Introduction to Machine Learning Neural Networks In practice

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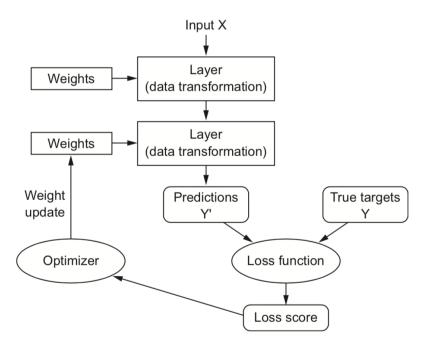
Overview

- Multiclass classification (general)
- Binary text classification
- Multiclass text classification
- Regression (of house prices)
- Multiclass image classification

Examples from Deep Learning with Python

Components of Neural Nets (recap)

- Layers of nodes: transform an input tensor to an output tensor
 - Each with (a tensor of) weights to be fitted to the training data
 - Many types: dense, convolutional, recurrent,...
- Loss function: Measures whether the model fits the training data
- Optimizer: How to update the network, e.g. SGD

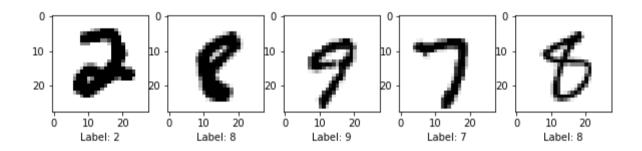


A first example: classifying digits

- This example is meant to introduce the main concepts. We'll cover them in more detail later.
- MNIST dataset contains 28x28 pixel images of handwritten digits (0-9)
- The goal is to classify each image as one of the possible digits
- We reshape the data to a 70000x28x28 tensor (n-dimensional matrix)
 X = X.reshape(70000, 28, 28)
- Traditional holdout uses the last 10,000 images for testing

- Retrieve from OpenML
- Reshape to 28x28 images
- Create train and test split

```
mnist = oml.datasets.get_dataset(554)
X, y = mnist.get_data(target=mnist.default_target_attribute);
X = X.reshape(70000, 28, 28)
X_train, X_test, y_train, y_test = train_test_split(X, y, train_size=600 00)
```



Training set: (60000, 28, 28) Test set: (10000, 28, 28) We can now build a simple neural network for MNIST:

- One dense hidden ReLU layer with 512 nodes
 - Input from a 28x28 matrix
- Output softmax layer with 10 nodes

```
from keras import models
from keras import layers

network = models.Sequential()
network.add(layers.Dense(512, activation='relu', input_shape=(28 * 28,)))
network.add(layers.Dense(10, activation='softmax'))
```

'Visualize' the model using summary()

• Also shows the number of model parameters (weights) that need to be learned

Layer (type)	Output Shape	Param #
dense_28 (Dense)	(None, 512)	401920
dense_29 (Dense)	(None, 10)	5130

Total params: 407,050

Trainable params: 407,050 Non-trainable params: 0

Compilation

We still need to specify how we want the network to be trained:

- Loss function: The objective function used to measure how well the model is doing, and steer itself in the right direction
 - e.g. Cross Entropy (*negative log likelihood* or *log loss*) for classification
- **Optimizer**: How to optimize the model weights in every iteration.
 - usually a <u>variant of stochastic gradient descent</u> (<u>http://ruder.io/optimizing-gradient-descent/index.html#momentum</u>)
 - RMSprop is a good all-round technique
- Metrics to monitor performance during training and testing.
 - e.g. accuracy

Cross-entropy loss (log loss)

