Técnicas de lA para Biologia

4 - Convolutional Networks

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Convolutional Networks

Summary

- What is convolution
- Convolution layers and neural networks (CNNs)
- Pooling
- Classification with convolutional networks
- CNN tutorial: Fashion MNIST classification with CNN and Keras

Convolutional Networks

Convolution

Definition:

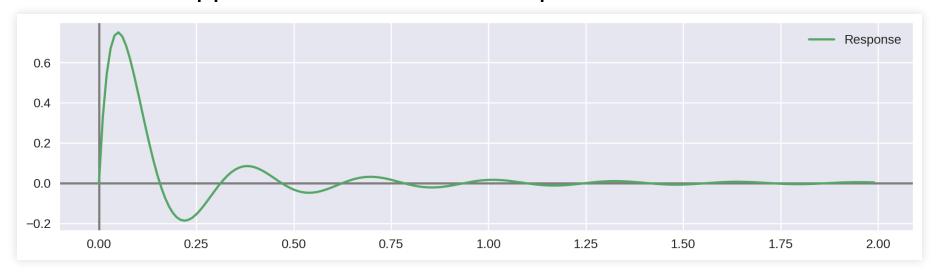
 Integral of the product of two functions, one of which was shifted and inverted

$$(f*g)(t) = \int_{-\infty}^{\infty} f(au)g(t- au)d au = \int_{-\infty}^{\infty} f(t- au)g(au)d au$$

 Used in many applications, such as probabilities or linear timeinvariant systems

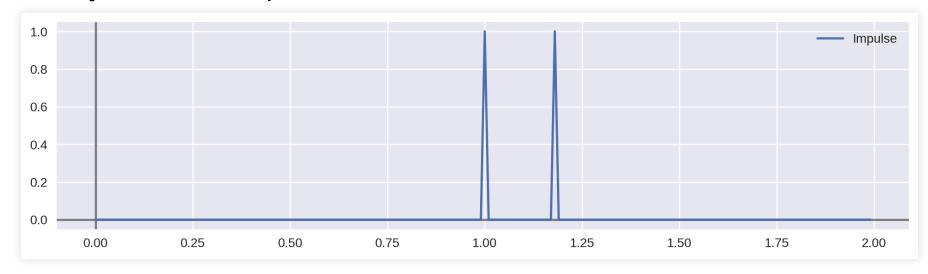
$$(f*g)(t) = \int_{-\infty}^{\infty} f(au)g(t- au)d au = \int_{-\infty}^{\infty} f(t- au)g(au)d au$$

Intuition: Suppose a LTIS with this response:



$$(f*g)(t) = \int_{-\infty}^{\infty} f(\tau)g(t-\tau)d au = \int_{-\infty}^{\infty} f(t-\tau)g(\tau)d au$$

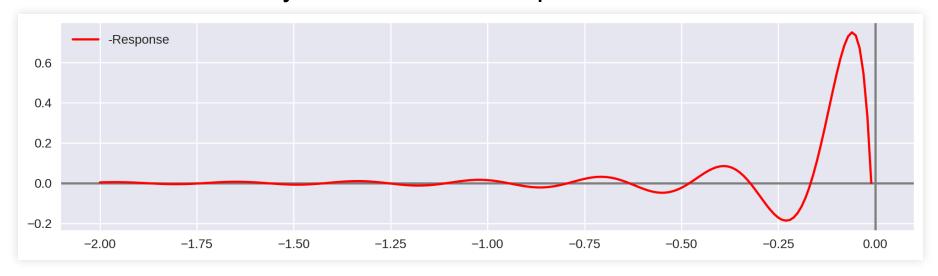
Subject to this impulse



How do we compute the output?

$$(f*g)(t) = \int_{-\infty}^{\infty} f(au)g(t- au)d au = \int_{-\infty}^{\infty} f(t- au)g(au)d au$$

