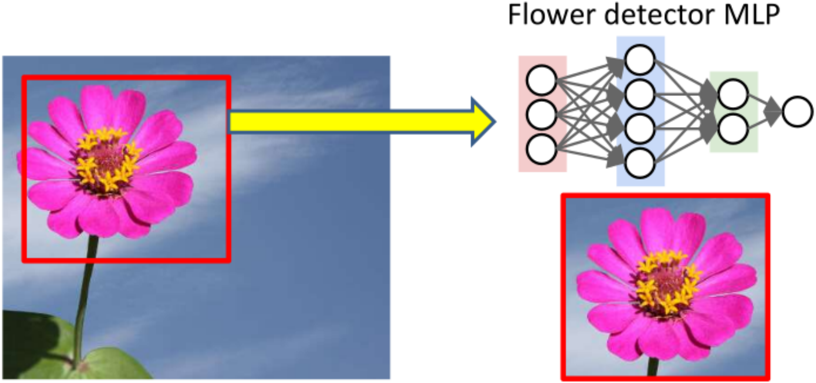

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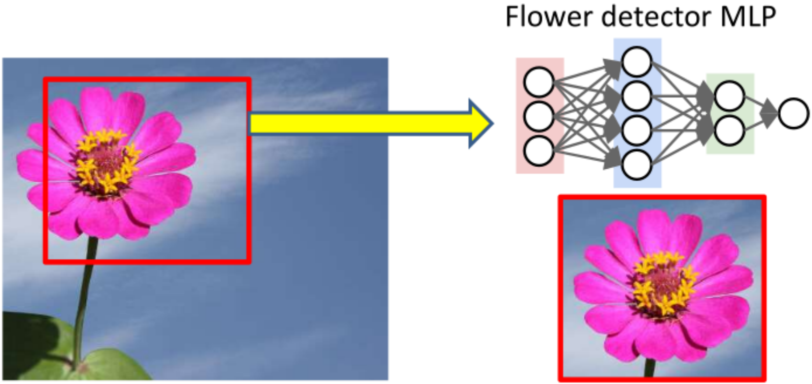

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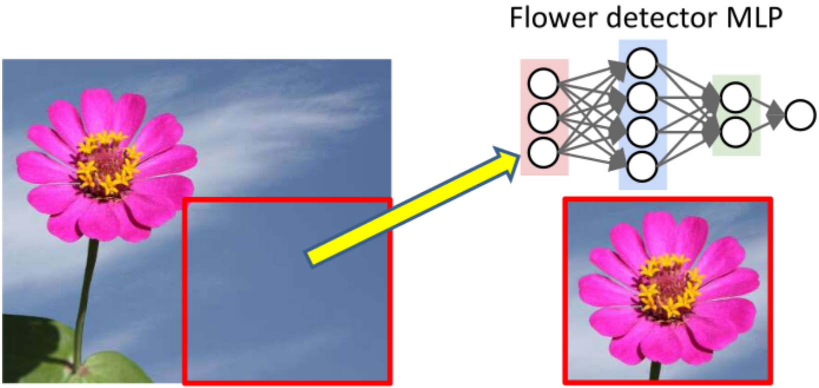

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Shared parameters of a Convolutional Layer

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

f	4	3	2	-5	3	5	2	5	5	6
g	1/3	1/3	1/3	→						

'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

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

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

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							

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

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

4	3	2	-5	3	5	2	5	5	6

1/3	1/3	1/3

??	3	0	0	1	10/3	4	4	16/3	??

What to do at boundaries?

Discrete Convolution: 1D case

4	3	2	-5	3	5	2	5	5	6

1/3	1/3	1/3

??	3	0	0	1	10/3	4	4	16/3	??

What to do at boundaries?

Possible Solution: 0-Padding

0	4	3	2	-5	3	5	2	5	5	6	0

1/3	1/3	1/3

??	3	0	0	1	10/3	4	4	16/3	??

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

What to do at boundaries?

Pad (often 0's)

7/3	3	0	0	1	10/3	4	4	16/3	11/3

Discrete Convolution: 1D case

4	3	2	-5	3	5	2	5	5	6

1/3	1/3	1/3

??	3	0	0	1	10/3	4	4	16/3	??

What to do at boundaries?

Possible Solution: 0-Padding

0	4	3	2	-5	3	5	2	5	5	6	0

1/3	1/3	1/3

??	3	0	0	1	10/3	4	4	16/3	??

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

What to do at boundaries?

