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Machine Learning for Neuroscience

ML4NS

# Convolutional Neural Networks (CNNs)

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## Feature Vectors

- Image data is represented as a two-dimensional grid of pixels, monochromatic or colour.
- Each pixel corresponds to one or multiple numerical values, respectively.
- Until now, most of the models that we have studied have ignored this rich structure and treated the data as vectors of numbers.

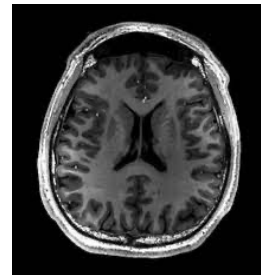
2

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## Images as vectors

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- Using images by *flattening* the images means overlooking the spatial relation between pixels.
- This deeply unsatisfying approach could be a very simple solution to feed the resulting one-dimensional vectors through a fully connected MLP or other probabilistic models.



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## Feeding images to the models as blocks

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- Because the MLP networks are invariant to the order of the features, we could get similar results regardless of whether we preserve an order corresponding to the spatial structure of the pixels or if we permute the columns of our design matrix before fitting the MLP's parameters.
- Preferably, we would leverage our prior knowledge that nearby pixels are typically related to each other to build efficient models for learning from image data.

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## Convolutional Neural Networks

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- Convolutional Neural Networks, or CNNs, are specialised neural networks that process data with a known grid-like topology.
- Examples include time series data, which can be thought of as a 1-D grid taking samples at regular intervals, and image data, which can be thought of as a 2-D grid of pixels.

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## CNNs

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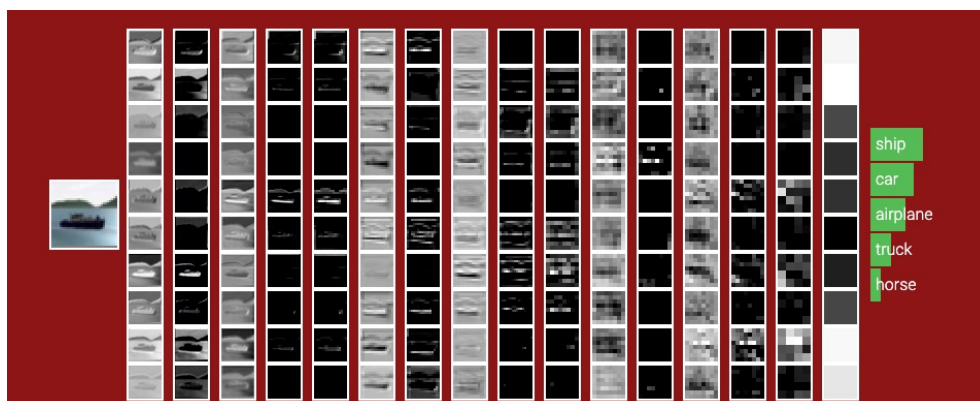


image source: <http://cs231n.stanford.edu/>

We will revisit this again in the following slides.

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## Convolution layer

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- Convolutional layers in CNN can be more accurately described as cross-correlations.
- They take an input (usually a grid or subset of the main image or input) and overlay or apply a kernel.
- The shape of the *kernel window* (or *convolution window*) is given by the height and width of the kernel.

Input		Kernel		Output																	
<table border="1" style="border-collapse: collapse;"> <tr><td>0</td><td>1</td><td>2</td></tr> <tr><td>3</td><td>4</td><td>5</td></tr> <tr><td>6</td><td>7</td><td>8</td></tr> </table>	0	1	2	3	4	5	6	7	8	*	<table border="1" style="border-collapse: collapse;"> <tr><td>0</td><td>1</td></tr> <tr><td>2</td><td>3</td></tr> </table>	0	1	2	3	=	<table border="1" style="border-collapse: collapse;"> <tr><td>19</td><td>25</td></tr> <tr><td>37</td><td>43</td></tr> </table>	19	25	37	43
0	1	2																			
3	4	5																			
6	7	8																			
0	1																				
2	3																				
19	25																				
37	43																				

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## CNN kernels

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Input		Kernel		Output																	
<table border="1" style="border-collapse: collapse;"> <tr><td>0</td><td>1</td><td>2</td></tr> <tr><td>3</td><td>4</td><td>5</td></tr> <tr><td>6</td><td>7</td><td>8</td></tr> </table>	0	1	2	3	4	5	6	7	8	*	<table border="1" style="border-collapse: collapse;"> <tr><td>0</td><td>1</td></tr> <tr><td>2</td><td>3</td></tr> </table>	0	1	2	3	=	<table border="1" style="border-collapse: collapse;"> <tr><td>19</td><td>25</td></tr> <tr><td>37</td><td>43</td></tr> </table>	19	25	37	43
0	1	2																			
3	4	5																			
6	7	8																			
0	1																				
2	3																				
19	25																				
37	43																				

