S&DS 365 / 665

Intermediate Machine Learning

Convolutional Neural Networks

February 4

Yale

Version of 2026/02/04 at 00:45

Reminders

- Assignment 1 due next Thursday (February 12)
- Assignment 2 posted next Wednesday
- Quiz 2 out, due this Friday

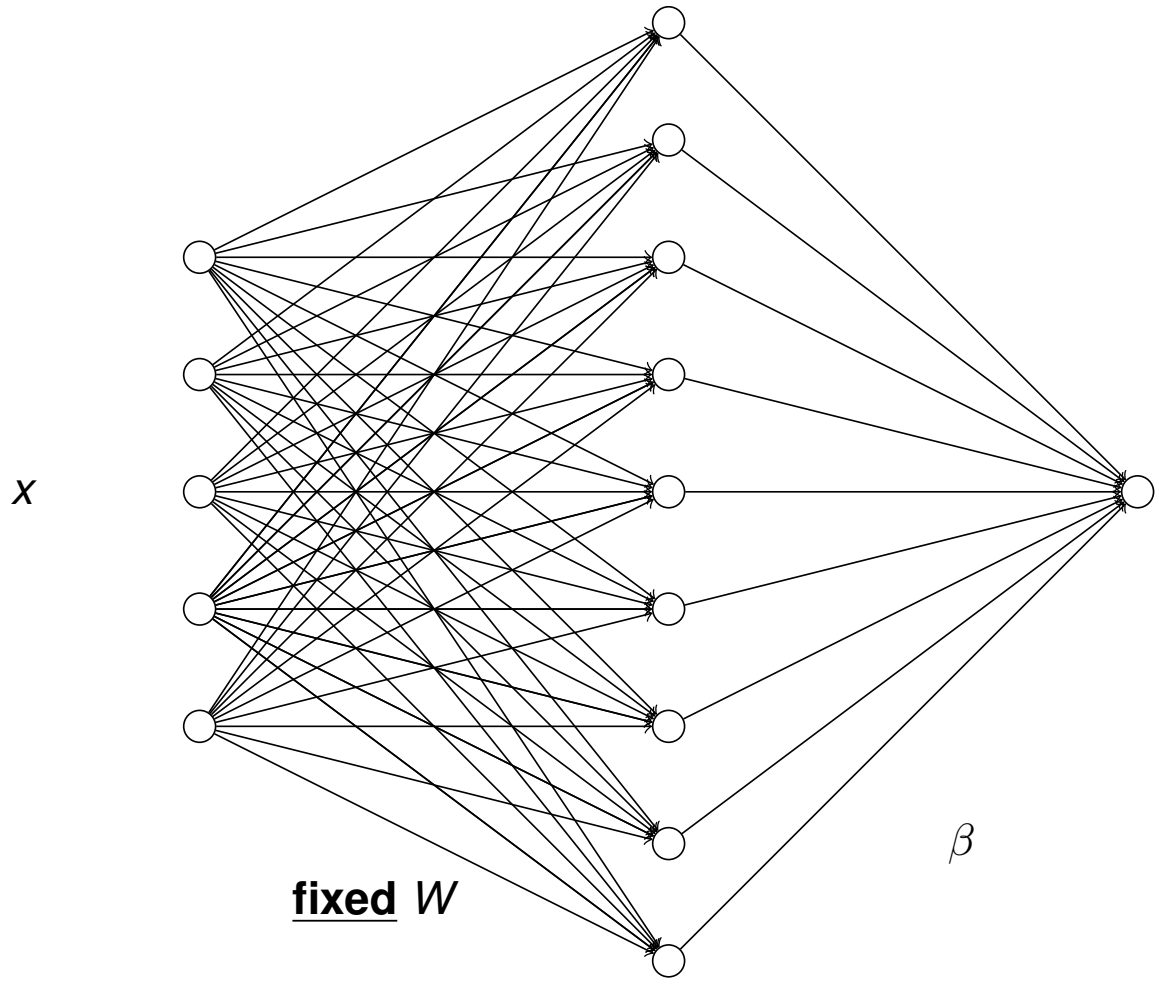
Random features

Fix the weights at their random initializations, for all but the last layer

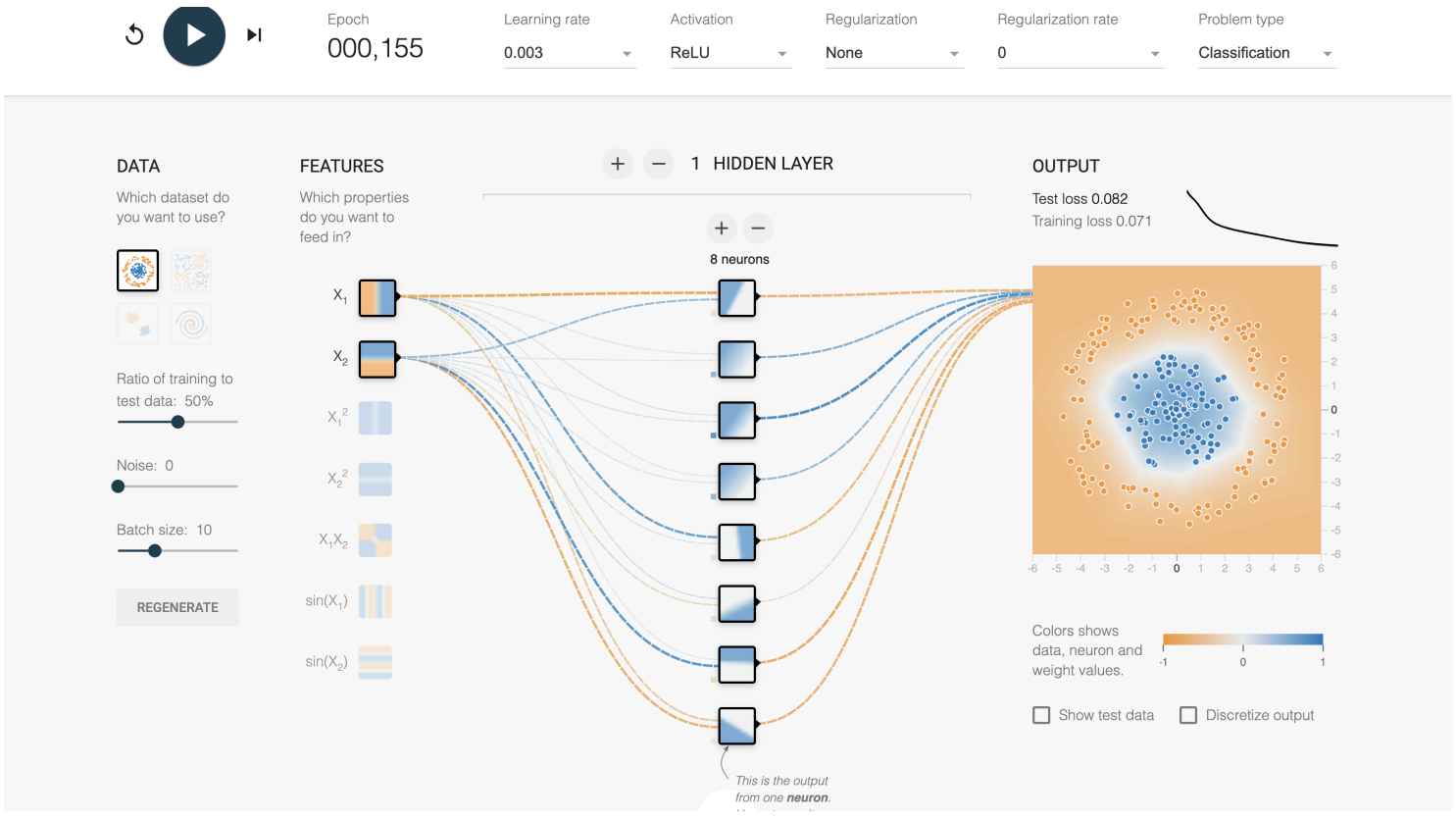
Just train the parameters β

This is called the *random features model*. It's a linear model with random covariates obtained from the hidden neurons.

Random features model



Demo



https://playground.tensorflow.org/

What's going on?

- These models are curiously robust to overfitting
- Why is this?
- Some insight: Kernels and double descent

OLS and minimal norm solution

OLS: $p < n$

$$\widehat{\beta} = (\mathbb{X}^T \mathbb{X})^{-1} \mathbb{X}^T Y$$

Minimal norm solution: $p > n$:

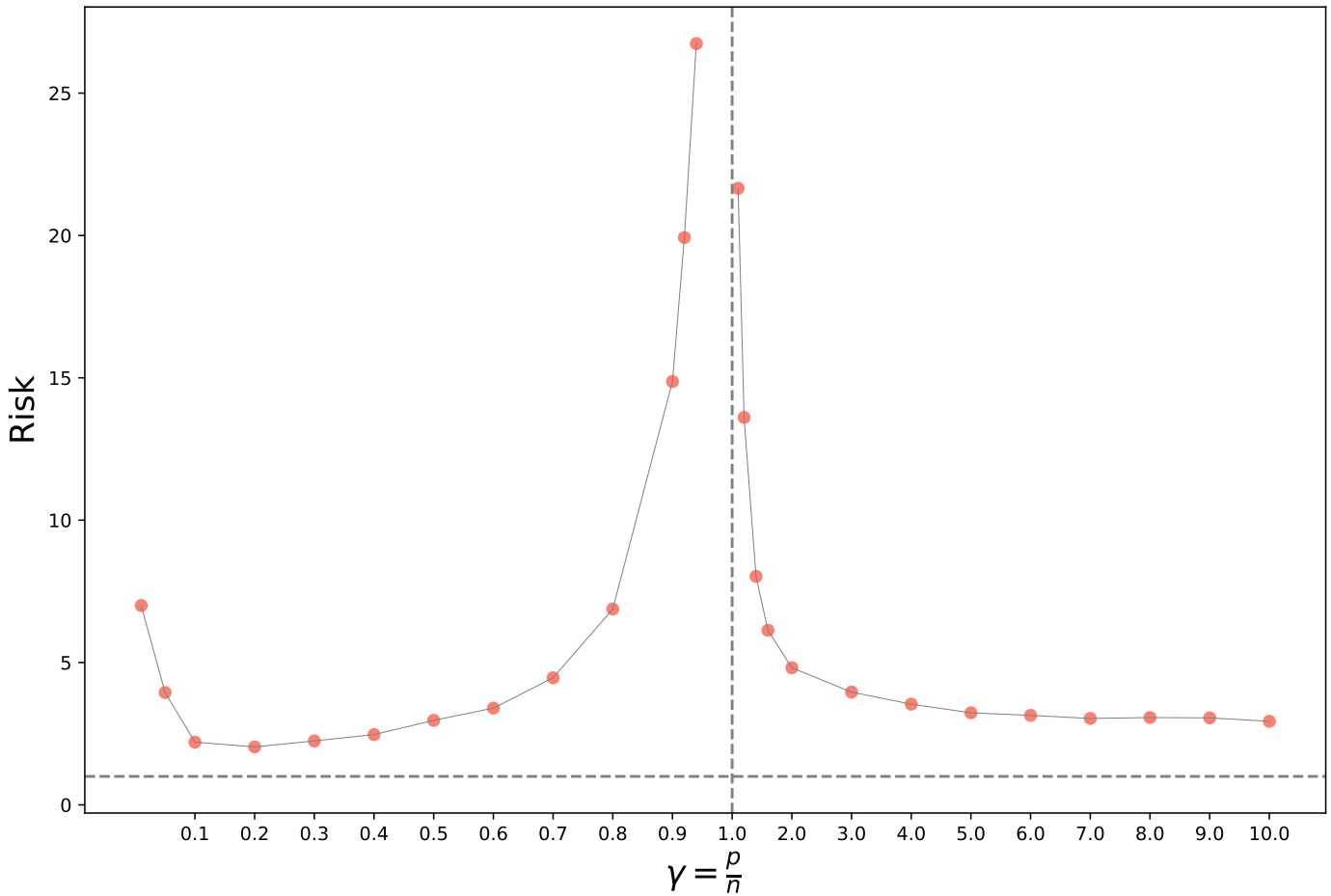
$$\widehat{\beta}_{\text{mn}} = \mathbb{X}^T (\mathbb{X}\mathbb{X}^T)^{-1} Y$$