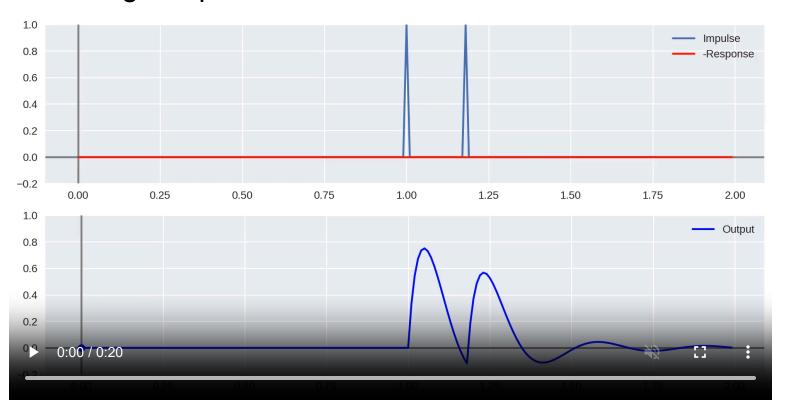
■ First we take the symmetric of the response:



How do we compute the response?

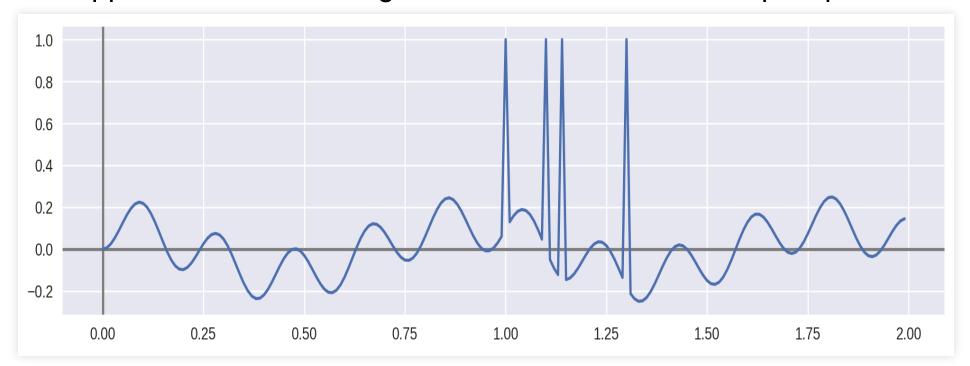
$$(fst g)(t)=\int_{-\infty}^{\infty}f(au)g(t- au)d au=\int_{-\infty}^{\infty}f(t- au)g(au)d au$$