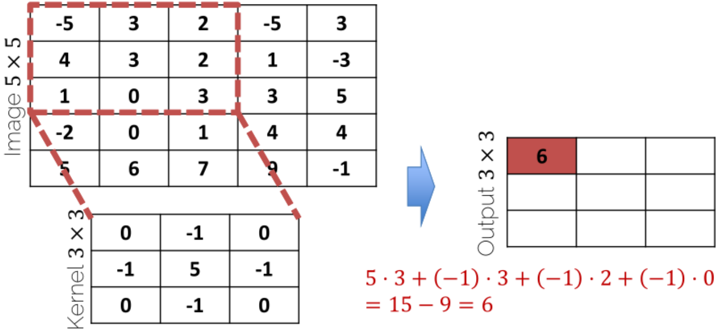
Pad (often 0's)

7/3	3	0	0	1	10/3	4	4	16/3	11/3

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

Discrete Convolution: 2D case

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



$$5 \cdot 3 + (-1) \cdot 3 + (-1) \cdot 2 + (-1) \cdot 0 + (-1) \cdot 4$$
$$= 15 - 9 = 6$$

Discrete Convolution: 2D case

Image 5 × 5

-5	3	2	-5	3
4	3	2	1	-3
1	0	3	3	5
-2	0	1	4	4
5	6	7	9	-1

Kernel 3 × 3

0	-1	0
-1	5	-1
0	-1	0

Output 3 × 3

6	1	

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

Discrete Convolution: 2D case

Image 5×5

-5	3	2	-5	3
4	3	2	1	-3
1	0	3	3	5
-2	0	1	4	4
5	6	7	9	-1

Kernel 3×3

0	-1	0
-1	5	-1
0	-1	0

Output 3×3

6	1	8

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

Discrete Convolution: 2D case

Image 5×5

-5	3	2	-5	3
4	3	2	1	-3
1	0	3	3	5
-2	0	1	4	4
5	6	7	9	-1

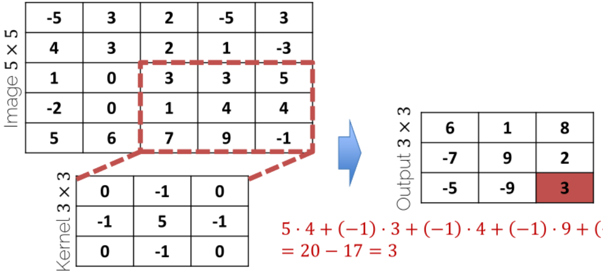
Kernel 3×3

0	-1	0
-1	5	-1
0	-1	0

Output 3×3

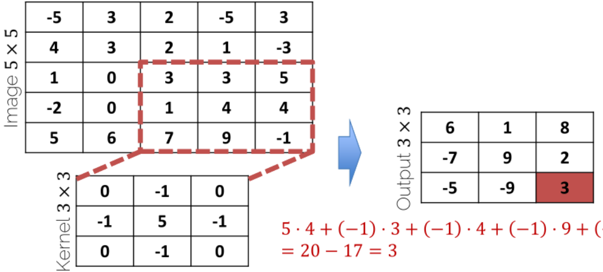
6	1	8
-7		

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



$$5 \cdot 4 + (-1) \cdot 3 + (-1) \cdot 4 + (-1) \cdot 9 + (-1) \cdot 1$$
$$= 20 - 17 = 3$$

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



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Discrete Convolution: 2D case

Image 5 × 5

-5	3	2	-5	3
4	3	2	1	-3
1	0	3	3	5
-2	0	1	4	4
5	6	7	9	-1

Kernel 3 × 3

0	-1	0
-1	5	-1
0	-1	0

Output 3 × 3

6	1	8
-7	9	2
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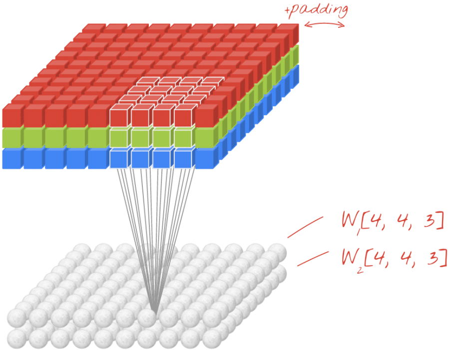
- Even in this case we could 0-pad the input grid for the feature map to have the same size of the input



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

$W_1[4, 4, 3]$
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$W[\underbrace{4, 4}_{\text{filter size}}, \underbrace{3}_{\text{input channels}}, \underbrace{2}_{\text{output channels}}]$

