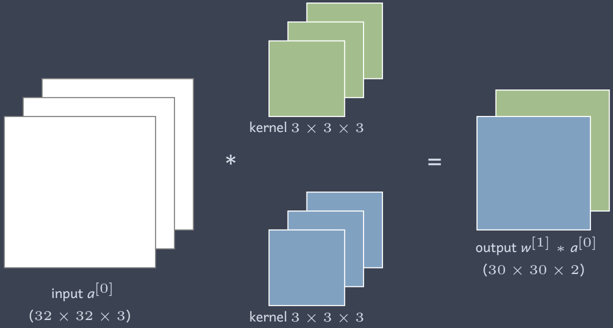
» Convolutional Layer

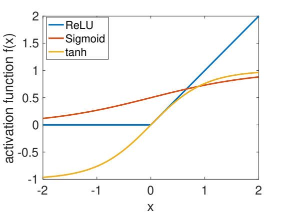
- Recall we can apply several filters to the same input and stack their outputs together. E.g.



- To get a complete convolutional layer we pass the elements of the output through a nonlinearity, usually after adding a bias.
  - Kernel weights $w^{[1]}$, input $a^{[0]}$, bias/offset $b^{[1]}$ (weights $w^{[1]}$ and bias $b^{[1]}$ are unknown parameters that need to be learned).
  - After convolution output is $w^{[1]} * a^{[0]}$
  - Add bias to get $z^{[1]} = w^{[1]} * a^{[0]} + b^{[1]}$
  - Final output $a^{[1]} = g(z^{[1]})$, for nonlinear *activation function* $g(\cdot)$. Note: $g(\cdot)$ is applied separately to each element of $z^{[1]}$.

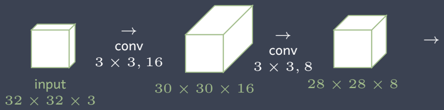
» Choice of Activation Function $g(\cdot)$

* ReLU (Rectified Linear Unit) $g(x) = \begin{cases} x & x \geq 0 \\ 0 & x < 0 \end{cases}$
* Almost universally used nowadays (older choices were sigmoid and tanh). Quick to compute, observed to work pretty well.
* But can lead to "dead" neurons where output is always zero $\rightarrow$ leaky ReLU



» Combining Convolutional Layers

* We can use the output from one convolution layer as the input to another convolution layer
* E.g. Suppose input to first layer is $32 \times 32 \times 3$ and convolve this with 16 kernels of size $3 \times 3 \times 3 \rightarrow$ output is $30 \times 30 \times 16$
* Now use this $30 \times 30 \times 16$ output as input to a second layer with 8 kernels fo size $3 \times 3 \times 16 \rightarrow$ output is $28 \times 28 \times 8$ tensor
* All layers use ReLU activation function. Stride is 1.
* Typical way of drawing this schematically:



* Notes:
  * "conv $3 \times 3, 16$" means convolutional layer with 3×3 kernel and 16 output channels.
  * Number of channels in each kernel must match number of input channels e.g. $3 \times 3 \times 3$ for 3 input channels and $3 \times 3 \times 16$ for 16 input channels, no choice here. So usually abbreviate to 3×3.
  * Depth of cube roughly indicates #output channels.

» Combining Convolutional Layers

Some more notes:

* No padding used, so output is smaller than input. Could keep the same using padding.
* Number of kernel weights/parameters for first layer is $16 \times 3 \times 3 \times 3 = 432$, and for second layer $8 \times 3 \times 3 \times 16 = 1152$
* Using equations:
    * Input $a^{[0]}$ to first layer, output is $a^{[1]} = g(w^{[1]} * a^{[0]} + b^{[1]})$
    * Input $a^{[1]}$ to second layer, output is $a^{[2]} = g(w^{[2]} * a^{[1]} + b^{[2]})$ where $w^{[1]}$, $w^{[2]}$ are layer kernel weights, $b^{[1]}$, $b^{[2]}$ layer bias parameters and $g(\cdot)$ is ReLU.