Now we integrate product at different time shifts



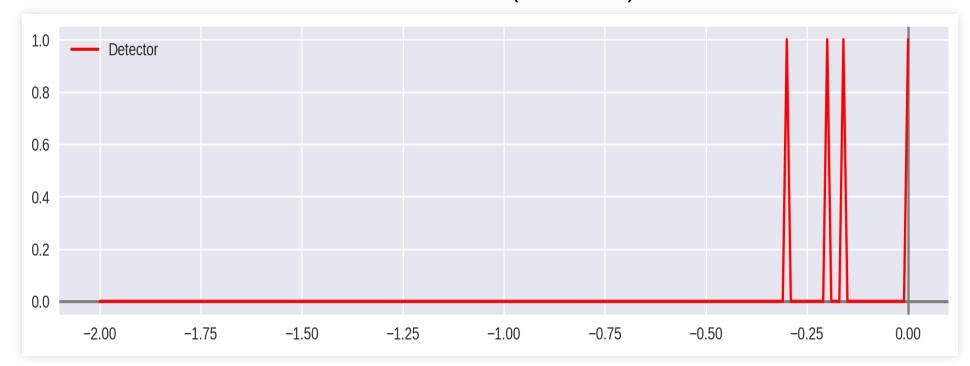
For finding patterns

Suppose we have this signal and want to detect the spike pattern



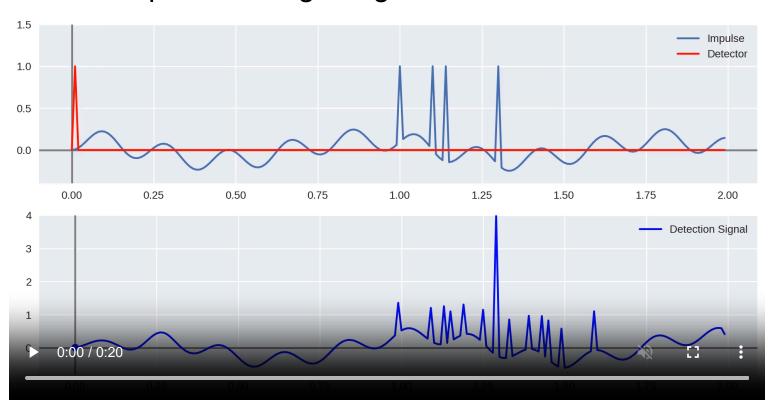
For finding patterns

We create this "detector" function (inverted)



$$(fst g)(t)=\int_{-\infty}^{\infty}f(au)g(t- au)d au=\int_{-\infty}^{\infty}f(t- au)g(au)d au$$

We detect the pattern integrating at different time shifts



Motivation:

- Use a kernel (w) to modify the input (x) and create a new function
 (s) using weighted values "around" the input
- E.g. a weighted average of most recent values in a time series, local features of an image, etc,

$$s(t) = (x*w)(t) = \sum_{m=-\infty}^{\infty} x(t)w(t-m)$$

- In practice, for CNN:
- The input is a finite, discrete set of values (assumed 0 everywhere else)
- The kernel is a finite set of parameters that will be learned
- The output will be tensor, typically of the same size and shape as the input

Two-dimensional convolution

We often use convolution in more than one dimension (e.g. for images)

$$S(i,j) = (I*K)(i,j) = \sum_m \sum_n I(m,n)K(i-m,j-n)$$

Since convolution is commutative, we often use:

$$S(i,j) = (I*K)(i,j) = \sum_m \sum_n I(i-m,j-n)K(m,n)$$

I.e. we index the kernel and the image around (i,j)

Convolutional networks

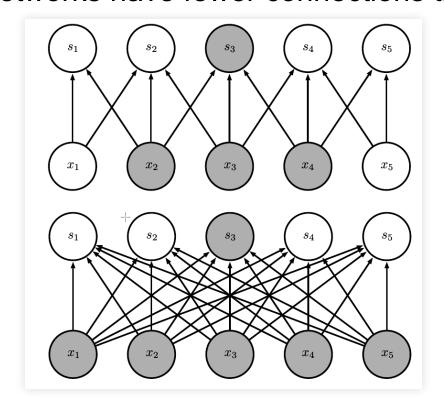
CNN

Motivation for convolutional networks

- Sparse interactions (sparse connectivity or sparse weights)
- Since the kernel is smaller than the input, we need fewer parameters
- Shared parameters
- Connections are sparse but the same parameters are used over all inputs
- Equivariance
- Convolutions are equivariant to some transformations
- I.e. applying the transformation (e.g. translation) to the input is the same as applying it to the convolution

Motivation: sparse interactions

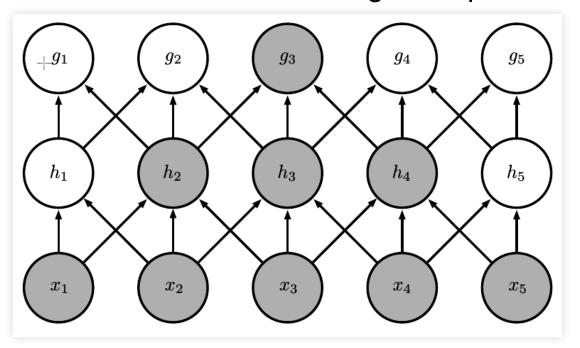
Convolutional networks have fewer connections than MLP