(1×0) + (2×1) + (4×2) + (5×3) = 25

(4×0) + (5×1) + (7×2) + (8×3) = 43

(3×0) + (4×1) + (6×2) + (7×3) = 37

Two-dimensional cross-correlation operation. The shaded portions are the first output element, as well as the input and kernel tensor elements used for the output computation:

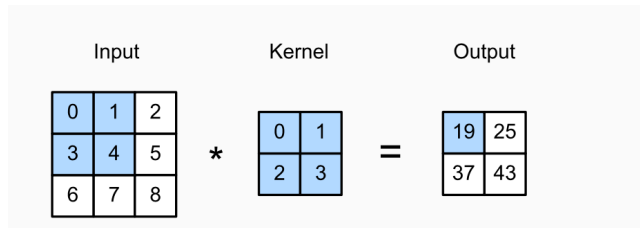
$$(0 \times 0) + (1 \times 1) + (3 \times 2) + (4 \times 3) = 19.$$

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## Sliding the kernel

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$$\begin{aligned}
 0 \times 0 + 1 \times 1 + 3 \times 2 + 4 \times 3 &= 19, \\
 1 \times 0 + 2 \times 1 + 4 \times 2 + 5 \times 3 &= 25, \\
 3 \times 0 + 4 \times 1 + 6 \times 2 + 7 \times 3 &= 37, \\
 4 \times 0 + 5 \times 1 + 7 \times 2 + 8 \times 3 &= 43.
 \end{aligned}$$

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## Example – edge detection: data

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```

tensor([[1., 1., 0., 0., 0., 0., 1., 1.],
        [1., 1., 0., 0., 0., 0., 1., 1.],
        [1., 1., 0., 0., 0., 0., 1., 1.],
        [1., 1., 0., 0., 0., 0., 1., 1.],
        [1., 1., 0., 0., 0., 0., 1., 1.],
        [1., 1., 0., 0., 0., 0., 1., 1.]])

```

```

X = torch.ones((6, 8))
X[:, 2:6] = 0
X

```

Code: GitHub - [PyTorch CNN\\_edge\\_detection\\_sample.ipynb](#)

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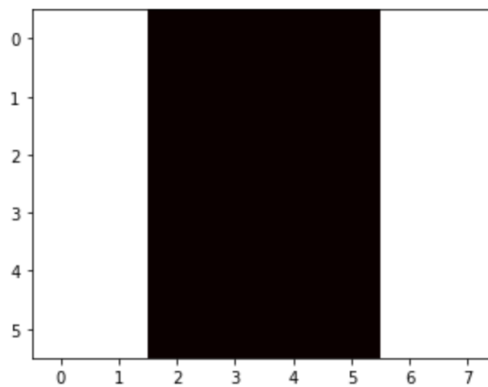
10

## Example – edge detection: data

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```
import matplotlib.pyplot as plt
import matplotlib.cm as cm
plt.imshow(X, cmap=plt.cm.hot)
plt.show()
```

✓ 0.1s



```
[[1., 1., 0., 0., 0., 0., 1., 1.],
 [1., 1., 0., 0., 0., 0., 1., 1.],
 [1., 1., 0., 0., 0., 0., 1., 1.],
 [1., 1., 0., 0., 0., 0., 1., 1.],
 [1., 1., 0., 0., 0., 0., 1., 1.],
 [1., 1., 0., 0., 0., 0., 1., 1.]]
```

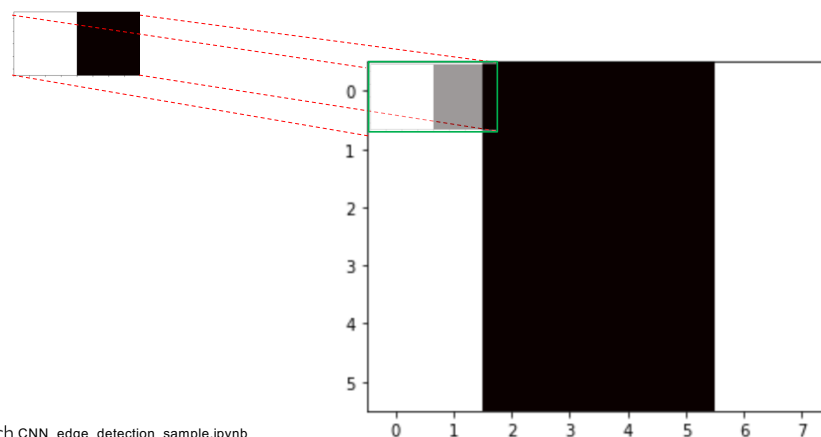
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## Example – edge detection: kernel