» Pooling Layer

- Pooling layers are used to reduce the size of matrices in tensor
- E.g. Suppose want to downsample 4×4 matrix to 2×2 matrix:

$$\begin{array}{|c|c|c|c|} \hline 1 & 2 & 3 & 4 \\ \hline 1 & 3 & 2 & 3 \\ \hline 3 & 2 & 1 & 4 \\ \hline 6 & 1 & 1 & 2 \\ \hline \end{array} \rightarrow \begin{array}{|c|c|} \hline & \\ \hline & \\ \hline \end{array}$$

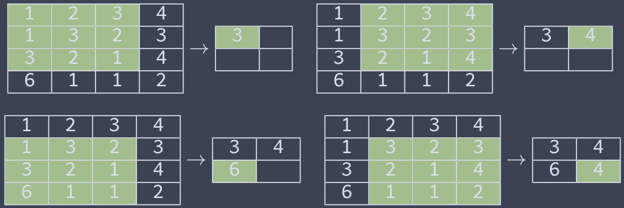
- Use *max-pooling* with 2×2 block size and stride 2:

$$\begin{array}{|c|c|c|c|} \hline 1 & 2 & 3 & 4 \\ \hline 1 & 3 & 2 & 3 \\ \hline 3 & 2 & 1 & 4 \\ \hline 6 & 1 & 1 & 2 \\ \hline \end{array} \rightarrow \begin{array}{|c|c|} \hline 3 & 4 \\ \hline 6 & 4 \\ \hline \end{array}$$

1. Partition input matrix into 2×2 blocks, stride of 2 means blocks don't overlap.
2. Calculate value of max element in each block.
3. Use max as value of corresponding output element.

» Pooling Layer

- E.g. Max-pooling with 3×3 block size and stride 1:



- But mostly use stride=block size $\rightarrow$ no overlap between blocks
- Pooling block size and stride must be chosen compatible with size of input matrix
- As well as max-pooling there is *average pooling* $\rightarrow$ output is average of elements in a block. But rarely used.

» Down-sampling Using Strided Convolution

- Recall that we can use strides > 1 in a convolutional layer $\rightarrow$ also reduces size of output
- E.g. Applying 2×2 kernel $\begin{bmatrix} 1 & -1 \\ 1 & -1 \end{bmatrix}$ with stride 2:

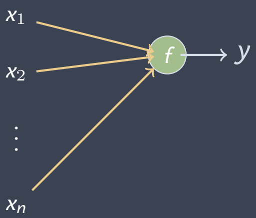
$$\begin{bmatrix} 1^{1} & 2^{-1} & 3 & 4 \\ 1^{1} & 3^{-1} & 2 & 3 \\ 3 & 2 & 1 & 4 \\ 6 & 1 & 1 & 2 \end{bmatrix} \rightarrow \begin{bmatrix} -3 & \\ & \end{bmatrix} \qquad \begin{bmatrix} 1 & 2 & 3^{1} & 4^{-1} \\ 1 & 3 & 2^{1} & 3^{-1} \\ 3 & 2 & 1 & 4 \\ 6 & 1 & 1 & 2 \end{bmatrix} \rightarrow \begin{bmatrix} -3 & -2 \\ & \end{bmatrix}$$

$$\begin{bmatrix} 1 & 2 & 3 & 4 \\ 1 & 3 & 2 & 3 \\ 3^{1} & 2^{-1} & 1 & 4 \\ 6^{1} & 1^{-1} & 1 & 2 \end{bmatrix} \rightarrow \begin{bmatrix} -3 & -2 \\ 6 & \end{bmatrix} \qquad \begin{bmatrix} 1 & 2 & 3 & 4 \\ 1 & 3 & 2 & 3 \\ 3 & 2 & 1^{1} & 4^{-1} \\ 6 & 1 & 1^{1} & 2^{-1} \end{bmatrix} \rightarrow \begin{bmatrix} -3 & -2 \\ 6 & -4 \end{bmatrix}$$