Goodfellow, Bengio, Courville, Deep Learning 2016

Motivation: sparse interactions

- Convolutional networks have fewer connections than MLP
- But deeper neurons can still have a large receptive field in the input

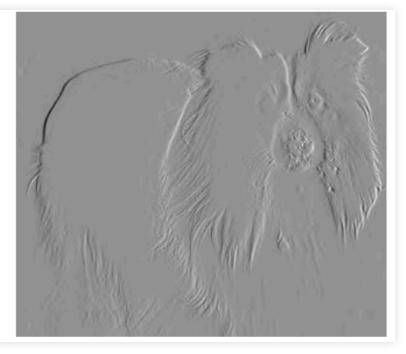


Goodfellow, Bengio, Courville, Deep Learning 2016

Motivation: parameter sharing

- The same parameter is used for many inputs
- E.g. edge detection by subtracting pixel on the left



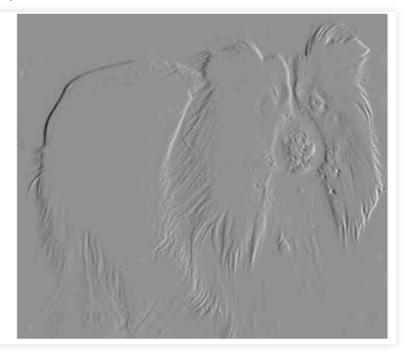


Goodfellow, Bengio, Courville, Deep Learning 2016

Motivation: equivariance

 Moving the input image is equivalent to moving the output of the convolution filter (the feature map)



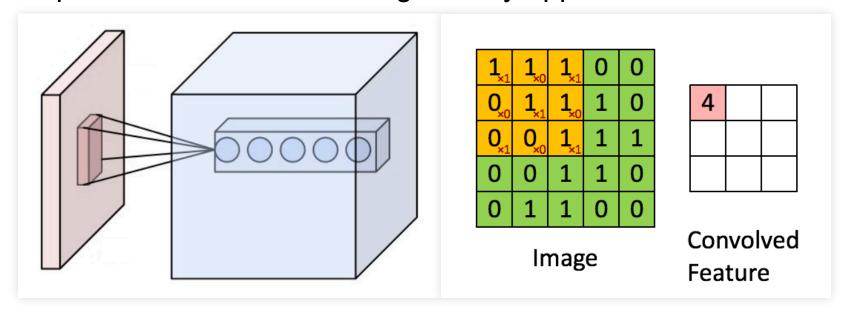


Goodfellow, Bengio, Courville, Deep Learning 2016



Receptive field and multiple filters

- Visual cortex neurons respond to a small receptive field in retina
- Neurons in convolution layers have this property
- Multiple convolution filters are generally applied



Images: Aphex34, CC-SA; UFLDL tutorial, Stanford (Ng et. al.)



Receptive field and multiple filters

- Multiple convolution filters are generally applied
- We generally represent convolution layers as 3D volumes of neurons (in image processing), stacking the different convolution filters

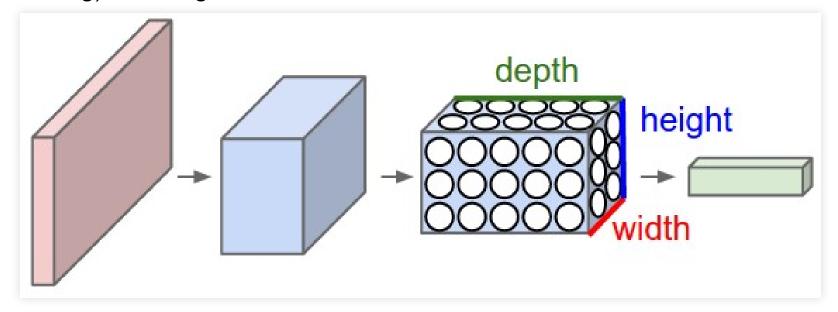
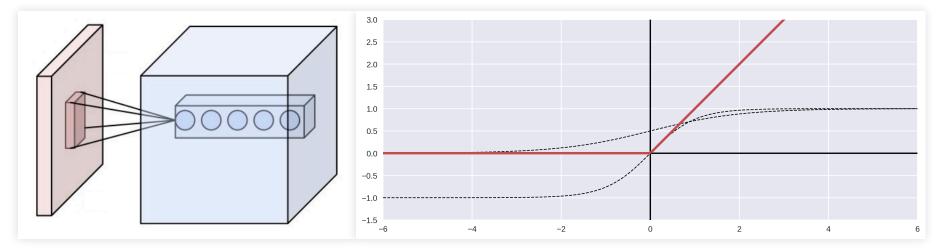