“Ridgeless regression”

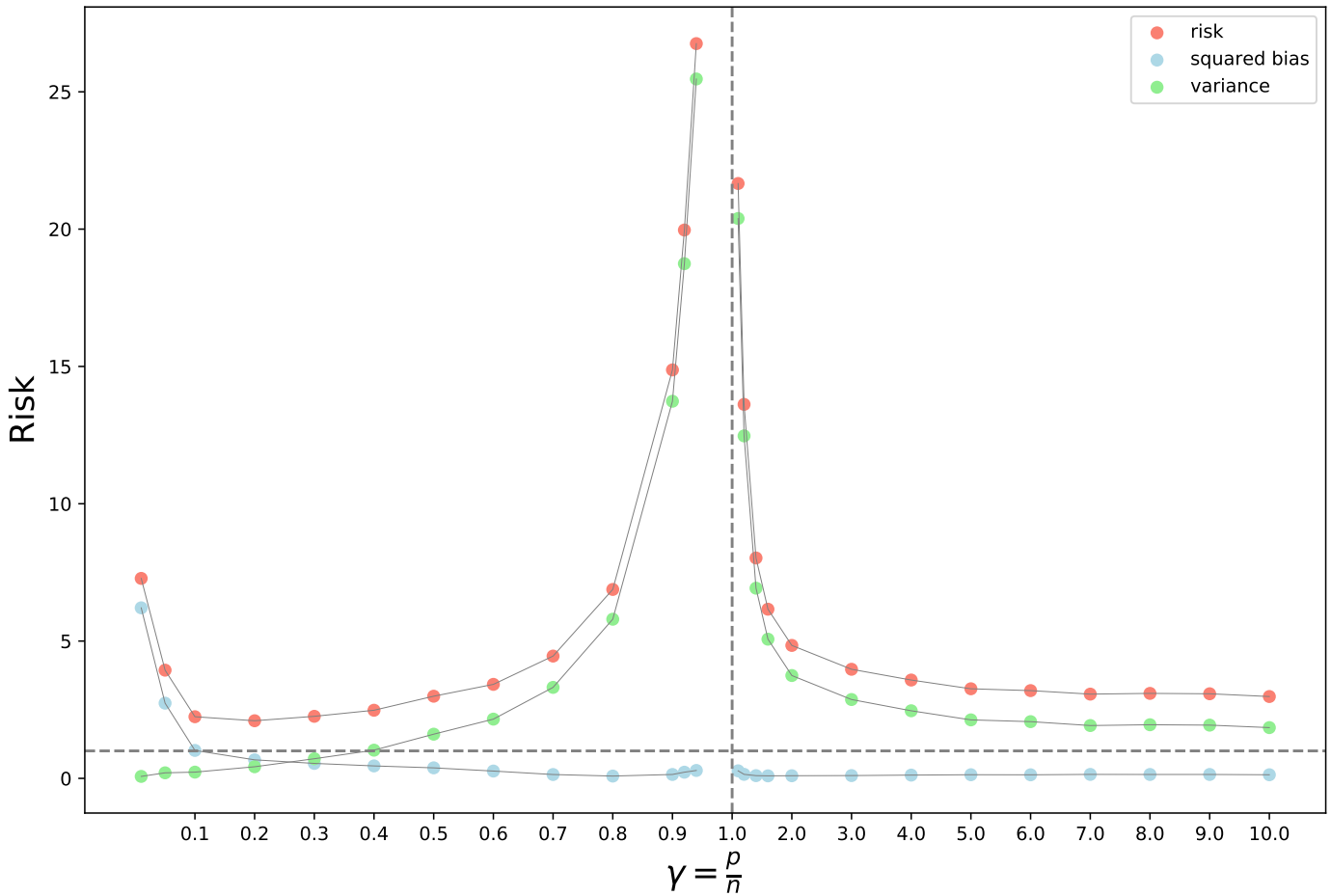
As λ decreases to zero, the ridge regression estimate:

- Converges to OLS in the “classical regime” $\gamma < 1$
- Converges to $\widehat{\beta}_{\text{mn}}$ in “overparameterized regime” $\gamma > 1$

Double descent



Double descent



Neural tangent kernel

The *neural tangent kernel (NTK)* has been useful in understanding the performance of large neural networks, and the dynamics of stochastic gradient descent training.

Neural tangent kernels (NTK)

A neural network is a parameterized function $f_\theta(x) \equiv f(x;\theta)$

We then define a *feature map*

$$x \mapsto \varphi(x) = \nabla_\theta f(x;\theta_0) = \begin{pmatrix} \dfrac{\partial f(x;\theta_0)}{\partial \theta_1} \\ \dfrac{\partial f(x;\theta_0)}{\partial \theta_2} \\ \vdots \\ \dfrac{\partial f(x;\theta_0)}{\partial \theta_p} \end{pmatrix}$$

This defines a Mercer kernel

$$K(x,x') = \varphi(x)^T \varphi(x') = \nabla_\theta f(x;\theta_0)^T \nabla_\theta f(x';\theta_0)$$

Neural tangent kernels (NTK)

This defines a Mercer kernel

$$K(x, x') = \varphi(x)^T \varphi(x') = \nabla_\theta f(x; \theta_0)^T \nabla_\theta f(x'; \theta_0)$$

What is the NTK for the random features model?

Neural tangent kernels (NTK)

The NTK for the random features model is

$$K(x, x') = h(x)^T h(x')$$

Neural tangent kernels (NTK)

Conversely, a deep neural network with a large number of neurons is approximately equivalent to a random features model!

Why?

NTK and SGD

- The dynamics of stochastic gradient descent for deep networks has been studied
- Upshot: As the number of neurons in the layers grows, the parameters in the network change very little during training, even though the training error quickly decreases to zero

NTK and random features

And, if the parameters only change by a small amount, a linear approximation can be used:

Let $\theta = \theta_0 + \beta$. Then

$$\begin{aligned} f(x, \theta) &\approx f(x, \theta_0) + \nabla_\theta f(x, \theta_0)^T \beta \\ &= \nabla_\theta f(x, \theta_0)^T \beta \end{aligned}$$

assuming that $f(x, \theta_0) = 0$

NTK and random features

This tells us that the neural network is (approximately) equivalent to a random features model!

The random features are $h(x) \equiv \nabla_\theta f(x, \theta_0)$

Note: These are *not* the neurons in the last layer of the network.

Summary

- Neural nets are layered linear models with nonlinearities added
- Trained using stochastic gradient descent with backprop
- A surprise in the risk properties: Double descent
- Kernel connection: NTK

Outline for CNNs

- Mechanics of convolutional networks
- Filters and pooling and flattening
- Example: Brain scans of mice
- Assignment 2: Convnets for MNIST
- Other examples

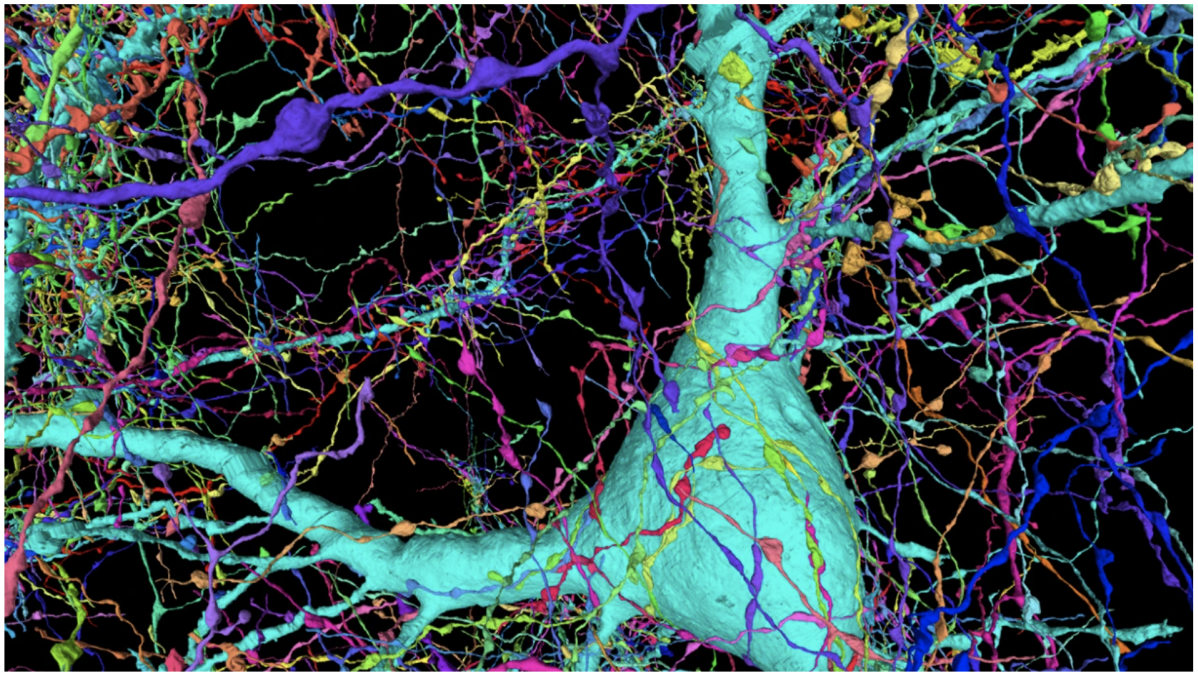
Deep learning and image analysis

TECHNOLOGY FEATURE | 20 September 2022

Five ways deep learning has transformed image analysis

From connectomics to behavioural biology, artificial intelligence is making it faster and easier to extract information from images.

