# 01\_deep\_autoencoders

September 29, 2021

## 1 Designing and training autoencoders using Python

In this notebook, we illustrate how to implement several of the autoencoder models introduced in the preceding section using Keras. We first load and prepare an image dataset that we use throughout this section because it makes it easier to visualize the results of the encoding process.

We then proceed to build autoencoders using deep feedforward nets, sparsity constraints, and convolutions and then apply the latter to denoise images.

Source: https://blog.keras.io/building-autoencoders-in-keras.html

## 1.1 Imports & Settings

```
[1]: %matplotlib inline
     from pathlib import Path
     import numpy as np
     from numpy.random import choice
     from numpy.linalg import norm
     import pandas as pd
     import tensorflow as tf
     from tensorflow.keras.layers import Input, Dense
     from tensorflow.keras import regularizers
     from tensorflow.keras.models import Model
     from tensorflow.keras.callbacks import TensorBoard, EarlyStopping, u
     →ModelCheckpoint
     from tensorflow.keras.datasets import fashion_mnist
     from sklearn.preprocessing import minmax_scale
     from sklearn.manifold import TSNE
     from scipy.spatial.distance import pdist, cdist
     import seaborn as sns
     import matplotlib.pyplot as plt
     from matplotlib.colors import ListedColormap
     from matplotlib.offsetbox import AnnotationBbox, OffsetImage
     from mpl_toolkits.axes_grid1 import make_axes_locatable
[2]: gpu_devices = tf.config.experimental.list_physical_devices('GPU')
     if gpu_devices:
         print('Using GPU')
         tf.config.experimental.set_memory_growth(gpu_devices[0], True)
         print('Using CPU')
    Using CPU
[3]: sns.set_style('whitegrid')
[4]: n_classes = 10 # all examples have 10 classes
     cmap = sns.color_palette('Paired', n_classes)
[5]: results_path = Path('results', 'fashion_mnist')
     if not results_path.exists():
         results_path.mkdir(parents=True)
```

### 1.2 Fashion MNIST Data

For illustration, we'll use the Fashion MNIST dataset, a modern drop-in replacement for the classic MNIST handwritten digit dataset popularized by Yann LeCun with LeNet in the 1990s. We also relied on this dataset in Chapter 12, Unsupervised Learning.

```
[6]: (X_train, y_train), (X_test, y_test) = fashion_mnist.load_data()
```

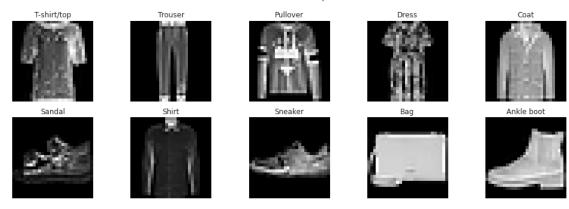
Keras makes it easy to access the 60,000 train and 10,000 test grayscale samples with a resolution of  $28 \times 28$  pixels:

### 1.2.1 Plot sample images

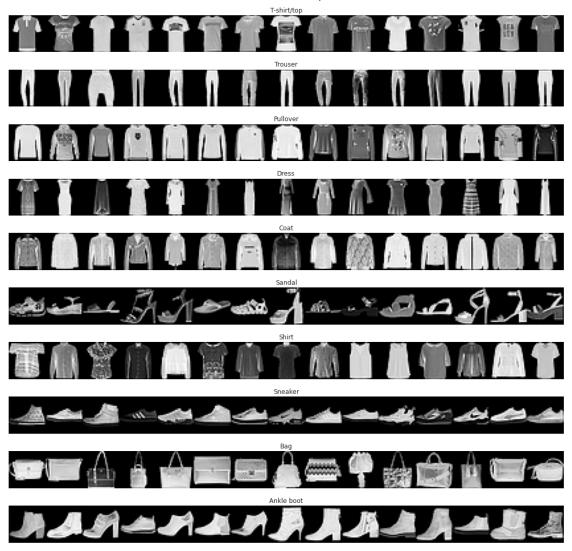
```
fig, axes = plt.subplots(nrows=2, ncols=5, figsize=(14, 5))
axes =axes.flatten()
for row, label in enumerate(classes):
    label_idx = np.argwhere(y_train == label).squeeze()
    axes[row].imshow(X_train[choice(label_idx)], cmap='gray')
    axes[row].axis('off')
    axes[row].set_title(class_dict[row])

fig.suptitle('Fashion MNIST Samples', fontsize=14)
fig.tight_layout()
fig.subplots_adjust(top=.85)
```

