Convolutional Neural Networks

Applied Machine Learning, KU

Daniel Murnane - May 6th, 2024

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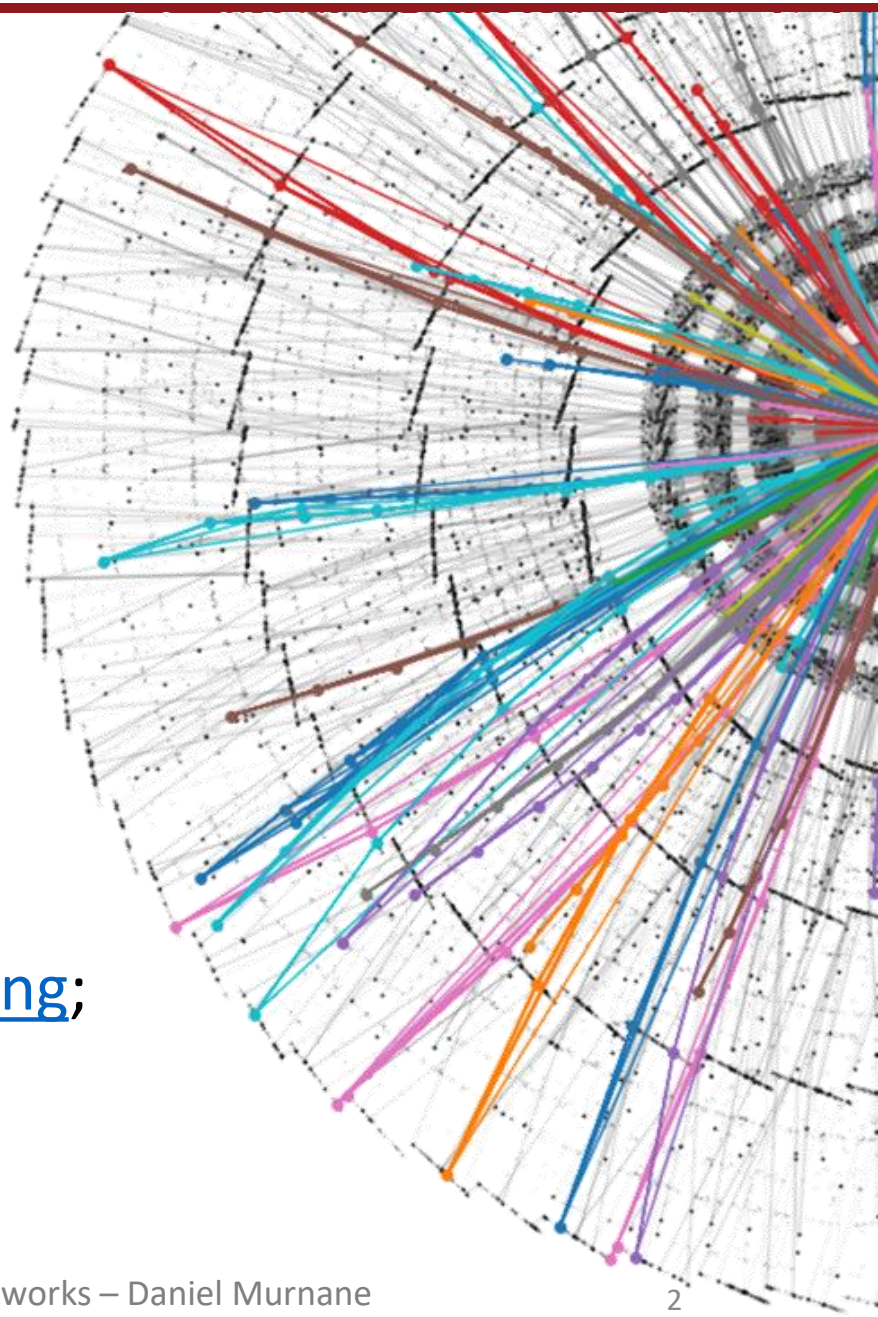
Introduction & Goals

- Nice to meet you!
- I work on ML for high energy physics @ NBI
- Goals for today:
  - Understand how to represent an image
  - See how images have traditionally been processed
  - Get intuition for the power of a convolution
  - Practice “convolution arithmetic”
  - Get a feeling for where CNNs fit into the rest of ML
  - See a few examples of CNNs in action
- Have borrowed content from MIT Intro to Deep Learning; and Julius Kirkegaard’s slides from 2022



Computer Vision

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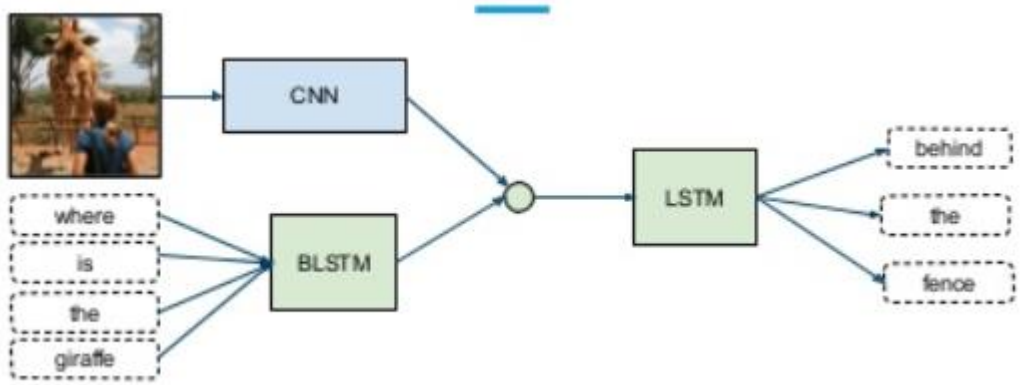
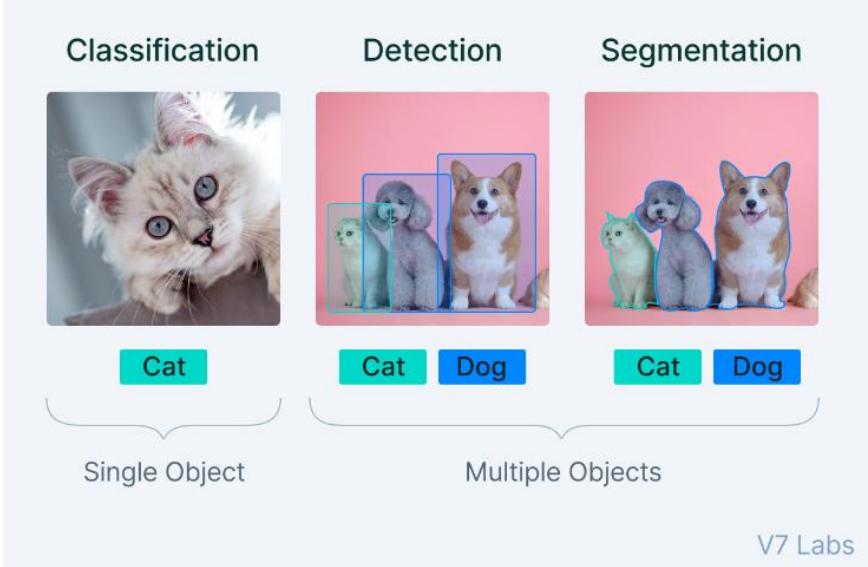
Modalities in ML

- So far, have seen “tabular data”
- Quick test for “tabularity”: Would this work well in Excel?
- The world contains more *modalities* than tabular:
  - **Images** (today!) – i.e. vision
  - Sequences (Wednesday afternoon!) – i.e. 1-dimensional time and/or causality
  - Point clouds and graphs (Wednesday morning!) – Multi-dimensional time and/or causality
- Most other modalities and senses can be represented as combinations of these:
  - Video = Images + Sequence
  - Robotic action = Tabular + Sequence/Graph
  - Audio = Images (waveform) or Sequence (fourier transform)
  - Biological & Chemical = Graph (Protein/DNA language models)
- Others might come along… Touch? Smell?
- The hot thing now is combining modalities – which is straightforward once you understand how to consume each individually



Computer Vision

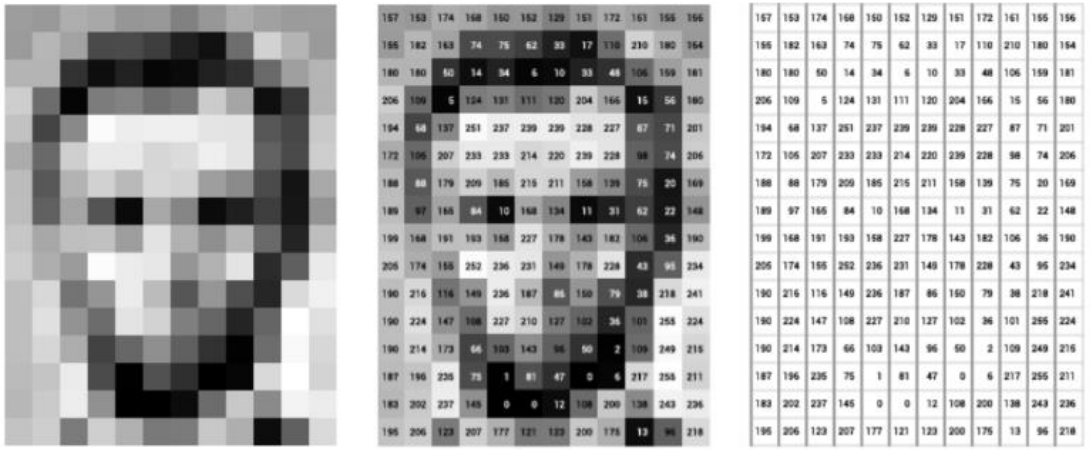
- Today's focus is vision
- Many diverse tasks: scene reconstruction, object detection, event detection, video tracking, object recognition, 3D pose estimation, learning, indexing, motion estimation, 3D scene modelling, and image restoration
- A beautiful template for the rest of machine learning
- Conventional CV: A huge collection of hand-engineered techniques on a task-by-task basis
- ML CV: A small set of models that can be used for many tasks



V7 Labs

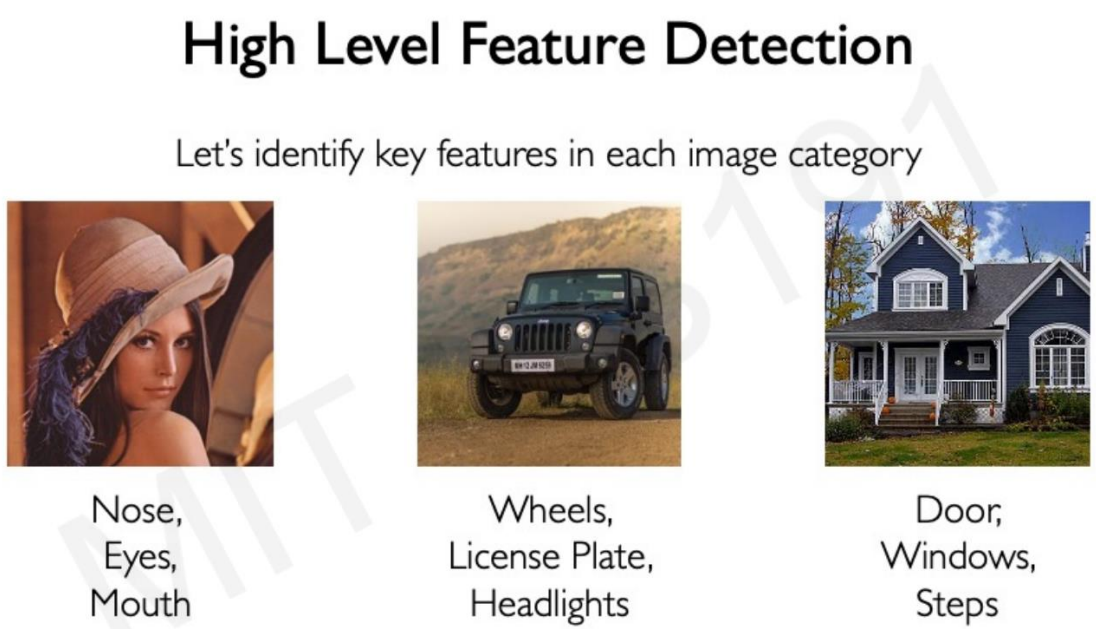
Images as Numbers

- Need way to consume images and apply functions to them
- Most typical way: represent each pixel as a vector
- Greyscale images only need a single value in the vector: the brightness of the pixel
- Colour images need 3 or 4 values in the vector: [R, G, B] or [C, M, Y, K]
- As in **every other ML project**, we normalize those inputs! Conventionally given to us as values [0, 255], therefore divide by 255



A Typical Computer Vision Task

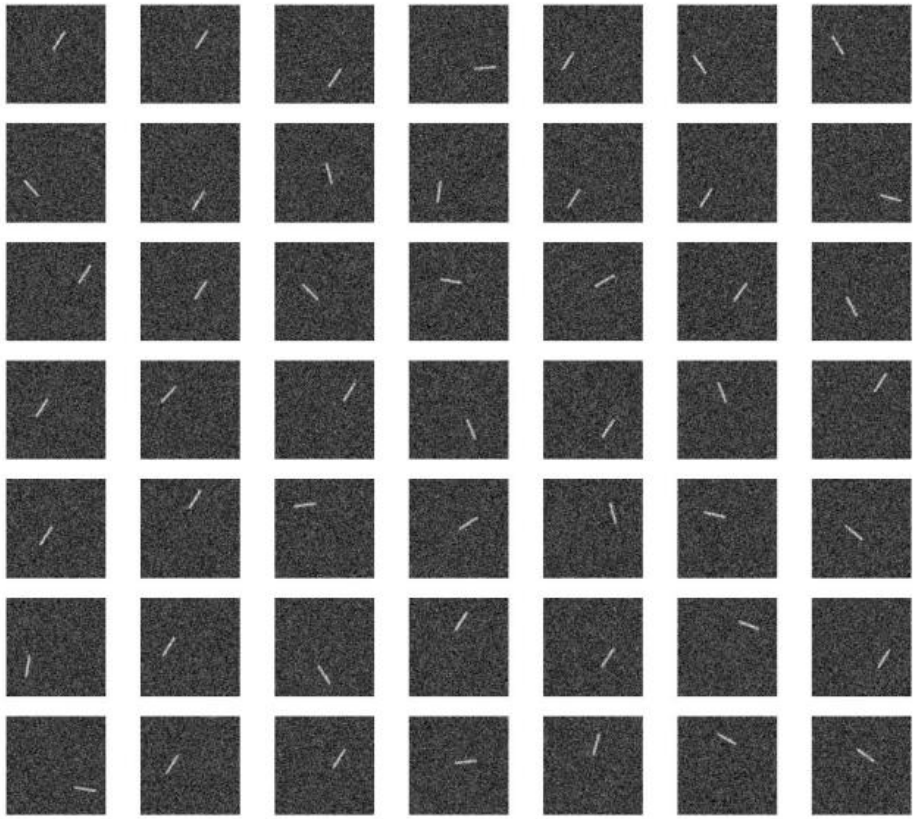
- Let's consider a typical task in CV: classification of the foreground object in an image
- How does a human do this?
- High level feature detection
- We are very sophisticated!
- Imagine if we had to look pixel-by-pixel…