Sandeep Ravindran



Neurons (teal) can have thousands of connections to other cells. Credit: Lichtman Lab, Harvard/Jain Group, Google

Notes

- Animations from tutorial “Let’s Code Convolutional Neural Network in plain NumPy: Mysteries of Neural Networks” by Piotr Skalski
- `https://towardsdatascience.com/lets-code-convolutional-neural-network-in-plain-numpy-ce48e732f5d5`
- To see the animations, view this pdf using Adobe Acrobat

Convolution

Mathematically, a *convolution* sweeps a function $K(u)$ over the values of another function f:

Continuous:

$$K \star f(x) = \int K(x-u)\, f(u)\, du$$

- Same operation we saw with smoothing kernels
- If K is a Gaussian bump, this blurs or smooths out the values.
- For CNNs, K will have small support, encode features of the input

---

We've seen this before...

Convolution

Mathematically, a *convolution* sweeps a function $K(u)$ over the values of another function f:

Discrete:

$$K \star f(x_j) = \sum_i K(x_j - x_i)\, f(x_i)$$

- Same operation we saw with smoothing kernels
- If K is a Gaussian bump, this blurs or smooths out the values.
- For CNNs, K will have small support, encode features of the input

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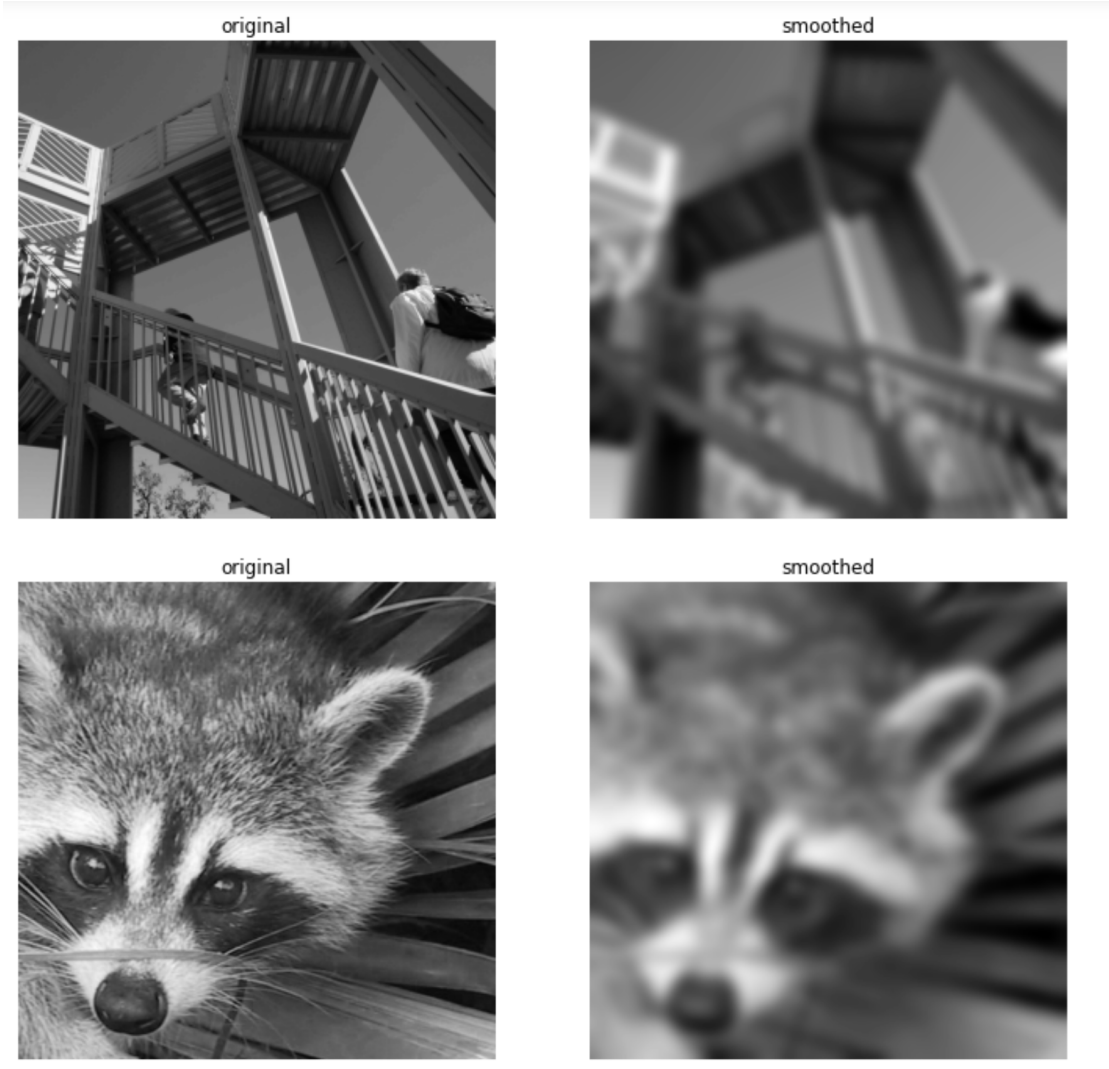
We've seen this before...

Examples

`convolve_demo.ipynb` gives examples



Principles

Some of the ideas behind convolutional neural networks (CNNs):

1. Parameter tying: Let neurons share the same weights
2. Kernel learning: The kernels should not be fixed, but rather *learned* from the data
3. Invariance: Doesn't matter where features are located

CNNs are most commonly used for images; can be used whenever data have some kind of spatial structure (e.g. DNA)

Tensors

A tensor is a multidimensional array*—like a matrix, but with more than just a pair of indices for row and column

In Python, tensors are represented in `numpy` using the type `numpy.ndarray` ("*n*-dimensional array")

TensorFlow also has built-in types to represent tensors

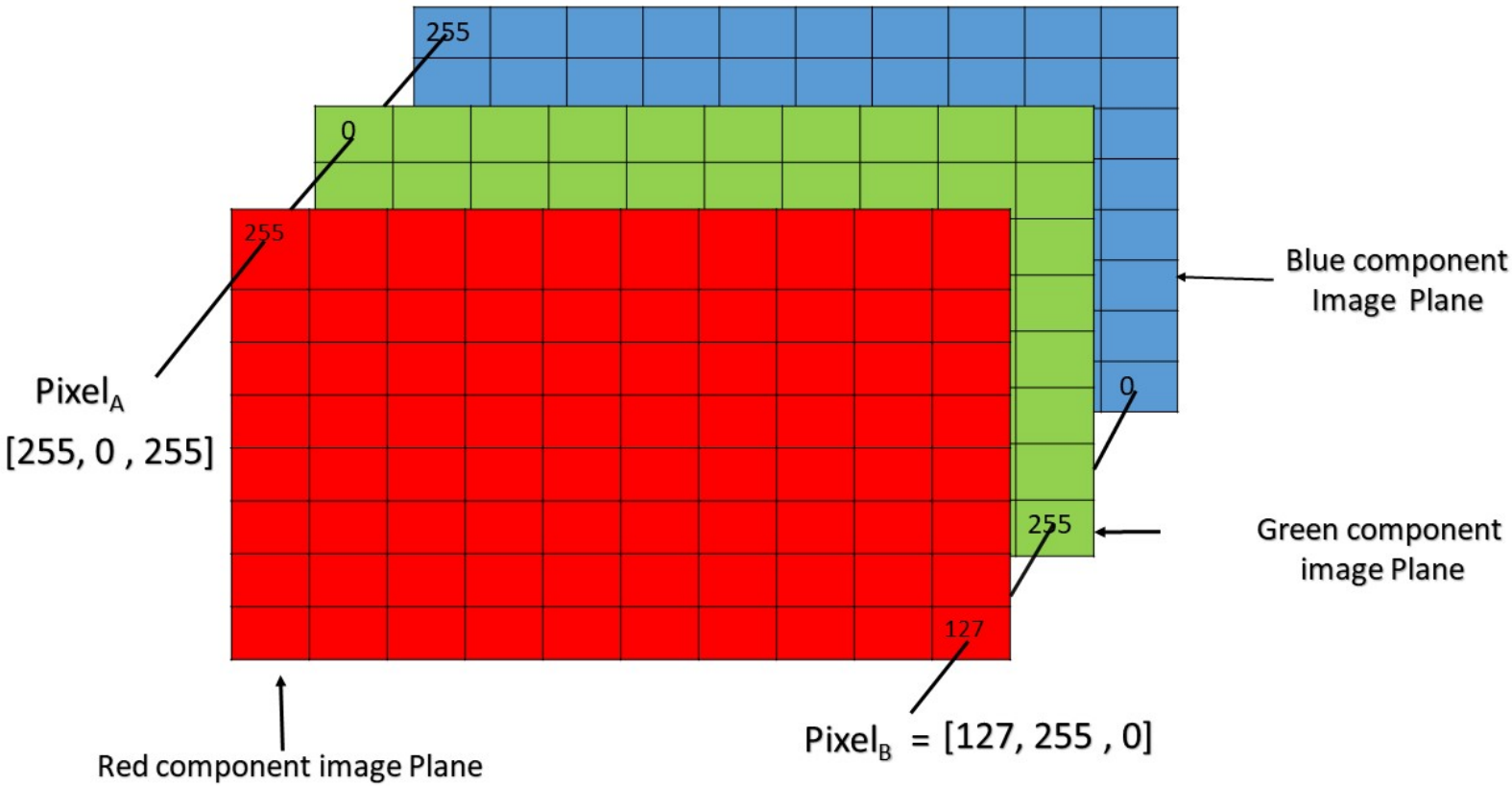
* In mathematics, there is a little more structure to tensors.