Fashion MNIST Samples



```
[11]: n_samples = 15
      fig, axes = plt.subplots(nrows=n_classes, figsize=(15, 15))
      axes =axes.flatten()
      for row, label in enumerate(classes):
          class_imgs = np.empty(shape=(image_size, n_samples * image_size))
          label_idx = np.argwhere(y_train == label).squeeze()
          class_samples = choice(label_idx, size=n_samples, replace=False)
          for col, sample in enumerate(class_samples):
              i = col * image_size
              class_imgs[:, i:i + image_size] = X_train[sample]
          axes[row].imshow(class_imgs, cmap='gray')
          axes[row].axis('off')
          axes[row].set_title(class_dict[row])
      fig.suptitle('Fashion MNIST Samples', fontsize=16)
      fig.tight_layout()
      fig.subplots_adjust(top=.95, bottom=0)
```



## 1.3 Reshape & normalize Fashion MNIST data

We reshape the data so that each image is represented by a flat one-dimensional pixel vector with  $28 \times 28 = 784$  elements normalized to the range of [0, 1]:

```
[12]: encoding_size = 32 # Size of encoding
[13]: def data_prep(x, size=input_size):
    return x.reshape(-1, size).astype('float32')/255
[14]: X_train_scaled = data_prep(X_train)
    X_test_scaled = data_prep(X_test)
```

```
[15]: X_train_scaled.shape, X_test_scaled.shape
```

```
[15]: ((60000, 784), (10000, 784))
```

## 1.4 Vanilla single-layer autoencoder

We start with a vanilla feedforward autoencoder with a single hidden layer to illustrate the general design approach using the functional Keras API and establish a performance baseline.

Encoding 28 x 28 images to a 32 value representation for a compression factor of 24.5

## 1.4.1 Single-layer Model

### Input Layer

```
[16]: input_ = Input(shape=(input_size,), name='Input')
```

**Dense Encoding Layer** The encoder part of the model consists of a fully-connected layer that learns the new, compressed representation of the input. We use 32 units for a compression ratio of 24.5:

**Dense Reconstruction Layer** The decoding part reconstructs the compressed data to its original size in a single step:

### Autoencoder Model

The thus defined encoder-decoder computation uses almost 51,000 parameters:

```
[20]: autoencoder.summary()
```

## Model: "Autoencoder"

Layer (type)	Output Shape	Param #
Input (InputLayer)	[(None, 784)]	0
Encoder (Dense)	(None, 32)	25120

Decoder (Dense) (None, 784) 25872

Total params: 50,992 Trainable params: 50,992 Non-trainable params: 0

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### 1.4.2 Encoder Model

The functional API allows us to use parts of the model's chain as separate encoder and decoder models that use the autoencoder's parameters learned during training.

The encoder just uses the input and hidden layer with about half of the total parameters:

[22]: encoder.summary()

Model: "Encoder"

Layer (type) Output Shape Param #

Input (InputLayer) [(None, 784)] 0

Encoder (Dense) (None, 32) 25120

Total params: 25,120 Trainable params: 25,120 Non-trainable params: 0

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Once we train the autoencoder, we can use the encoder to compress the data.

### 1.4.3 Decoder Model

The decoder consists of the last autoencoder layer, fed by a placeholder for the encoded data:

## Placeholder for encoded input

### Extract last autoencoder layer

```
[24]: decoder_layer = autoencoder.layers[-1](encoded_input)
```

Define Decoder Model

[26]: decoder.summary()

Model: "model"

Total params: 25,872 Trainable params: 25,872 Non-trainable params: 0

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### 1.4.4 Compile the Autoencoder Model

```
[27]: autoencoder.compile(optimizer='adam', loss='mse')
```

### 1.4.5 Train the autoencoder

We compile the model to use the Adam optimizer (see Chapter 17, Deep Learning) to minimize the MSE between the input data and the reproduction achieved by the autoencoder. To ensure that the autoencoder learns to reproduce the input, we train the model using the same input and output data:

### Create early\_stopping callback

## Create TensorBard callback to visualize network performance

Create checkpoint callback

```
[30]: filepath = (results_path / 'autencoder.32.weights.hdf5').as_posix()
[31]: checkpointer = ModelCheckpoint(filepath=filepath,
                          monitor='val_loss',
                          save_best_only=True,
                          save_weights_only=True,
                          mode='auto')
   Fit the Model To avoid running time, you can load the pre-computed results in the 'model'
   folder (see below)
[32]: training = autoencoder.fit(x=X_train_scaled,
                       y=X_train_scaled,
                       epochs=100,
                       batch_size=32,
                       shuffle=True,
                       validation_split=.1,
                       callbacks=[tb_callback, early_stopping,_
    →checkpointer])
   Epoch 1/100
   val_loss: 0.0174
   Epoch 2/100
   val_loss: 0.0146
   Epoch 3/100
   1688/1688 [============= ] - 2s 1ms/step - loss: 0.0137 -
   val_loss: 0.0134
   Epoch 4/100
   val_loss: 0.0132
   Epoch 5/100
   val_loss: 0.0130
   Epoch 6/100
   1688/1688 [============= ] - 2s 1ms/step - loss: 0.0128 -
   val_loss: 0.0129
   Epoch 7/100
   val_loss: 0.0128
   Epoch 8/100
   1688/1688 [============= ] - 2s 1ms/step - loss: 0.0127 -
   val_loss: 0.0128
   Epoch 9/100
```

1688/1688 [============== ] - 2s 1ms/step - loss: 0.0127 -

val\_loss: 0.0128

```
Epoch 10/100
val_loss: 0.0127
Epoch 11/100
val loss: 0.0127
Epoch 12/100
val loss: 0.0127
Epoch 13/100
val_loss: 0.0127
Epoch 14/100
val_loss: 0.0127
Epoch 15/100
val_loss: 0.0127
Epoch 16/100
val loss: 0.0128
Epoch 17/100
val_loss: 0.0127
```

## 1.4.6 Reload weights from best-performing model

```
[33]: autoencoder.load_weights(filepath)
```

## 1.4.7 Evaluate trained model

Training stops after some 20 epochs with a test RMSE of 0.1122:

# 1.4.8 Encode and decode test images

[34]: 'MSE: 0.0127 | RMSE 0.1125'

To encode data, we use the encoder we just defined, like so:

```
[35]: encoded_test_img = encoder.predict(X_test_scaled)
encoded_test_img.shape
```

```
[35]: (10000, 32)
```

The decoder takes the compressed data and reproduces the output according to the autoencoder training results:

```
[36]: decoded_test_img = decoder.predict(encoded_test_img) decoded_test_img.shape
```

[36]: (10000, 784)

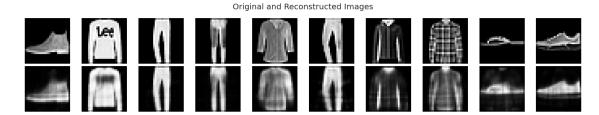
Compare Original with Reconstructed Samples The following figure shows ten original images and their reconstruction by the autoencoder and illustrates the loss after compression:

```
fig, axes = plt.subplots(ncols=n_classes, nrows=2, figsize=(20, 4))
for i in range(n_classes):

    axes[0, i].imshow(X_test_scaled[i].reshape(image_size, image_size),
    cmap='gray')
    axes[0, i].axis('off')

    axes[1, i].imshow(decoded_test_img[i].reshape(28, 28) , cmap='gray')
    axes[1, i].axis('off')

fig.suptitle('Original and Reconstructed Images', fontsize=20)
fig.tight_layout()
fig.subplots_adjust(top=.85)
fig.savefig(results_path / 'reconstructed', dpi=300)
```



### 1.5 Combine training steps into function

The helper function train\_autoencoder just summarizes some repetitive steps.

## 1.6 Autoencoders with Sparsity Constraints

## 1.6.1 Encoding Layer with L1 activity regularizer

The addition of regularization is fairly straightforward. We can apply it to the dense encoder layer using Keras' activity\_regularizer, as follows:

### 1.6.2 Decoding Layer

```
[41]: autoencoder_l1 = Model(input_, decoding_l1)
```

### 1.6.3 Autoencoder Model

```
[42]: autoencoder_11.summary()
   Model: "model_1"
   Layer (type)
                       Output Shape
                                         Param #
   ______
   Input (InputLayer)
                      [(None, 784)]
   Encoder_L1 (Dense)
                       (None, 32)
                                         25120
   Decoder L1 (Dense)
                   (None, 784)
    ------
   Total params: 50,992
   Trainable params: 50,992
   Non-trainable params: 0
```

```
[43]: autoencoder_l1.compile(optimizer='adam', loss='mse')
```