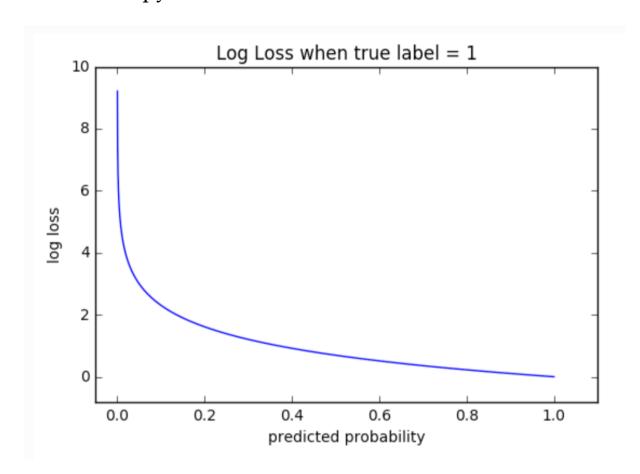
- Measures how similar the actual and predicted probability distributions are
 - Compute cross-entropy $H(y, \hat{y})$ between true y and predicted \hat{y}
 - Sum up over all training samples

$$H(y, \hat{y}) = -\sum_{c=1}^{C} y_c \log(\hat{y}_c)$$

• For binary classification, this simplifies to

$$-\sum_{c=0,1} y_c \log(\hat{y}_c) = -(y \log(\hat{y}) + (1-y) \log(1-\hat{y}))$$

Cross-entropy loss



Preprocessing

- Neural networks are sensitive to scaling, so always scale the inputs
- The network expects the data in shape (n, 28 * 28), so we also need to reshape
- We also need to categorically encode the labels
 - e.g. '4' becomes [0,0,0,0,1,0,0,0,0,0]

```
from keras.utils import to_categorical
y_train = to_categorical(y_train)
y_test = to_categorical(y_test)
```

Training

Training (fitting) is done by **stochastic gradient descent** (SGD).

Optimizes the model parameters (weights)

Prediction

We can now call predict or predict_proba to generate predictions

Evaluation

Evaluate the trained model on the entire test set

Overfitting

- Our test set accuracy is quite a bit lower than our training set accuracy
- We've already seen many choices (moving pieces) that can still be optimized:
 - Number of layers
 - Number of nodes per layer
 - Activation functions
 - Loss function (and hyperparameters)
 - SGD optimizer (and hyperparameters)
 - Batch size
 - Number of epochs
- We'll get back to this soon

Text data: preprocessing

- We can't just input text into a neural net, we need to create tensors
- First, create a *dictionary* of words (e.g. 10000 more frequent words)
 - Every word is replaced with an ID (0..10000)
 - Less frequent words replaced with '?'
- We also cannot input categories (!), we need one-hot-encoding:
 - 10000 features, '1.0' if the word occurs
- Word embeddings (word2vec):
 - Map each word to a dense vector that represents it (it's embedding)
 - *Embedding* layer: pre-trained layer that looks up the embedding in a dictionary
 - Converts 2D tensor of word indices (zero-padded) to 3D tensor of embeddings
- Let's do One-Hot-Encoding for now. We'll come back to *Embedding* layers.

IMDB movie reviews

- Dataset: 50,000 IMDB reviews, labeled positive (1) or negative (0)
 - Included in Keras, with a 50/50 train-test split
- Each row is one review, with only the 10,000 most frequent words retained
- Each word is replaced by a *word index* (word ID)

```
Encoded review: [1, 14, 22, 16, 43, 530, 973, 1622, 1385, 65]
Original review: ? this film was just brilliant casting location scenery story
```

```
# Custom implementation of one-hot-encoding
def vectorize_sequences(sequences, dimension=10000):
    results = np.zeros((len(sequences), dimension))
    for i, sequence in enumerate(sequences):
        results[i, sequence] = 1. # set specific indices of results[i]
    to 1s
        return results
x_train = vectorize_sequences(train_data)
x_test = vectorize_sequences(test_data)

Encoded review: [1, 14, 22, 16, 43, 530, 973, 1622, 1385, 65]
One-hot-encoded review: [0. 1. 1. 0. 1. 1. 1. 1. 1.]
Label: 1.0
```