The Almighty Filter

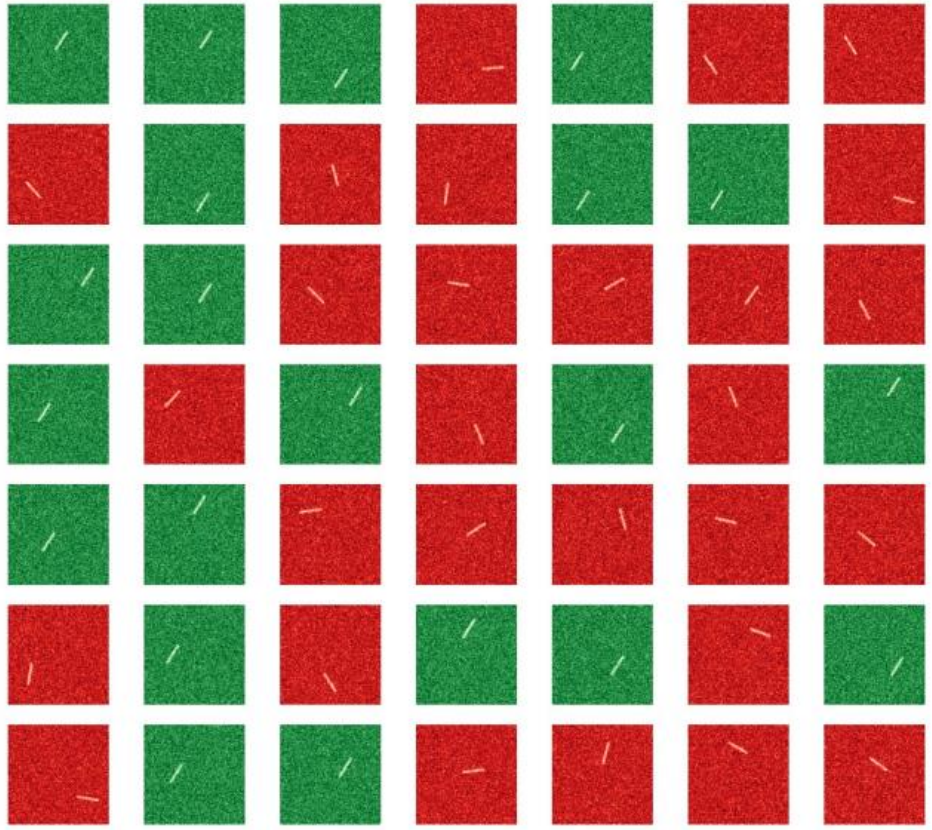
- Consider a very simple classification problem:

Find images with angle:



The Almighty Filter

- Consider a very simple classification problem:
- Note that we don't care where the feature is *within* the image



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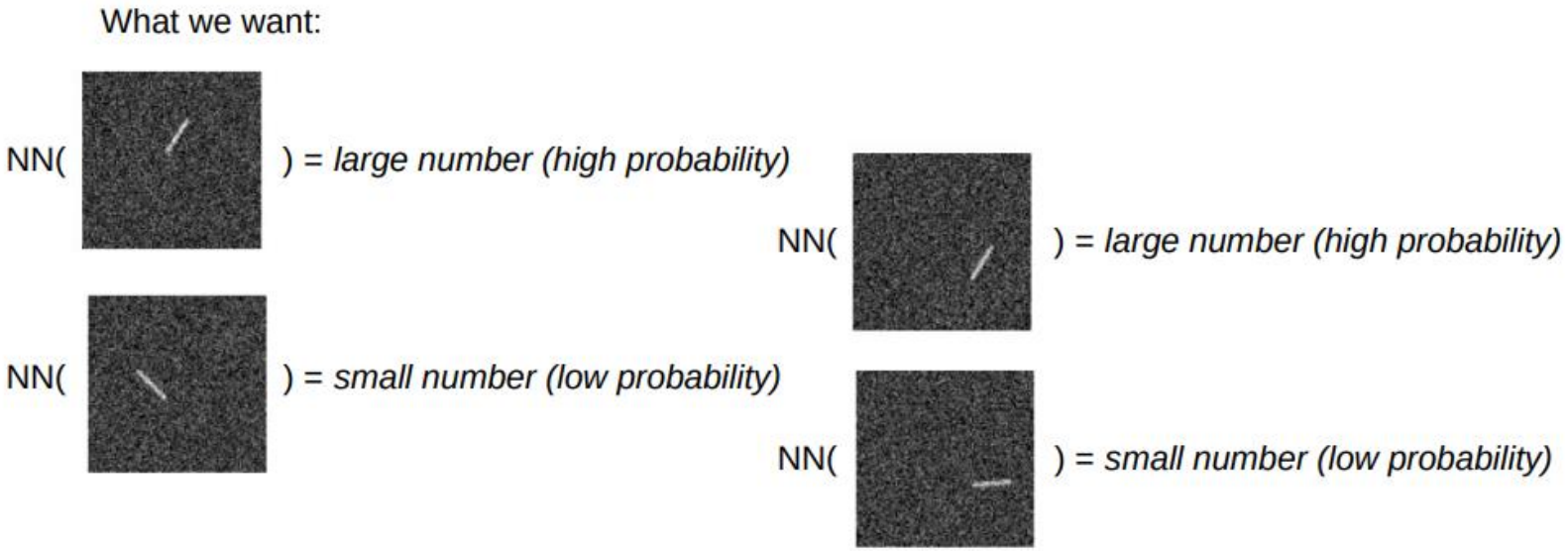
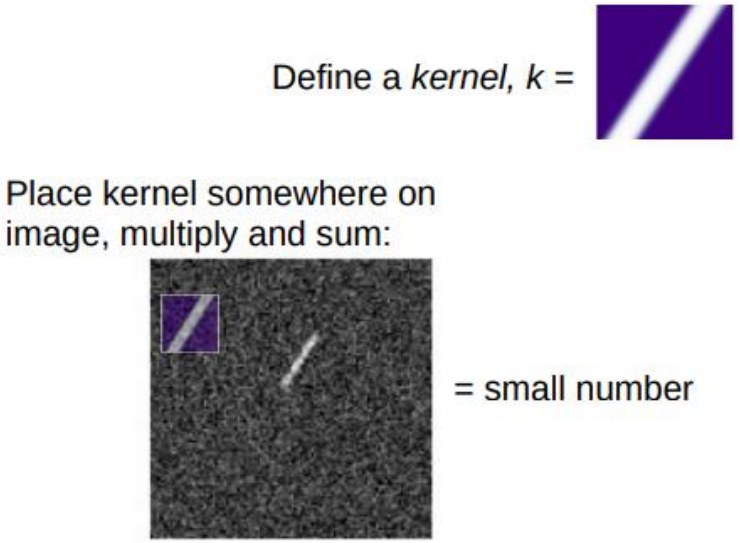


The Almighty Filter

- A “kernel”, or a “filter” is a hypothesis about a feature of interest to the task
- We are hand-engineering here, so we can use our intuition
- A kernel is a matrix of the same size of the neighbourhood of pixels we want to “test our hypothesis” on

The Almighty Filter



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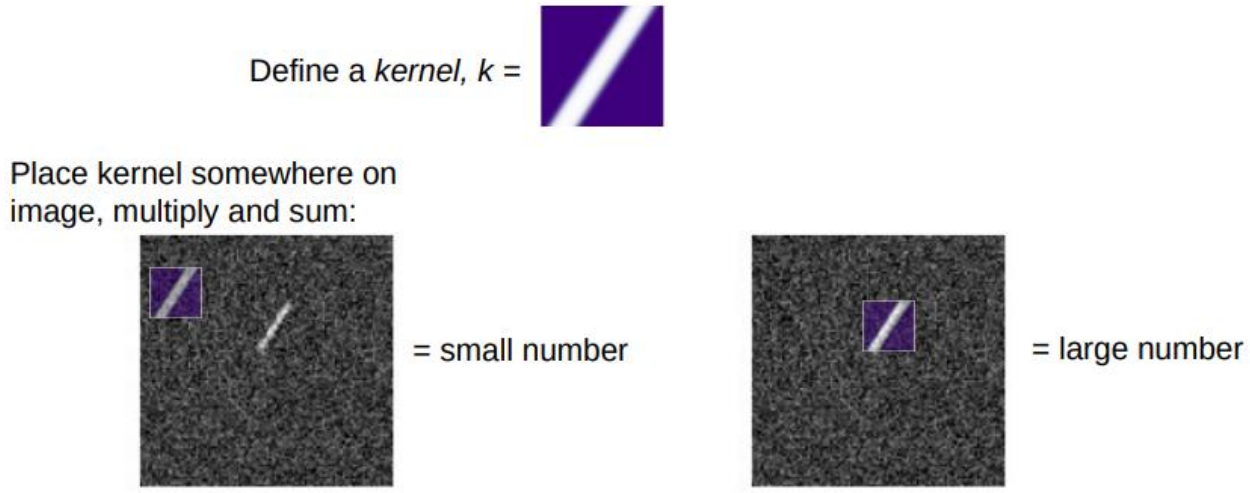

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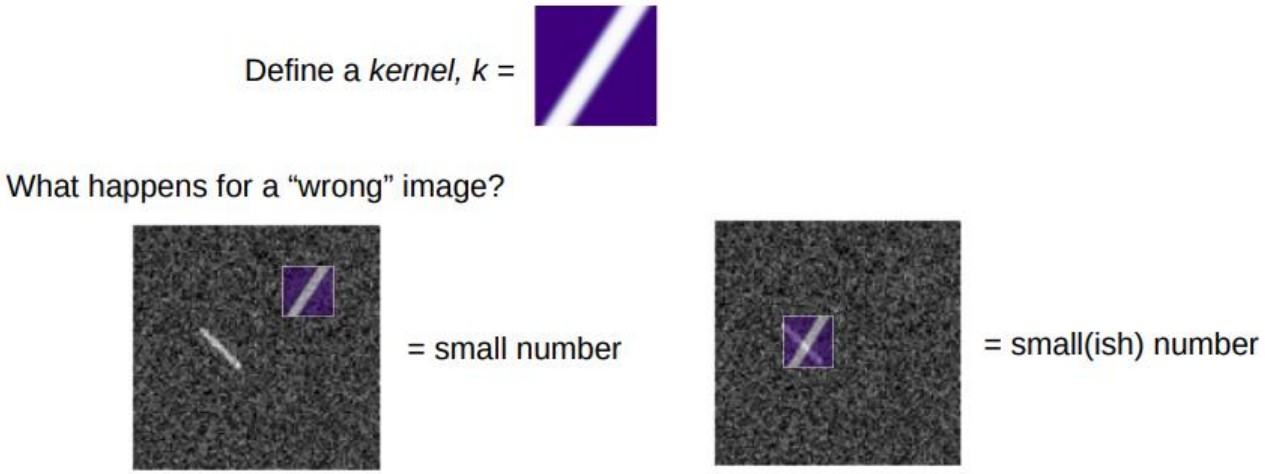

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The Almighty Filter

- Applying the filter is actually just a sum over elementwise multiplication:

Image neighbourhood

Filter

$$\sum\left(\begin{bmatrix} 0.1 & 0.1 & 0.9 \\ 0.1 & 0.9 & 0.1 \\ 0.9 & 0.1 & 0.1 \end{bmatrix} \cdot \begin{bmatrix} 0.1 & 0.1 & 0.9 \\ 0.1 & 0.9 & 0.1 \\ 0.9 & 0.1 & 0.1 \end{bmatrix}\right) = \sum\left(\begin{bmatrix} 0.01 & 0.01 & 0.81 \\ 0.01 & 0.81 & 0.01 \\ 0.81 & 0.01 & 0.01 \end{bmatrix}\right) = 2.43$$