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```
K = torch.tensor([[1.0, -1.0]])
```

Code: GitHub - [PyTorch CNN\\_edge\\_detection\\_sample.ipynb](#)

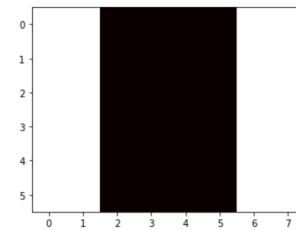
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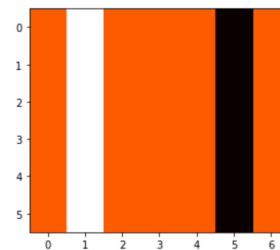
## Example – edge detection: result

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```
[1., 1., 0., 0., 0., 0., 1., 1.],
[1., 1., 0., 0., 0., 0., 1., 1.],
[1., 1., 0., 0., 0., 0., 1., 1.],
[1., 1., 0., 0., 0., 0., 1., 1.],
[1., 1., 0., 0., 0., 0., 1., 1.],
[1., 1., 0., 0., 0., 0., 1., 1.]]
```



```
[ 0., 1., 0., 0., 0., -1., 0.],
[ 0., 1., 0., 0., 0., -1., 0.],
[ 0., 1., 0., 0., 0., -1., 0.],
[ 0., 1., 0., 0., 0., -1., 0.],
[ 0., 1., 0., 0., 0., -1., 0.],
[ 0., 1., 0., 0., 0., -1., 0.]]
```

Code: GitHub -  PyTorch CNN\_edge\_detection\_sample.ipynb

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## Learning a kernel

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- Designing an edge detector by finite differences  $[1, -1]$  is neat if we know this is precisely what we are looking for.
- However, as we look at larger kernels and consider successive layers of convolutions, it might be impossible to specify precisely what each filter should be doing manually.

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## Learning a kernel through training

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- We can learn the kernel that generated  $\mathbf{Y}$  from  $\mathbf{X}$  by looking only at the input-output pairs. We first construct a convolutional layer and initialise its kernel as a random tensor.
- Next, in each iteration, we will use the squared error to compare  $\mathbf{Y}$  with the convolutional layer output.
- We can then calculate the gradient to update the kernel.

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## Example: how to learn a kernel

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```
# Construct a two-dimensional convolutional layer with 1 output channel and a
# kernel of shape (1, 2). For the sake of simplicity, we ignore the bias here
# adapted from https://d2l.ai/chapter_convolutional-neural-networks/conv-layer.html

conv2d = nn.LazyConv2d(1, kernel_size=(1, 2), bias=False)

# The two-dimensional convolutional layer uses four-dimensional input and
# output in the format of (example, channel, height, width), where the batch
# size (number of examples in the batch) and the number of channels are both 1
X = X.reshape((1, 1, 6, 8))
Y = Y.reshape((1, 1, 6, 7))
lr = 3e-2 # Learning rate

for i in range(10):
    Y_hat = conv2d(X)
    l = (Y_hat - Y) ** 2
    conv2d.zero_grad()
    l.sum().backward()
    # Update the kernel
    conv2d.weight.data[:] -= lr * conv2d.weight.grad
    if (i + 1) % 2 == 0:
        print(f'epoch {i + 1}, loss {l.sum():.3f}')
```

✓ 0.6s


epoch 2, loss 1.373

epoch 4, loss 0.240

epoch 6, loss 0.044

epoch 8, loss 0.009

epoch 10, loss 0.002

Code: GitHub -  PyTorch CNN\_edge\_detection\_sample.ipynb

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## Example: how to learn a kernel: result

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```

X
[24] ✓ 0.3s
... tensor([[[[1., 1., 0., 0., 0., 0., 1., 1.],
               [1., 1., 0., 0., 0., 0., 1., 1.],
               [1., 1., 0., 0., 0., 0., 1., 1.],
               [1., 1., 0., 0., 0., 0., 1., 1.],
               [1., 1., 0., 0., 0., 0., 1., 1.],
               [1., 1., 0., 0., 0., 0., 1., 1.]]]]])

Y
[25] ✓ 0.3s
... tensor([[[[ 0.,  1.,  0.,  0.,  0., -1.,  0.],
               [ 0.,  1.,  0.,  0.,  0., -1.,  0.],
               [ 0.,  1.,  0.,  0.,  0., -1.,  0.],
               [ 0.,  1.,  0.,  0.,  0., -1.,  0.],
               [ 0.,  1.,  0.,  0.,  0., -1.,  0.],
               [ 0.,  1.,  0.,  0.,  0., -1.,  0.]]]]])

conv2d.weight.data
[23] ✓ 0.6s
... tensor([[[[ 0.9975, -0.9905]]]])

```

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## CNNs so far

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- The core computation required for a convolutional layer is a cross-correlation operation.
- We saw that a simple nested for-loop is all that is required to compute its value.
- If we have multiple input and output channels, we perform a matrix-matrix operation between channels.