Image: CS231n Stanford (Fei-Fei Li et. al.)



Nonlinear tranformation

 A convolution is a linear transformation, so in CNN the convolution filter generally feeds into a nonlinear response (usually ReLU)





Hyperparameters of a convolution layer

- Depth: the number of filters being learned
- Stride: How the receptive field "jumps"
- Padding: to prevent output from shrinking

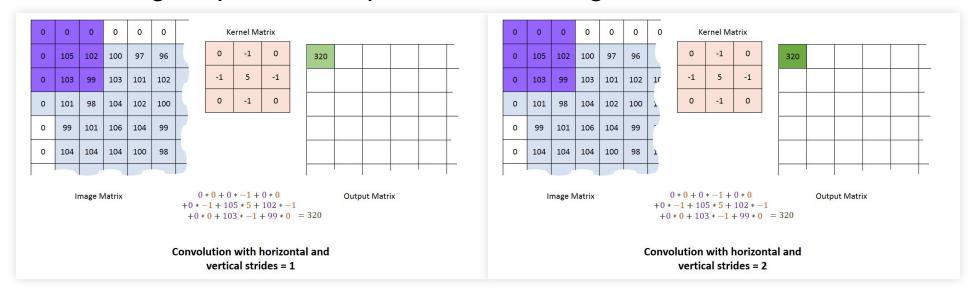
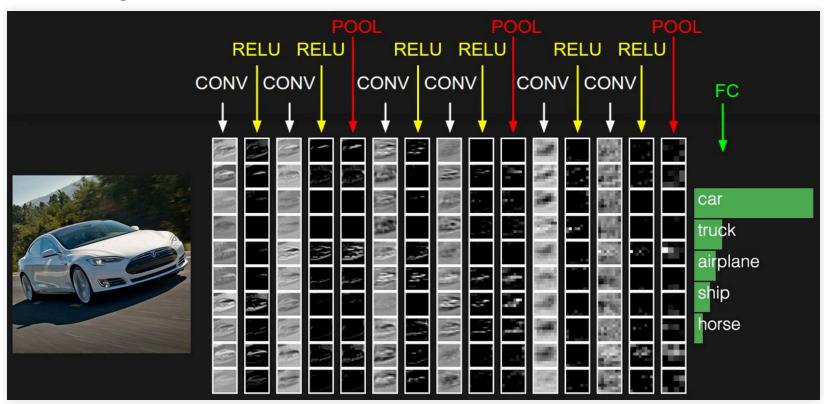


Image: Machine learning guru, http://machinelearninguru.com



Example: convolution network

- Stanford (CS231, Fei-Fei Li et. al.)
- http://cs231n.github.io/convolutional-networks/



Convolutional networks

Pooling

Pooling

Typical architecture of a convolutional layer

- Convolutions: several convolutions in parallel, generating a set of linear activations
- Nonlinear activation: applied to each linear output (typically ReLU)
- (detector stage)
- Pooling: aggregates the outputs in a single output for each region

