6 - Representation Learning

André Lamúrias

Motivation

Motivation

Features are very important

- Example: long division using Arabic or Roman numerals
- In machine learning, the right representation makes all the difference
- Deep learning can be seen as stacked feature extractors, until the final classification
  - The top layer could even be replaced by another type of model, in theory

Representation learning

- Supervised learning with limited data can lead to overfitting
- But learning the best representation can be done with unlabelled data
  - Unsupervised and semi-supervised learning can help find the right features

Motivation

"Meta-priors": what makes a good representation?

Representation Learning; Bengio, Courville, Vincent, 2013

- **Manifolds:**
  - Actual data is distributed in a subspace of all possible feature value combinations
- **Disentanglement:**
  - Data is generated by combination of independent factors (e.g. shape, color, lighting, ...)
- **Hierarchical organization of explanatory factors:**
  - Concepts that explain reality can be composed of more elementar concepts (e.g. edges, shapes, patterns)
- **Semi-supervised learning:**
  - Unlabelled data is more numerous and can be used to learn structure

Motivation

"Meta-priors": what makes a good representation?

Representation Learning; Bengio, Courville, Vincent, 2013

- Shared factors:
  - Important features for one problem may also be important for other problems (e.g. image recognition)
- Sparsity:
  - Each example may contain only some of the relevant factors (ears, tail, legs, wings, feet)
- Smoothness:
  - The function we are learning outputs similar y for similar x

Motivation

"Meta-priors": what makes a good representation?

Representation Learning; Bengio, Courville, Vincent, 2013

- If we can capture these regularities, we can extract useful features from our data
- These features can be reused in different problems, even with different data

Unsupervised Pretraining

Unsupervised Pretraining

Greedy layer-wise unsupervised pretraining

- Greedy: optimizes each part independently
- Layer-wise: pretraining is done one layer at a time
  - E.g. train autoencoder, discard decoder, use encoding as input for next layer (another autoencoder)
- Unsupervised: each layer is trained without supervision (e.g. autoencoder)
- Pretraining: the goal is to initialize the network
  - It is followed by fine-tuning with backpropagation
  - Or by training of a classifier "on top" of the pretrained layers

Unsupervised Pretraining

Why should this work?

- Initialization has regularizing effect

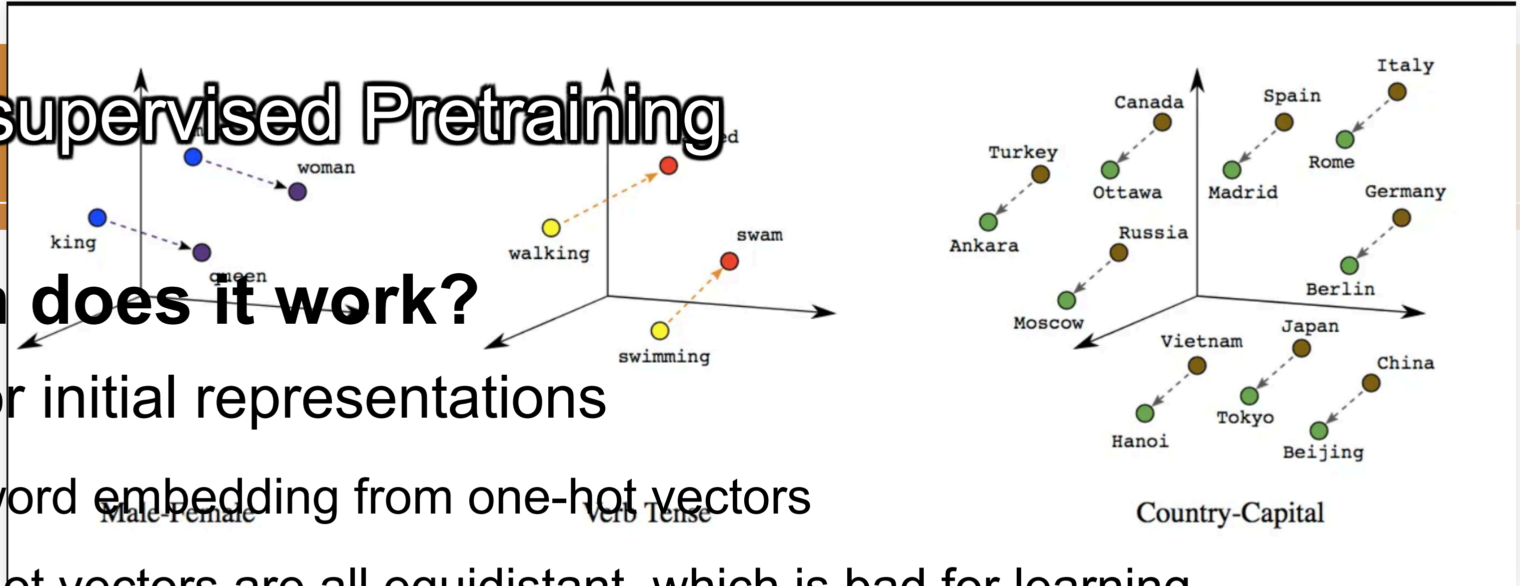
- Initially thought as a way to find different local minima, but this does not seem to be the case (ANN do not generally stop at minima)
- It may be that pretraining allows the network to reach a different region of the parameter space

Unsupervised Pretraining

When does it work?