  $\rightarrow$ for 4×4 input the output is reduced to 2×2
- Often works well, e.g. see Striving For Simplicity: The All Convolutional Net https://arxiv.org/pdf/1412.6806.pdf
- Not quite the same as using (2,2) kernel with stride 1 and same padding followed by (2,2) max-pooling:
  - (2,2) kernel with stride 1 and same padding does 16 convolutions whereas (2,2) kernel with stride 2 calcs only 4 convolutions (so faster, computationally cheaper)
  - Max-pooling combines info from all 4 convolutions involving 2×2 block whereas (2,2) kernel with stride 2 only uses info from 1 convolution per 2×2 block (uses less info)

» Fully-Connected Layer

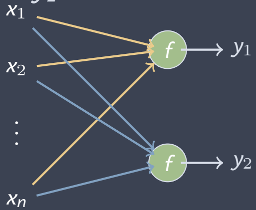
- *Fully-connected (FC) layer* = one layer of MLP. Called *dense* layer in keras.
- Each output is a function of a weighted sum of all of the inputs
  - Input is vector x (*not* a tensor or matrix). Output is $y = f(w^T x)$, w are weights/parameters, $f(\cdot)$ is nonlinear function.



- If input is output from a convolution layer, i.e. a tensor, need to *flatten* it before it can be used as input to FC layer.
  - flattening $\rightarrow$ take all elements of tensor and write them as a list/array
  - e.g. two channels $\begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix}, \begin{bmatrix} 4 & 5 \\ 6 & 7 \end{bmatrix} \rightarrow [1, 2, 3, 4, 4, 5, 6, 7]$.

» Fully-Connected Layer

- A FC-layer can have multiple outputs e.g. Input x and two output $y_1 = f(w^T x)$, $y_2 = f(v^T x)$. Here w is weight vector for y_1, v the weight vector for y_2.

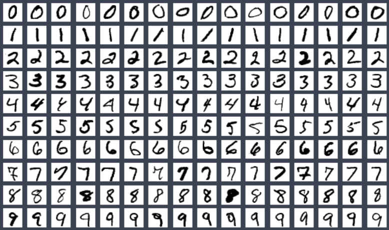


- If input vector x has n elements and have m outputs then FC-layer has $n \times m$ parameters.
  - Suppose have $h_0 \times w_0 \times c_0$ input and $h_1 \times w_1 \times c_1$ output.
  - Convolution layer has $c_1 \times k \times k \times c_0$ parameters for $k \times k$ kernel
  - FC-layer has $h_0 \times w_0 \times c_0 \times h_1 \times w_1 \times c_1$ parameters
  - $h_0 = w_0 = 32$, $c_0 = 32$, $h_1 = w_1 = 32$, $c_1 = 32$, conv 3×3 layer has 9216 parameters, FC layer has 10^9 parameters.
- Common to use FC-layer as the last layer in a ConvNet i.e. the layer which generates the (smallish number of) final outputs.
- How to choose nonlinear function $f(\cdot)$?
  - Common choice: *softmax*.
  - Recall softmax = multi-class logistic regression model.

» Convolutional Network Example

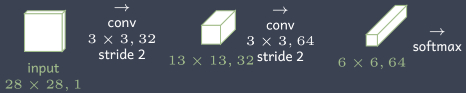
MNIST Dataset[1]

- Training data: 60K images of handwritten digits 0-9. Test data 10K images
- Each image is 28×28 pixels, gray scale
- Task is to predict which digit an image shows.
- Widely studied, relatively easy task. Best performance to date is 99.8% accuracy using ConvNet



[1] https://en.wikipedia.org/wiki/MNIST_database#cite_note-Gradient-9

» Convolutional Network Example



- Uses strides to downsample the image.
  - Input $28 \times 28 \times 1 \rightarrow 13 \times 13 \times 32 \rightarrow 6 \times 6 \times 64$
- Number of channels increases as we move through network ($1 \rightarrow 32 \rightarrow 64$), size of image decreases ($28 \times 28 \rightarrow 13 \times 13 \rightarrow 6 \times 6$)
- We use final softmax layer/logistic regression to map from ConvNet features to final output (flatten step not shown in schematic)
  - Output is $10 \times 1 \rightarrow$ there are 10 classes, corresponding to digits 0-9, elements of output vector are probability of each class. To make prediction pick the class with highest probability.