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## Padding and Stride

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- A tricky issue when applying convolutional layers is that we tend to lose pixels on the perimeter of our image.

0	1	2
3	4	5
6	7	8

Kernel

0	1
2	3

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## Padding

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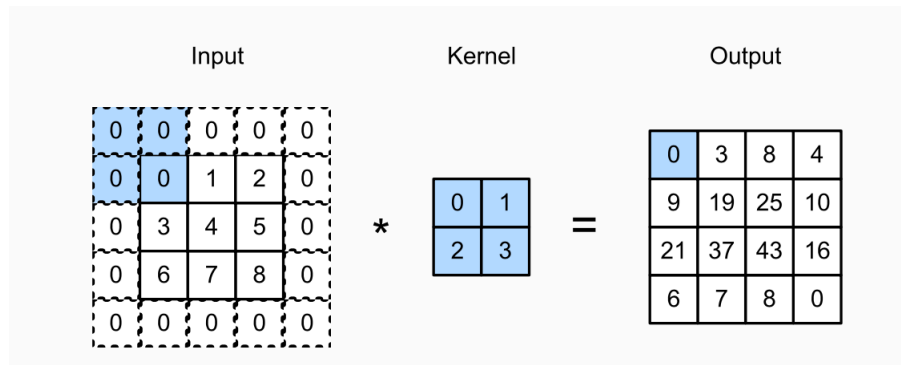
- Since we typically use small kernels for any given convolution, we might only lose a few pixels, but this can add up as we apply many successive convolutional layers.
- One straightforward solution to this problem is to add extra pixels of filler around the boundary of our input image, thus increasing the effective size of the image.
- Typically, we set the values of the extra pixels to zero.

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## Padding: example

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## Choice of padding size

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- CNNs commonly use convolution kernels with odd height and width values, such as 1, 3, 5, or 7.
- Choosing odd kernel sizes has the benefit that we can preserve the dimensionality while padding with the same number of rows on top and bottom and the same number of columns on left and right.
- For any two-dimensional tensor  $X$ , when the kernel's size is odd and the number of padding rows and columns on all sides are the same, an output with the same height and width as the input is produced.

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## Stride

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- When computing the cross-correlation, we start with the convolution window at the upper-left corner of the input tensor and then slide it over all locations both down and to the right.
- We have been sliding one element at a time in the previous examples.

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## Stride

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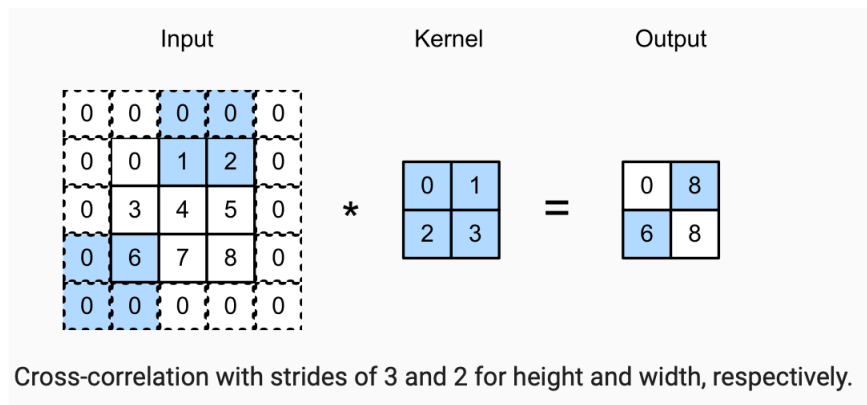
- Sometimes, either for computational efficiency or because we wish to down sample, we move our window more than one element at a time, skipping the intermediate locations.
- This is particularly useful if the convolution kernel is large since it captures a large area of the underlying image.
- We refer to the number of rows and columns traversed per slide as *stride*.

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## Stride: example

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## Choice of padding

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- Padding can increase the height and width of the output.
- This is often used to give the output the same height and width as the input to avoid undesirable shrinkage of the output.
- Moreover, it ensures that all pixels are used equally frequently.
- Typically, we pick symmetric padding on both sides of the input height and width.