- Poor initial representations
  - E.g. word embedding from one-hot vectors
  - One-hot vectors are all equidistant, which is bad for learning
  - Unsupervised pretraining helps find representations that are more useful
- Example: (Large) Language Models
  - Known as self-supervised learning, latent representations are called word embeddings

Unsupervised Pretraining



https://developers.google.com/machine-learning/crash-course/embeddings/translating-to-a-lower-dimensional-space

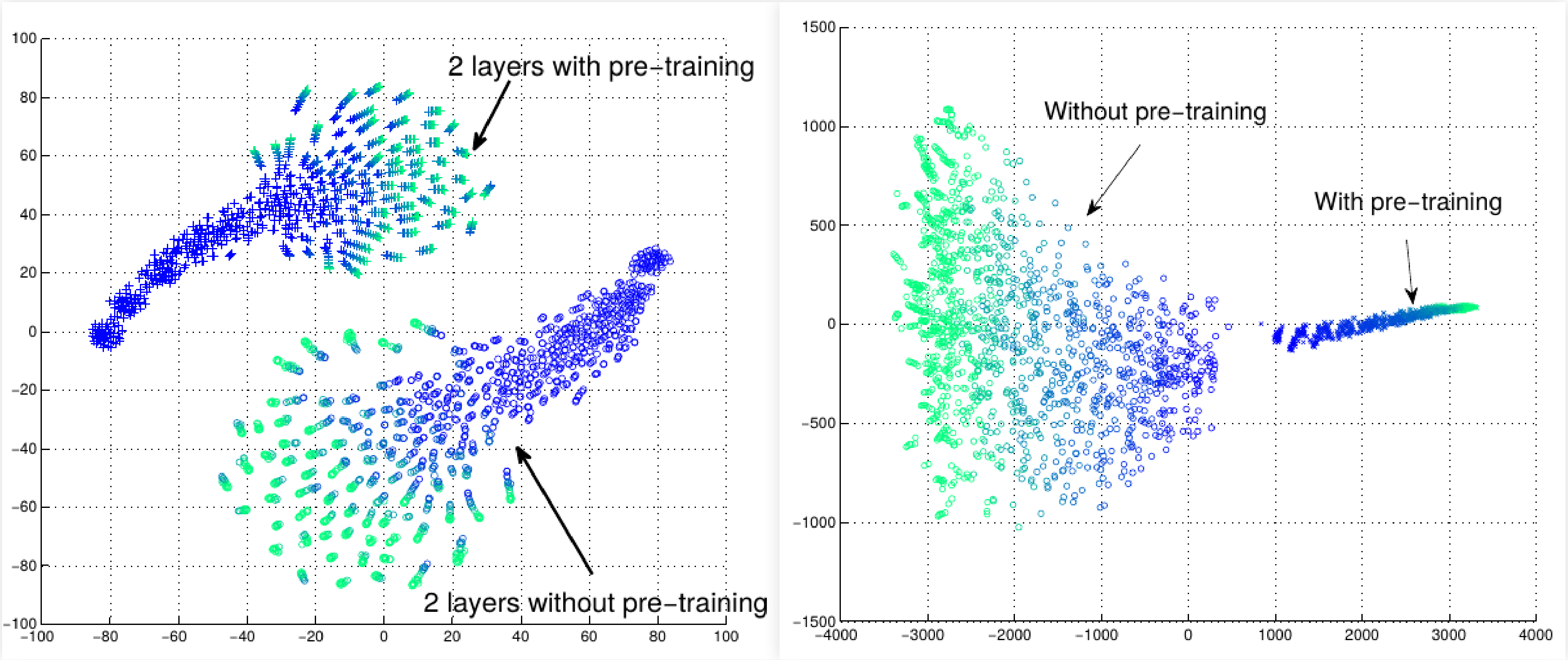
When does it work?

- Poor initial representations
  - E.g. word embedding from one-hot vectors
  - One-hot vectors are all equidistant, which is bad for learning
  - Unsupervised pretraining helps find representations that are more useful
- Regularization, for few labelled examples
  - If labelled data is scarce, there is greater need for regularization and unsupervised pretraining can use unlabelled data for this
- Example: Training trajectories with and without pretraining
  - Concatenate vector of outputs for all test set at different iterations
  - (50 nertworks with and without pretraining)
  - Project into 2D (tSNE and ISOMAP)

Unsupervised Pretraining

- Regularizing effect

- Ehrlan et. al. 2010: output vectors for all data, reduce dimensionality, plot



t-Distributed Stochastic Neighbor Embedding and ISOMAP

Unsupervised Pretraining

Unsupervised pretraining is historically important

- It was the first practical method for training deep networks
- Most DL problems habed abandoned it because of ReLU and dropout, which allows efficient supervised training and regularization of the whole network
  - For very small datasets, other methods outperform neural networks
  - e.g. Bayesian methods
- Another disadvantage: having two training stages makes it harder to adjust Hyperparameters
- Commonly used in some applications, such as natural language processing
  - Unsupervised pretraining with billions of examples to learn good word representations

Transfer Learning

Two different tasks with shared relevant factors

- Shared lower level features:
  - E.g. distinguish between cats and dogs, or between horses and donkeys
  - The low level features are mostly the same, only the higher level classification layers need to change
- Shared higher level representations:
  - E.g. speech recognition
  - The high level generation of sentences is the same for different speakers
  - However, the low level feature extraction may need to be tailored to each speaker

Domain adaptation

Same underlying function but different domains

- We want to model the same mapping from input to output, but are using different sets of examples
- E.g. sentiment analysis
  - Model was trained on customer reviews for movies and songs
  - Now we need to do the same for electronics
  - There should be only one mapping from words to happy or unhappy, but we are training on different sets with different words
  - This is one example where unsupervised training (DAE - denoising autoencoders) can help