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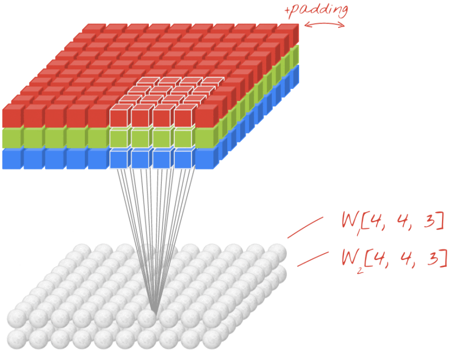

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filter size — input channels — output channels

- 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

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  - In other words, each filter produces an output channel, which are stacked atop each other

Outline

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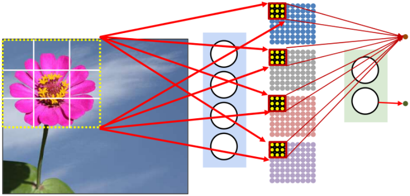

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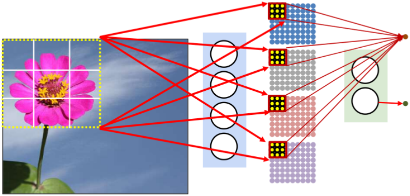

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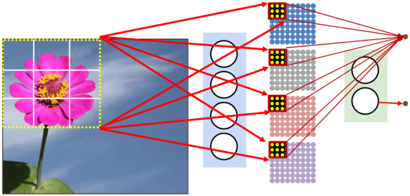

- Each neuron in the second convolutional layer is performing the equivalent of a convolution of a 9×9 filter!
- Total parameters per filter: 9 in the first layer, and 9 in the second layer. 18 vs 81!!

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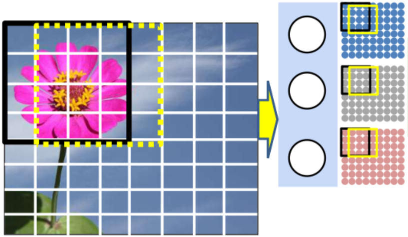
Advantage of Distributed Convolution

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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- Its usage depends on the semantic of the input!

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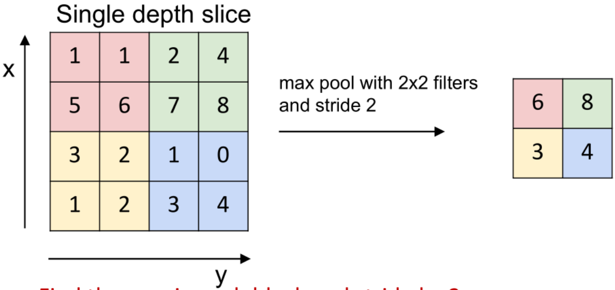
For these reasons pooling layers usually follow convolutional layers

Max/Mean Pooling

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



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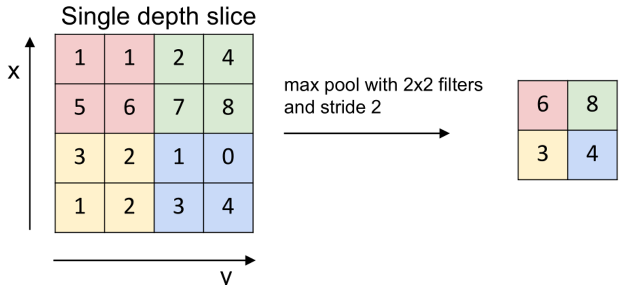

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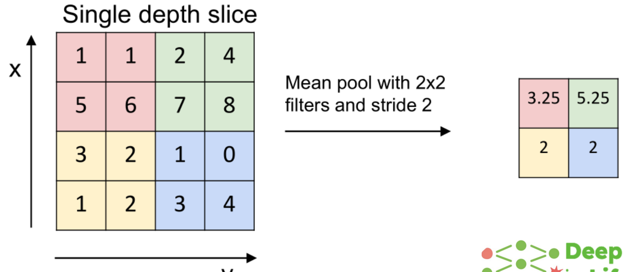