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## Multiple Input and Multiple Output Channels

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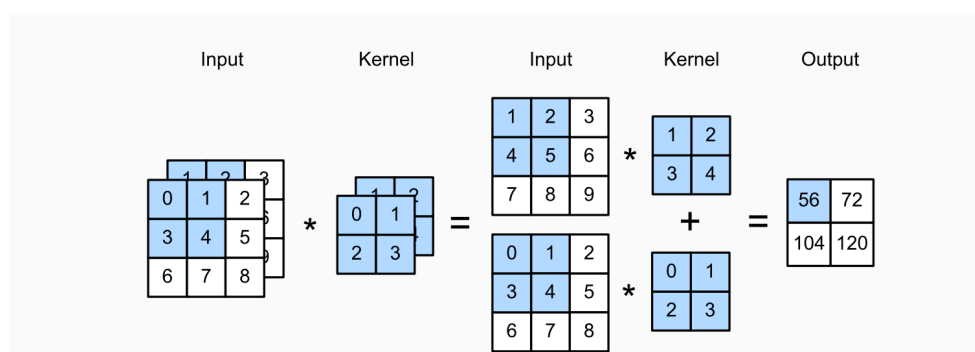
- Multiple channels can comprise each image (e.g., colour images have the standard RGB channels to indicate the amount of red, green and blue) , and we can have convolutional layers for multiple channels.
- When the input data contains multiple channels, we need to construct a convolution kernel with the same number of input channels as the input data so that it can perform cross-correlation with the input data.

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## Multiple Input Channels: example

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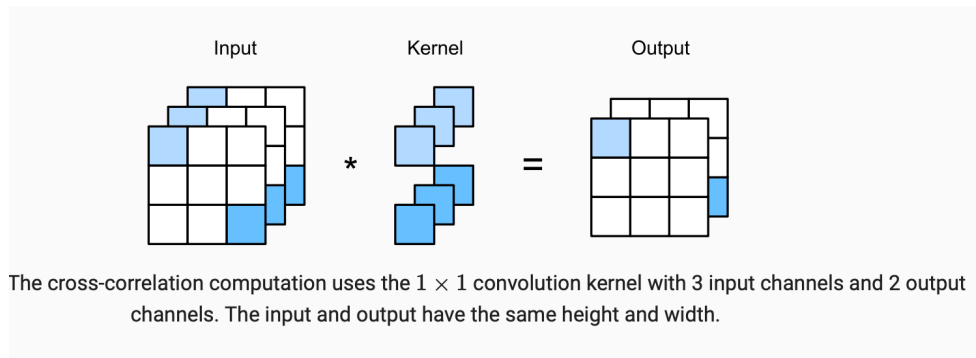


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## Multiple Output Channel: example (1x1 convolution)

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## CNN Channels

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- Channels allow us to combine the best of both worlds: MLPs, which allow for significant nonlinearities, and convolutions, which allow for *localised* analysis of features.
- In particular, channels allow the CNN to reason with multiple features, such as edge and shape detectors at the same time.
- They also offer a practical trade-off between the drastic parameter reduction arising from translation invariance and locality and the need for expressive and diverse models in computer vision.

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## Pooling

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- In many cases our ultimate task asks some global question about the image, e.g., *does it contain a lesion?*
- Consequently, the units of our final layer should be sensitive to the entire input.
- By gradually aggregating information, yielding coarser and coarser maps, we accomplish this goal of ultimately learning a global representation, while keeping all the advantages of convolutional layers at the intermediate layers of processing.

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## CNN – deep layers

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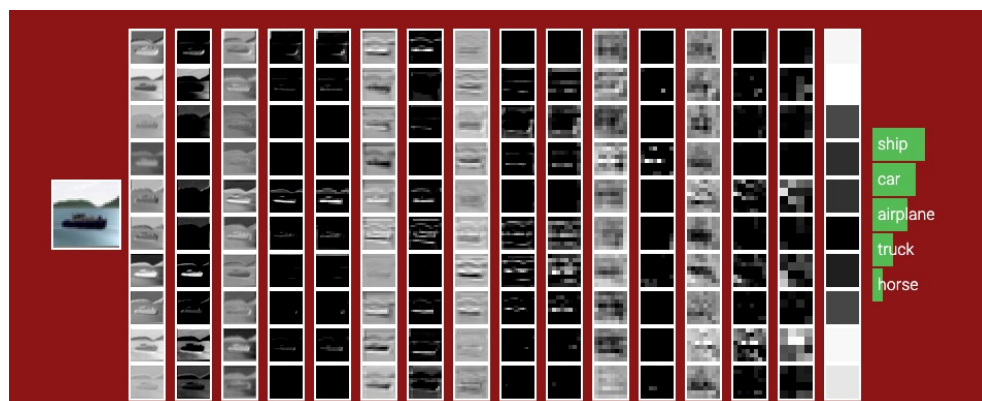