Concept Drift

Similar to Transfer learning or domain adaptation

- But occurs when the change is gradual over time

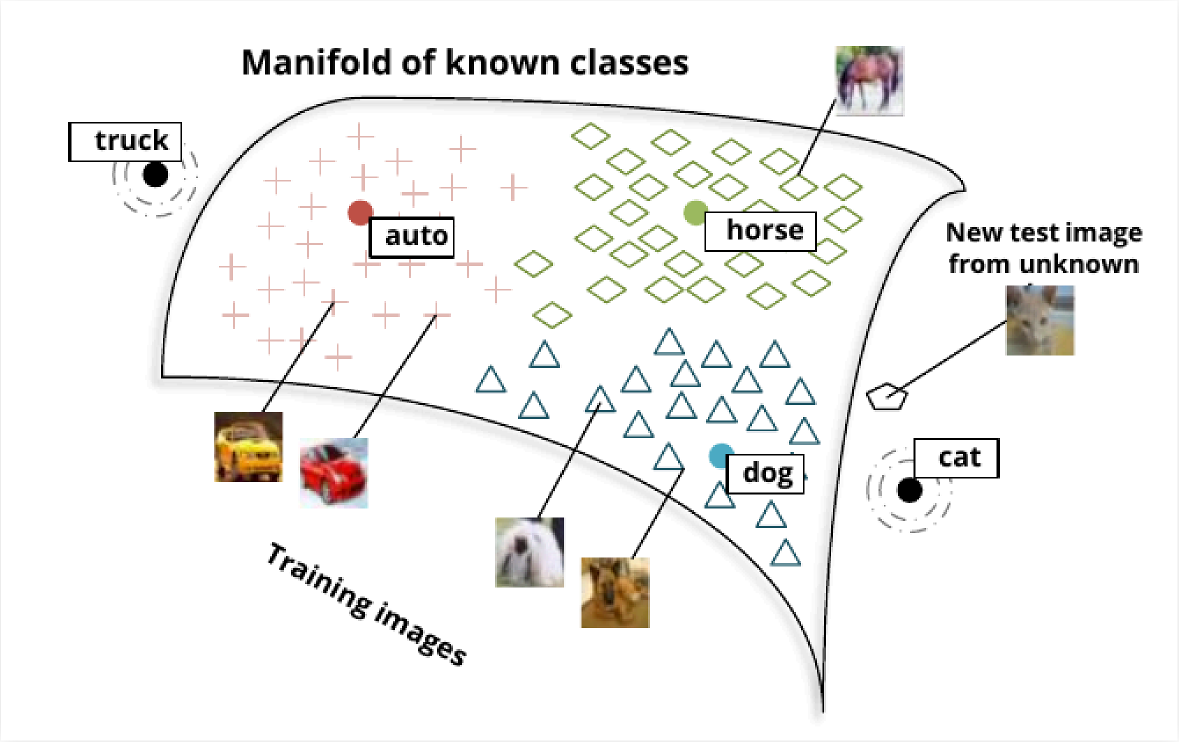
- E.g. as the brand becomes more popular, customer base changes from specialized to general

Use previous experience in new conditions

- The common idea is that we can use what was learned before to help learn now
- Extreme examples: one-shot learning and zero-shot learning
- Zero-shot learning: no labelled examples of new classes are necessary
  - Everything was learned on other classes or unsupervised
- One-shot learning: use only one labelled example to learn new dataset
  - The rest was learned on other data

Transfer Learning

- Zero-shot learning, example:
  - Unsupervised learning of word manifold, supervised mapping of known images
  - A new image is mapped to word manifold



Socher et. al. Zero-Shot Learning Through Cross-Modal Transfer (2013)

Summary

Representation learning

Summary

- Improve learning from poor representations
  - Find the best features
- Regularization or feature extraction with unlabelled data
- Historically important in deep learning
  - Still used in NLP (self-supervised learning)
- Transfer learning (often supervised)

Further reading

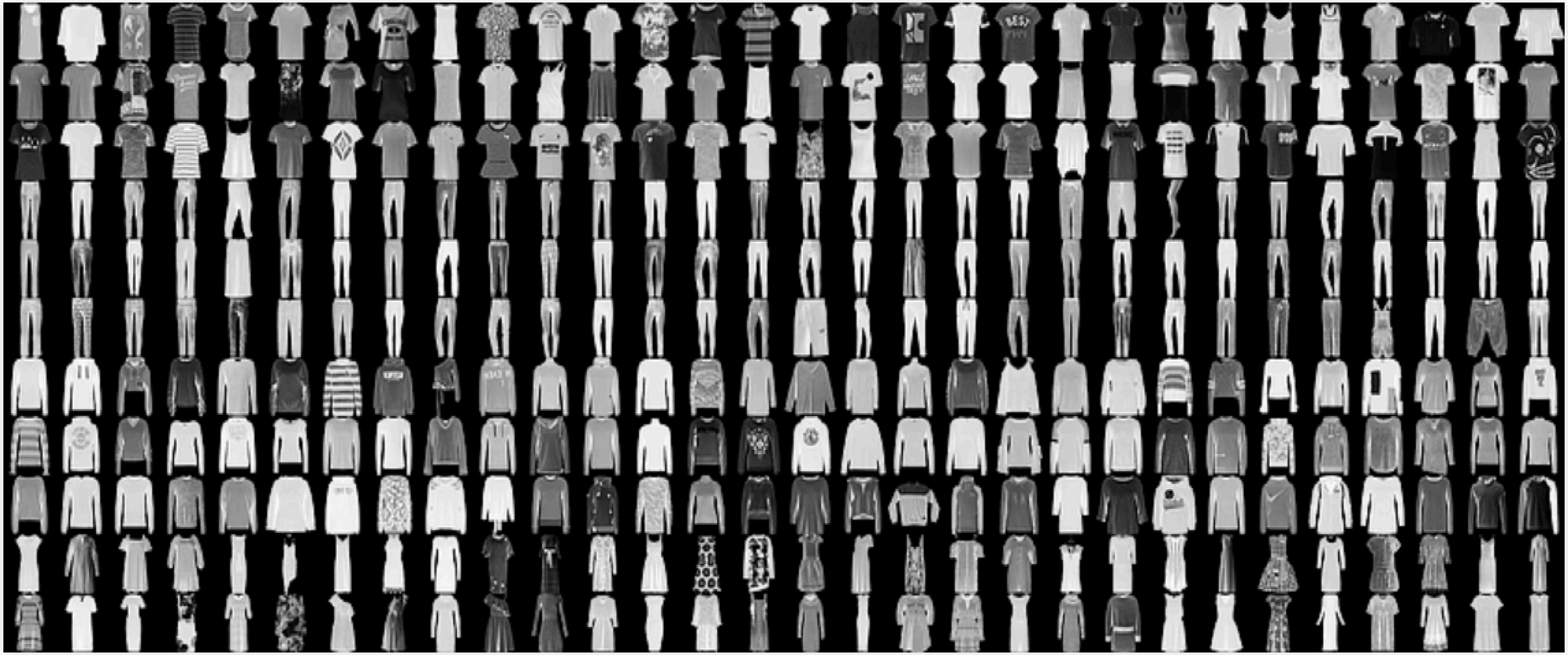
- Goodfellow et.al, Deep learning, Chapter 15 (and 8.7.4)
- Bengio et. al. Representation Learning: A Review and New Perspectives, 2013