Tensors

```
x = np.array(np.arange(24)).reshape(2,3,4)
print(x)
print(x[:,:,0])
```

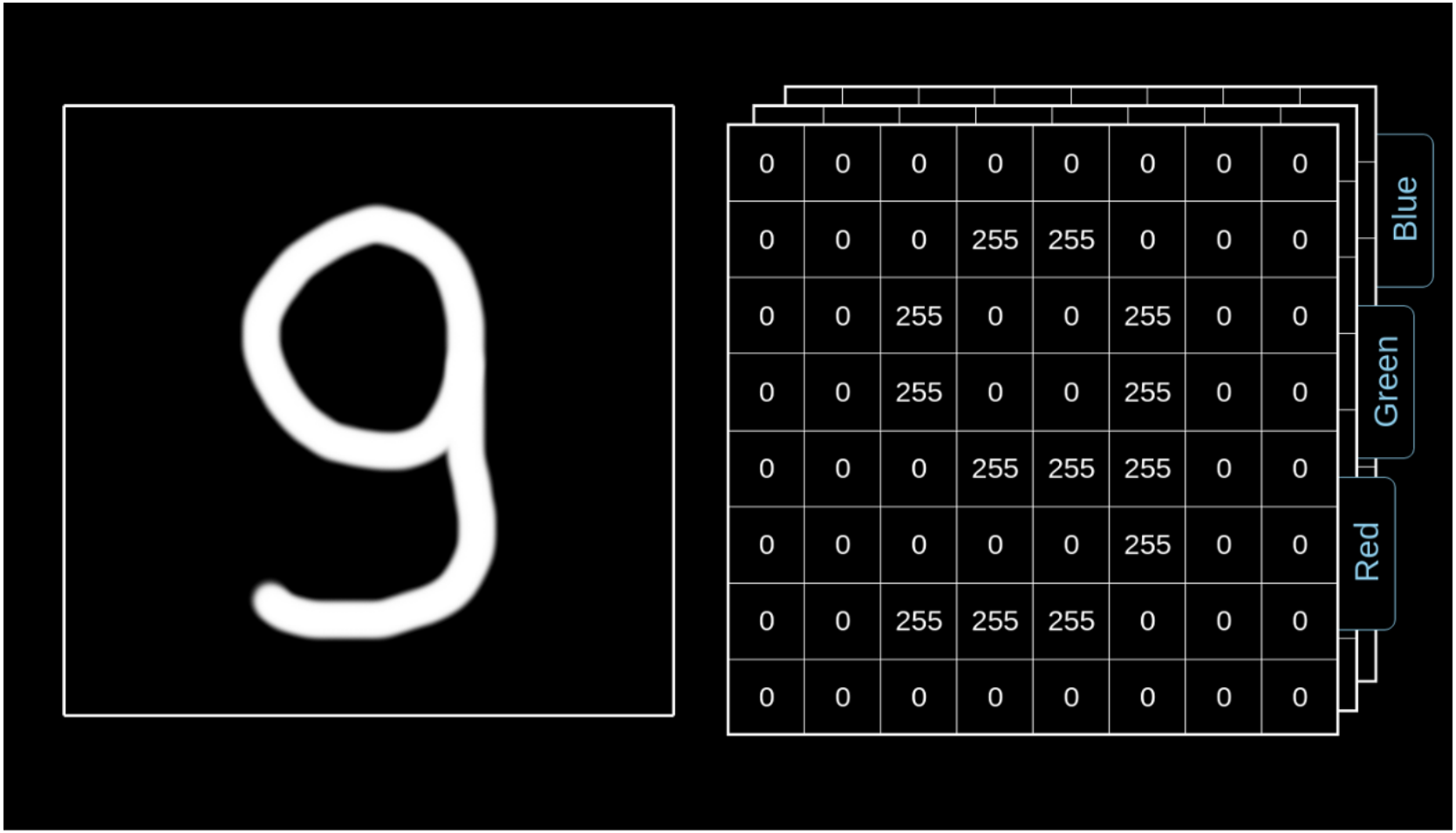
```
[[[ 0  1  2  3]
  [ 4  5  6  7]
  [ 8  9 10 11]]

 [[12 13 14 15]
  [16 17 18 19]
  [20 21 22 23]]]

[[ 0  4  8]
 [12 16 20]]
```

Images as tensors: Channels



Pixel of an RGB image are formed from the corresponding pixel of the three component images

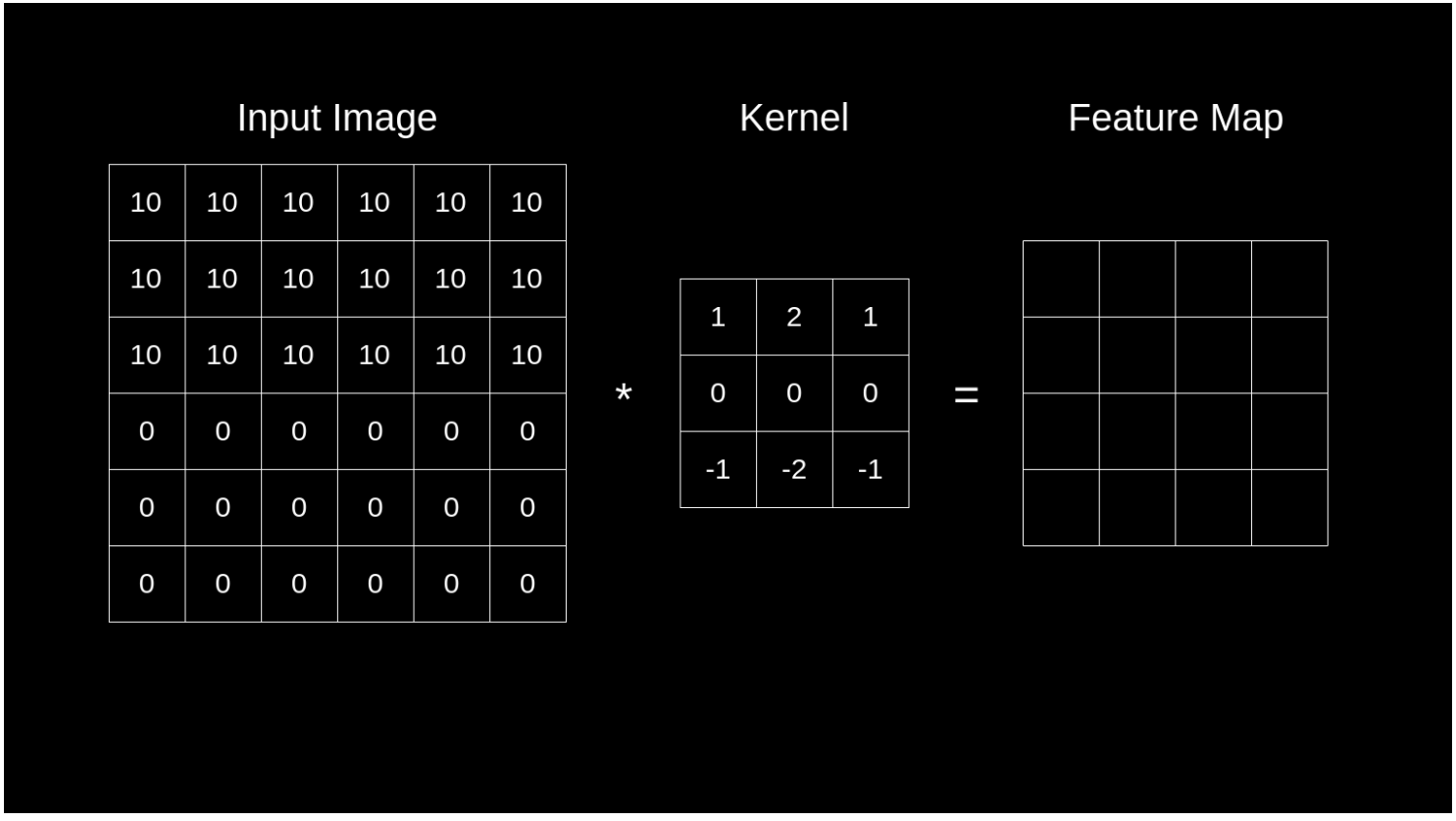
Images as tensors: Channels



Convolutional layer

- In a convolutional layer, a set of *kernels* are “swept over” or convolved over the input
- The kernels are themselves tensors with entries that are trained weights
- The output after convolving the kernel over the input tensor is called a *feature map*
- A convolutional layer is equivalent to a standard fully connected layer, but where the weights are constrained to be sparse and shared (or “tied”) across different neurons

Convolutional layer



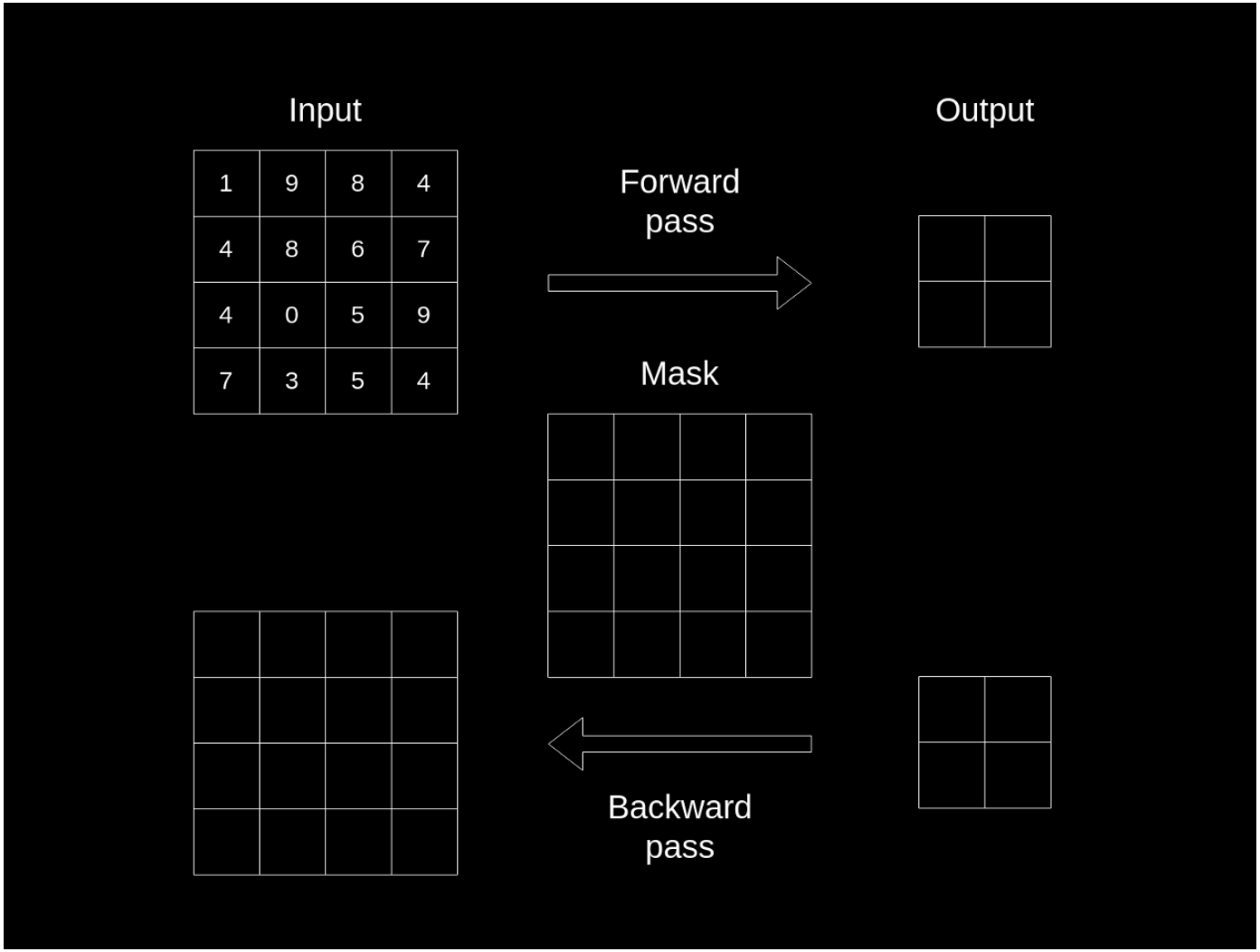
Adding a nonlinearity

- So far everything is linear
- An activation function is used to add a nonlinearity
- Each filter also has an intercept (a single number), added before applying the activation function
- The same activation function is used for all of the kernels in a layer