image source: <http://cs231n.stanford.edu/>

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## Deeper layers in CNNs

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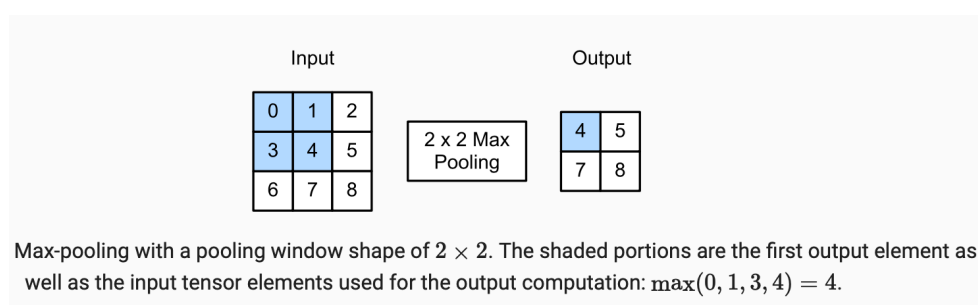
- The deeper we go in the network, the larger the receptive field (relative to the input) to which each hidden node is sensitive.
- Reducing spatial resolution accelerates this process since the convolution kernels cover a larger effective area.
- In early layers, kernels learn simple patterns such as edges and corners.
- In deeper layers of a multilayer CNN, kernels learn more abstract patterns, such as shapes, objects, or specific parts of objects.
- Overall, convolution layers capture increasingly abstract features layer by layer.
- Pooling layers help the model to be more robust to minor input variations.

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## Maximum Pooling and Average Pooling

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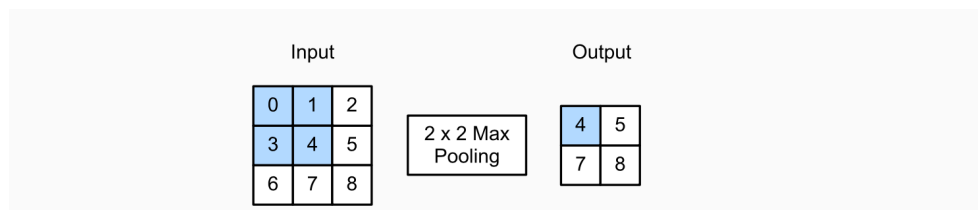
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## Pooling

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- Like convolutional layers, *pooling* operators consist of a fixed-shape window that is slid over all regions in the input according to its stride, computing a single output for each location traversed by the fixed-shape window (sometimes known as the *pooling window*).



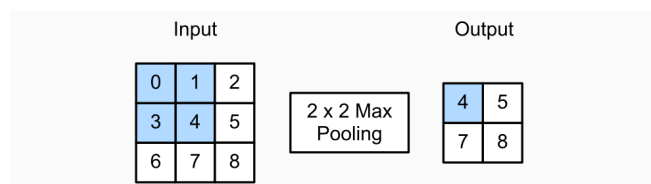
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## Max-pooling and average-pooling

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- However, unlike the cross-correlation computation of the inputs and kernels in the convolutional layer, the pooling layer contains no parameters (**there is no kernel**).
- Instead, pooling operators are deterministic, typically calculating either the maximum or the average value of the elements in the pooling window.
- These operations are called *maximum pooling* (*max-pooling* for short) and *average pooling*, respectively.

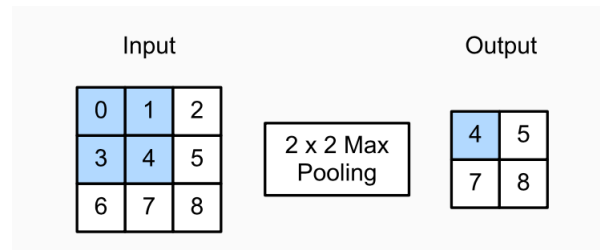


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## Max-pooling: revisiting the example

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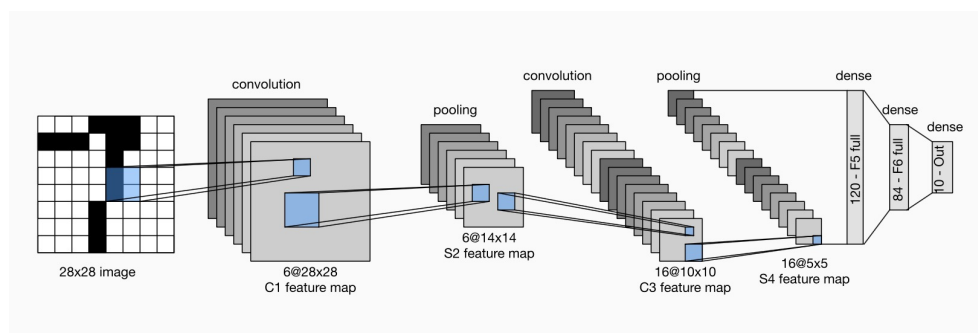
$$\begin{aligned}\max(0, 1, 3, 4) &= 4, \\ \max(1, 2, 4, 5) &= 5, \\ \max(3, 4, 6, 7) &= 7, \\ \max(4, 5, 7, 8) &= 8.\end{aligned}$$

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## Convolutional Neural Networks: example LeNet