Building the network

- We can solve this problem using a network of *Dense* layers and the *ReLU* activation function.
- How many layers? How many hidden units for layer?
 - Start with 2 layers of 16 hidden units each
 - We'll optimize this soon
- Output layer: single unit with *sigmoid* activation function
 - Close to 1: positive review, close to 0: negative review
 - Also vectorize the labels: from 0/1 to float

```
model = models.Sequential()
model.add(layers.Dense(16, activation='relu', input_shape=(10000,)))
model.add(layers.Dense(16, activation='relu'))
model.add(layers.Dense(1, activation='sigmoid'))
model.compile(optimizer='rmsprop', loss='binary_crossentropy', metrics=['accuracy'])
```

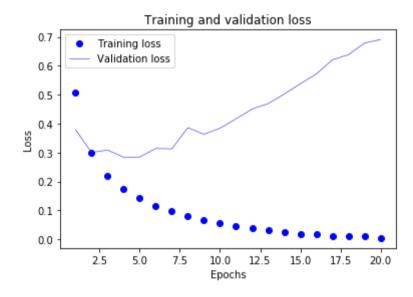
For more control, you can explictly create the optimizer, loss, and metrics:

Model selection

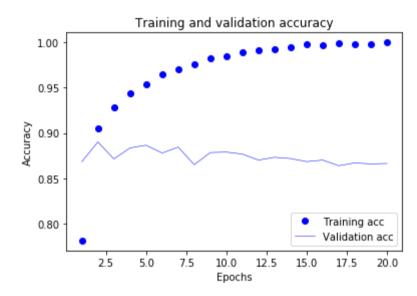
- How many epochs do we need for training?
- Take a validation set of 10,000 samples from the training set
- Train the neural net and track the loss after every iteration on the validation set
 - This is returned as a History object by the fit() function
- We start with 20 epochs in minibatches of 512 samples

We can now retrieve visualize the loss on the validation data

- The training loss keeps decreasing, due to gradient descent
- The validation loss peaks after a few epochs, after which the model starts to overfit



We can also visualize the accuracy, with similar findings



Early stopping

One simple technique to avoid overfitting is to use the validation set to 'tune' the optimal number of epochs

• In this case, we could stop after 4 epochs

Predictions

Out of curiosity, let's look at a few predictions:

Review 0: ? please give this one a miss br br ? ? and the rest of the cas t rendered terrible performances the show is flat flat flat br br i don't know how michael madison could have allowed this one on his plate he almos t seemed to know this wasn't going to work out and his performance was qui te ? so all you madison fans give this a miss Predicted positiveness: [0.016]

Review 16: ? from 1996 first i watched this movie i feel never reach the end of my satisfaction i feel that i want to watch more and more until now my god i don't believe it was ten years ago and i can believe that i almos t remember every word of the dialogues i love this movie and i love this n ovel absolutely perfection i love willem ? he has a strange voice to spell the words black night and i always say it for many times never being bored i love the music of it's so much made me come into another world deep in my heart anyone can feel what i feel and anyone could make the movie like this i don't believe so thanks thanks

Predicted positiveness: [0.927]

Takeaways

- Neural nets require a lot of preprocessing to create tensors
- Dense layers with ReLU activation can solve a wide range of problems
- Binary classification can be done with a Dense layer with a single unit, sigmoid activation, and binary cross-entropy loss
- Neural nets overfit easily
- Many design choices have an effect on accuracy and overfitting. Try:
 - 1 or 3 hidden layers
 - more or fewer hidden units (e.g. 64)
 - MSE loss instead of binary cross-entropy
 - tanh activation instead of ReLU

Wrapping Keras models as scikit-learn estimators

- Model selection can be tedious in pure Keras
- We can use all the power of scikit-learn by wrapping Keras models