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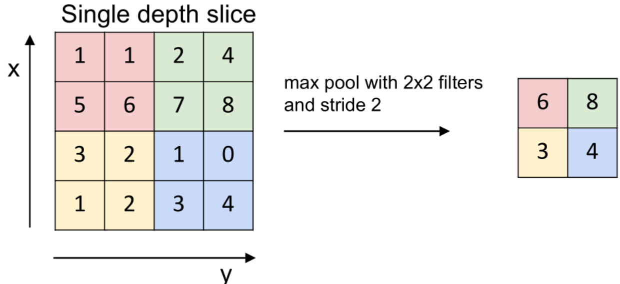

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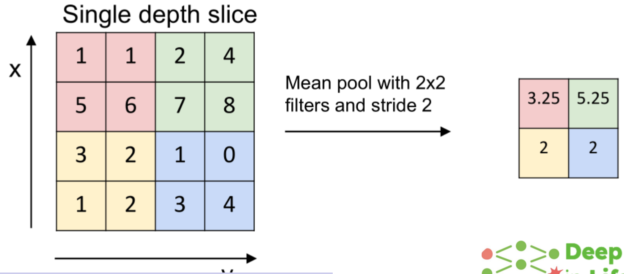
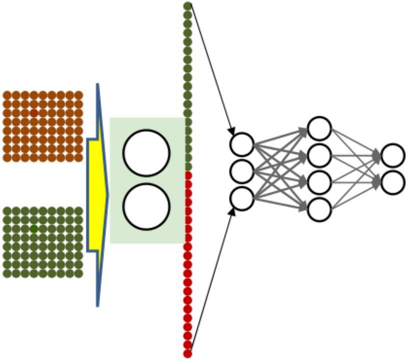


An $N \times N$ picture compressed by a $F \times F$ pooling filter extent with stride S results in an output map of size $\left\lceil \frac{(N-F)}{S} \right\rceil + 1$

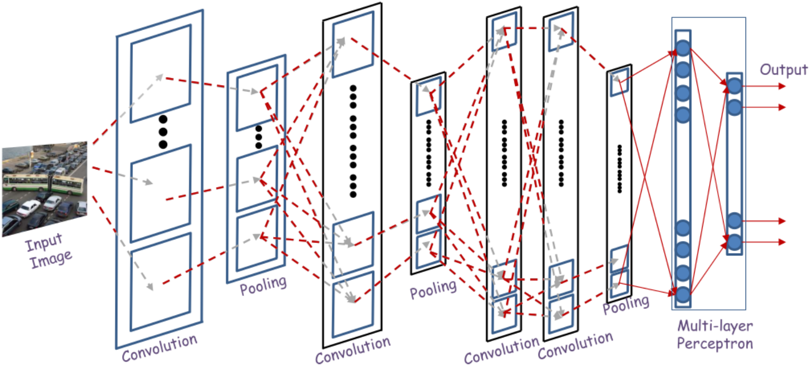
– Typically do not zero pad

Terminology

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



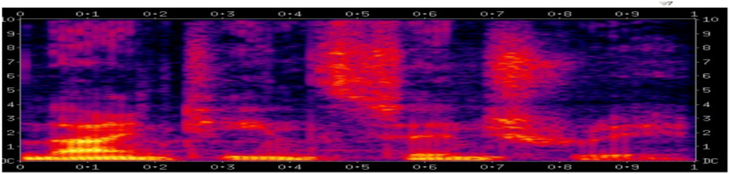
Typical CNN



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

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

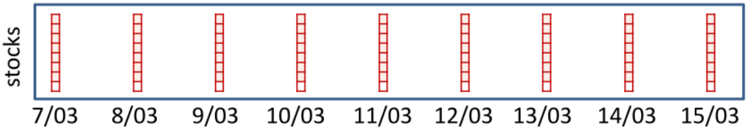
What are they talking about?

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

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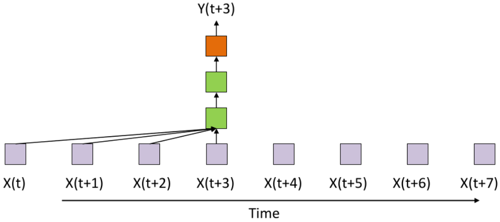
- Problem: Increasing much the input "history" can make the network too complex



A CNN looking at the last few past temporal steps

Infinite dependency

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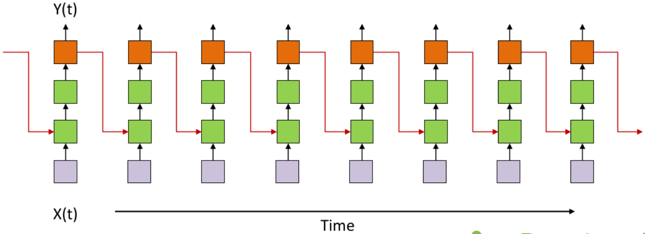
- $Y(0)$ produces $Y(1)$, which produces $Y(2)$ ... till potentially $Y(\infty)$. If we unroll it, we have something like:



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

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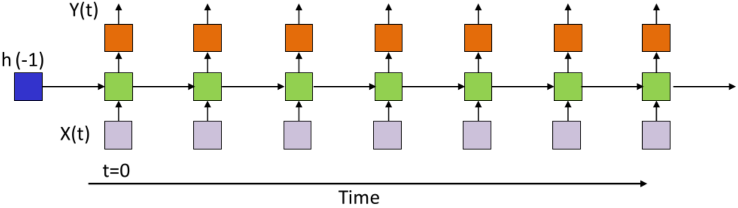
This is a fully recurrent neural network! Or simply a recurrent neural network (RNN)

Recurrent Neural Networks



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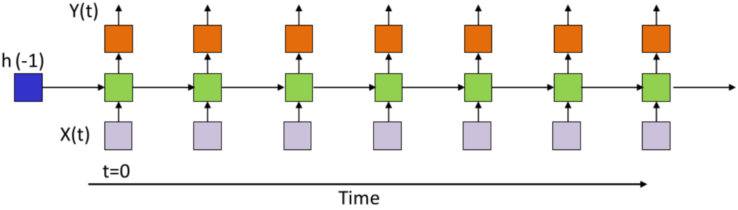

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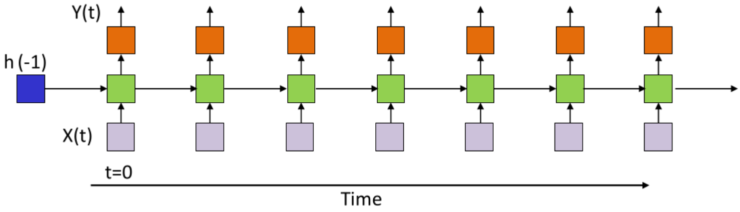

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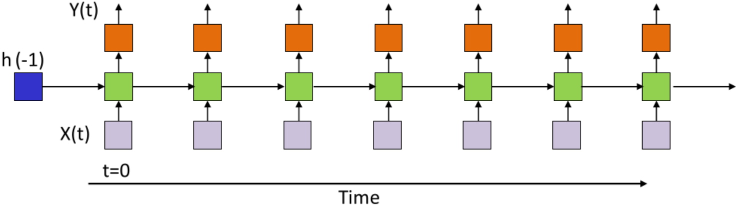

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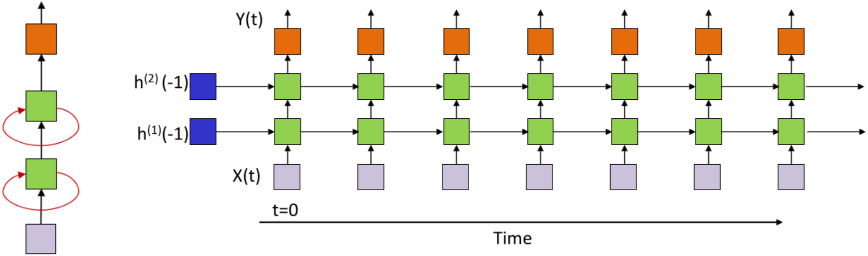
- We can add multiple recurrent layers

Rolled view



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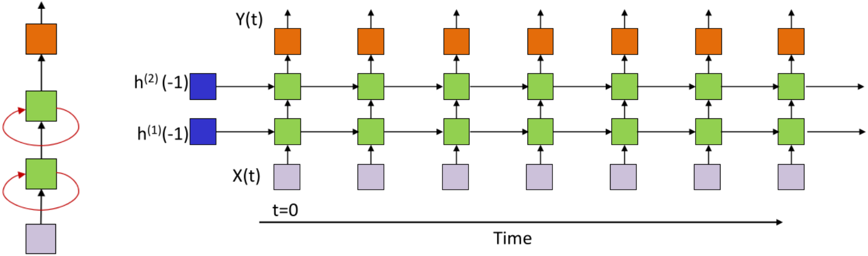