The Almighty Filter

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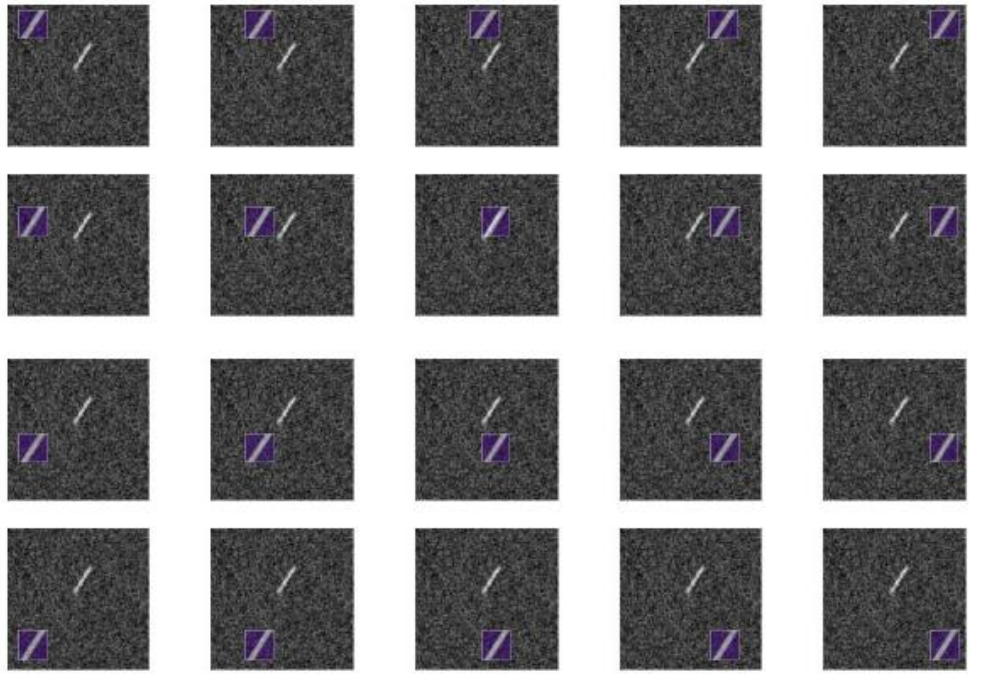
Image neighbourhood

Filter

$$\sum\left(\begin{bmatrix} 0.9 & 0.1 & 0.1 \\ 0.1 & 0.9 & 0.1 \\ 0.1 & 0.1 & 0.9 \end{bmatrix} \cdot \begin{bmatrix} 0.1 & 0.1 & 0.9 \\ 0.1 & 0.9 & 0.1 \\ 0.9 & 0.1 & 0.1 \end{bmatrix}\right) = \sum\left(\begin{bmatrix} 0.09 & 0.01 & 0.09 \\ 0.01 & 0.81 & 0.01 \\ 0.09 & 0.01 & 0.09 \end{bmatrix}\right) = 1.21$$

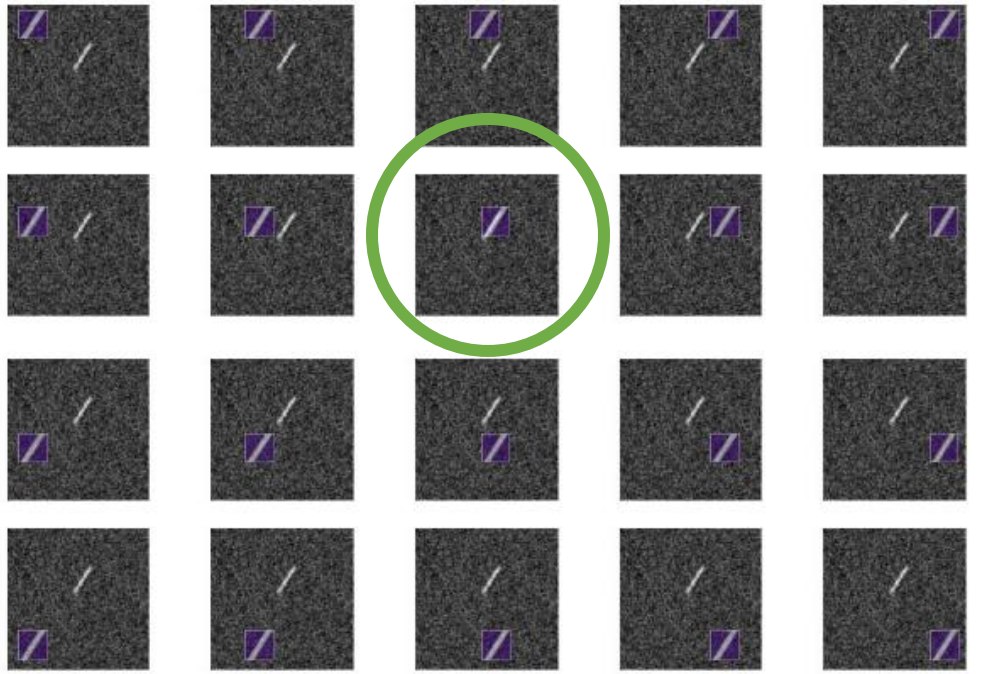
Max Pooling

- Let's slide the filter across all neighbourhoods in the image
- Keep track of the filter score for each neighbourhood

$Max($  $)$

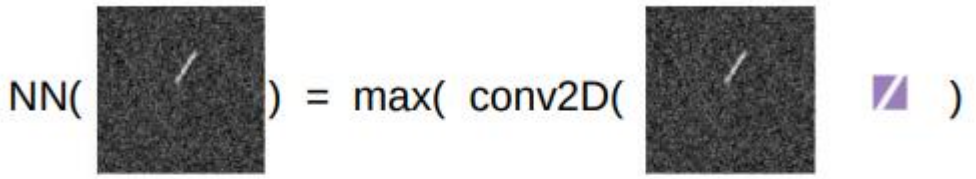
Max Pooling

- Let's slide the filter across all neighbourhoods in the image
- Keep track of the filter score for each neighbourhood
- Find the maximum score across the whole image

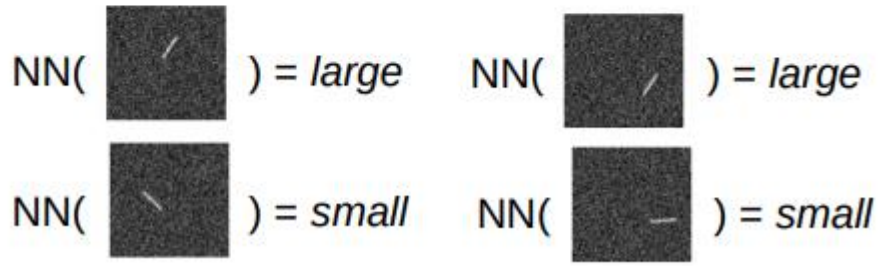
$Max($  $)$

Convolutional Filter

This is precisely what a convolution does!



We have our function!
Indeed:

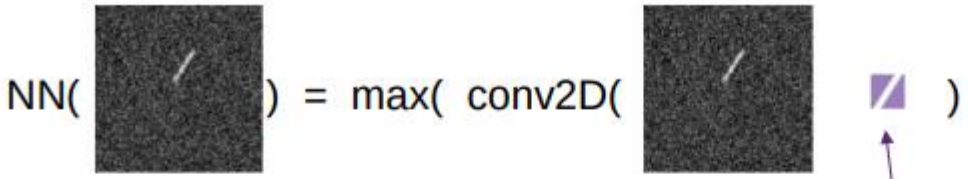


- But, we haven't trained anything!
- This is a "hand-crafted" filter:

0.1	0.1	0.9
0.1	0.9	0.1
0.9	0.1	0.1

- What if we made the 9 values in the matrix learnable parameters?
- Then we could find the filter that minimises a loss function

Trainable Convolutional Filter



We handcrafted the kernel. In CNNs we train to choose the best kernels

```
net = nn.Sequential(nn.Conv2d(1, 1, 11),
                    nn.AdaptiveMaxPool2d(1),
                    nn.Linear(1, 1))
```

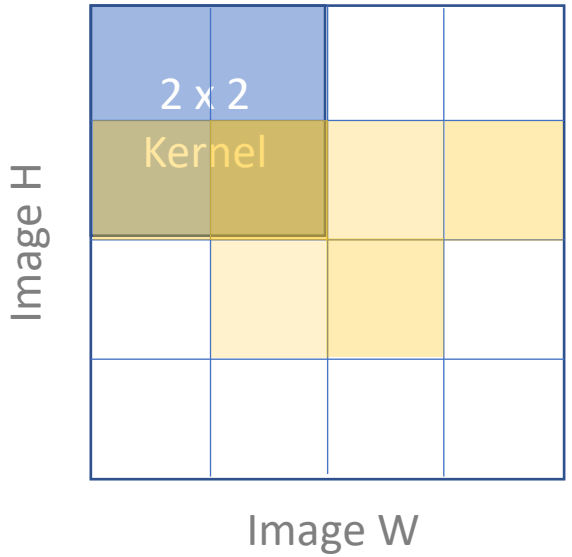
```
# Soft-max probabilities -> cross entropy
p = torch.exp(pred) / (torch.exp(pred) + torch.exp(-pred))
loss = -torch.mean(labels * torch.log(p) + (1 - labels) * torch.log(1 - p))  # (this can be done smarter!,
                                                                             # no reason to take exp, then log)
```

Run code!

(slightly smarter than ours!, albeit noisy)

Adding a Latent Space

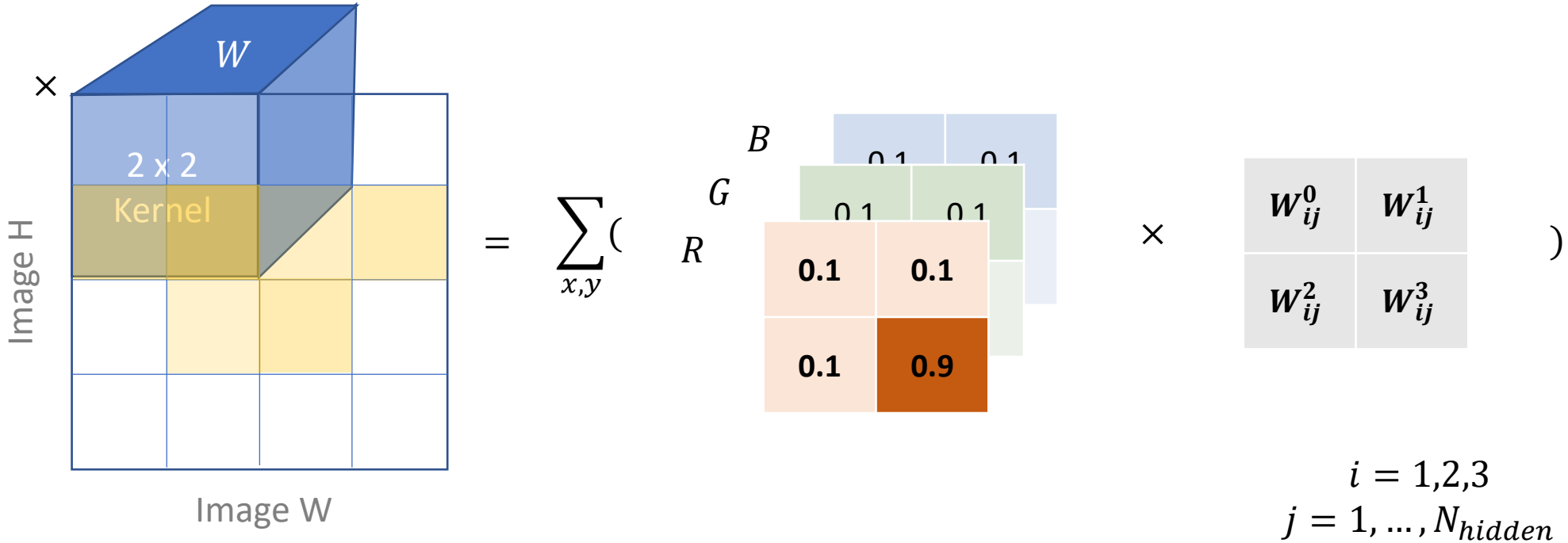
- Currently everything is “flat” – each pixel multiplied by a single learnable parameter



- But recall neural networks can learn *many* parameters

Adding a Latent Space

- We can add as much depth to the convolution as we want
- This is a bit hard to understand! There are two levels of matrices…



$$i = 1,2,3$$
$$j = 1, \ldots, N_{hidden}$$

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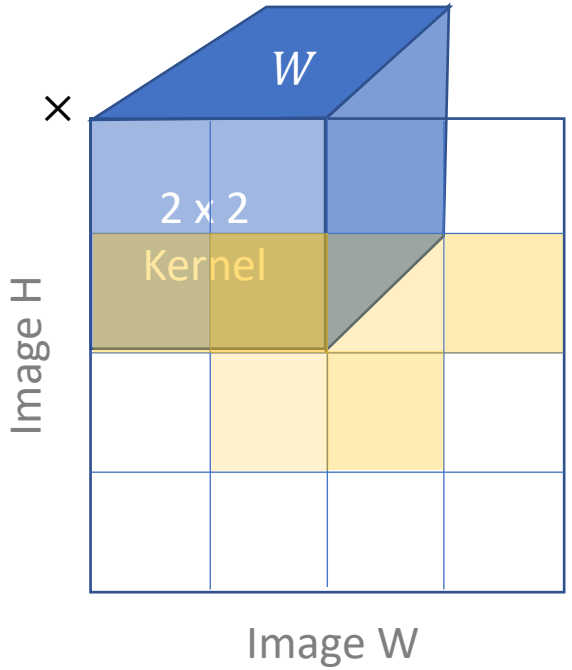

$$= \sum_{x,y} \Big(\begin{matrix} W^0_{2j} & W^1_{2j} \\ W^0_{1j} & W^1_{1j} \end{matrix} \; \begin{matrix} W^1_{2j} \\ W^3_{2j} \end{matrix} \; \begin{matrix} W^3_{1j} \end{matrix} \; \begin{matrix} W^0_{0j} & W^1_{0j} \\ W^2_{0j} & W^3_{0j} \end{matrix} \Big)$$

R G B

$$i = 1,2,3$$
$$j = 1, \dots, N_{hidden}$$

Why not just use a feedforward layer?

- You might ask…
- We have this magical block box: fully-connected, feedforward neural network
- We know it can approximate any function, provided it is wide and deep enough
- Why not simply feed in the list of pixels as “tabular data” and run through a FFNN?
- First answer: Translational invariance

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ORIGINAL CONTRIBUTION

Multilayer Feedforward Networks are Universal Approximators

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Technische Universität Wien

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(*Received* 16 *September* 1988; *revised and accepted* 9 *March* 1989)

Abstract—*This paper rigorously establishes that standard multilayer feedforward networks with as few as one hidden layer using arbitrary squashing functions are capable of approximating any Borel measurable function from one finite dimensional space to another to any desired degree of accuracy, provided sufficiently many hidden units are available. In this sense, multilayer feedforward networks are a class of universal approximators.*

Keywords—Feedforward networks, Universal approximation, Mapping networks, Network representation capability, Stone-Weierstrass Theorem, Squashing functions, Sigma-Pi networks, Back-propagation networks.