### 1.6.4 Encoder & Decoder Models

```
[44]: encoder_l1 = Model(inputs=input_, outputs=encoding_l1, name='Encoder')

[45]: encoded_input = Input(shape=(encoding_size,), name='Decoder_Input')
    decoder_l1_layer = autoencoder_l1.layers[-1](encoded_input)
    decoder_l1 = Model(inputs=encoded_input, outputs=decoder_l1_layer)
```

### 1.6.5 Train Model

```
[46]: path = (results_path / 'autencoder_11.32.weights.hdf5').as_posix()
   autoencoder 11, mse = train autoencoder(path, autoencoder 11)
   Epoch 1/100
   val_loss: 0.0224
   Epoch 2/100
   1688/1688 [============== ] - 2s 929us/step - loss: 0.0199 -
   val_loss: 0.0186
   Epoch 3/100
   1688/1688 [============== ] - 2s 919us/step - loss: 0.0177 -
   val loss: 0.0174
   Epoch 4/100
   val_loss: 0.0167
   Epoch 5/100
   1688/1688 [============= ] - 2s 930us/step - loss: 0.0164 -
   val_loss: 0.0163
   Epoch 6/100
   1688/1688 [============= ] - 2s 941us/step - loss: 0.0161 -
   val_loss: 0.0162
   Epoch 7/100
   val_loss: 0.0158
   Epoch 8/100
   val loss: 0.0157
   Epoch 9/100
   val_loss: 0.0156
   Epoch 10/100
   1688/1688 [============= ] - 2s 1ms/step - loss: 0.0153 -
   val_loss: 0.0153
   Epoch 11/100
```

```
val_loss: 0.0153
Epoch 12/100
1688/1688 [============= ] - 2s 922us/step - loss: 0.0150 -
val loss: 0.0151
Epoch 13/100
1688/1688 [============= ] - 2s 917us/step - loss: 0.0149 -
val_loss: 0.0150
Epoch 14/100
1688/1688 [============= ] - 2s 917us/step - loss: 0.0148 -
val_loss: 0.0150
Epoch 15/100
1688/1688 [=============== ] - 2s 919us/step - loss: 0.0148 -
val loss: 0.0148
Epoch 16/100
1688/1688 [============== ] - 2s 912us/step - loss: 0.0147 -
val_loss: 0.0148
Epoch 17/100
val loss: 0.0148
Epoch 18/100
1688/1688 [=============== ] - 2s 917us/step - loss: 0.0146 -
val_loss: 0.0148
Epoch 19/100
val_loss: 0.0149
Epoch 20/100
1688/1688 [============= ] - 2s 919us/step - loss: 0.0145 -
val_loss: 0.0146
Epoch 21/100
1688/1688 [============== ] - 2s 931us/step - loss: 0.0145 -
val_loss: 0.0146
Epoch 22/100
1688/1688 [============= ] - 2s 916us/step - loss: 0.0144 -
val loss: 0.0148
Epoch 23/100
1688/1688 [=============== ] - 2s 925us/step - loss: 0.0144 -
val loss: 0.0145
Epoch 24/100
1688/1688 [============= ] - 2s 935us/step - loss: 0.0144 -
val_loss: 0.0144
Epoch 25/100
val_loss: 0.0146
Epoch 26/100
1688/1688 [=============== ] - 2s 920us/step - loss: 0.0143 -
val_loss: 0.0147
Epoch 27/100
```

### 1.6.6 Evaluate Model

The input and decoding layers remain unchanged. In this example, with a compression of factor 24.5, regularization negatively affects performance with a test RMSE of 0.0.1229.

### 1.7 Deep Autoencoder

To illustrate the benefit of adding depth to the autoencoder, we build a three-layer feedforward model that successively compresses the input from 784 to 128, 64, and 34 units, respectively:

### 1.7.1 Define three-layer architecture

```
[50]: input_ = Input(shape=(input_size,))
    x = Dense(128, activation='relu', name='Encoding1')(input_)
    x = Dense(64, activation='relu', name='Encoding2')(x)
    encoding_deep = Dense(32, activation='relu', name='Encoding3')(x)

x = Dense(64, activation='relu', name='Decoding1')(encoding_deep)
    x = Dense(128, activation='relu', name='Decoding2')(x)
    decoding_deep = Dense(input_size, activation='sigmoid', name='Decoding3')(x)
```

```
[51]: autoencoder_deep = Model(input_, decoding_deep)
autoencoder_deep.compile(optimizer='adam', loss='mse')
```

The resulting model has over 222,000 parameters, more than four times the capacity of the preceding single-layer model:

## [52]: autoencoder\_deep.summary()

Model: "model\_3"

Layer (type)	Output Shape	Param #
input_1 (InputLayer)	[(None, 784)]	0
Encoding1 (Dense)	(None, 128)	100480
Encoding2 (Dense)	(None, 64)	8256
Encoding3 (Dense)	(None, 32)	2080
Decoding1 (Dense)	(None, 64)	2112
Decoding2 (Dense)	(None, 128)	8320
Decoding3 (Dense)	(None, 784)	101136
Total params: 222,384		

\_\_\_\_\_

## 1.7.2 Encoder & Decoder Models

Trainable params: 222,384 Non-trainable params: 0

```
[53]: encoder_deep = Model(inputs=input_, outputs=encoding_deep, name='Encoder')
[54]: encoded_input = Input(shape=(encoding_size,), name='Decoder_Input')
```

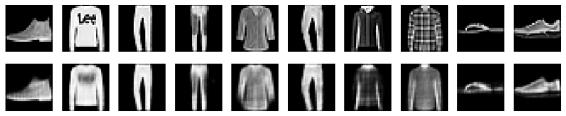
```
x = autoencoder_deep.layers[-3](encoded_input)
   x = autoencoder_deep.layers[-2](x)
   decoded = autoencoder_deep.layers[-1](x)
   decoder_deep = Model(inputs=encoded_input, outputs=decoded)
[55]: decoder_deep.summary()
   Model: "model_4"
           Output Shape
   Layer (type)
                                 Param #
   ______
   Decoder_Input (InputLayer) [(None, 32)]
   _____
                  (None, 64)
   Decoding1 (Dense)
                                  2112
   -----
   Decoding2 (Dense)
                   (None, 128)
                                  8320
   Decoding3 (Dense) (None, 784)
                                 101136
   ______
   Total params: 111,568
   Trainable params: 111,568
   Non-trainable params: 0
   1.7.3 Train Model
[56]: path = (results_path / 'autencoder_deep.32.weights.hdf5').as_posix()
[57]: autoencoder_deep, mse = train_autoencoder(path, autoencoder_deep)
   Epoch 1/100
   val_loss: 0.0183
   Epoch 2/100
   val_loss: 0.0157
   Epoch 3/100
   val_loss: 0.0146
   Epoch 4/100
   val_loss: 0.0136
   Epoch 5/100
   val_loss: 0.0130
   Epoch 6/100
   1688/1688 [============= ] - 2s 1ms/step - loss: 0.0126 -
```

```
val_loss: 0.0127
Epoch 7/100
1688/1688 [============= ] - 2s 1ms/step - loss: 0.0123 -
val loss: 0.0124
Epoch 8/100
val loss: 0.0121
Epoch 9/100
1688/1688 [============= ] - 2s 1ms/step - loss: 0.0117 -
val_loss: 0.0119
Epoch 10/100
1688/1688 [============== ] - 2s 1ms/step - loss: 0.0115 -
val_loss: 0.0117
Epoch 11/100
1688/1688 [============= ] - 2s 1ms/step - loss: 0.0113 -
val_loss: 0.0115
Epoch 12/100
1688/1688 [============= ] - 2s 1ms/step - loss: 0.0112 -
val_loss: 0.0113
Epoch 13/100
1688/1688 [============= ] - 2s 1ms/step - loss: 0.0110 -
val loss: 0.0112
Epoch 14/100
1688/1688 [============== ] - 2s 1ms/step - loss: 0.0109 -
val_loss: 0.0112
Epoch 15/100
1688/1688 [============= ] - 2s 1ms/step - loss: 0.0108 -
val_loss: 0.0109
Epoch 16/100
1688/1688 [============= ] - 2s 1ms/step - loss: 0.0107 -
val_loss: 0.0109
Epoch 17/100
1688/1688 [============= ] - 2s 1ms/step - loss: 0.0107 -
val_loss: 0.0108
Epoch 18/100
val loss: 0.0110
Epoch 19/100
1688/1688 [============== ] - 2s 1ms/step - loss: 0.0105 -
val_loss: 0.0109
Epoch 20/100
1688/1688 [============== ] - 2s 1ms/step - loss: 0.0105 -
val_loss: 0.0106
Epoch 21/100
1688/1688 [============= ] - 2s 1ms/step - loss: 0.0104 -
val_loss: 0.0108
Epoch 22/100
1688/1688 [============ ] - 2s 1ms/step - loss: 0.0104 -
```

```
val_loss: 0.0106
Epoch 23/100
1688/1688 [============= ] - 2s 1ms/step - loss: 0.0103 -
val loss: 0.0105
Epoch 24/100
val loss: 0.0105
Epoch 25/100
1688/1688 [============= ] - 2s 1ms/step - loss: 0.0102 -
val_loss: 0.0104
Epoch 26/100
1688/1688 [============== ] - 2s 1ms/step - loss: 0.0102 -
val_loss: 0.0106
Epoch 27/100
1688/1688 [============= ] - 2s 1ms/step - loss: 0.0101 -
val_loss: 0.0103
Epoch 28/100
1688/1688 [============= ] - 2s 1ms/step - loss: 0.0101 -
val_loss: 0.0103
Epoch 29/100
1688/1688 [============= ] - 2s 1ms/step - loss: 0.0100 -
val loss: 0.0104
Epoch 30/100
1688/1688 [============== ] - 2s 1ms/step - loss: 0.0100 -
val_loss: 0.0103
Epoch 31/100
1688/1688 [============= ] - 2s 1ms/step - loss: 0.0099 -
val_loss: 0.0102
Epoch 32/100
1688/1688 [============= ] - 2s 1ms/step - loss: 0.0099 -
val_loss: 0.0102
Epoch 33/100
1688/1688 [============= ] - 2s 1ms/step - loss: 0.0099 -
val_loss: 0.0101
Epoch 34/100
val loss: 0.0102
Epoch 35/100
1688/1688 [============== ] - 2s 1ms/step - loss: 0.0098 -
val_loss: 0.0101
Epoch 36/100
val_loss: 0.0100
Epoch 37/100
1688/1688 [============= ] - 2s 1ms/step - loss: 0.0097 -
val_loss: 0.0100
Epoch 38/100
1688/1688 [============= ] - 2s 1ms/step - loss: 0.0097 -
```