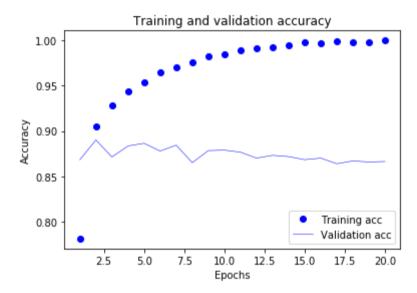
Grid search results

Out[12]:

		mean_test_score	mean_train_score
param_epochs	param_hidden_size		
1	32	0.89	0.94
	64	0.89	0.93
	256	0.89	0.93
5	32	0.88	0.97
	64	0.88	0.97
	256	0.88	0.97
10	32	0.87	0.99
	64	0.87	0.99
	256	0.87	0.99

Go a bit deeper: 3 hidden layers

• Not really worth it, very similar results



Multi-class classification (topic classification)

- Dataset: 11,000 news stories, 46 topics
 - Included in Keras, with a 50/50 train-test split
- Each row is one news story, with only the 10,000 most frequent words retained
- Each word is replaced by a *word index* (word ID)

```
News wire: ? ? said as a result of its december acquisition of space co it expects earnings per share in 1987 of 1 15 to 1 30 dlrs per share up fr om 70 cts in 1986 the company said pretax net should rise to nine to 10 ml n dlrs from six mln dlrs in 1986 and rental operation revenues to 19 to 22 mln dlrs from 12 5 mln dlrs it said cash flow per share this year should be 2 50 to three dlrs reuter 3 Encoded: [1, 2, 2, 8, 43, 10, 447, 5, 25, 207, 270, 5, 3095, 111, 16, 36 9, 186, 90, 67, 7] Topic: 3
```

Preparing the data

- We have to vectorize the data again (using one-hot-encoding)
- We have to vectorize the labels as well, also using one-hot-encoding
 - We can use Keras' to_categorical again
 - This yields a vector of 46 floats (0/1) for every sample

```
from keras.utils.np_utils import to_categorical
x_train = vectorize_sequences(train_data)
x_test = vectorize_sequences(test_data)
one_hot_train_labels = to_categorical(train_labels)
one_hot_test_labels = to_categorical(test_labels)
```

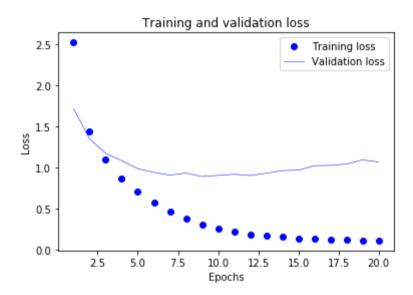
Building the network

- 16 hidden units may be too limited to learn 46 topics, hence we use 64 in each layer
- *Information bottleneck*: Every layer can drop some information, which can never be recovered by subsequent layers
- The output layer now needs 46 units, one for each topic
 - We use softmax activation for the output to get probabilities]
- The loss function is now categorical_crossentropy

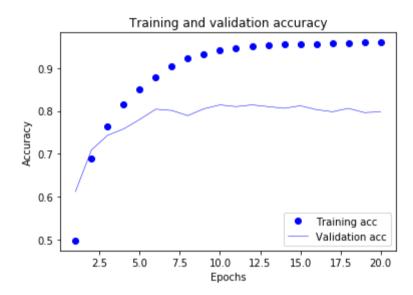
Model selection

- Take a validation set from the training set
- Fit again with 20 epochs

Loss curve:



Accuracy curve. Overfitting starts after about 8 epochs



Retrain with early stopping after 8 epochs and validate

Information bottleneck

- What happens if we create an information bottleneck on purpose
 - Use only 4 hidden units in the second layer
- Accuracy drops dramatically!
- We are trying to learn 64 separating hyperplanes from a 4-dimensional representation
 - It manages to save a lot of information, but also loses a lot