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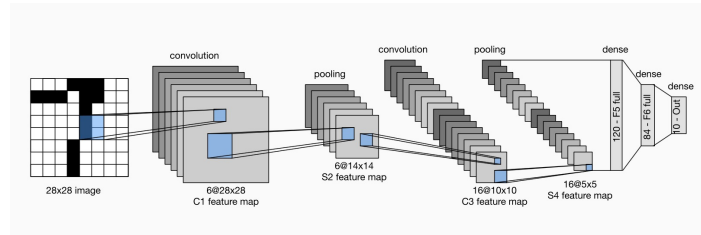
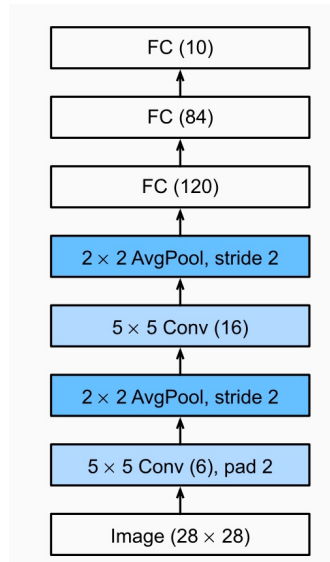


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## Compressed notion for LeNet-5

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## Example of a practical model: VGG-19

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- In practice, you use models such as VGG;
  - VGG: Very Deep Convolutional Networks for Large-Scale Image Recognition by Karen Simonyan, Andrew Zisserman, ICLR 2015, <https://arxiv.org/pdf/1409.1556>

```

Input: 224×224 RGB Image
↓
[Conv3-64] → [Conv3-64] → [MaxPool]
↓
[Conv3-128] → [Conv3-128] → [MaxPool]
↓
[Conv3-256] → [Conv3-256] → [Conv3-256] → [Conv3-256] → [MaxPool]
↓
[Conv3-512] → [Conv3-512] → [Conv3-512] → [Conv3-512] → [MaxPool]
↓
[Conv3-512] → [Conv3-512] → [Conv3-512] → [Conv3-512] → [MaxPool]
↓
[FC-4096] → [FC-4096] → [FC-1000] → [Softmax]

```

Note: [Conv3-64] denotes a convolutional layer with a 3×3 kernel and 64 filters; [MaxPool] denotes a max-pooling layer; [FC-4096] denotes a fully connected layer with 4096 units.

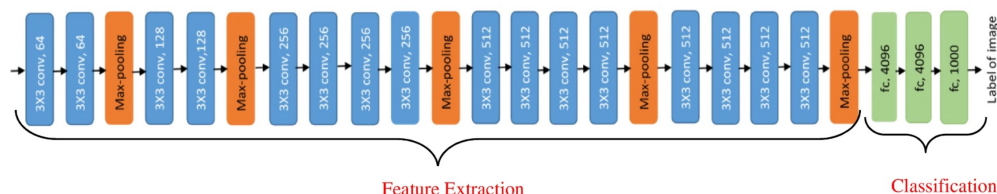


Image source: Bansal, M., Kumar, M., Sachdeva, M. et al. Transfer learning for image classification using VGG19: Caltech-101 image data set. *J Ambient Intell Human Comput* 14, 3609–3620 (2023). <https://doi.org/10.1007/s12652-021-03488-z>

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## CNN Autoencoder

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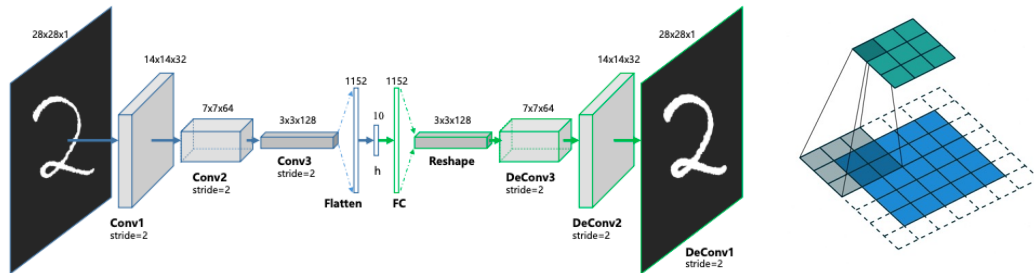


image source: <https://towardsdatascience.com/convolutional-autoencoders-for-image-noise-reduction-32fce9fc1763>

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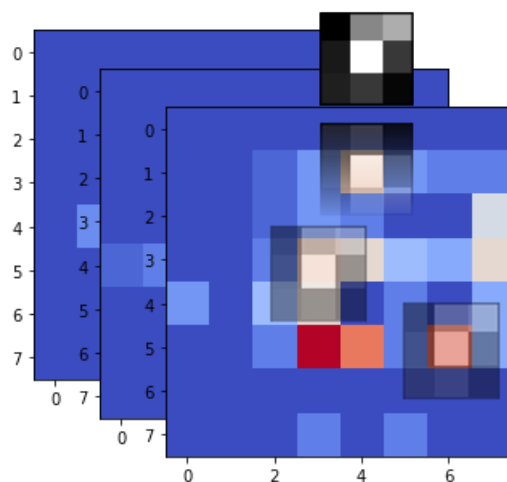
## More examples

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A sample filter which mainly focuses on the middle and top right areas out of data.