Exercise 1: transfer learning Fashion MNIST to MNIST

Exercise

Transfer learning

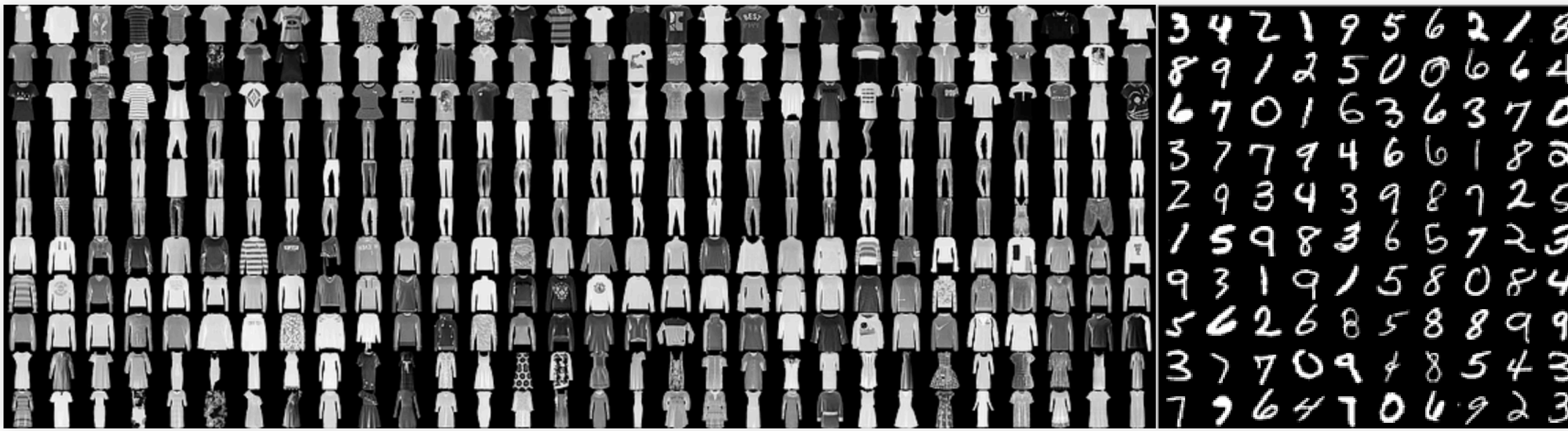
- Use network trained on Fashion MNIST



Exercise

Transfer learning

- Use network trained on Fashion MNIST



- Use Keras functional API and pre-trained model

Transfer learning

- Using pre-trained model:

- Create same graph as model we trained last week
- Load weights from last week's trained model
- Fix weights of convolutional part (won't be retrained)
- Recreate the dense classifier and train it on MNIST

Exercise

Prepare dataset

- Same process as last week, but with MNIST instead of Fashion MNIST

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

((trainX, trainY), (testX, testY)) = keras.datasets.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
```

Exercise

- Keras functional API
  - Layer objects are callable (implement `__call__` method)
  - Receive tensors as arguments, return tensors
  - `Input` instantiates a Keras tensor (shaped like the data)
  - Naming layers helps finding them again in the model
- We start by recreating the original model architecture

```
inputs = Input(shape=(28,28,1),name='inputs')
layer = Conv2D(32, (3, 3), padding="same", input_shape=(28,28,1))(inputs)
layer = Activation("relu")(layer)
layer = BatchNormalization(axis=-1)(layer)
layer = Conv2D(32, (3, 3), padding="same")(layer)
layer = Activation("relu")(layer)
layer = BatchNormalization(axis=-1)(layer)
layer = MaxPooling2D(pool_size=(2, 2))(layer)
layer = Dropout(0.25)(layer)
...
```

Exercise

- Chain layers as in the original model
- Create the old model and compile it
- Load previous weights and disable training in the old model
- Note: `Flatten` layer named for use in new model

```
...
features = Flatten(name='features')(layer)
layer = Dense(512)(features)
layer = Activation("relu")(layer)
layer = BatchNormalization()(layer)
layer = Dropout(0.5)(layer)
layer = Dense(10)(layer)
layer = Activation("softmax")(layer)

old_model = Model(inputs = inputs, outputs = layer)
old_model.compile(optimizer=SGD(), loss='mse')
old_model.load_weights('fashion_model')
for layer in old_model.layers:
    layer.trainable = False
```

Exercise

- Create new dense layers for new model
  - The input for this layer is the `"features"` layer in old model
- Then create the new model with:
  - Old model `inputs` as input
  - New softmax layer as output
- This chains old CNN to new dense layer

```
layer = Dense(512)(old_model.get_layer('features').output)
layer = Activation("relu")(layer)
layer = BatchNormalization()(layer)
layer = Dropout(0.5)(layer)
layer = Dense(10)(layer)
layer = Activation("softmax")(layer)
model = Model(inputs = old_model.get_layer('inputs').output, outputs = layer)
```

Exercise

- Now train