Takeaways

- For a problem with *C* classes, the final Dense layer needs *C* units
- Use softmax activation and categorical_crossentropy loss
- Information bottleneck: when classifying many classes, the hidden layers should be large enough
- Many design choices have an effect on accuracy and overfitting. Try:
 - 1 or 3 hidden layers
 - more or fewer hidden units (e.g. 128)

Regression

- Dataset: 506 examples of houses and sale prices (Boston)
 - Included in Keras, with a 1/5 train-test split
- Each row is one house price, described by numeric properties of the house and neighborhood
- Small dataset, non-normalized features

Preprocessing

- Neural nets work a lot better if we normalize the features first.
- Keras has no built-in support so we have to do this manually (or with scikit-learn)
 - Again, be careful not to look at the test data during normalization

```
mean, std = train_data.mean(axis=0), train_data.std(axis=0)
train_data -= mean
train_data /= std
test_data -= mean
test_data /= std
```

Building the network

- This is a small dataset, so easy to overfit
 - We use 2 hidden layers of 64 units each
- Use smaller batches, more epochs
- Since we want scalar output, the output layer is one unit without activation
- Loss function is Mean Squared Error (bigger penalty)
- Evaluation metric is Mean Absolute Error (more interpretable)
- We will also use cross-validation, so we wrap the model building in a function, so that we can call it multiple times

Cross-validation

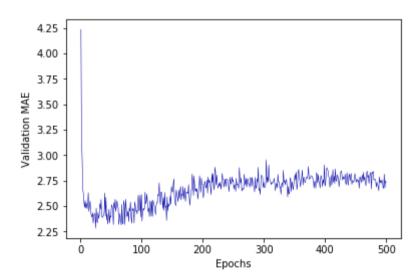
- Keras does not have support for cross-validation
- Luckily we can wrap a Keras model as a scikit-learn estimate
- We can also implement cross-validation ourselves (see notebook)
- Generally speaking, cross-validation is tricky with neural nets
 - Some fold may not converge, or fluctuate on random initialization

```
clf = KerasClassifier(build_model)
score = cross_val_score(clf, train_data, train_targets, scoring='neg_mea
n_absolute_error', cv=4, fit_params={'epochs': 100, 'batch_size':1, 'ver
bose':0});
```

MAE: 2.5091171695454286

Train for longer (500 epochs) and keep track of loss after every epoch (see code in notebook)

The model starts overfitting after epoch 80



Retrain with optimized number of epochs

Takeaways

- Regression is usually done using MSE loss and MAE for evaluation
- Input data should always be scaled (independent from the test set)
- Small datasets:
 - Use cross-validation
 - Use simple (non-deep) networks
 - Smaller batches, more epochs

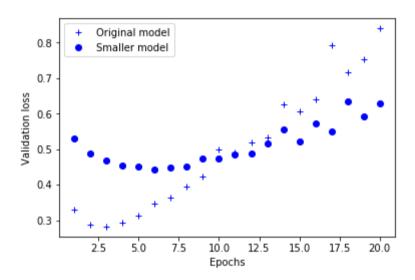
Regularization: build smaller networks

- The easiest way to avoid overfitting is to use a simpler model
- The number of learnable parameters is called the model *capacity*
- A model with more parameters has a higher memorization capacity
 - The entire training set can be stored in the weights
 - Learns the mapping from training examples to outputs
- Forcing the model to be small forces it to learn a compressed representation that generalizes better
 - Always a trade-off between too much and too little capacity
- Start with few layers and parameters, incease until you see diminisching returns

Let's try this on our movie review data, with 4 units per layer

```
smaller_model = models.Sequential()
smaller_model.add(layers.Dense(4, activation='relu', input_shape=(10000
,)))
smaller_model.add(layers.Dense(4, activation='relu'))
smaller_model.add(layers.Dense(1, activation='sigmoid'))
```

The smaller model starts overfitting later than the original one, and it overfits more *slowly*