» Convolutional Network Example

* We'll use Python keras package for ConvNets (its a front end to tensorflow)

```
import numpy as np
from tensorflow import keras
from tensorflow.keras import regularizers
from keras.layers import Dense, Flatten, Conv2D, MaxPooling2D, Dropout

num_classes = 10
input_shape = (28, 28, 1)

# Load MNIST dataset
(x_train, y_train), (x_test, y_test) = keras.datasets.mnist.load_data()
# Scale images to the [0, 1] range
x_train = x_train.astype("float32") / 255
x_test = x_test.astype("float32") / 255
# Make sure images have shape (28, 28, 1)
x_train = np.expand_dims(x_train, -1)
x_test = np.expand_dims(x_test, -1)

model = keras.Sequential()
#3x3 kernel with stride 2, 32 output channels.
model.add(Conv2D(32, kernel_size=(3, 3), strides=(2,2), input_shape=input_shape, activation="relu"))
#3x3 kernel with stride 2, 64 output channels.
model.add(Conv2D(64, kernel_size=(3, 3), strides=(2,2), activation="relu"))
# use CNN output as input to a Logistic regression classifier. Regularise logistic loss with L2 penalty.
model.add(Flatten())
model.add(Dense(num_classes, activation='softmax',activity_regularizer=regularizers.l2(0.01)))
model.summary()

model.compile(loss="categorical_crossentropy", optimizer='adam', metrics=["accuracy"])
model.fit(x_train, y_train, batch_size=32, epochs=5, validation_split=0.2)
score = model.evaluate(x_test, y_test, verbose=0)
print("Test loss: %f accuracy: %f"%(score[0],score[1]))
```

* Note: use regularisation on FC-layers but usually not on convolutional layers. Why?

» Convolutional Network Example

* Typical output:

```
_________________________________________________________________
Layer (type) Output Shape Param #
=================================================================
conv2d (Conv2D) (None, 13, 13, 32) 320
_________________________________________________________________
conv2d_1 (Conv2D) (None, 6, 6, 64) 18496
_________________________________________________________________
flatten (Flatten) (None, 2304) 0
_________________________________________________________________
dense (Dense) (None, 10) 23050
=================================================================
Total params: 41,866
Trainable params: 41,866
Non-trainable params: 0
_________________________________________________________________
Epoch 1/5
3000/3000 [==============================] - 6s 2ms/step - loss: 0.1927 - accuracy: 0.9447 - val_loss: 0.0916 -
val_accuracy: 0.9765
Epoch 2/5
3000/3000 [==============================] - 6s 2ms/step - loss: 0.0788 - accuracy: 0.9788 - val_loss: 0.0755 -
val_accuracy: 0.9814
Epoch 3/5
3000/3000 [==============================] - 6s 2ms/step - loss: 0.0584 - accuracy: 0.9850 - val_loss: 0.0700 -
val_accuracy: 0.9820
Epoch 4/5
3000/3000 [==============================] - 6s 2ms/step - loss: 0.0466 - accuracy: 0.9882 - val_loss: 0.0723 -
val_accuracy: 0.9819
Epoch 5/5
3000/3000 [==============================] - 6s 2ms/step - loss: 0.0384 - accuracy: 0.9908 - val_loss: 0.0616 -
val_accuracy: 0.9858
Test loss: 0.051263 accuracy: 0.987100
```

* Achieves 98.7% accuracy on test data, model takes about 30s to train
* Baseline for comparison:
  * Logistic regression: 73s to train, achieves 92% accuracy
  * Kernelised SVM: 711s to train, achieves 94% accuracy

» Convolutional Network Example

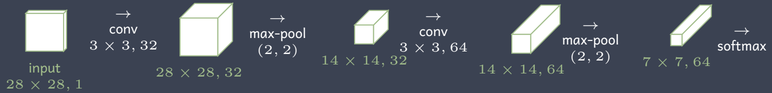
* Can also use dropouts rather than L_2 penalty for regularisation $\rightarrow$ using dropouts is popular in ConvNets

```
model = keras.Sequential()
model.add(Conv2D(32, kernel_size=(3, 3), strides=(2,2), input_shape=input_shape, activation="relu"))
model.add(Conv2D(64, kernel_size=(3, 3), strides=(2,2), activation="relu"))
model.add(Dropout(0.5))
model.add(Flatten())
model.add(Dense(num_classes, activation='softmax'))
```

* Again, note that use regularisation on FC-layers but usually not on convolutional layers.