1. INTRODUCTION

It has been nearly twenty years since Minsky and Papert (1969) conclusively demonstrated that the simple two-layer perceptron is incapable of usefully representing or approximating functions outside a very narrow and special class. Although Minsky and Papert left open the possibility that multilayer networks might be capable of better performance, it has only been in the last several years that researchers have begun to explore the ability of multilayer feedforward networks to approximate general mappings from one finite dimensional space to another. Recently, this research has virtually exploded with impressive successes across a wide variety of applications. The scope of these applications is too broad to mention useful specifics here; the interested reader is referred to the proceedings of recent IEEE Conferences on Neural Networks (1987, 1988) for a sampling of examples.

The apparent ability of sufficiently elaborate feedforward networks to approximate quite well nearly any function encountered in applications leads one to wonder about the ultimate capabilities of such networks. Are the successes observed to date reflective of some deep and fundamental approximation capability, or are they merely flukes, resulting from selective reporting and a fortuitous choice of problems? Are multilayer feedforward networks in fact inherently limited to approximating only some fairly special class of functions, albeit a class somewhat larger than the lowly perceptron? The purpose of this paper is to address these issues. We show that multilayer feedforward networks with as few as one hidden layer are indeed capable of universal approximation in a very precise and satisfactory sense.

Advocates of the virtues of multilayer feedforward networks (e.g., Hecht-Nielsen, 1987) often cite Kolmogorov's (1957) superposition theorem or its more recent improvements (e.g., Lorentz, 1976) in support of their capabilities. However, these results require a *different* unknown transformation (g in Lorentz's notation) for each continuous function to be represented, while specifying an exact upper limit to the number of intermediate units needed for the representation. In contrast, quite specific squashing functions (e.g., logistic, hyperbolic tangent) are used in practice, with necessarily little regard for the function being approximated and with the number of hidden units increased *ad libitum* until some desired level of approximation accuracy is reached. Al-

White's participation was supported by a grant from the Guggenheim Foundation and by National Science Foundation Grant SES-8806990. The authors are grateful for helpful suggestions by the referees.

Requests for reprints should be sent to Halbert White, Department of Economics, D-008, UCSD, La Jolla, CA 92093.

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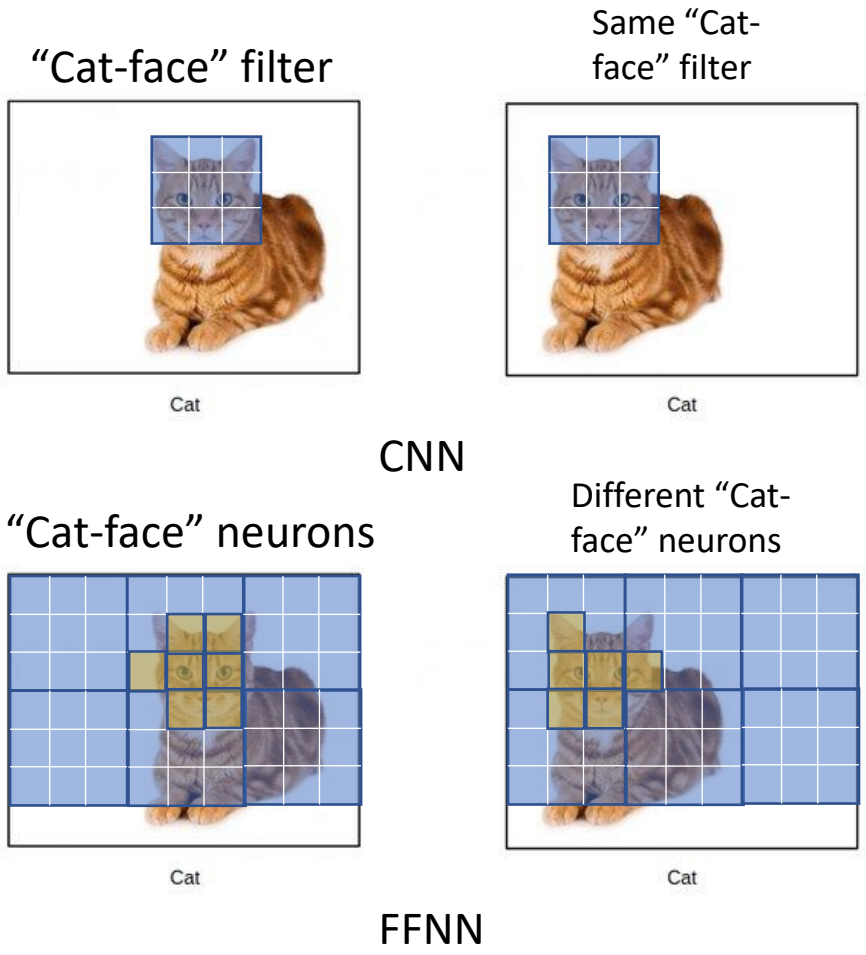
[Hornick et al, 1989]

Symmetries, Invariances & Inductive Bias

- We *know* that the location of a feature shouldn't matter in an image – we can translate a cat in x and y and it's still a cat
- In a CNN, the *same* convolutional filter is applied in each neighbourhood (aka "shared weights"), so will find a cat in any part of the image: it is translationally invariant
- A FFNN, on the other hand, has a dedicated parameter for *each* pixel – it has no concept of "nearness" or a "neighbourhood"
- We have introduced an "inductive bias" by choosing a function (the filter) that is translationally invariant
- A CNN is able to train with *much* less data than a FFNN, and is less prone to overfitting: Because we used our human intuition of translational symmetry



Convolutional Neural Networks

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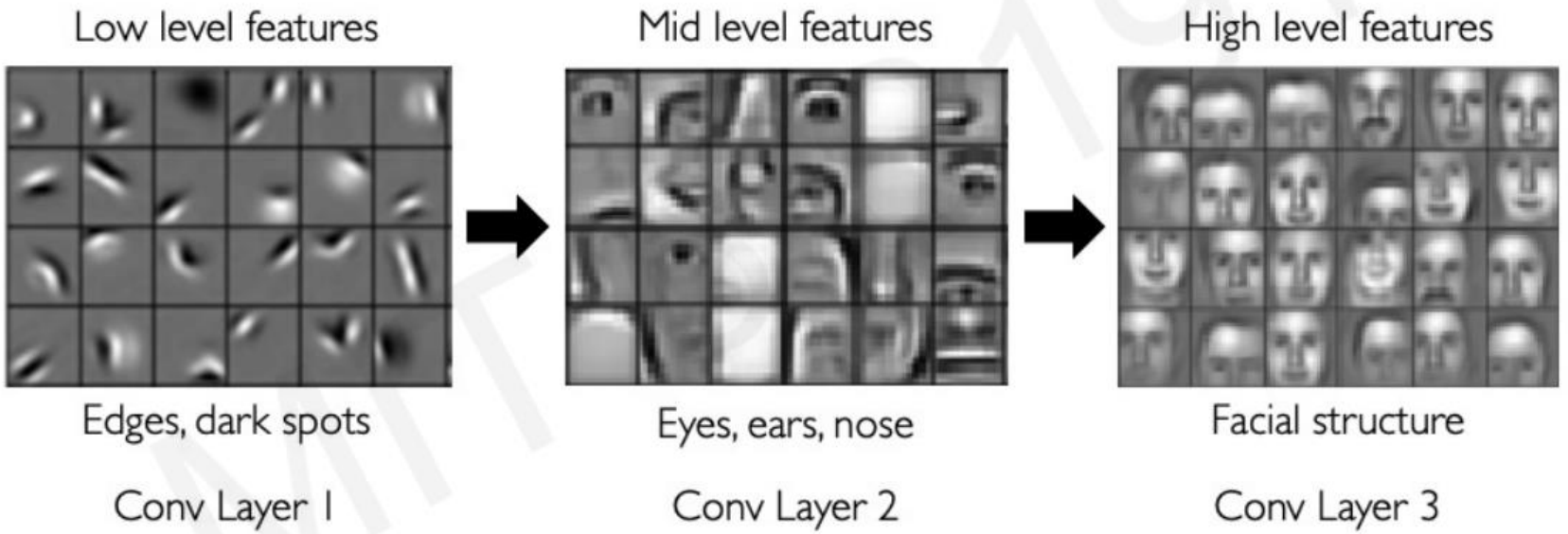
Hierarchy and Scale-dependent Features

- Our filter from earlier didn't seem to represent any recognisable object
- But it might be an "edge" or a "corner", which are important low level features in many objects
- Our knowledge of scale is another inductive bias that we can introduce into the CNN architecture

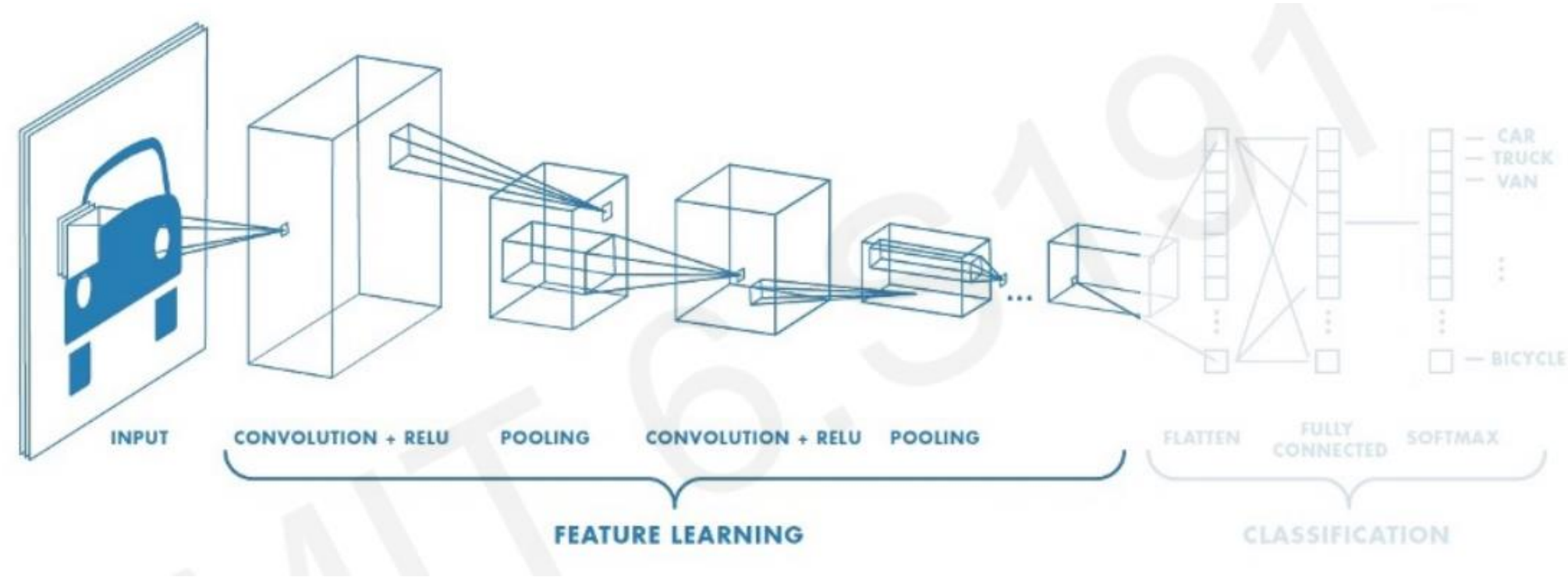


A Typical CNN Architecture

- We can handle scale by having convolutions of increasing size, each one applied to the output of the previous convolution
- Recall the pattern: $MaxPool\left(ReLU\left(Conv2D\left(x_{ij}\right)\right)\right)$: encoder
- Note: We added a non-linearity here – this allows the NN to universally approximate
- We stack multiple encoders to learn features

A Typical CNN Architecture

- We stack multiple encoders to learn features



Convolution Arithmetic

- Let's look at a couple of examples to understand the specifics

CONV2D

PyTorch

CLASS torch.nn.Conv2d(*in_channels*, *out_channels*, *kernel_size*, *stride=1*, *padding=0*, *dilation=1*, *groups=1*, *bias=True*, *padding_mode='zeros'*, *device=None*, *dtype=None*) [SOURCE]

- The Conv2D class is simply an implementation of the kernel/filter that we invented earlier, but it has a few bells and whistles that you need to understand

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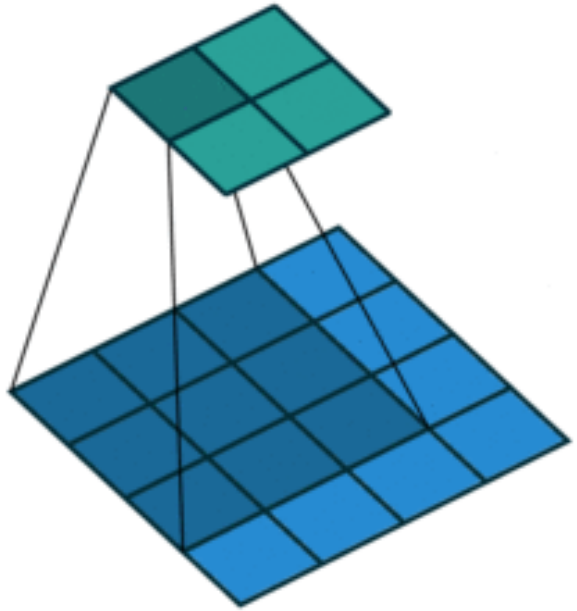
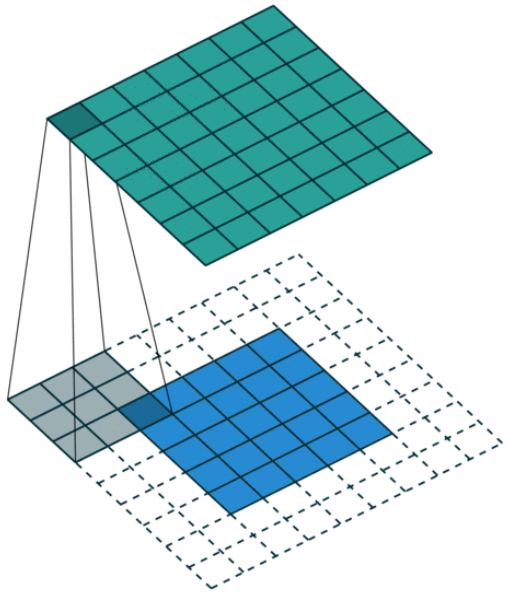
Kernel Size