Pooling

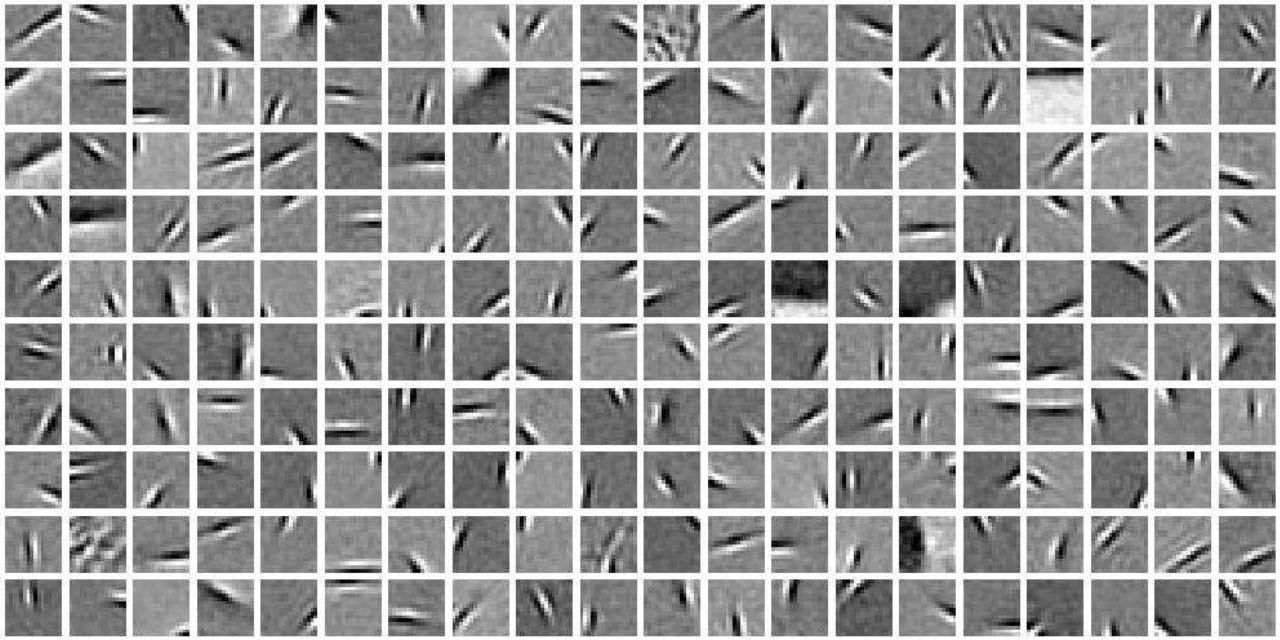
- The point of a convolutional layer is to learn “features” of the input
- We don’t care too much exactly where they appear
- *Pooling* the feature map reduces the dimension and encodes the approximate location of features
- Two common types: max pooling and average pooling
- When using max pooling, to update weights in backpropagation, the locations of the features can be noted

Pooling


Input
Output
1 9 8 4
4 8 6 7
4 0 5 9
7 3 5 4
Forward pass
Mask
Backward pass

How features are built up

- Filters in the first layer may look like this:



- Filters in second layer can then capture more complex shapes

How features are built up

- Each kernel has a weight for each spatial position and channel
- Features from previous layers are recorded in the channels
- So the next layer can have a kernel that says

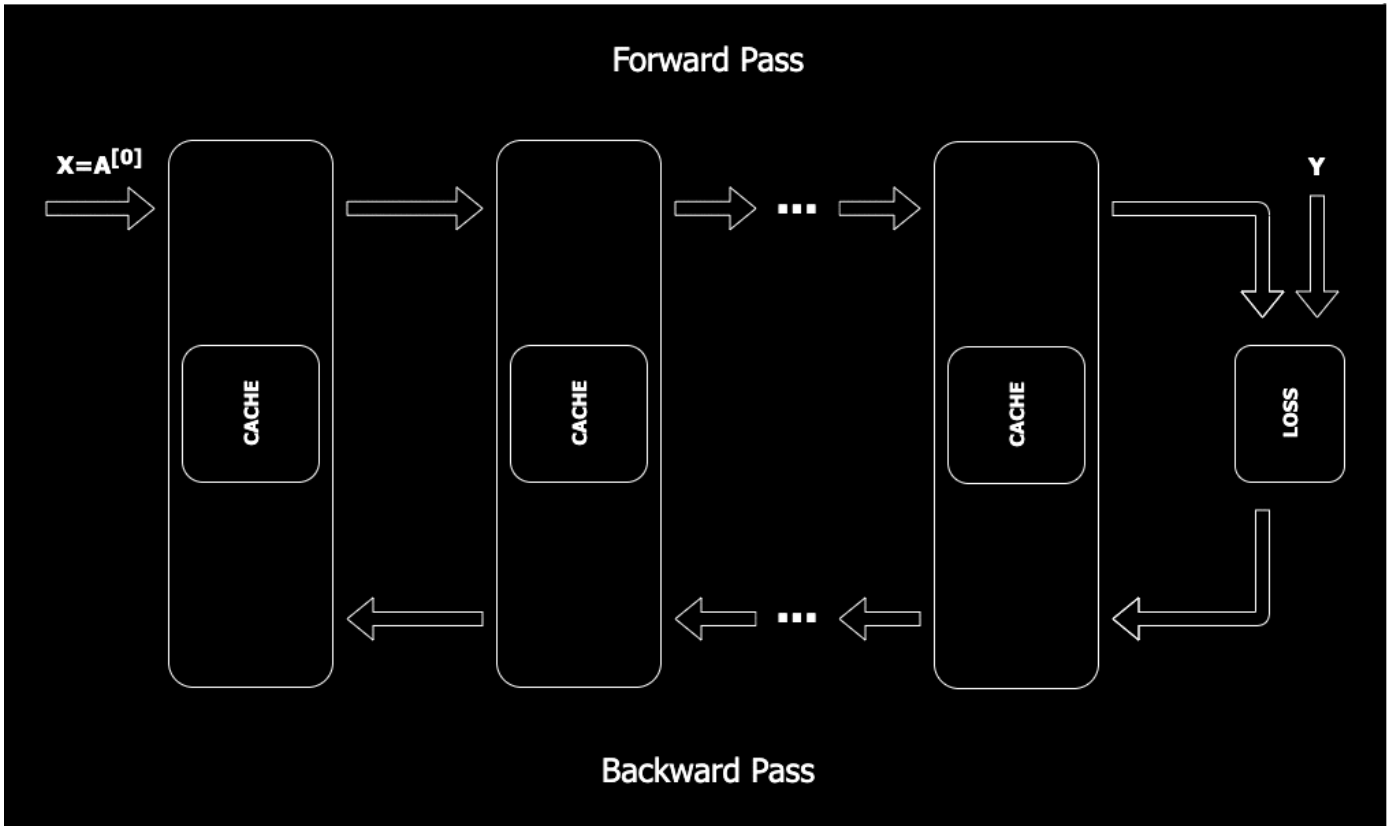
  “Oh, I see that feature 17 (a horizontal edge) from the previous layer is active in position (1,1), feature 42 (a vertical edge) is active in position (1,2)” to capture “corners”

- This enables compound features to be built up

Pooling and backpropagation

- A forward pass through the layers is used to make predictions, and store intermediate results to be used later
- A backward pass propagates the errors in prediction back through the layers, and computes changes to the weights for the gradient step

Forward and backward passes



Applying kernels across channels

- Each kernel (filter) has the same number of channels as the input tensor
- A kernel is applied at each location by multiplying component-wise and then summing
- The feature map for each kernel is then one channel in the output tensor
- So, the number of channels in the output is the number of kernels

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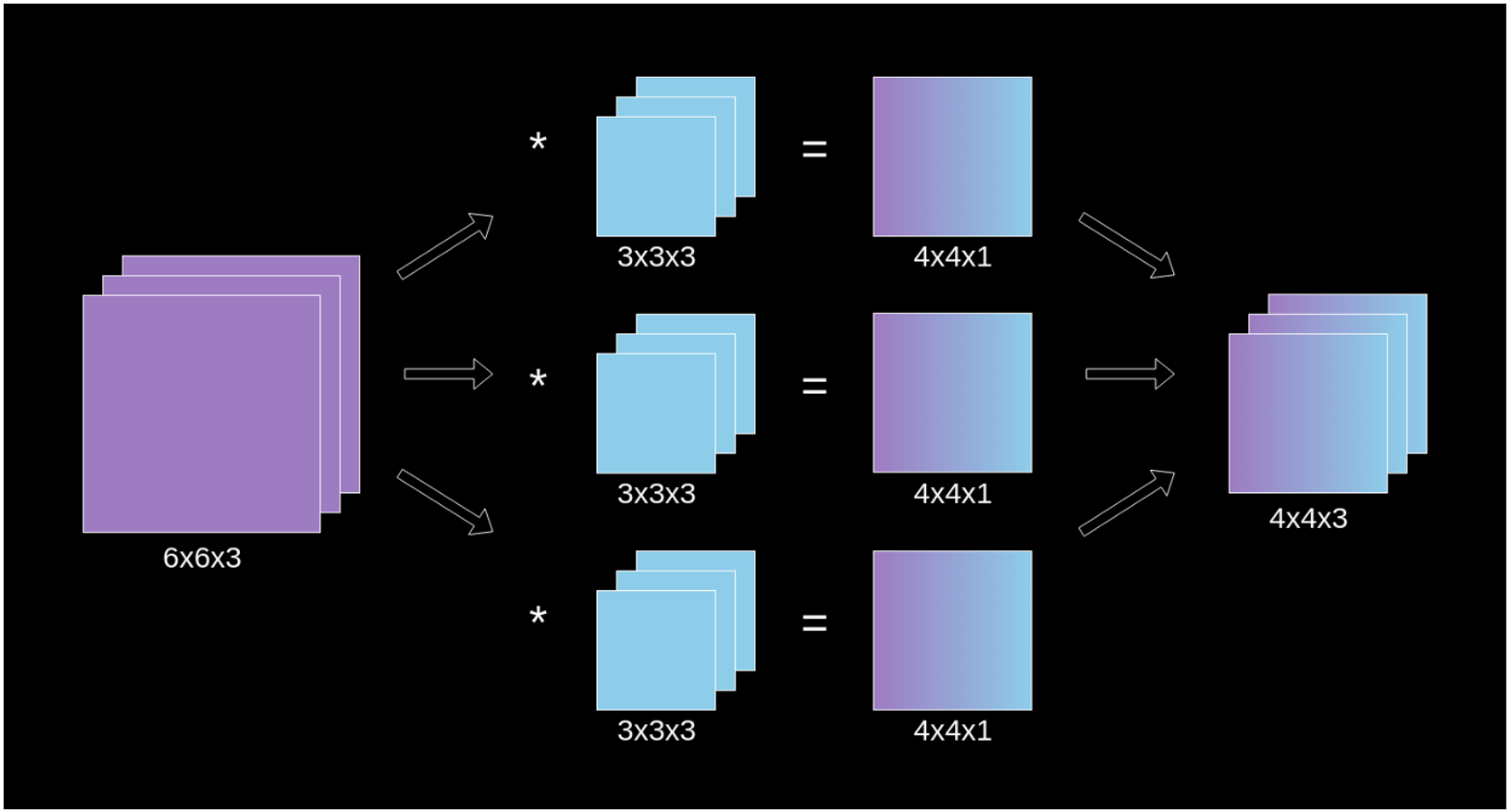
Filter is synonomous with kernel in today's discussion