» Convolutional Network Example

An alternative (but v similar) architecture:



- Use “same” padding in conv layers → output is same size as input.
- Use max-pool to downsample, stride=kernel size=2
- $28 \times 28 \times 1 \rightarrow 28 \times 28 \times 32 \rightarrow 14 \times 14 \times 32 \rightarrow 14 \times 14 \times 64 \rightarrow 8 \times 8 \times 64$
- Using same padding plus max-pool like this is currently popular ... but that might well change
- Python keras code:

```
model = keras.Sequential()
model.add(Conv2D(32, kernel_size=(3, 3), input_shape=input_shape, padding=”same”,activation=”relu”))
model.add(MaxPooling2D(pool_size=(2, 2)))
model.add(Conv2D(64, kernel_size=(3, 3), padding=”same”, activation=”relu”))
model.add(MaxPooling2D(pool_size=(2, 2)))
model.add(Flatten())
model.add(Dense(num_classes, activation=’softmax’,activity_regularizer=regularizers.l2(0.01)))
model.summary()
```

» Convolutional Network Example

* Typical output:

```
_________________________________________________________________
Layer (type) Output Shape Param #
=================================================================
conv2d (Conv2D) (None, 28, 28, 32) 320
_________________________________________________________________
max_pooling2d (MaxPooling2D) (None, 14, 14, 32) 0
_________________________________________________________________
conv2d_1 (Conv2D) (None, 14, 14, 64) 18496
_________________________________________________________________
max_pooling2d_1 (MaxPooling2 (None, 7, 7, 64) 0
_________________________________________________________________
flatten (Flatten) (None, 3136) 0
_________________________________________________________________
dense (Dense) (None, 10) 31370
=================================================================
Total params: 50,186
Trainable params: 50,186
Non-trainable params: 0
_________________________________________________________________
Epoch 1/5
3000/3000 [==============================] - 21s 7ms/step - loss: 0.1490 - accuracy: 0.9565 - val_loss: 0.0627 -
val_accuracy: 0.9854
Epoch 2/5
3000/3000 [==============================] - 22s 7ms/step - loss: 0.0570 - accuracy: 0.9850 - val_loss: 0.0527 -
val_accuracy: 0.9886
Epoch 3/5
3000/3000 [==============================] - 22s 7ms/step - loss: 0.0432 - accuracy: 0.9898 - val_loss: 0.0567 -
val_accuracy: 0.9849
Epoch 4/5
3000/3000 [==============================] - 22s 7ms/step - loss: 0.0345 - accuracy: 0.9920 - val_loss: 0.0504 -
val_accuracy: 0.9877
Epoch 5/5
3000/3000 [==============================] - 21s 7ms/step - loss: 0.0284 - accuracy: 0.9941 - val_loss: 0.0474 -
val_accuracy: 0.9901
Test loss: 0.044836 accuracy: 0.989100
```

* Achieves 98.9% accuracy on test data
* Takes 100s to train (longer than when use strides to downsample, why?)

» Cross-validation

* Training by minimising cost function and using cross-validation to select hyperparameters (not just regularisation penalty but also number of convolutional output channels etc) is best practice
* But ...
* ... it often takes ages to train ConvNets. Even in above v easy example it takes a minute or so, with bigger networks and more data training can easily take days even with a good GPU rig
* So *k*-fold cross-validation usually impractical, just takes too long
* Instead often just keep a hold-out test set and use that to evaluate hyperparameter choices. Also often only evaluate only a few hyperparameter values as otherwise takes too long.
* Its not great, but we have little choice. Also means you can see many conflicting/random views on web for how to approach the same ML task.