A sample filter which focuses almost on an L shape area (not equally) from the data.

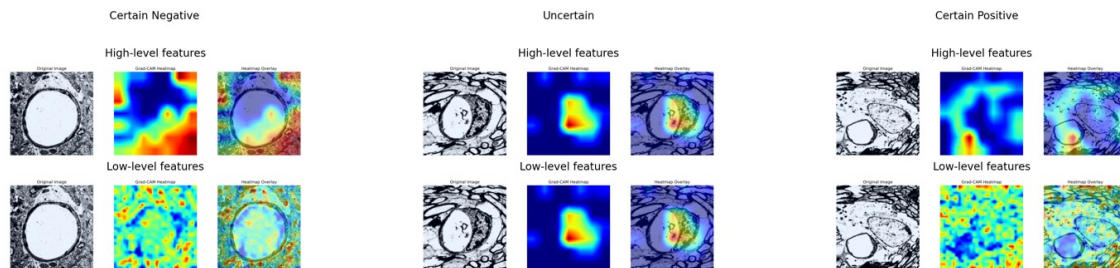


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## CNN Example: VGG model for cell microscopy data analysis

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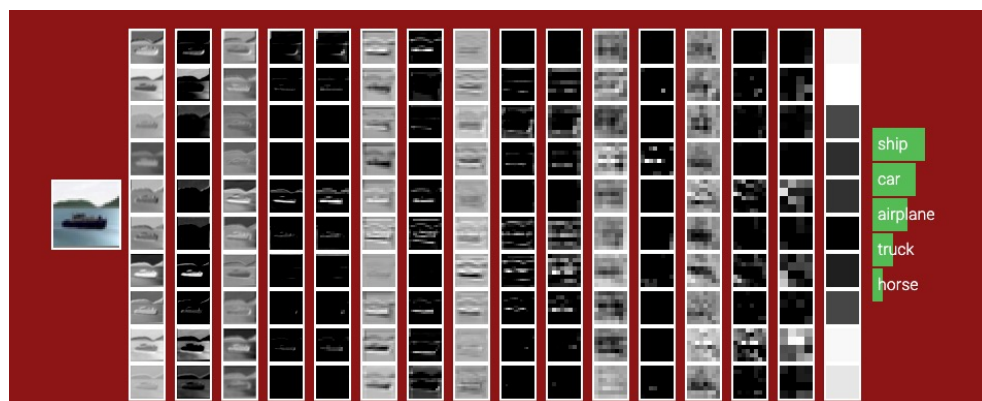
( Nan Fletcher-Lloyd, 2025)

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## Revisiting the initial example

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image source: <http://cs231n.stanford.edu/>

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## Review questions

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In a CNN network, what technique has been used if a method generates results shown in section (b) from the data grid shown in section (a)?

12	10	3	2
8	6	1	0
4	7	5	7
4	6	6	8

(a)



12	3
7	8

(b)

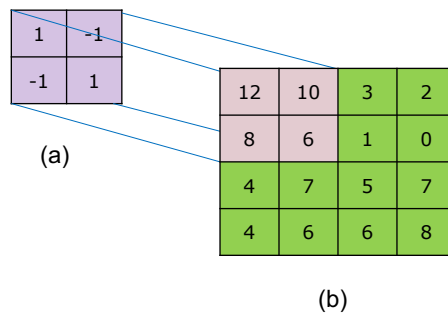
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Q2

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In a CNN network, if we have the kernel shown in (a) and want to apply to the data shown (b) with a stride of 2, what padding size would you recommend?



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Q3

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- Which operation reduces the spatial dimensions of an image in CNNs?
- A) Convolution
  - B) Pooling
  - C) Padding
  - D) Fully connected layer

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Q4

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- What does "padding" in CNNs achieve?
  - A) Reduces the computational cost of the network
  - B) Prevents overfitting during training
  - C) Maintains the spatial dimensions of the input
  - D) Enhances gradient descent optimisation

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Q5

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- What is the receptive field in CNNs?
  - A) The total number of filters used in a layer
  - B) The region of the input image that affects a single output value
  - C) The activation map produced by a convolution
  - D) The number of the kernel applied during convolution

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If you have any questions

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- Please feel free to arrange a meeting or email ([p.barnaghi@imperial.ac.uk](mailto:p.barnaghi@imperial.ac.uk)) - my office: 928, Sir Michael Uren Research Hub, White City Campus.

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