```
NUM_EPOCHS = 5
BS=512
opt = SGD(lr=1e-2, momentum=0.9)
model.compile(loss="categorical_crossentropy",
              optimizer=opt, metrics=["accuracy"])
model.summary()
H = model.fit(trainX, trainY,validation_data=(testX, testY),
             batch_size=BS, epochs=NUM_EPOCHS)
```

- Summary:

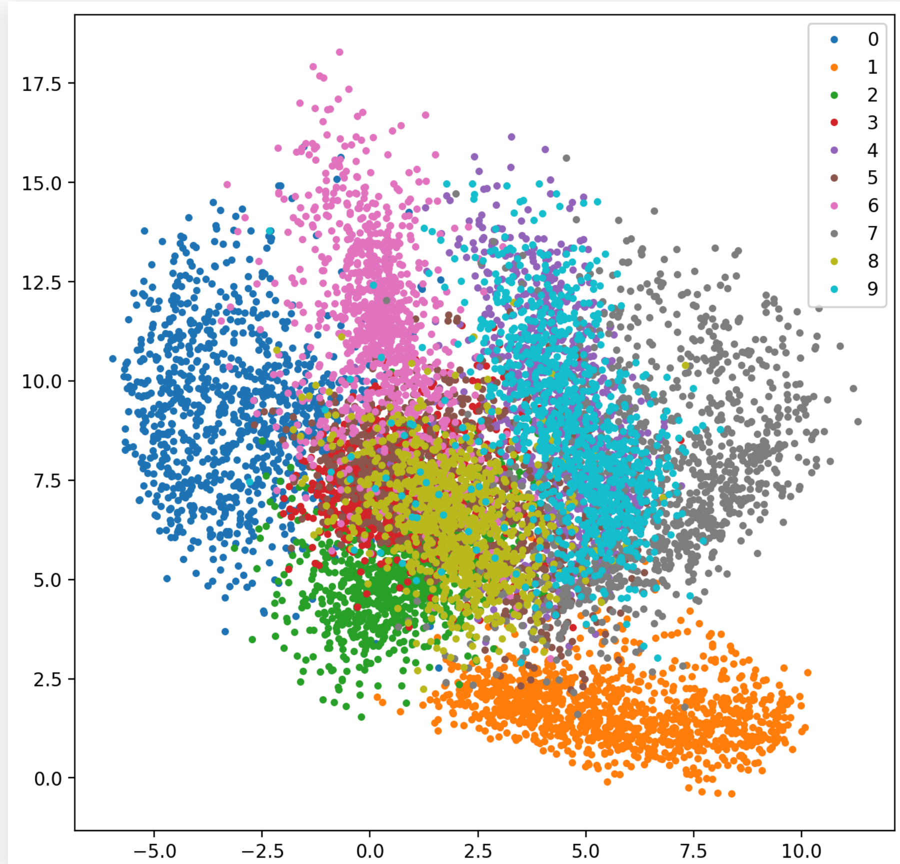
```
Total params: 1,679,082
Trainable params: 1,612,298
Non-trainable params: 66,784
```

- Compare with training all model from the start

Exercise 2: dimension reduction with autoencoder

Autoencoder

- Project MNIST data set into 2D



Autoencoder

- Need some extra layers:

```
from tensorflow.keras.layers import UpSampling2D,Reshape
```

- Encoder:

```
def autoencoder():
  inputs = Input(shape=(28,28,1),name='inputs')
  layer = Conv2D(32, (3, 3), padding="same", input_shape=(28,28,1))(inputs)
  layer = Activation("relu")(layer)
  layer = BatchNormalization(axis=-1)(layer)
  #[...] parts missing here!
  layer = MaxPooling2D(pool_size=(2, 2))(layer)
  #[...] parts missing here!
  layer = Conv2D(8, (3, 3), padding="same")(layer)
  layer = Activation("relu")(layer)
  layer = BatchNormalization(axis=-1)(layer)

  layer = Flatten()(layer)
  features = Dense(2,name='features')(layer)
```

Autoencoder

- Decoder:

```
layer = BatchNormalization()(features)
layer = Dense(8*7*7,activation="relu")(features)
layer = Reshape((7,7,8))(layer)
layer = Conv2D(8, (3, 3), padding="same")(layer)
layer = Activation("relu")(layer)
layer = BatchNormalization(axis=-1)(layer)
layer = Conv2D(16, (3, 3), padding="same")(layer)
layer = Activation("relu")(layer)
layer = BatchNormalization(axis=-1)(layer)
layer = UpSampling2D(size=(2,2))(layer)
[...]
layer = Conv2D(32, (3, 3), padding="same")(layer)
layer = Activation("relu")(layer)
layer = BatchNormalization(axis=-1)(layer)
layer = Conv2D(1, (3, 3), padding="same")(layer)
layer = Activation("sigmoid")(layer)
autoencoder = Model(inputs = inputs, outputs = layer)
encoder = Model(inputs=inputs,outputs=features)
return autoencoder,encoder
```

Suggestions

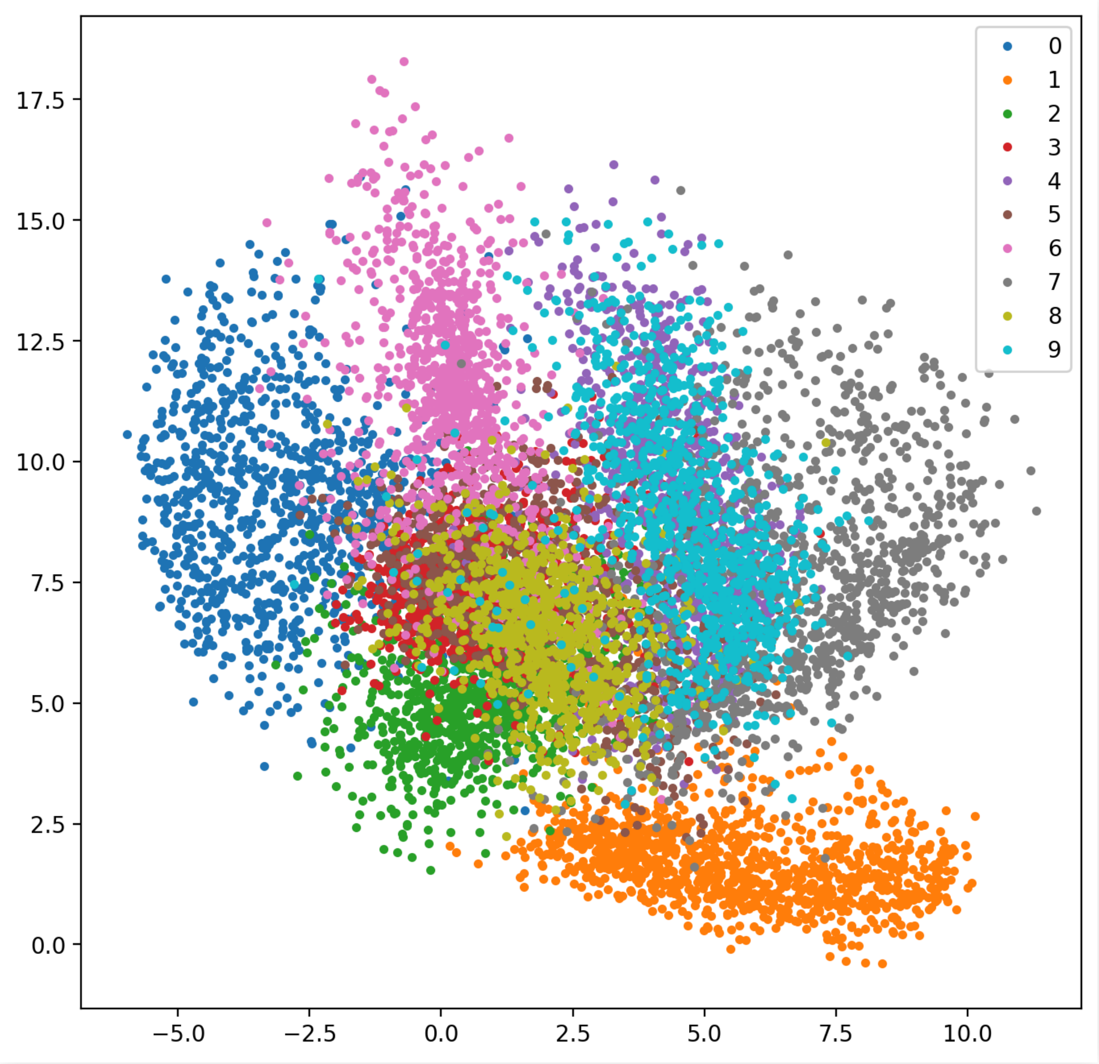
- Architecture:
  - Convolution layer with 32 filters, followed by pooling
  - Convolution layer with 32 filters, then convolution layer with 16 filters, then pooling
  - Convolution layer with 16 filters, then convolution layer with 8 filters, then pooling
  - Dense layer with 2 neurons and linear output, then dense layer with 8*7*7 neurons (relu) and reshape
  - Convolutions in reverse (8, 16, 16, 32 and 32 filters), and upsampling
  - A final convolution of 1 filter for the (sigmoid) output.
- Training: takes some time (40 epochs or more...)
  - Details weigh little on the loss function
- Save weights after training!

Autoencoder

- Check representation, plot in 2D:

```
def plot_representation():
    ae,enc = autoencoder()
    ae.load_weights('mnist_autoencoder.h5')
    encoding = enc.predict(testX)
    plt.figure(figsize=(8,8))
    for cl in np.unique(testY):
        mask = testY == cl
        plt.plot(encoding[mask,0],encoding[mask,1],'.',label=str(cl))
    plt.legend()
```

Autoencoder



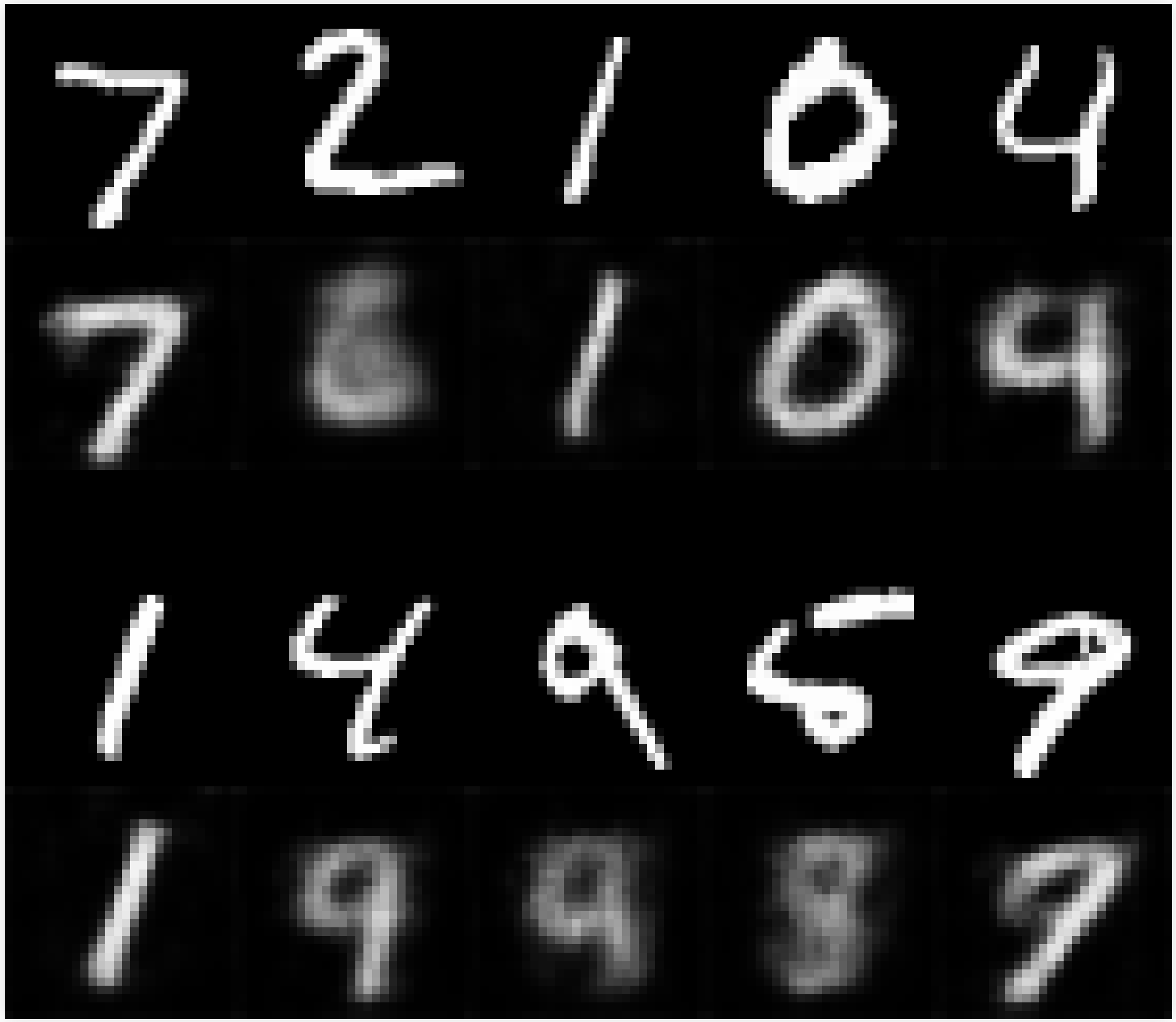
Autoencoder

- Check reconstruction:

```
from skimage.io import imsave

def check_images():
    ae,enc = autoencoder()
    ae.load_weights('mnist_autoencoder.h5')
    imgs = ae.predict(testX[:10])
    for ix in range(10):
        imsave(f'T03_{ix}_original.png',testX[ix])
        imsave(f'T03_{ix}_restored.png',imgs[ix])
```

Autoencoder

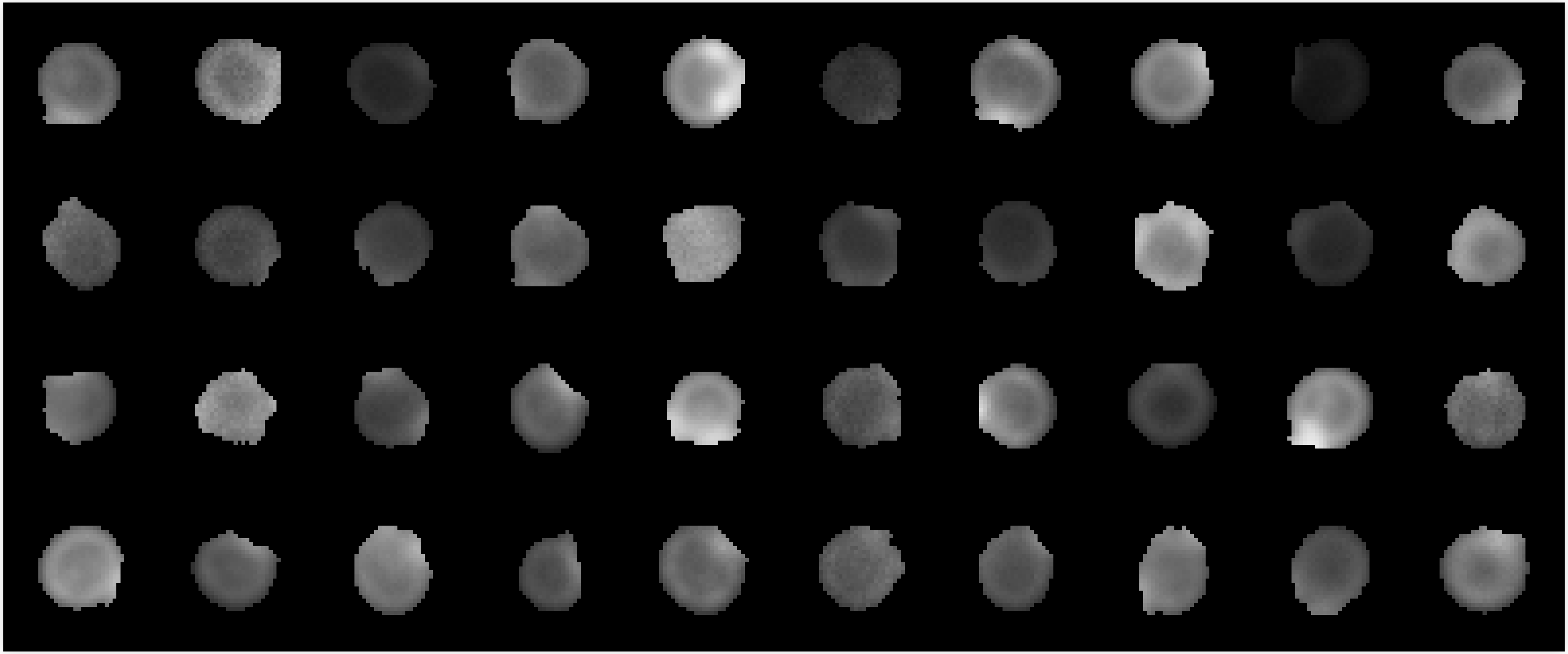


Assignment 1

Assignment 1

Context: image classification

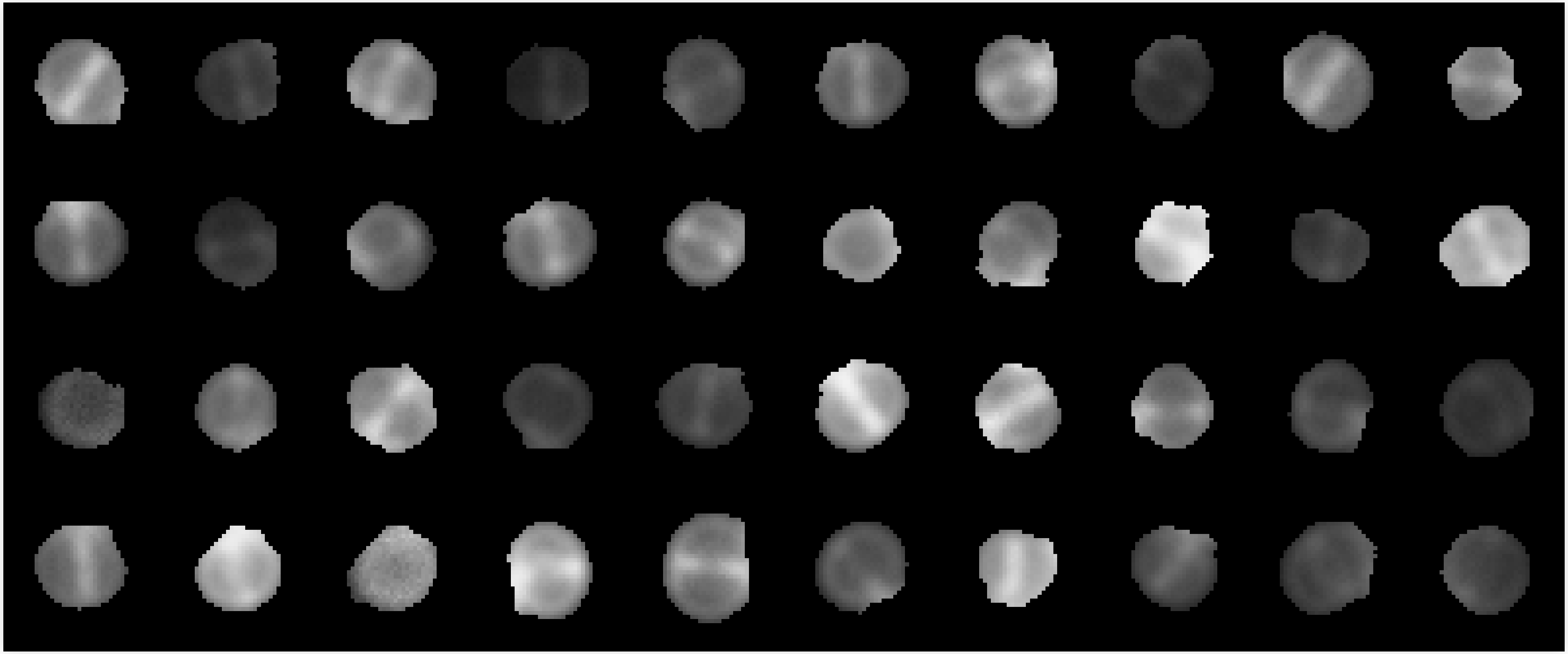
- Super-resolution fluorescence microscopy images of bacteria
- Stage 0: before division starts



Assignment 1

Context: image classification

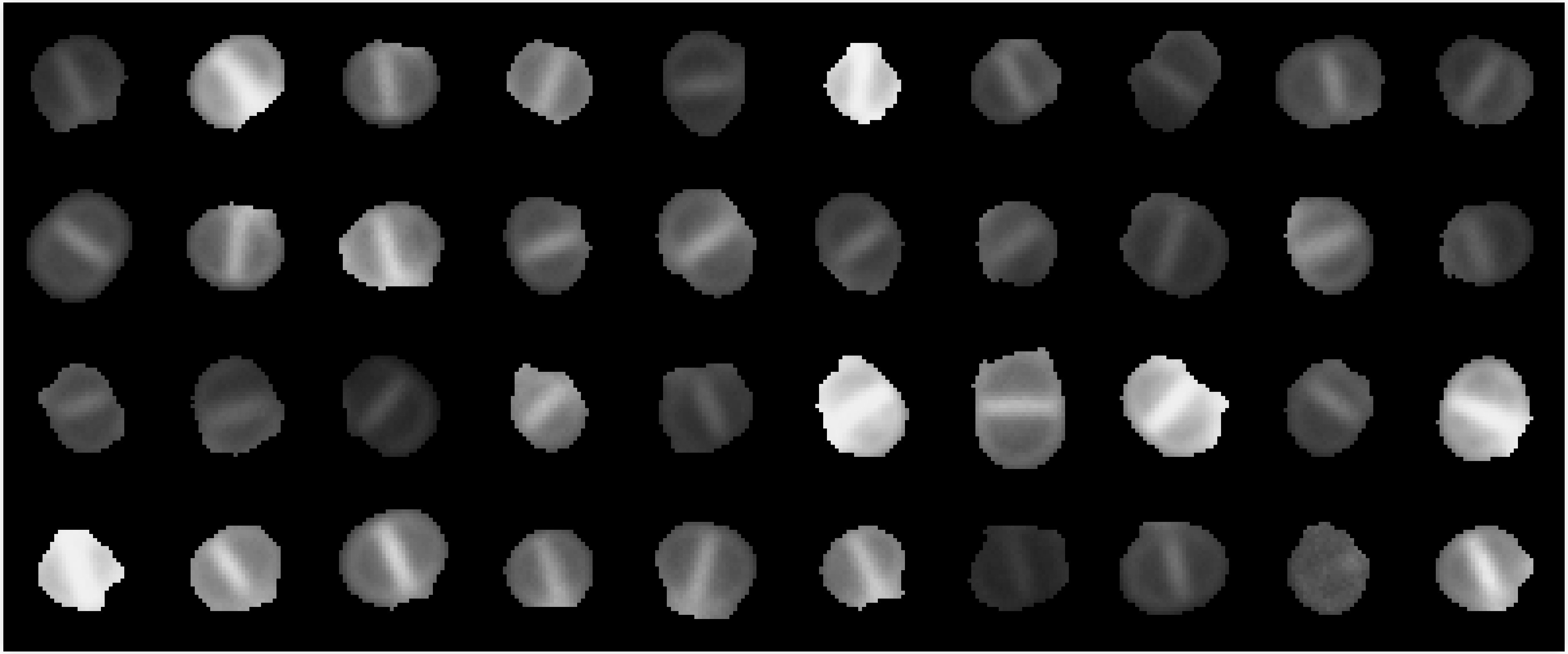
- Super-resolution fluorescence microscopy images of bacteria
- Stage 1: septum starts to form



Assignment 1

Context: image classification

- Super-resolution fluorescence microscopy images of bacteria
- Stage 2: septum is formed, before cell splits



Assignment 1

- Data:400 labelled images, 3892 unlabelled images
  - (40x40 pixels, grayscale)

```
data = np.load('data.npz')
X_u = data['unlabelled'].astype("float32") / 255.0
X_l = data['labelled'].astype("float32") / 255.0
Y_l = keras.utils.to_categorical(data['labels'],3)
```

- Tasks: experiment, justify and discuss architectures for
  - A classifier using the 400 labelled images (300 train, 100 validation)
  - An autoencoder with 3892 unlabelled images (use the 400 for validation)
  - A simpler classifier using the encoded representations of the 400 labelled images (300 train, 100 validation)
- Similar to the exercises we have done so far.
- Deadline: March 29 (ideally)