# C3W5\_Capstone\_Project

August 31, 2021

# 1 Capstone Project

# 1.1 Probabilistic generative models

#### 1.1.1 Instructions

In this notebook, you will practice working with generative models, using both normalising flow networks and the variational autoencoder algorithm. You will create a synthetic dataset with a normalising flow with randomised parameters. This dataset will then be used to train a variational autoencoder, and you will used the trained model to interpolate between the generated images. You will use concepts from throughout this course, including Distribution objects, probabilistic layers, bijectors, ELBO optimisation and KL divergence regularisers.

This project is peer-assessed. Within this notebook you will find instructions in each section for how to complete the project. Pay close attention to the instructions as the peer review will be carried out according to a grading rubric that checks key parts of the project instructions. Feel free to add extra cells into the notebook as required.

#### 1.1.2 How to submit

When you have completed the Capstone project notebook, you will submit a pdf of the notebook for peer review. First ensure that the notebook has been fully executed from beginning to end, and all of the cell outputs are visible. This is important, as the grading rubric depends on the reviewer being able to view the outputs of your notebook. Save the notebook as a pdf (File -> Download as -> PDF via LaTeX). You should then submit this pdf for review.

### 1.1.3 Let's get started!

We'll start by running some imports below. For this project you are free to make further imports throughout the notebook as you wish.

```
In [1]: import tensorflow as tf
    import tensorflow_probability as tfp
    tfd = tfp.distributions
    tfb = tfp.bijectors
    tfpl = tfp.layers

import numpy as np
    import matplotlib.pyplot as plt
    %matplotlib inline
```

For the capstone project, you will create your own image dataset from contour plots of a transformed distribution using a random normalising flow network. You will then use the variational autoencoder algorithm to train generative and inference networks, and synthesise new images by interpolating in the latent space.

# The normalising flow

- To construct the image dataset, you will build a normalising flow to transform the 2-D Gaussian random variable  $z=(z_1,z_2)$ , which has mean **0** and covariance matrix  $\Sigma=\sigma^2\mathbf{I}_2$ , with  $\sigma=0.3$ .
- This normalising flow uses bijectors that are parameterised by the following random variables:

```
-\theta \sim U[0,2\pi)
- a \sim N(3,1)
```

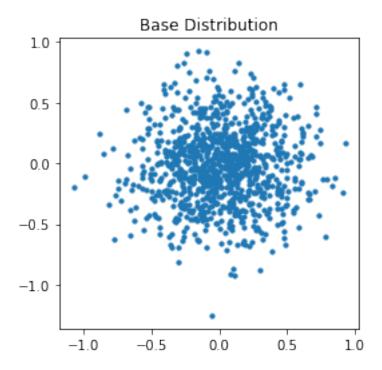
The complete normalising flow is given by the following chain of transformations: \*  $f_1(z) = (z_1, z_2 - 2)$ , \*  $f_2(z) = (z_1, \frac{z_2}{2})$ , \*  $f_3(z) = (z_1, z_2 + az_1^2)$ , \*  $f_4(z) = Rz$ , where R is a rotation matrix with angle  $\theta$ , \*  $f_5(z) = \tanh(z)$ , where the tanh function is applied elementwise.