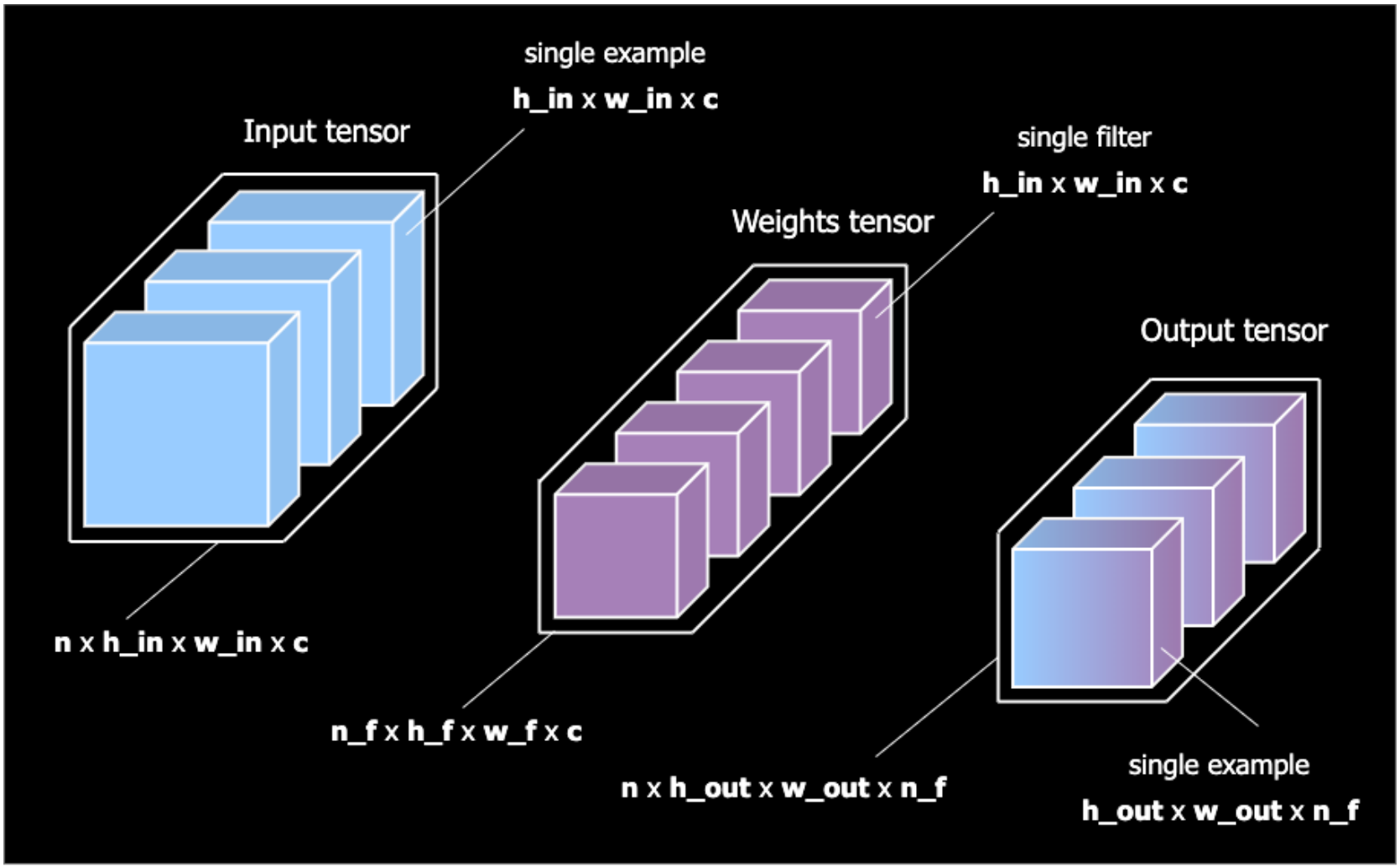
Applying kernels across channels



Convolutional layer: Tensor shapes

- Data points are processed in “mini-batches” of n items
- The first dimension of the input and output tensors at each layer is always n
- The last dimension of the output is the number of kernels (filters)

Convolutional layer: Tensor shapes

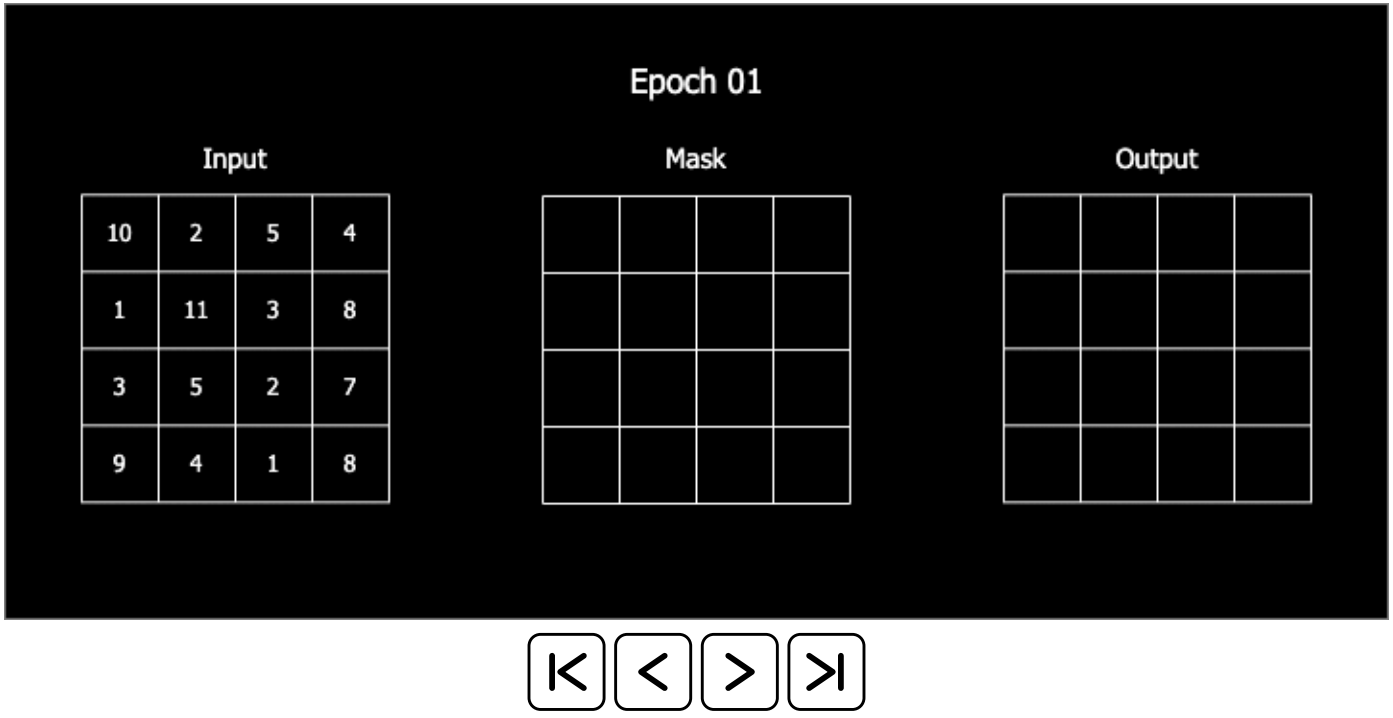


Dropout

- "Dropout" is a type of regularization that is easy to incorporate
- Idea: Randomly zero out entries in a tensor
- Helps guard against overfitting
- Usual form:
  - Independently zero out each entry with probability ε
  - Divide by $(1 - \varepsilon)$

Equivalent to a type of ridge penalization: https://arxiv.org/abs/1307.1493, and approximate Bayesian averaging: http://proceedings.mlr.press/v48/gal16.pdf