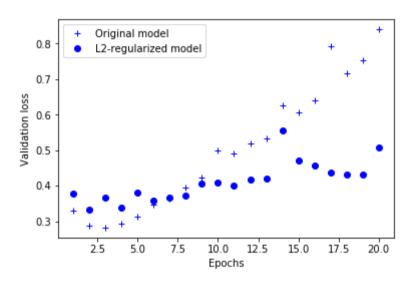


Regularization: Weight regularization

- As we did many times before, we can also add weight regularization to our loss function
- L1 regularization: leads to *sparse networks* with many weights that are 0
- L2 regularization: leads to many very small weights
 - Also called weight decay in neural net literature
- In Keras, add kernel_regularizer to every layer

from keras import regularizers

L2 regularized model is much more resistant to overfitting, even though both have the same number of parameters



You can also try L1 loss or both at the same time

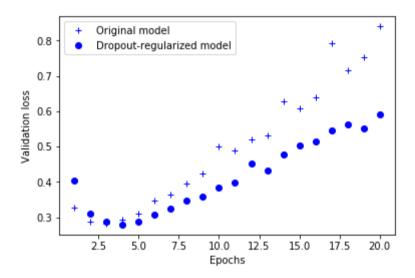
```
from keras import regularizers
```

```
# L1 regularization
regularizers.11(0.001)
# L1 and L2 regularization at the same time
regularizers.11_12(11=0.001, 12=0.001)
```

Regularization: dropout

- One of the most effective and commonly used regularization techniques
- Breakes up accidental non-significant learned patterns
- Randomly set a number of outputs of the layer to 0
- *Dropout rate*: fraction of the outputs that are zeroed-out
 - Usually between 0.2 and 0.5
- Nothing is dropped out at test time, but the output values are scaled down by the dropout rate
 - Balances out that more units are active than during training
- In Keras: add Dropout layers between the normal layers

Dropout finds a better model, and overfits more slowly as well

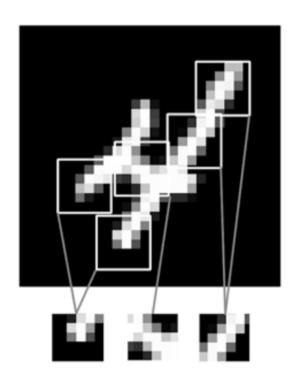


Regularization recap

- Get more training data
- Reduce the capacity of the network
- Add weight regularization
- Add dropout
- Either start with a simple model and add capacity
- Or, start with a complex model and then regularize by adding weight regularization and dropout

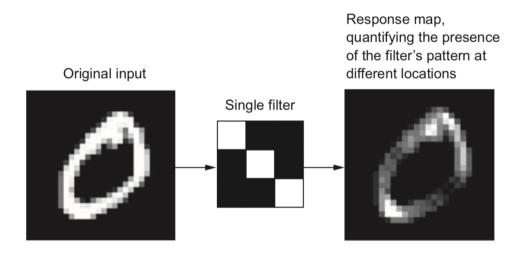
Convolutional neural nets

- When processing image data, we want to discover 'local' patterns (between nearby pixels)
 - edges, lines, structures
- Consider *windows* (or *patches*) of pixels (e.g 5x5)



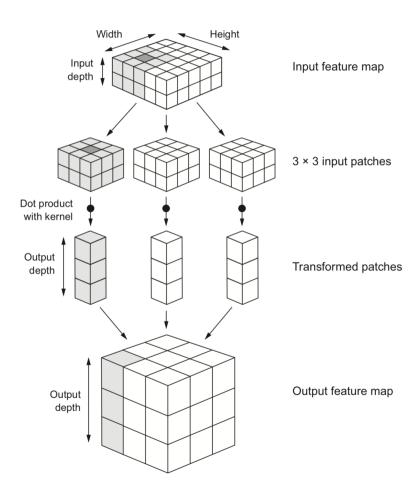
Convolution

- Slide an $n \times n$ filter (or kernel) over $n \times n$ patches of the input feature map
- Replace pixel values with the convolution of the kernel with the underlying image patch