- Consider the convolution on the right
- Our input image is 4 x 4
- The “kernel size” is the “receptive field” of the convolution: how big is the matrix?
- The kernel size is 3 x 3 (it is conventionally square)



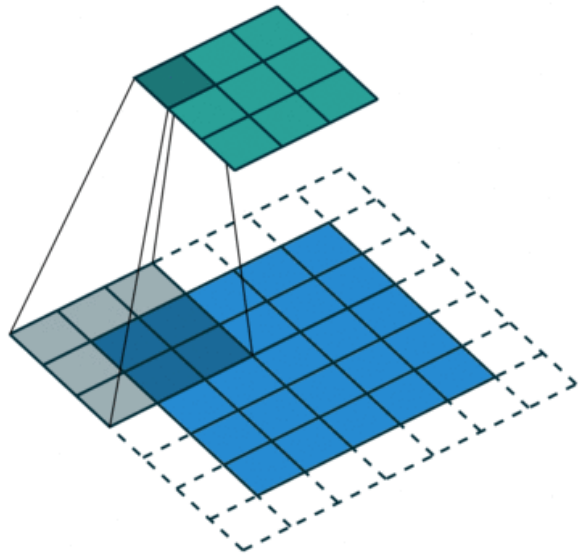
Padding

- Notice in the previous slide that our output is smaller than the input: *we don't necessarily want this!*
- To give us back our precious pixels, we can add some dummy pixels to the input
- See the example on the right has output size equal to input size



Stride

- Pixels side-by-side are likely to contain very similar information
- It may be a waste of computational resources to consider the neighbourhood of *every single pixel*
- Assuming it's enough that a pixel is in the neighbourhood of *some* convolution, we can set a stride: the number of pixels to slide along
- Here we stride by 2 pixels

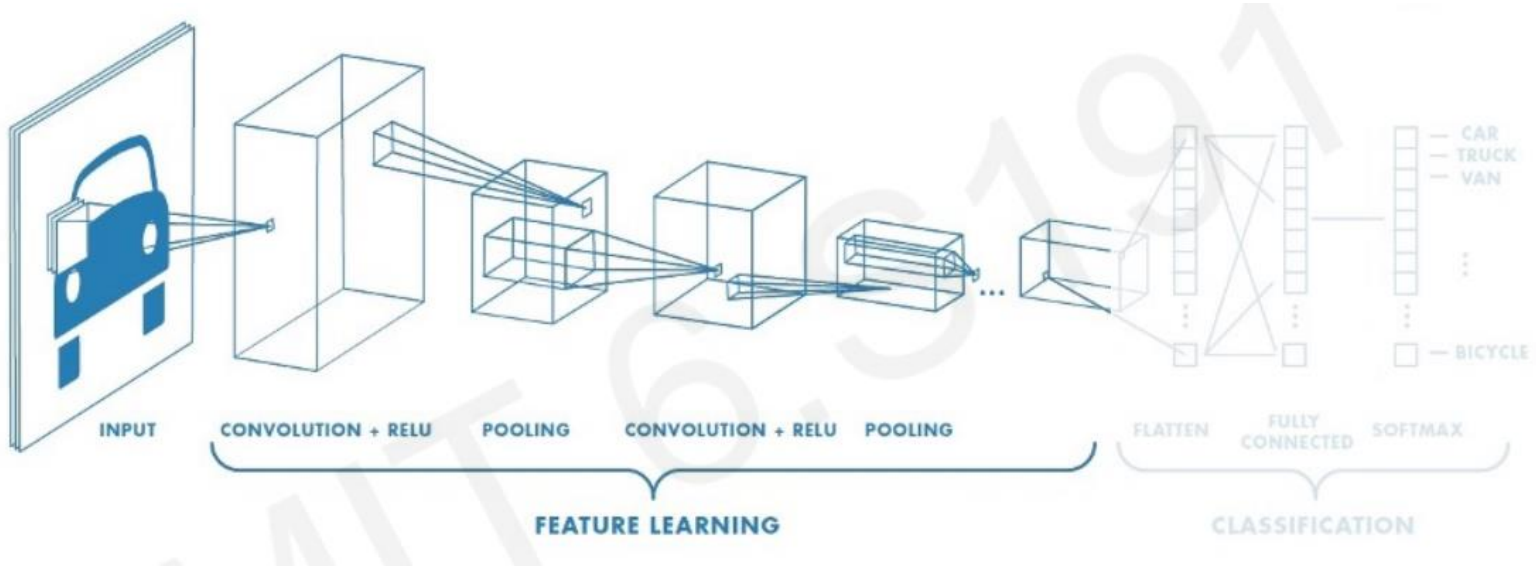


Example

- Consider the following:
  - Max Pool of kernel size = 4, stride = 1, padding = 0; applied to
  - Convolution of kernel size = 3, stride = 2, padding = 1; applied to
  - An image of 256 x 256 pixels
- What is the output size?

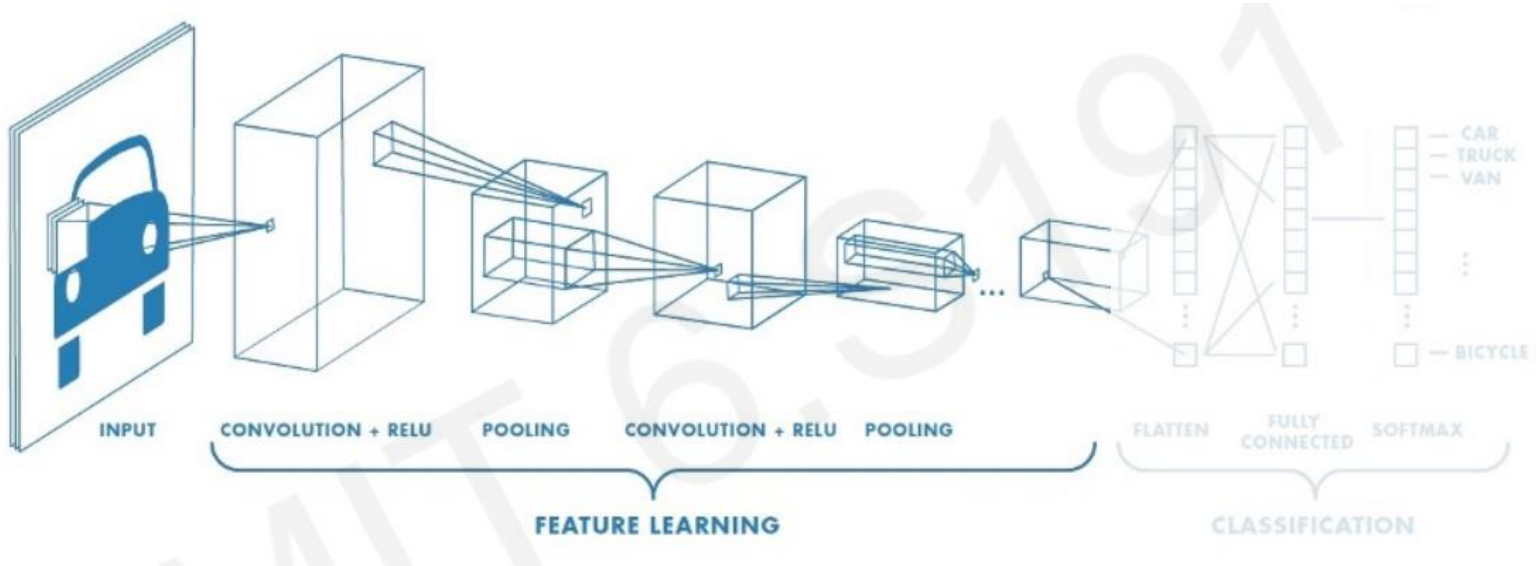
Back to the Typical Architecture

- Typically, we want to grow our receptive field (by using stride and maxpooling to downsample the image), and deepen the latent space
- This is based on the intuition that there are a small number of complex ideas/features that can fully capture an image



Back to the Typical Architecture

- Okay, so we have convolved and pooled our way to a tiny image with a big latent space
- What happens at the end??
- It depends…



Case Studies

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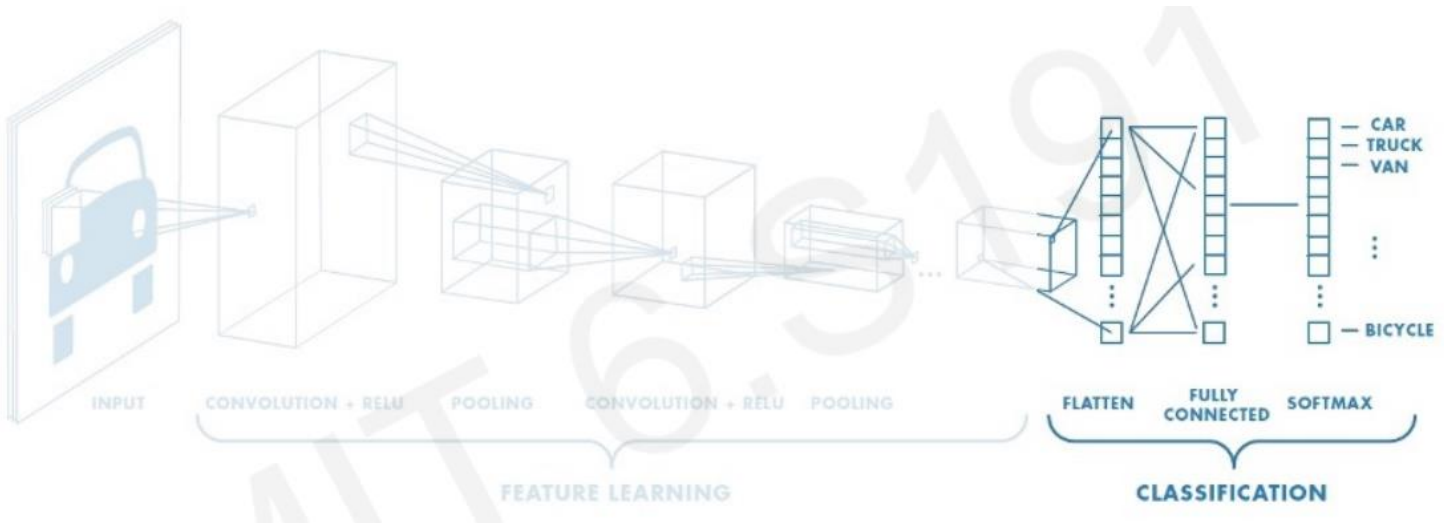
Classification

- The classic task: classification (or regression)
- As in all classification, we need to transform our $x \times y \times h$ encoded image into a prediction vector (for example, where the entries are class probabilities)
- Simple idea: just line up all the rows of pixels into one big vector (aka “flatten the image”) and pass through a FFNN



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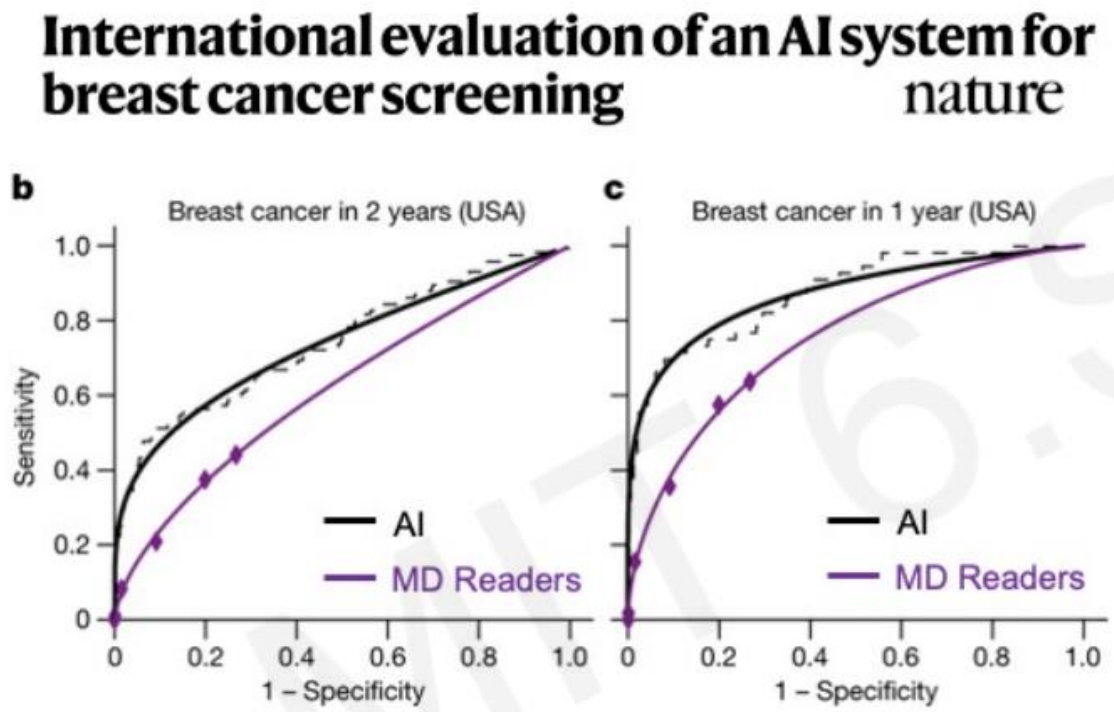
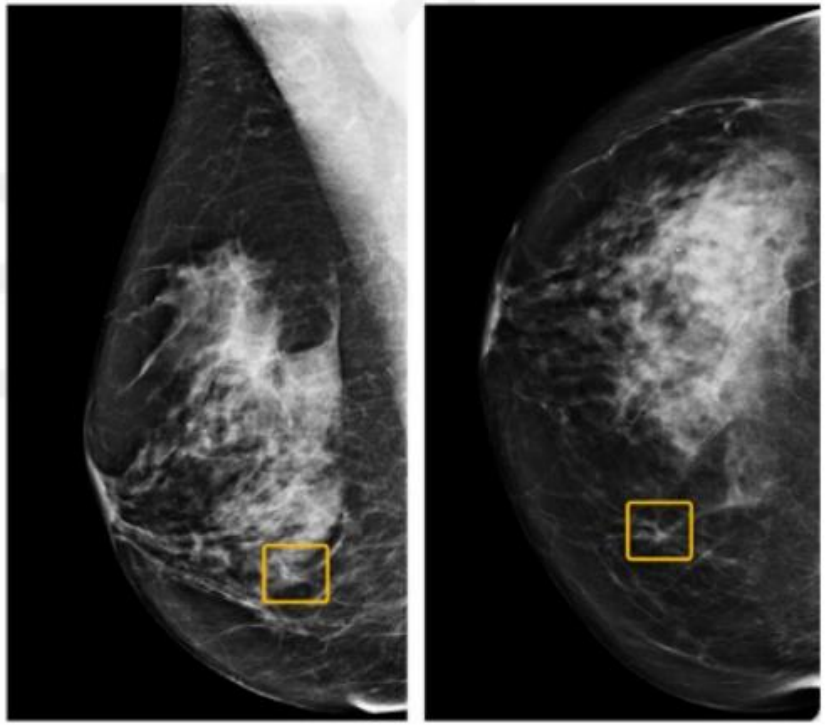
- Simple idea: just line up all the rows of pixels into one big vector (aka "flatten the image") and pass through a FFNN
- But didn't you say this doesn't work very well? Once we have learned features with convolutions and downsampled the image, it works extremely well. Doesn't work well on the raw input pixels