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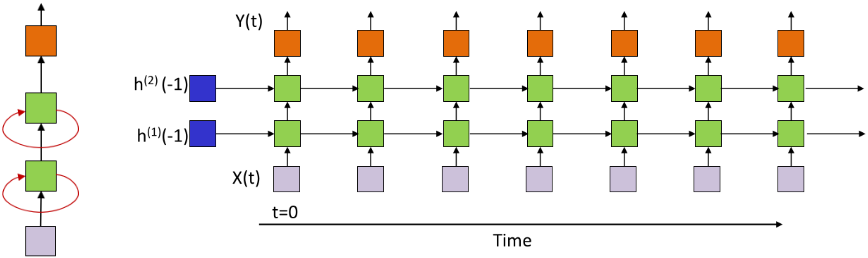

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- All columns are identical and share parameters

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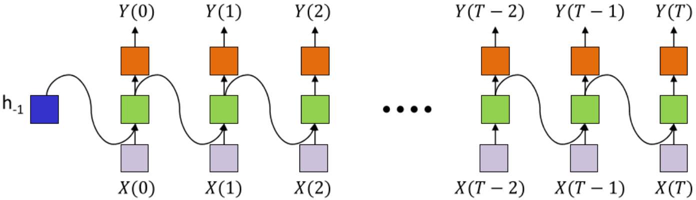
- Back Propagation Through Time (BPTT) !

Back Propagation Through Time - main cases



- In general, we have a sequence of $T + 1$ inputs $\boldsymbol{X}(0), \dots, \boldsymbol{X}(T)$
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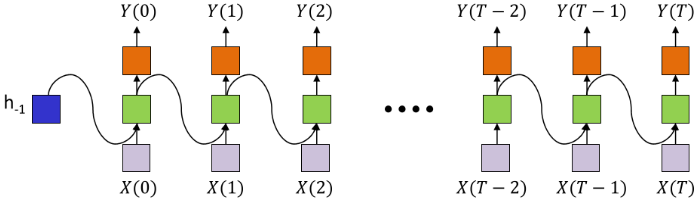

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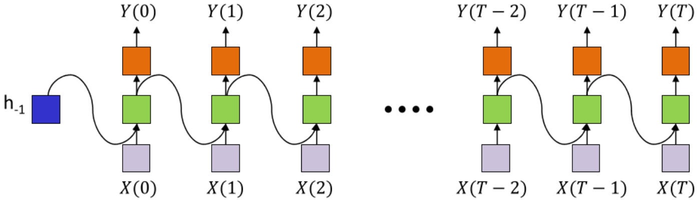
- **Case 1**: We are interested to all the intermediate outputs (e.g., predicting the trend of an index through the time)

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
- **Case 1**: We are interested to all the intermediate outputs (e.g., predicting the trend of an index through the time)
  - We will compute the error between the sequence of desired outputs over time $\boldsymbol{d}(0), \ldots \boldsymbol{d}(T)$ and the corresponding predictions $\boldsymbol{Y}(0), \ldots, \boldsymbol{Y}(T)$

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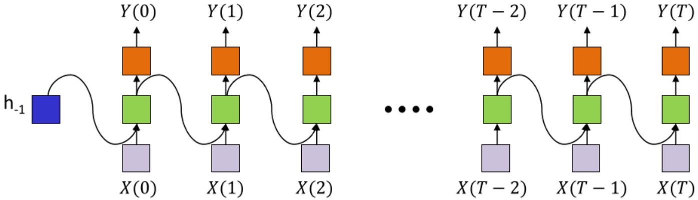

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  - We will compute the error between the sequence of desired outputs over time $\boldsymbol{d}(0), \dots \boldsymbol{d}(T)$ and the corresponding predictions $\boldsymbol{Y}(0), \dots, \boldsymbol{Y}(T)$
  - In principle, this is not just the sum of the errors at individual times

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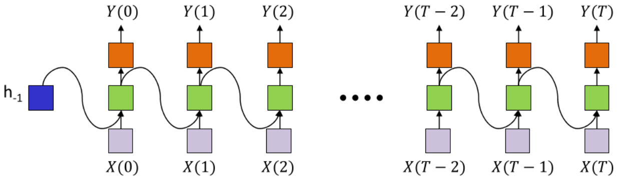

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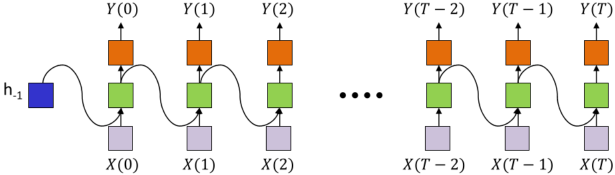

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The long-term dependency problem

- 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

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.