Convolutional layers: Feature maps

- We slide *d* filters across the input image in parallel, producing a (1x1xd) output per patch, reassembled into the final *feature map* with *d* channels.
- The filters are randomly initialized, we want to *learn* the optimal values



Undersampling

- Sometimes, we want to *downsample* a high-resolution image
 - Faster processing, less noisy (hence less overfitting)
- One approach is to *skip* values during the convolution
 - Distance between 2 windows: *stride length*
- Example with stride length 2 (without padding):

			1	
1	2			
3	4			
			3	
		J		

Max-pooling

- Another approach to shrink the input tensors is *max-pooling*:
 - Run a filter with a fixed stride length over the image
 - Usually 2x2 filters and stride length 2
 - The filter returns the *max* (or *avg*) of all values
- Agressively reduces the number of weights (less overfitting)
- Information from every input node spreads more quickly to output nodes
 - In pure convnets, one input value spreads to 3x3 nodes of the first layer, 5x5 nodes of the second, etc.
 - You'd need much deeper networks, which are much harder to train

Convolutional nets in practice

- Let's model MNIST again, this time using convnets
- Conv2D for 2D convolutional layers
 - Default: 32 filters, randomly initialized (from uniform distribution)
- MaxPooling2D for max-pooling
 - 2x2 pooling reduces the number of inputs by a factor 4

Observe how the input image is reduced to a 3x3x64 feature map

Layer (type)	Output	Shape	Param #
conv2d_4 (Conv2D)	(None,	26, 26, 32)	320
max_pooling2d_3 (MaxPooling2	(None,	13, 13, 32)	0
conv2d_5 (Conv2D)	(None,	11, 11, 64)	18496
max_pooling2d_4 (MaxPooling2	(None,	5, 5, 64)	0
conv2d_6 (Conv2D)	(None,	3, 3, 64)	36928 =======

Total params: 55,744

Trainable params: 55,744
Non-trainable params: 0

Compare to the architecture without max-pooling:

• Output layer is a 22x22x64 feature map!

Layer (type)	Output Shape	Param #
conv2d_7 (Conv2D)	(None, 26, 26, 32)	320
conv2d_8 (Conv2D)	(None, 24, 24, 64)	18496
conv2d_9 (Conv2D)	(None, 22, 22, 64)	36928

Total params: 55,744

Trainable params: 55,744 Non-trainable params: 0

- To classify the images, we still need a Dense and Softmax layer.
- We need to flatten the 3x3x36 feature map to a vector of size 576

```
model.add(layers.Flatten())
model.add(layers.Dense(64, activation='relu'))
model.add(layers.Dense(10, activation='softmax'))
```

Layer (type)	Output	Shape	Param #
conv2d_4 (Conv2D)	(None,	26, 26, 32)	320
<pre>max_pooling2d_3 (MaxPooling2</pre>	(None,	13, 13, 32)	0
conv2d_5 (Conv2D)	(None,	11, 11, 64)	18496
max_pooling2d_4 (MaxPooling2	(None,	5, 5, 64)	0
conv2d_6 (Conv2D)	(None,	3, 3, 64)	36928
flatten_1 (Flatten)	(None,	576)	0
dense_30 (Dense)	(None,	64)	36928
dense_31 (Dense)	(None,	10)	650 =======

Total params: 93,322

Trainable params: 93,322
Non-trainable params: 0

- Train and test as usual (takes about 5 minutes):
- Compare to the 97,8% accuracy of the earlier dense architecture

Exercises

- Build simple feed-forward neural net for Fashion MNIST
- Build a convolutional neural net and compare the results
- Try to improve the model with further finetuning
- Upload your best models to OpenML and compare with the best models there
 - Wrap Keras models in KerasClassifier
- Try to build better models for the IMDB and News wire datasets