Classification: Breast Cancer Screening



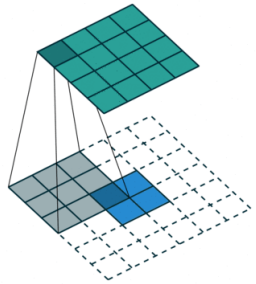
CNN-based system outperformed expert radiologists at detecting breast cancer from mammograms

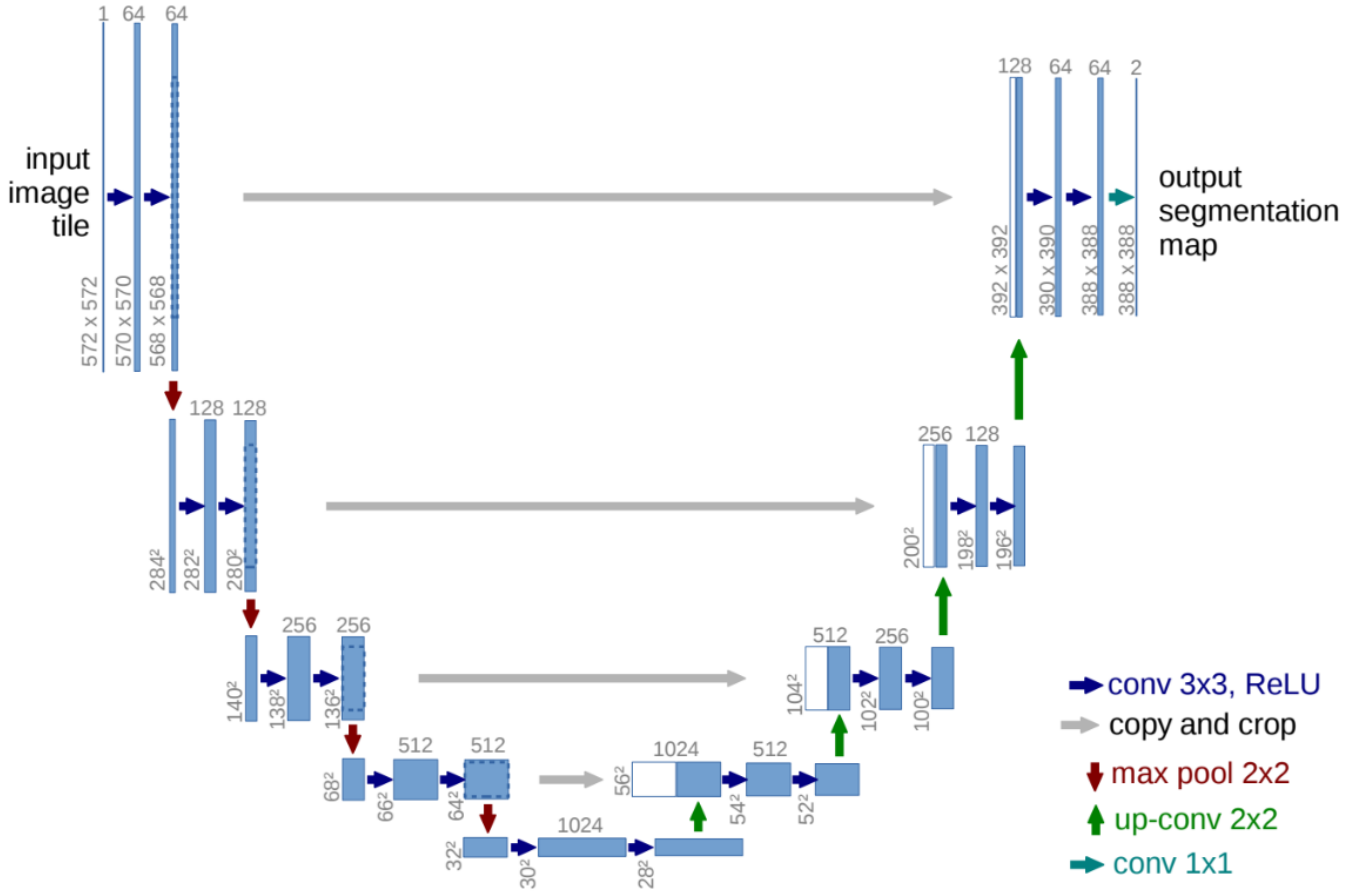


Breast cancer case missed by radiologist but detected by AI

Instance and Semantic Segmentation

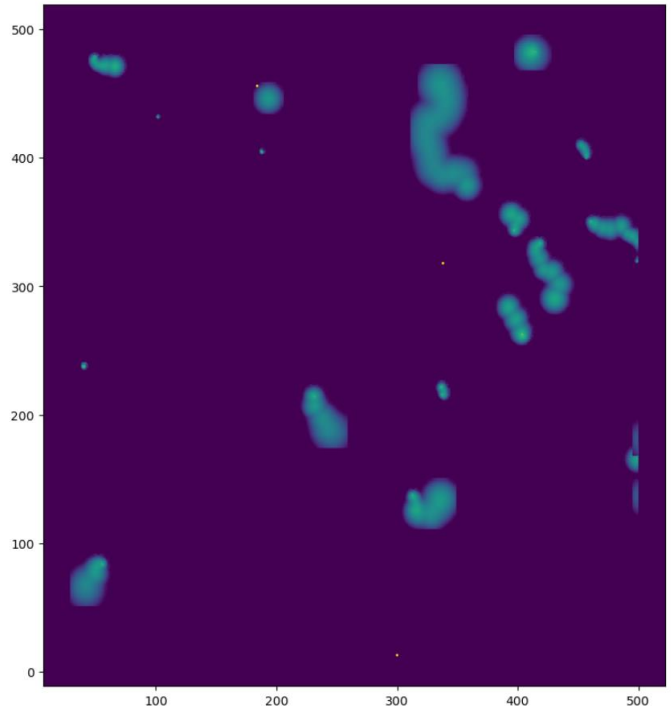
- What if we want to label all the objects in an image, and find their location?
- This is segmentation: rather than a classification for the image, give a classification for *each pixel*
- But this requires returning an output the same size as the input image
- Enter the “Unet”: allows a large receptive field, while still returning the original dimensions
- Contains a “transposed convolution”

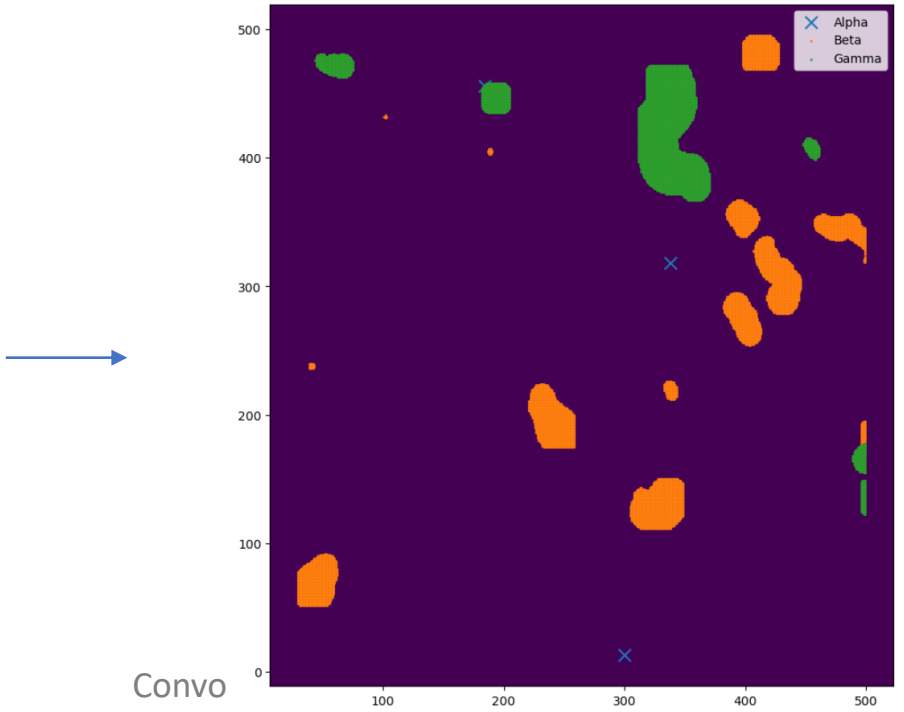




Semantic Segmentation: Tritium Detection

- Given the fallout of a nuclear disaster, can you detect radioactive decays from soil in a silicon charge-couple device?
- We hope so! This is a semantic segmentation problem:



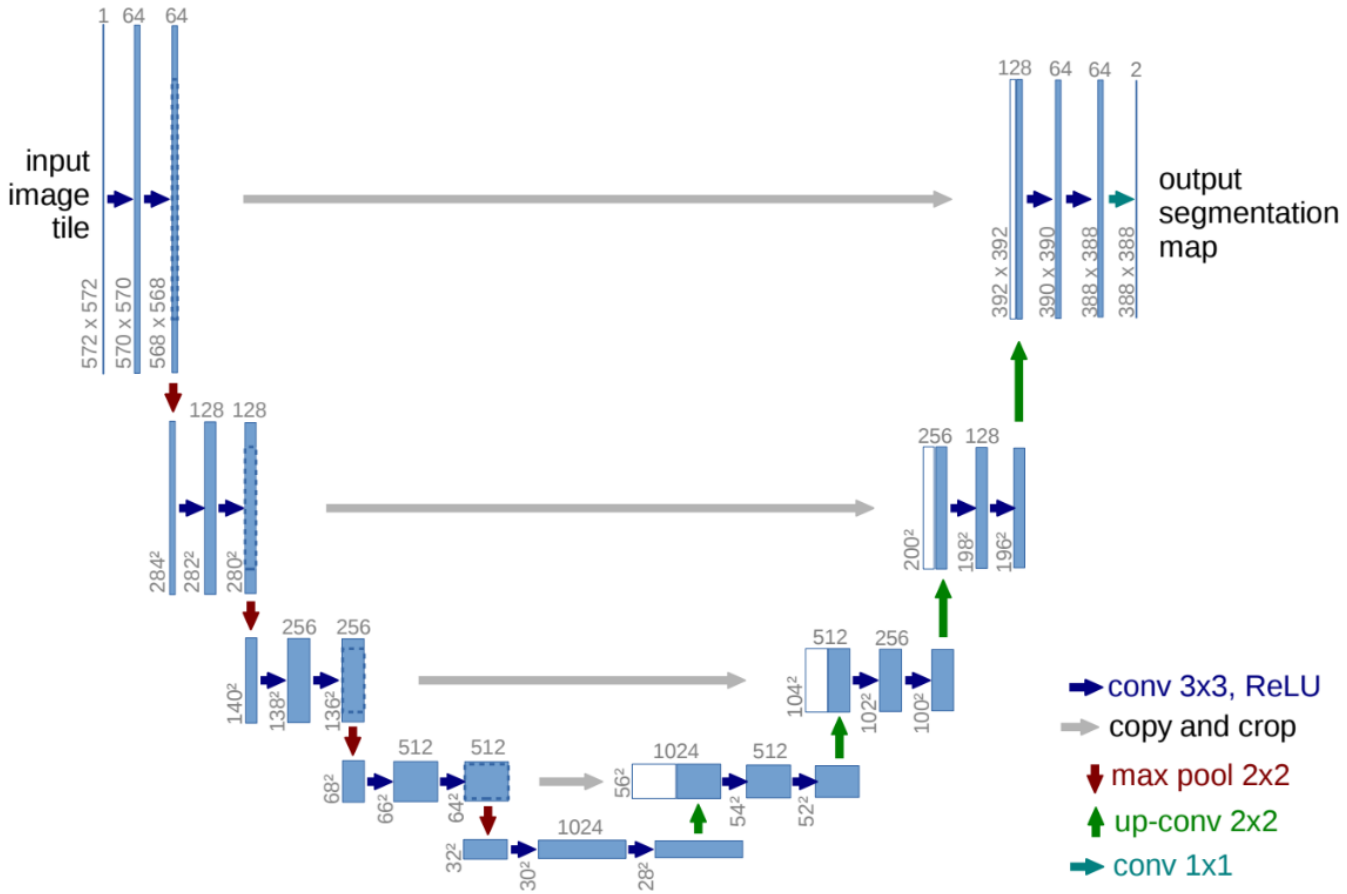


UNIVE
COPE

Convo

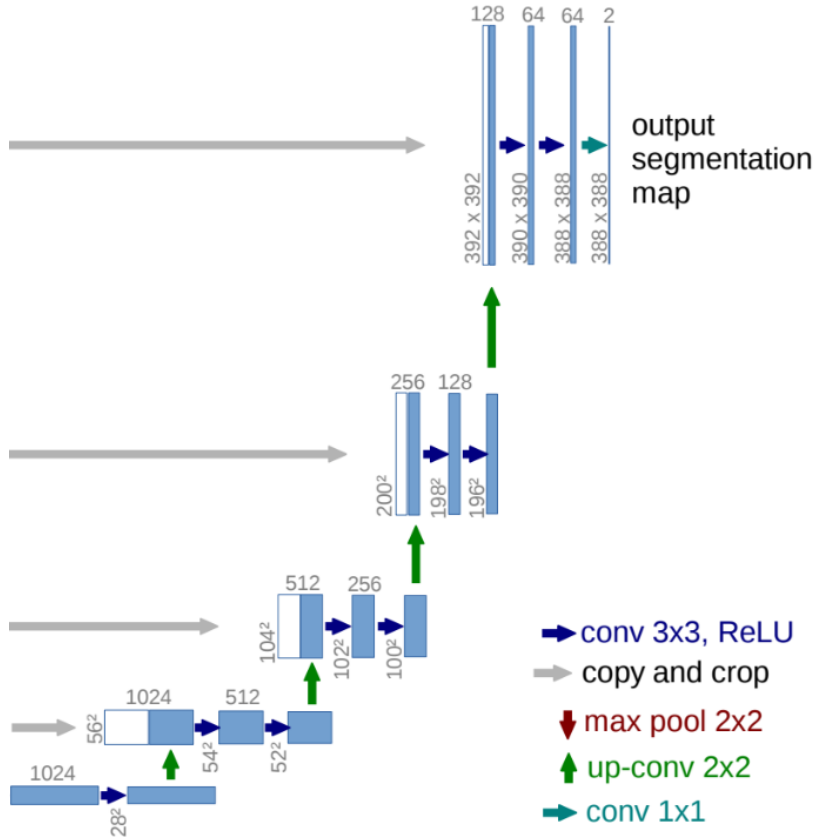
Generative Models

- Recall the Unet: it goes all the way down to a single “pixel” of very large latent space
- Called the “bottleneck” – used to capture information about the whole image
- The grey arrows are “residual connections”: simply concatenate/sum two latent spaces together! Simple but powerful



Generative Models

- Recall the Unet: it goes all the way down to a single “pixel” of very large latent space
- Called the “bottleneck” – used to capture information about the whole image
- We can train a network that *starts* at the bottleneck to perform transposed convolutions and *generate* an image
- **Many** different ways to train, but they almost always rely on bottleneck→transposed convolution

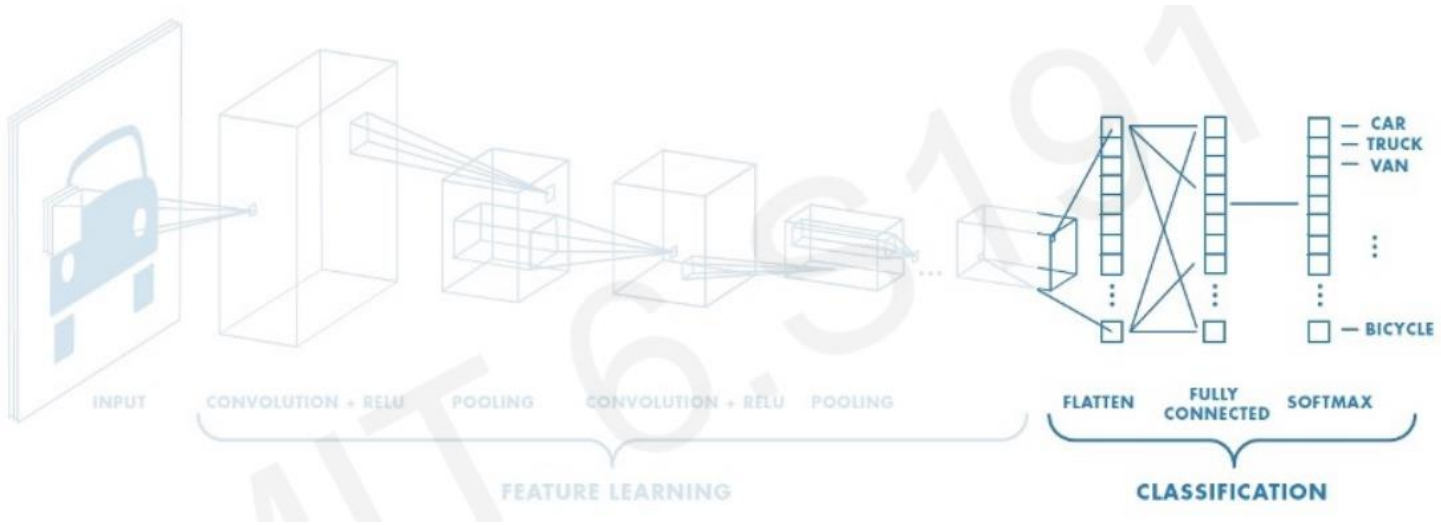


Generative Models

- CycleGAN is a sophisticated sequence of transposed convolutions and bottlenecks

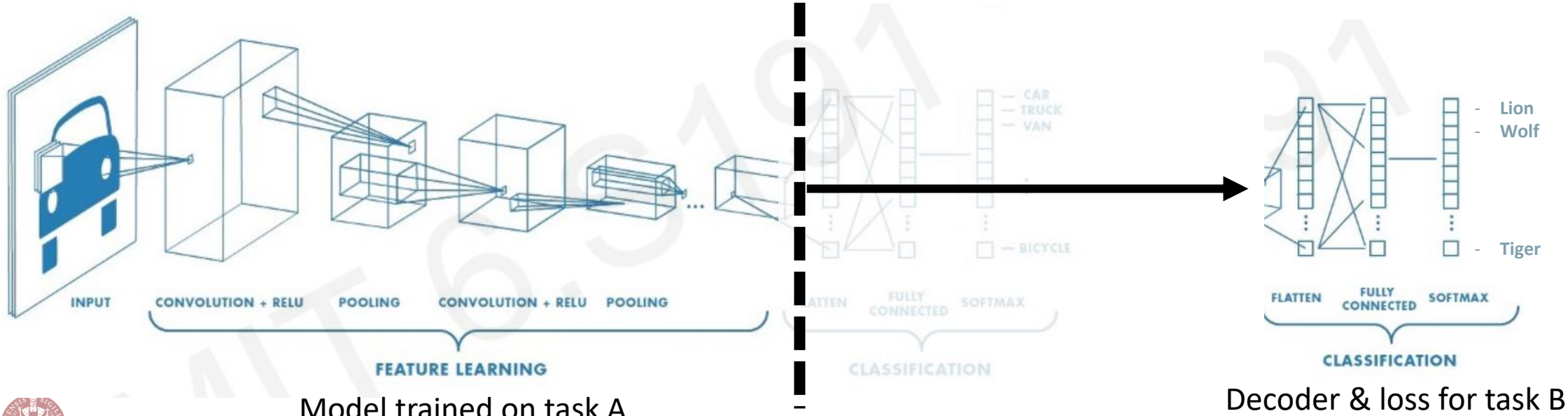
Transfer Learning with Feature Extraction

- What if we spend $1million training a cat/dog classifier, then realise we actually want to classify lions and wolves – or worse: aeroplanes, boats and cars



Transfer Learning with Feature Extraction

- What if we spend $1million training a cat/dog classifier, then realise we actually want to classify lions and wolves – or worse: aeroplanes, boats and cars
- Intuition: the features learned from a cat picture (edges for example) are relevant for other image classifiers
- We can slice off the final task-specific layer of a model and still use its feature layers

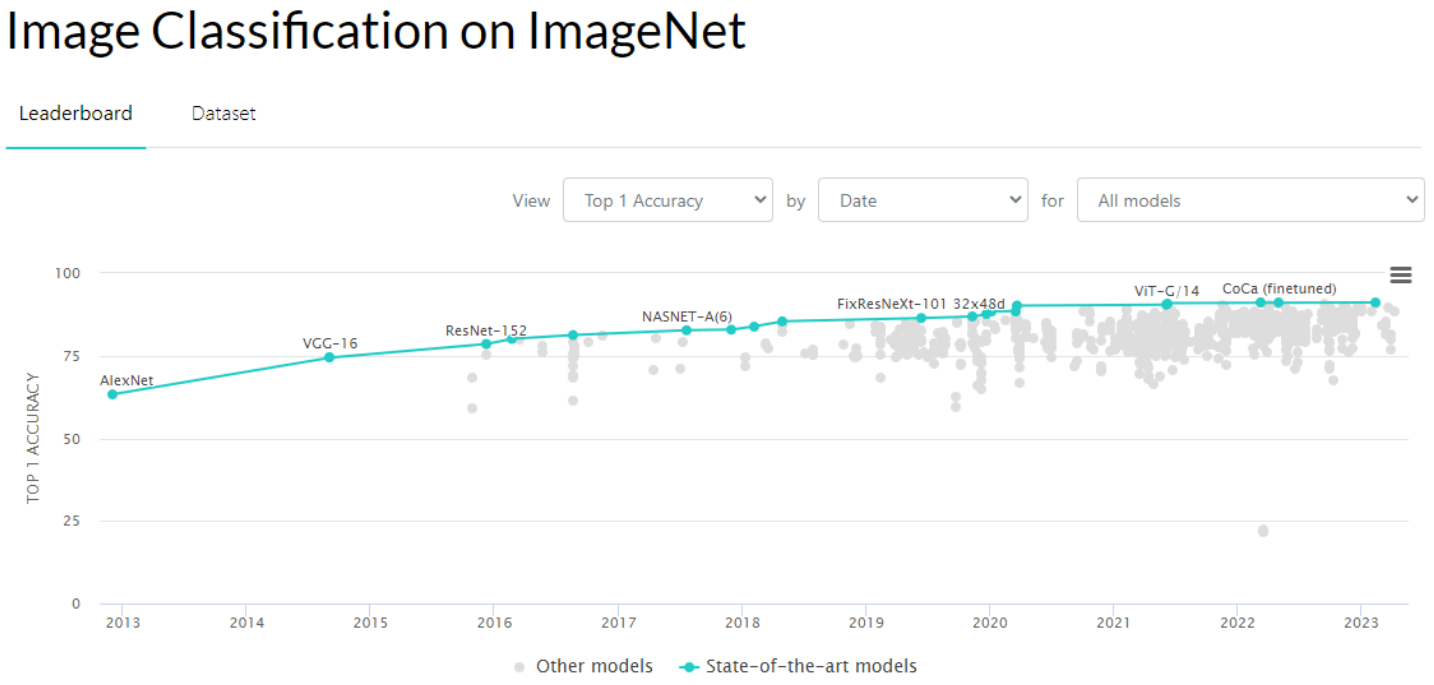


Model trained on task A

Decoder & loss for task B

Transfer Learning: ImageNet

- ImageNet has 14 million images, with 20,000 (!!!) classes
- There are many publicly available CNNs trained on ImageNet that have feature layers for transfer learning
- ResNet is a classic model that combines convolutions and residual connections




```
import torch
model = torch.hub.load('pytorch/vision:v0.10.0', 'resnet18', pretrained=True)
```

Other Dimensions of Convolution: Sequences & Videos

- We have only talked about 2D convolutions, but →
- If we have a sequence of scalar measurements (e.g. histogram), where nearby measurements should be related somehow, then we can use a 1D convolution
- If we have a sequence of vector measurements, then we can use a 2D convolution
- If we have a sequence of 2D measurements (e.g. video), then we can use a 3D convolution
- In principle, could go ever higher!