Dropout

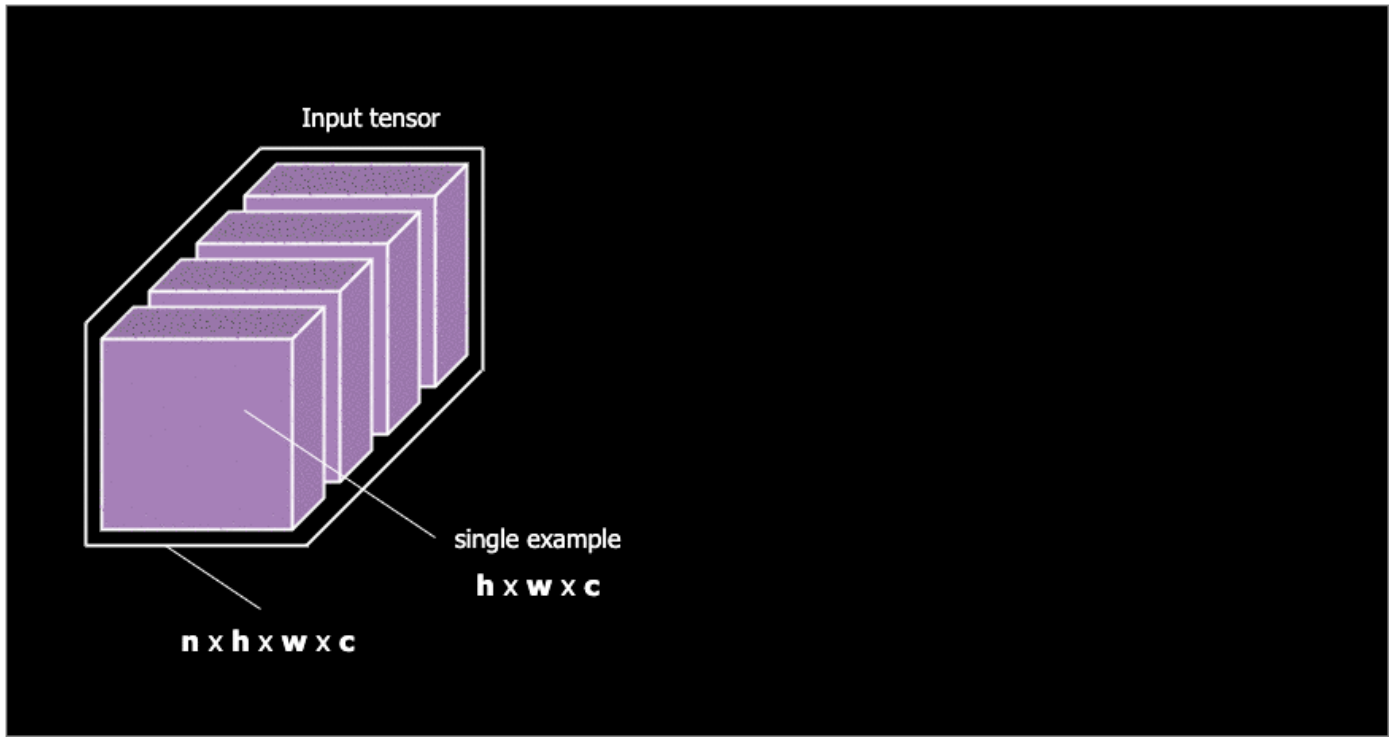


This illustrates something a bit different than the standard dropout

Flattening

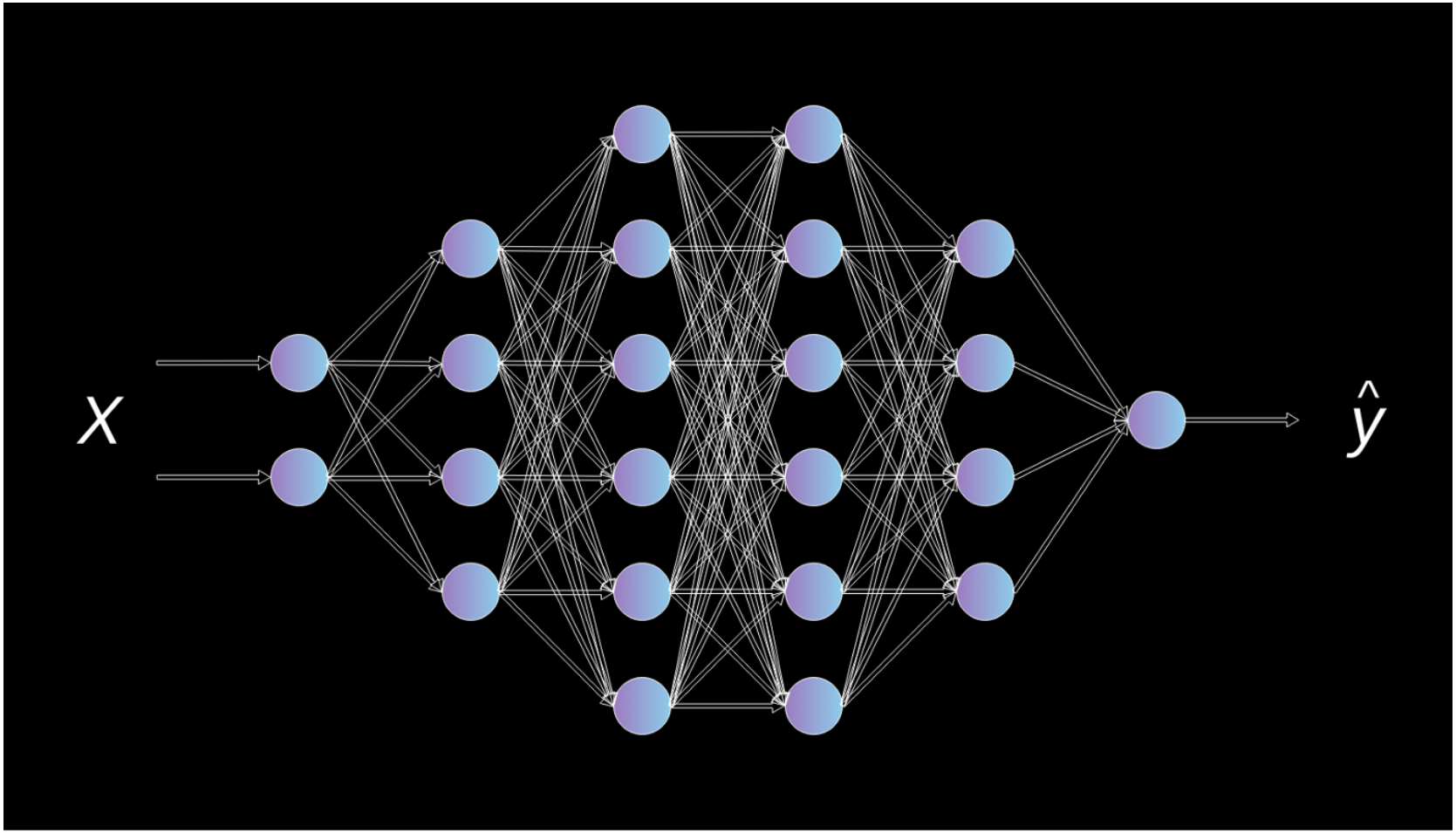
- After one or more convolutional layers, we usually add “dense” layers
- These are the standard types of layers in a neural network, with each output neuron connected to each input neuron, with a tuneable weight
- In CNNs, the convolutional layers build up a set of “features” and then these features are used to make a prediction