Pooling

Pooling: aggregating outputs

Example: max pooling

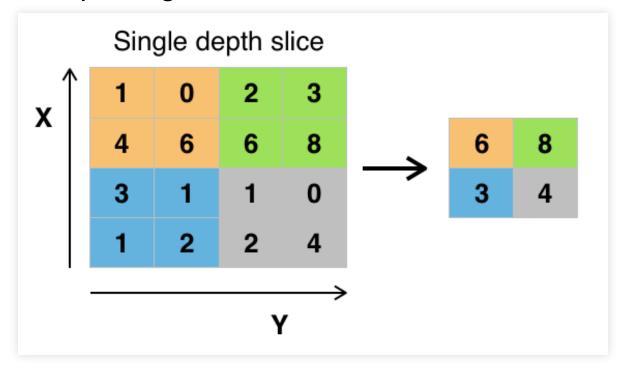


Image: Aphex34, CC-SA

Pooling

Pooling: aggregating outputs

- Typical pooling functions:
- Max pooling, average pooling, L 2 norm pooling: $\sqrt{\sum x_i^2}$
- Pooling makes model nearly invariant to small shifts in input

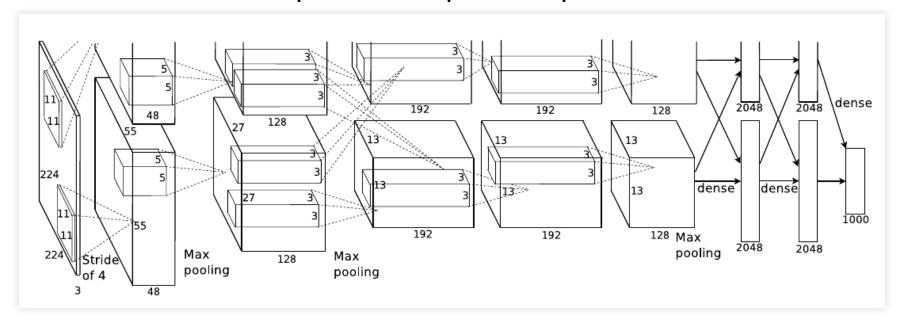
Pooling Stride

- We may want to regulate the overlap of pooling regions
- If the stride is equal to the size of the regions, then there is no overlap
- Stride also reduces the dimension
- (pooling of stride 1, with padding, preserves dimension)

Classification with CNN

For classification, conv layers combined with MLP

- Fully connected layers at the end to predict class for example
- Forces fixed-sized input and output not spacial



Alex Krizhevsky, Ilya Sutskever, Geoffrey E. Hinton, 2012

Convolutional networks

Tutorial: Keras Sequential API

Building a model with Keras

Start by importing classes:

```
from tensorflow.keras.optimizers import SGD
from tensorflow.keras.models import Sequential
from tensorflow.keras.layers import BatchNormalization,Conv2D,MaxPooling2D,
from tensorflow.keras.layers import Activation, Flatten, Dropout, Dense
```

Building a model with Keras

Create a Sequential model and add layers

```
model = Sequential()
model.add(Conv2D(32, (3, 3), padding="same", input_shape=(28,28,1)))
model.add(Activation("relu"))
...
model.add(MaxPooling2D(pool_size=(2, 2)))
model.add(Conv2D(64, (3, 3), padding="same"))
...
model.add(Flatten())
model.add(Dense(512))
model.add(Activation("relu"))
model.add(BatchNormalization())
model.add(Dense(10))
model.add(Dense(10))
model.add(Activation("softmax"))
```

Side note:

- (Current consensus, but some opinions may vary)
- Use batch normalization after activation so that input of following layer is standardized
- Use dropout after all batch normalizations
- Otherwise you may need to compensate the rescaling of dropout when shifting to prediction mode
- Dropout may have some benefits in convolution layers but in that case it is not the same as dropout in dense layers

Compiling the model

Now we can train the model and save the weights.