PyTorch

Convolution Layers

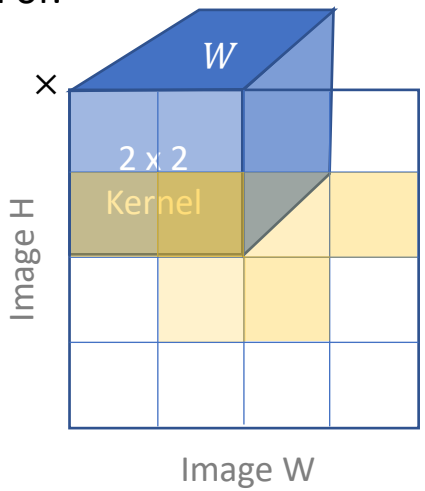
`nn.Conv1d`

`nn.Conv2d`

`nn.Conv3d`

Other Dimensions of Convolution: Sequences & Videos

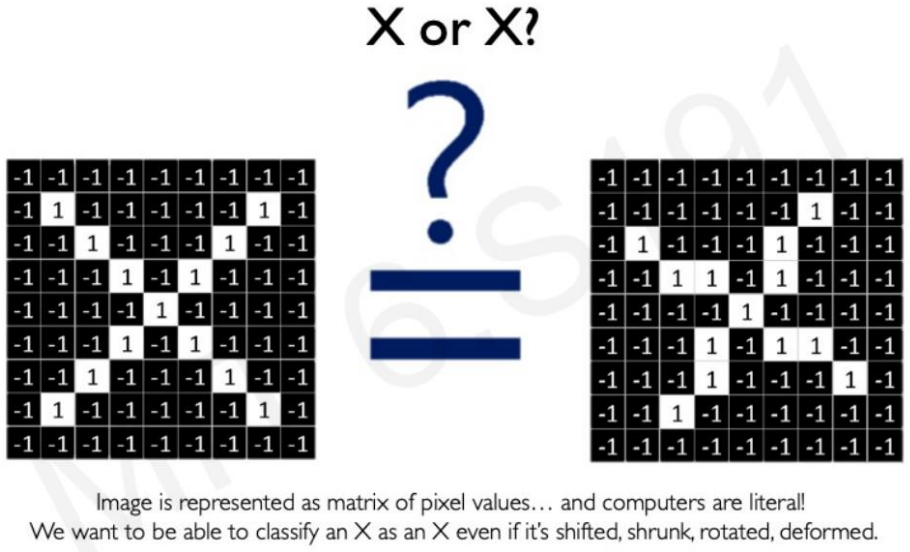
- We can perform a 3D convolution across $[t, x, y]$
- That is, instead of:

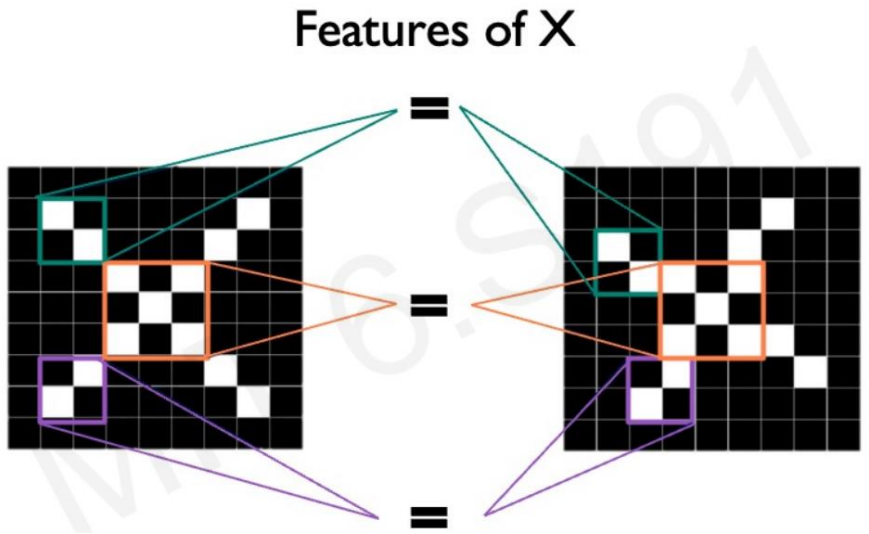


- We need to use a $t \times x \times y \times h$ tensor to multiply each time-pixel
- This might capture concepts that are not static, e.g. emotions…

Data Augmentation & Learned Symmetries

- We know we have translational invariance (the sliding kernel!)
- Do we have rotational invariance? Dilation invariance? *Lorentz invariance?*
- The MIT course certainly seems to think so…

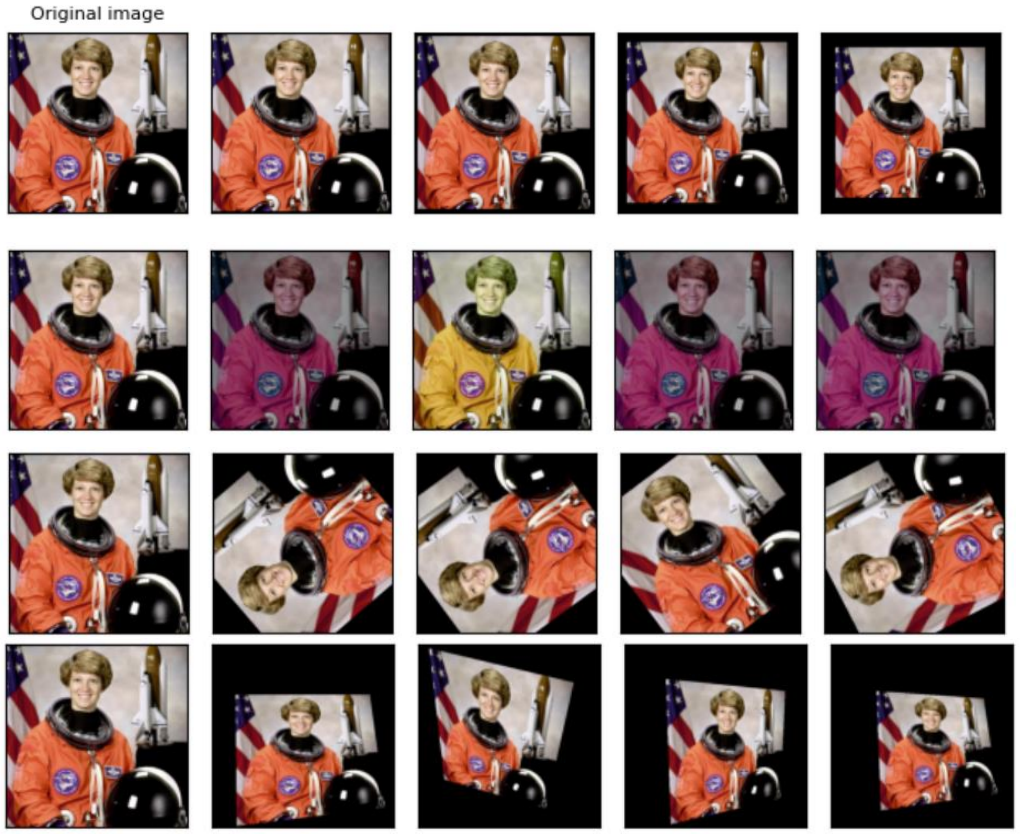




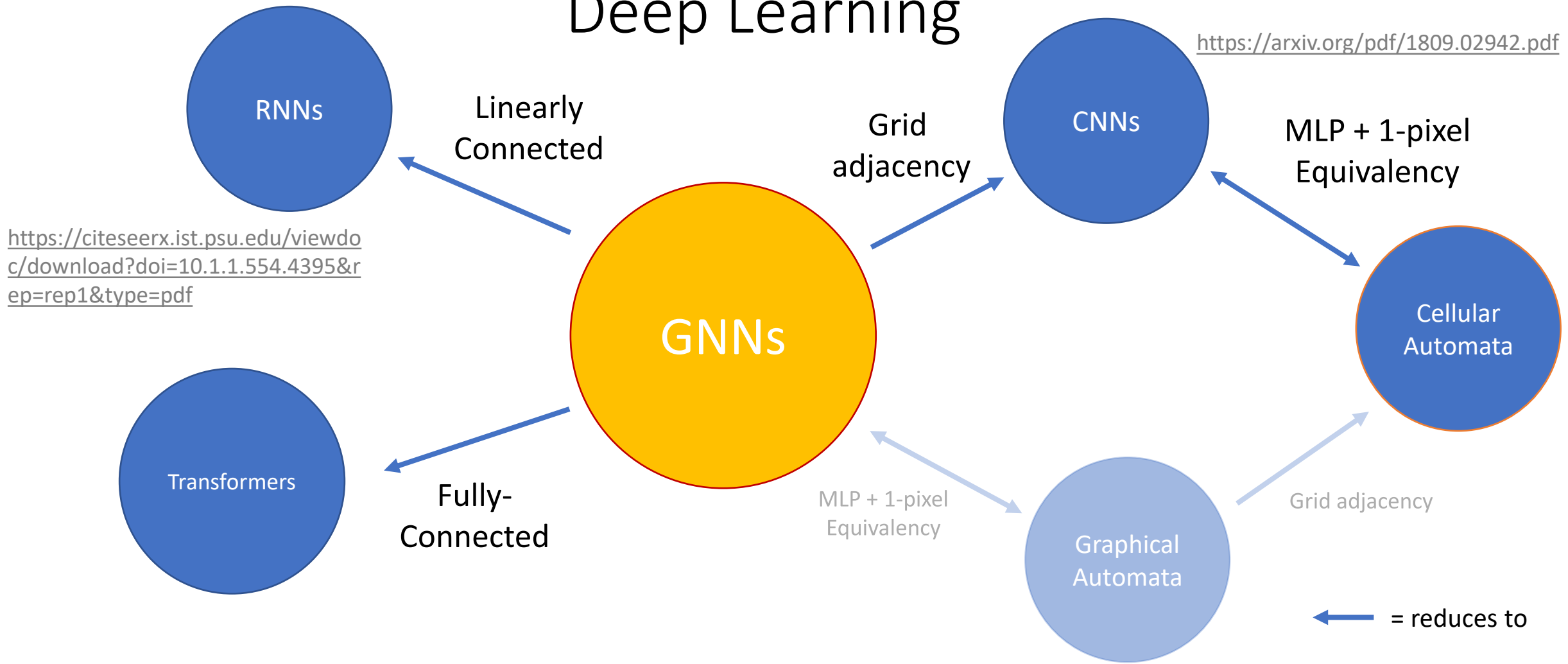
Data Augmentation & Learned Symmetries

- In fact, we don't have these other symmetries "hard-coded" in, like we do with translation
- If we want to include them, we need to learn them: Enter data augmentation
- Principle: In training, randomly transform image samples with rotations, noise, dilations, colour changes, etc.
- Practice: Use a `Transform` function

```
transformed_dataset = FaceLandmarksDataset(csv_file='data/faces/face_landmarks.csv',
                                           root_dir='data/faces/',
                                           transform=transforms.Compose([
                                               Rescale(256),
                                               RandomCrop(224),
                                               ToTensor()
                                           ]))
```



CNNs in The Landscape of Geometric Deep Learning



https://github.com/murnanedaniel/GNN-as-Transformer-as-GNN/blob/main/0-Transformer_vs_GNN_Annotated.ipynb
https://arxiv.org/pdf/2012.09699.pdf

Key Take-aways

- The convolution is a building block in almost any architecture applied to vision and video
- Convolution arithmetic is kind of a pain, but that's what `print(tensor.shape)` statements are for
- Convolutions can also be applied to sequential data, can learn symmetries in augmented data, and can segment images
- These days: Always start with a pre-trained model – it's a free lunch!
- The humble CNN proves the value of many ideas in ML: symmetry, hierarchy, inductive bias, data augmentation, generative models, etc.

CNN FAQ

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Where do the hidden channels come in?

- Recall our toy model

Image neighbourhood

Filter

$$\sum\left(\begin{bmatrix} 0.1 & 0.1 & 0.9 \\ 0.1 & 0.9 & 0.1 \\ 0.9 & 0.1 & 0.1 \end{bmatrix} \cdot \begin{bmatrix} 0.1 & 0.1 & 0.9 \\ 0.1 & 0.9 & 0.1 \\ 0.9 & 0.1 & 0.1 \end{bmatrix}\right) = \sum\left(\begin{bmatrix} 0.01 & 0.01 & 0.81 \\ 0.01 & 0.81 & 0.01 \\ 0.81 & 0.01 & 0.01 \end{bmatrix}\right) = 2.43$$

Where do the hidden channels come in?

- Recall our toy model

Image neighbourhood Filter

$$\sum\left(\begin{array}{|c|c|c|}\hline 0.1 & 0.1 & 0.9 \\ \hline 0.1 & 0.9 & 0.1 \\ \hline 0.9 & 0.1 & 0.1 \\ \hline\end{array} \cdot \begin{array}{|c|c|c|}\hline 0.1 & 0.1 & 0.9 \\ \hline 0.1 & 0.9 & 0.1 \\ \hline 0.9 & 0.1 & 0.1 \\ \hline\end{array}\right) = \sum\left(\begin{array}{|c|c|c|}\hline 0.01 & 0.01 & 0.81 \\ \hline 0.01 & 0.81 & 0.01 \\ \hline 0.81 & 0.01 & 0.01 \\ \hline\end{array}\right) = 2.43$$

- The window ("kernel size") is 3x3, but the input shape (in each pixel) is just one number, and the output shape (for each pixel) is just one number

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Where do the hidden channels come in?

- Recall our toy model

Image neighbourhood Filter

$$\sum_{ij}\left(\begin{array}{ccc} 0.1 & 0.1 & 0.9 \\ 0.1 & 0.9 & 0.1 \\ 0.9 & 0.1 & 0.1 \end{array} \cdot \begin{array}{ccc} 0.1 & 0.1 & 0.9 \\ 0.1 & 0.9 & 0.1 \\ 0.9 & 0.1 & 0.1 \end{array}\right) = \sum_{ij}\left(\begin{array}{ccc} 0.01 & 0.01 & 0.81 \\ 0.01 & 0.81 & 0.01 \\ 0.81 & 0.01 & 0.01 \end{array}\right) = 2.43$$

- The window ("kernel size") is 3x3, but the input shape (in each pixel) is just one number, and the output shape (in each pixel) is just one number

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Where do the hidden channels come in?

- To make a CNN more powerful, we need to be able to take in any number of features (e.g. color) and we want *many* filter channels in a convolution. That is, we need input length and output length
- Our general convolution is thus

$$\sum_{ij} x_{ij}^{M} W_{ij}^{MN} = \sum_{ij} m_{ij}^{N} = h^{N}$$

where x_{ij}^{M} is the input window, W_{ij}^{MN} is the learnable kernel with the ij^{th} entry an $M \times N$ matrix. M is input shape (e.g. 3 colors), N is output shape, i is the window rows, j is the window columns

When do I do max pooling?

- Max pooling and the convolutional kernel are **completely separate**, and we don't even need to do pooling
- They both use a "window" system, of looking at neighborhoods of pixels, but the window size of the kernel does not have to be the same size as the max pooling window size
- **Max** pooling is just one choice of pooling. Any kind of aggregation will work: mean, sum, min, or even more exotic kinds like variance

But does the pooling reduce the image size?

- If we pad our image on the border, and slide the kernel or pooling window one pixel at a time, **our output array will be the same shape as the input array:** the kernel and pooling do not inherently down-sample an image
- It is only when we increase the stride (the number of pixels we move the window each time) that the output shape gets reduced
- Either kernel and/or pooling use windows, so they can both use stride, and thus can both be used to down-sample an image. Which one you use to down-sample is part intuition, part trial-and-error