### 1.7.4 Evaluate Model

Training stops after 54 epochs and results in a  $\sim 10\%$  reduction of the test RMSE to 0.1026. Due to the low resolution, it is difficult to visually note the better reconstruction.



### 1.7.5 Compute t-SNE Embedding

We can use the t-distributed Stochastic Neighbor Embedding (t-SNE) manifold learning technique, see Chapter 12, Unsupervised Learning, to visualize and assess the quality of the encoding learned by the autoencoder's hidden layer.

If the encoding is successful in capturing the salient features of the data, the compressed representation of the data should still reveal a structure aligned with the 10 classes that differentiate the observations.

We use the output of the deep encoder we just trained to obtain the 32-dimensional representation of the test set:

Since t-SNE can take a long time to run (~15-20 min), we are providing pre-computed results

```
[62]: # alternatively, compute the result yourself
tsne = TSNE(perplexity=25, n_iter=5000)
train_embed = tsne.fit_transform(encoder_deep.predict(X_train_scaled))
```

### Persist result

```
[64]: # store results given computational intensity (different location to avoid

→overwriting the pre-computed results)

# pd.DataFrame(train_embed).to_hdf('tsne.h5', 'autoencoder_deep')
```

### Load pre-computed embeddings

```
[]: # Load the pre-computed results here: train_embed = pd.read_hdf(results_path / 'tsne.h5', 'autoencoder_deep')
```

### Visualize Embedding

```
[65]: def plot_embedding(X, y=y_train, title=None, min_dist=0.1, n_classes=10,__
       X = minmax scale(X)
         inner = outer = 0
         for c in range(n_classes):
             inner += np.mean(pdist(X[y == c]))
              outer += np.mean(cdist(X[y == c], X[y != c]))
         fig, ax = plt.subplots(figsize=(14, 10))
         ax.axis('off')
         ax.set_title(title + ' | Distance: {:.2%}'.format(inner/outer))
          sc = ax.scatter(*X.T, c=y, cmap=ListedColormap(cmap), s=5)
          shown_images = np.ones((1, 2))
         images = X_train.reshape(-1, 28, 28)
         for i in range(0, X.shape[0]):
              dist = norm(X[i] - shown_images, axis=1)
              if (dist > min_dist).all():
                  shown_images = np.r_[shown_images, [X[i]]]
                  imagebox = AnnotationBbox(OffsetImage(images[i],
```

The following figure shows that t-SNE manages to separate the 10 classes well, suggesting that the encoding is useful as a lower-dimensional representation that preserves key characteristics of the data:

[66]: plot\_embedding(X=train\_embed, title='t-SNE & Deep Autoencoder')