- The saved weights can be loaded with
- model.load weights(file name)

Monitoring

The fit method returns a history object (parameters, model, etc)

```
In: history.history
Out:
    {'acc': [0.7736167, ...],
    'loss': [0.6834171069622039, ...],
    'val_acc': [0.1974, ...],
    'val_loss': [2.1077217151641845, ...]}
```

Convolutional networks

Tutorial: Regression and CNN

Regression with the Auto MPG Data Set

- Predict the fuel consumption of cars
- Auto MPG Data Set, available at the UCI repository
- Some pointers:
- Shuffle the data before splitting into training and validation sets
- Target: first column, MPG (miles per gallon)
- Standardize features and target value
- Standardizing target centers the output and minimizes numerical problems
- Only 392 examples. Use 300 for training and 92 for validation.
- Linear output for the last neuron (only one neuron)
- Mean squared error loss function for training
- Try different activations and learning parameters (rate, momentum)

Regression with the Auto MPG Data Set

■ Load, standardize, use 300 for train and rest for validation:

```
data = np.loadtxt('AutoMPG.tsv', skiprows=1)
np.random.shuffle(data)
means = np.mean(data,axis=0)
stds = np.std(data,axis=0)
data = (data-means)/stds

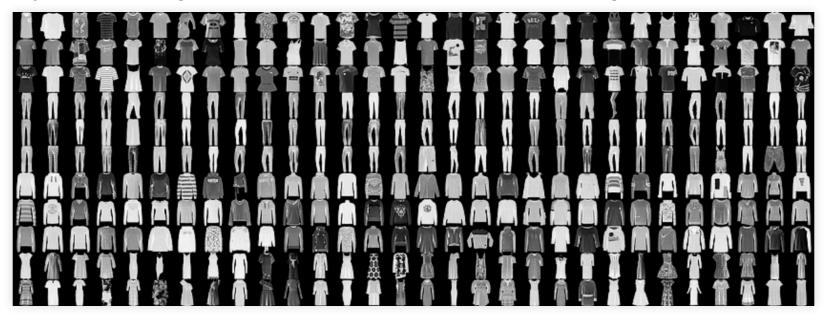
valid_Y = data[300:,0]
valid_X = data[300:,1:]

Y = data[:300,0]
X = data[:300,1:]
```

Fashion MNIST

https://github.com/zalandoresearch/fashion-mnist

Grayscale images, 28x28, 10 classes of clothing



Import the dataset and set up the data

```
from tensorflow import keras
((trainX, trainY), (testX, testY)) = keras.datasets.fashion_mnist.load_data()
trainX = trainX.reshape((trainX.shape[0], 28, 28, 1))
testX = testX.reshape((testX.shape[0], 28, 28, 1))
trainX = trainX.astype("float32") / 255.0
testX = testX.astype("float32") / 255.0
# one-hot encode the training and testing labels
trainY = keras.utils.to_categorical(trainY, 10)
testY = keras.utils.to_categorical(testY, 10)
```

One-hot encoding for encoding multi-class.

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

 Softmax will output vectors with sum of 1 and with probabilities of belonging to each class

Model for this exercise:

- First stack:
- Two convolution layers with 3 imes3 kernel, padding "same", 32 filters, ReLU activation and batch normalization
- ullet Max pooling of size 2 imes 2 and same stride
- Optional: you can try adding dropout layer with 25% dropout probability (but results seem to be worse)
- Second stack: Identical to first but with 64 filters
- Dense layer of 512 neurons with ReLU activation, batch normalization and dropout of 50%
- Softmax layer with 10 neurons.
- Use the SGD optimizer and about 25 epochs, save after fitting
- Optional: Experiment changing the model and optimizers

Convolutional networks

Summary

Convolutional networks

Summary

- Convolutions
- Convolution layers
- Classification with convolutional networks
- CNN tutorial using the Keras sequential API

Further reading:

- Goodfellow et.al, Deep learning, Chapter 9
- Tensorflow Keras API
- https://www.tensorflow.org/guide/keras