Flattening

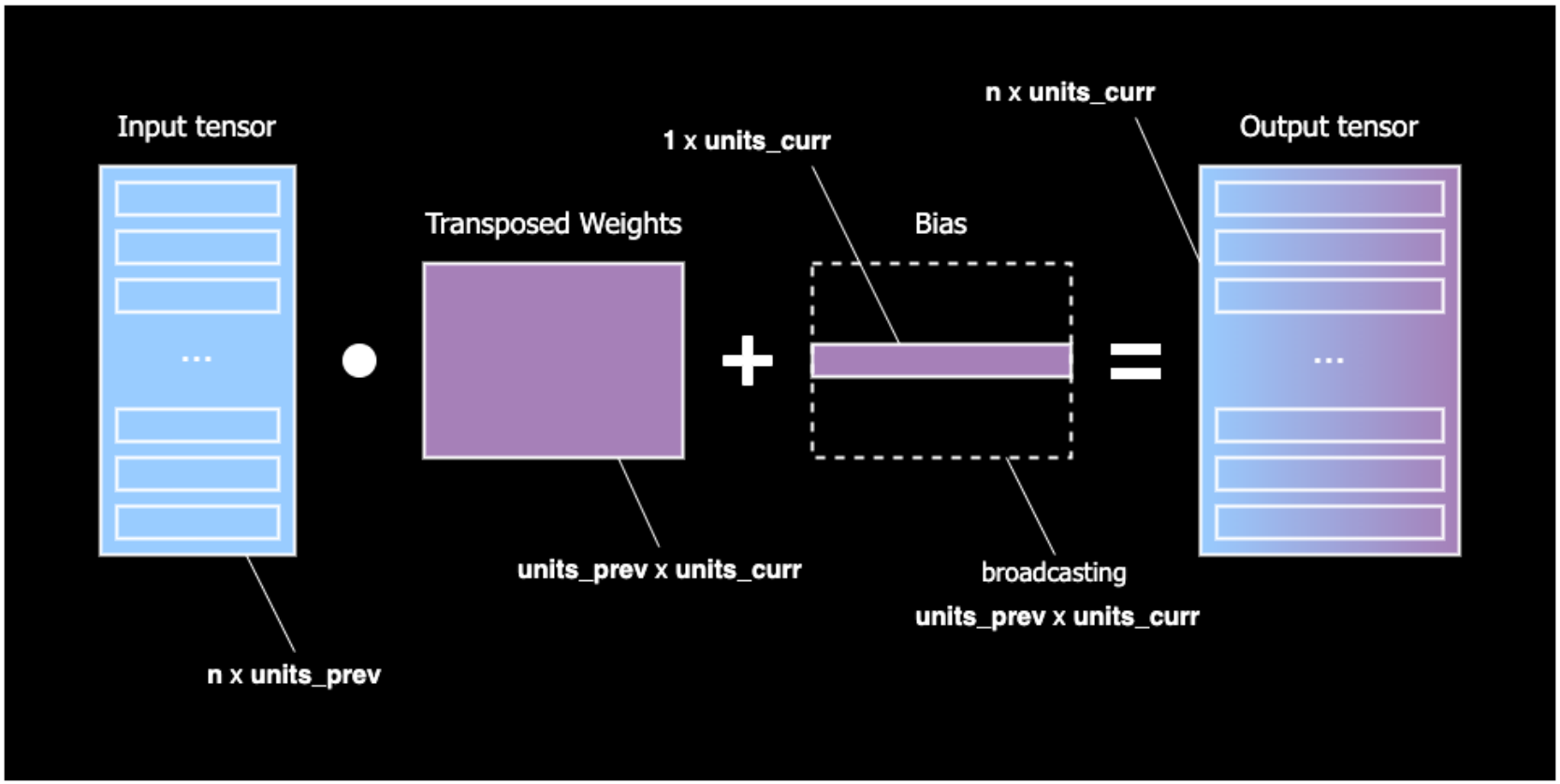


This is the same as the `numpy.flatten()` operation

Dense layers



Dense operations

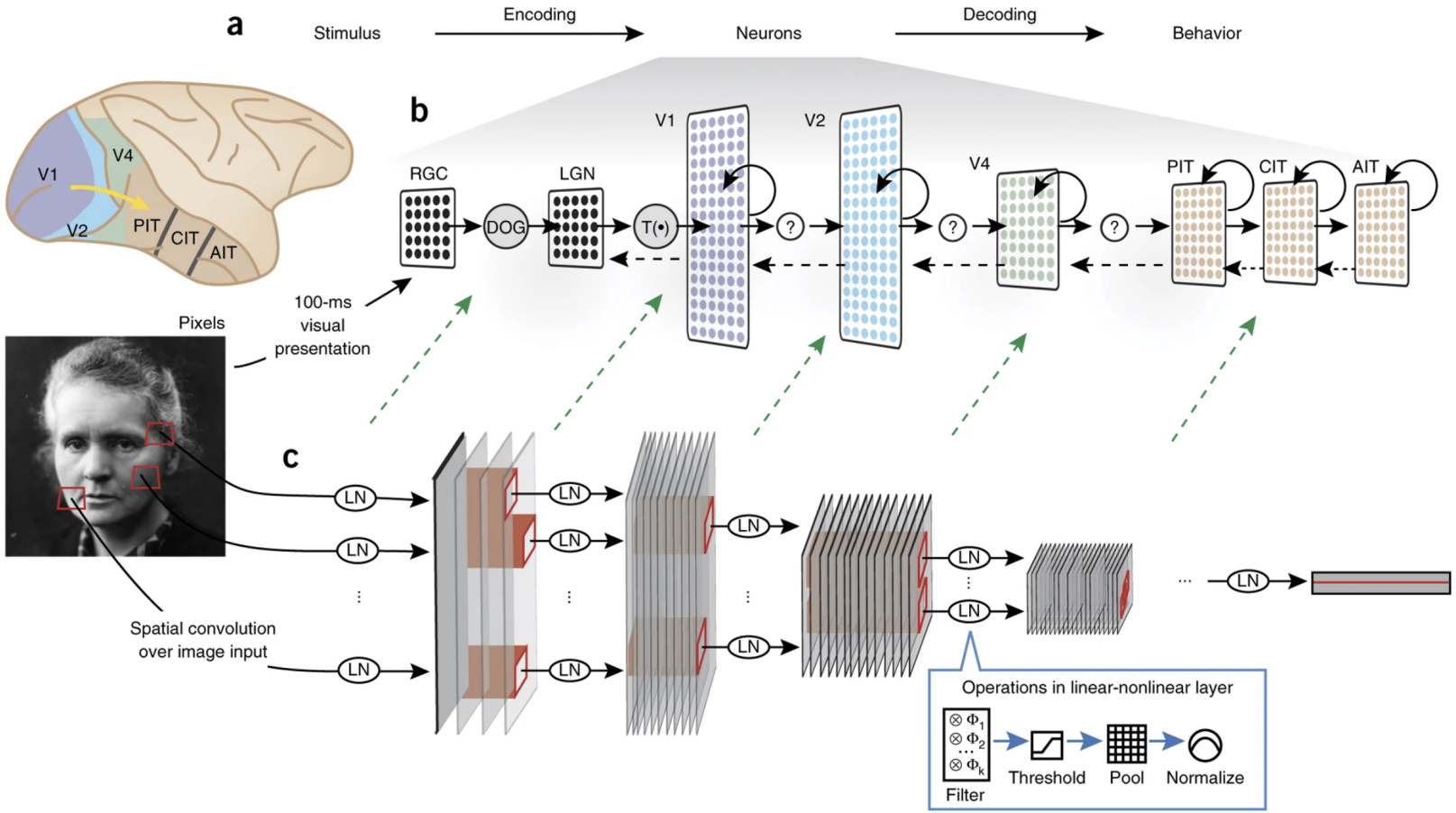


Again, this is not showing the use of an activation function

CNNs: Biological analogies

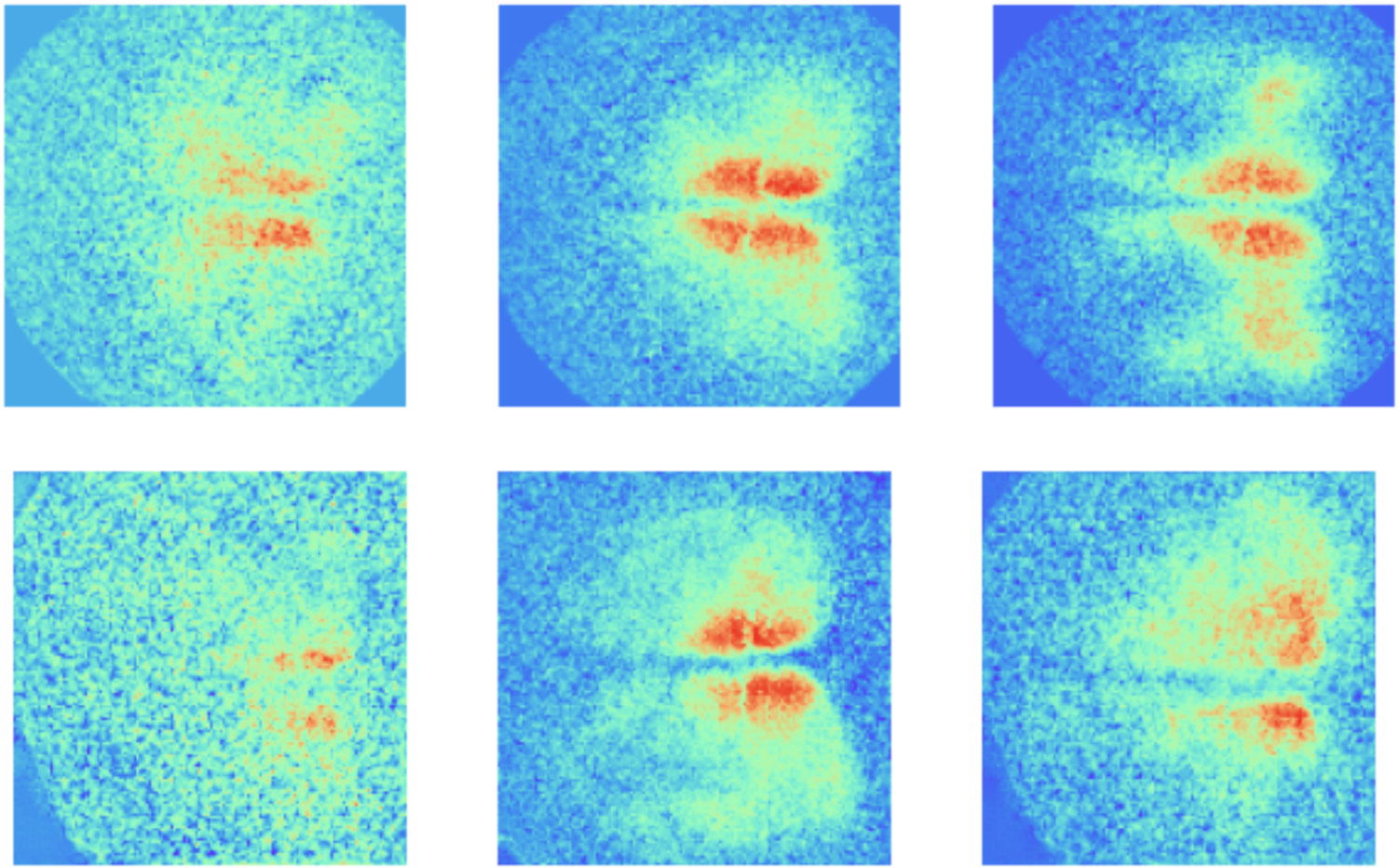
- It has been argued that common architectures for CNNs used for image processing mirror the organization and function of visual cortex in many species

CNNs: Biological analogies



Using goal-driven deep learning models to understand sensory cortex, Yamins and DiCarlo, 2016, https://www.nature.com/articles/nn.4244

Task: Real or Fake?



Task: Real or Fake?

- The real images are optical images of neural activity at the surface of the cortex in transgenic mice
- The fake images were generated by a “deconvolutional” neural network trained as part of a GAN

Example CNN

```
model = models.Sequential()
model.add(layers.Conv2D(32, (5, 5), activation='relu', input_shape=(128, 128, 1)))
model.add(layers.MaxPooling2D((4, 4)))
model.add(layers.Flatten())
model.add(layers.Dense(2))
model.summary()
```

```
Model: "sequential"
_________________________________________________________________
Layer (type)                 Output Shape              Param #
=================================================================
conv2d (Conv2D)              (None, 124, 124, 32)      832
_________________________________________________________________
max_pooling2d (MaxPooling2D) (None, 31, 31, 32)        0
_________________________________________________________________
flatten (Flatten)            (None, 30752)             0
_________________________________________________________________
dense (Dense)                (None, 2)                 61506
=================================================================
Total params: 62,338
Trainable params: 62,338
Non-trainable params: 0
_________________________________________________________________
```

Example CNN

First layer:

- Input: 128×128 images, 1 channel
- First layer: 32 filters, each of size 5×5
- Output of first layer: tensor of shape $124 \times 124 \times 32$
- Number of parameters: $(5 \times 5 + 1) \times 32 = 832$
- Activation function: ReLU
- Output of first layer: tensor of shape $124 \times 124 \times 32$

Example CNN

Second layer:

- Maximum of 4×4 regions in feature map
- Output: Tensor of shape $31 \times 31 \times 32$ since 124/4 = 31
- Number of parameters: Zero!

Example CNN

Third layer:

- Flattened version of previous layer
- Number of neurons: $31 \times 31 \times 32 = 30{,}752$
- Number of parameters: Zero!

Example CNN

Final layer:

- Dense connections
- Two neurons in output (“class 0” and “class 1”)
- Number of parameters: $(30{,}752 + 1) \times 2 = 61{,}506$

Example CNN

Overall:

- Number of parameters: $832 + 61{,}506 = 62{,}338$
- Most come from dense layer (98.7%)

A model with two convolutional layers

```
model = models.Sequential()
model.add(layers.Conv2D(32, (5, 5), activation='relu', input_shape=(128, 128, 1)))
model.add(layers.MaxPooling2D((4, 4)))
model.add(layers.Conv2D(32, (2, 2), activation='relu'))
model.add(layers.MaxPooling2D((4,4)))
model.add(layers.Flatten())
model.add(layers.Dense(128, activation='relu'))
model.add(layers.Dense(2))
model.summary()
```

```
Model: "sequential_11"
_________________________________________________________________
Layer (type)                 Output Shape              Param #
=================================================================
conv2d_20 (Conv2D)           (None, 124, 124, 32)      832
_________________________________________________________________
max_pooling2d_20 (MaxPooling (None, 31, 31, 32)        0
_________________________________________________________________
conv2d_21 (Conv2D)           (None, 30, 30, 32)        4128
_________________________________________________________________
max_pooling2d_21 (MaxPooling (None, 7, 7, 32)          0
_________________________________________________________________
flatten_11 (Flatten)         (None, 1568)              0
_________________________________________________________________
dense_17 (Dense)             (None, 128)               200832
_________________________________________________________________
dense_18 (Dense)             (None, 2)                 258
=================================================================
Total params: 206,050
Trainable params: 206,050
Non-trainable params: 0
_________________________________________________________________
```

Summary for today

- A convolutional layer applies a set of kernels (filters) across the input
- Each kernel is a tensor of smaller dimension than the input
- The values of the kernels are learned by backpropagation
- Successive convolutional layers build increasingly rich features
- The convolutional layers define a set of features that are then used to make predictions in one or more dense layers
- CNNs are attractive whenever the data have spatial structure where the same features might appear at many different locations