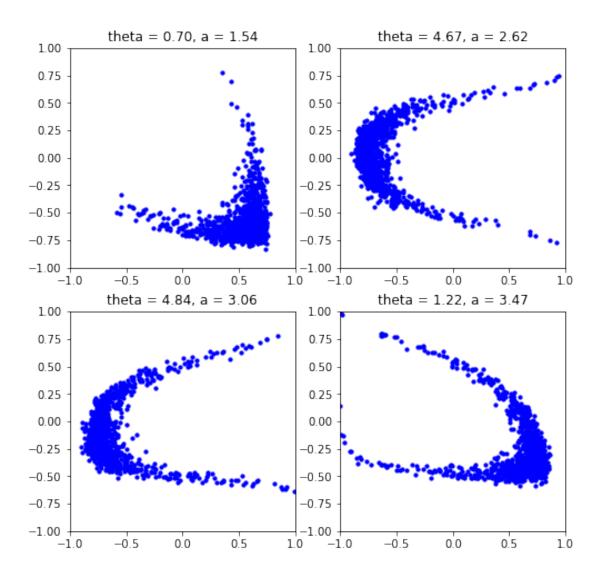
The transformed random variable x is given by  $x = f_5(f_4(f_3(f_2(f_1(z)))))$ . \* You should use or construct bijectors for each of the transformations  $f_i$ , i = 1, ..., 5, and use tfb.Chain and tfb.TransformedDistribution to construct the final transformed distribution. \* Ensure to implement the log\_det\_jacobian methods for any subclassed bijectors that you write. \* Display a scatter plot of samples from the base distribution. \* Display 4 scatter plot images of the transformed distribution from your random normalising flow, using samples of  $\theta$  and a. Fix the axes of these 4 plots to the range [-1,1].

```
In [2]: mu = 0
        sigma = 0.3
        base_distribution = tfd.MultivariateNormalDiag(loc=[mu, mu], scale_diag=[sigma, sigma]
In [3]: import math
        theta_dist = tfd.Uniform(low=0, high=2*math.pi)
        a_dist = tfd.Normal(loc=3, scale=1.)
In [4]: class F3Bijector(tfb.Bijector):
            def __init__(self, a, name='F3', **kwargs):
                self.a = a
                super(F3Bijector, self).__init__(
                    is_constant_jacobian=True,
                    forward_min_event_ndims=0,
                    name=name,
                     **kwargs)
            def _forward(self, x):
                x = tf.cast(x, tf.float32)
                return tf.concat([x[..., :1], x[..., 1:] + self.a * tf.pow(<math>x[..., :1], 2)], ax
```

```
def _inverse(self, y):
                y = tf.cast(y, tf.float32)
                return tf.concat([y[..., :1], y[..., 1:] - self.a * tf.pow(y[..., :1], 2)], ax
            def _forward_log_det_jacobian(self, x):
                return tf.constant(0., x.dtype)
In [5]: class RotationBijector(tfb.Bijector):
            def __init__(self, theta, name='Rotation', **kwargs):
                super(RotationBijector, self).__init__(
                    is_constant_jacobian=True,
                    forward_min_event_ndims=1,
                    validate_args=False,
                    name=name,
                     **kwargs)
                self.rotation_matrix = tf.convert_to_tensor([[tf.cos(theta), -tf.sin(theta)],
                                                         [tf.sin(theta), tf.cos(theta)]], dtype
            def _forward(self, x):
                x = tf.cast(x, tf.float32)
                return tf.linalg.matvec(self.rotation_matrix, x)
            def _inverse(self, y):
                y = tf.cast(y, tf.float32)
                return tf.linalg.matvec(tf.transpose(self.rotation_matrix), y)
            def _forward_log_det_jacobian(self, x):
                return tf.constant(0., x.dtype)
In [6]: def get_bjiectors_chain(a, theta):
            bjiectors = []
            bjiectors.append(tfb.Shift([0., -2.])) # f1
            bjiectors.append(tfb.Scale([1, 0.5])) # f2
            bjiectors.append(F3Bijector(a)) # f3
            bjiectors.append(RotationBijector(theta)) # f4
            bjiectors.append(tfb.Tanh()) # f5
            return tfb.Chain(list(reversed(bjiectors)))
In [7]: def get_transformed_distribution(distribution, a, theta):
            return tfd.TransformedDistribution(distribution=distribution, bijector=get_bjiector
In [40]: def display_samples_from_base_distribution(n_samples):
             z = base_distribution.sample(n_samples).numpy().squeeze()
             plt.figure(figsize=(4, 4))
             plt.scatter(z[:, 0], z[:, 1], s=10)
             plt.title("Base Distribution")
             plt.show()
```

In [41]: display\_samples\_from\_base\_distribution(n\_samples)





# 1.2 2. Create the image dataset

- You should now use your random normalising flow to generate an image dataset of contour plots from your random normalising flow network.
  - Feel free to get creative and experiment with different architectures to produce different sets of images!
- First, display a sample of 4 contour plot images from your normalising flow network using 4 independently sampled sets of parameters.
  - You may find the following get\_densities function useful: this calculates density values for a (batched) Distribution for use in a contour plot.
- Your dataset should consist of at least 1000 images, stored in a numpy array of shape (N, 36, 36, 3). Each image in the dataset should correspond to a contour plot of a transformed dis-

tribution from a normalising flow with an independently sampled set of parameters s, T, S, b. It will take a few minutes to create the dataset.

- As well as the get\_densities function, the get\_image\_array\_from\_density\_values function will help you to generate the dataset.
  - This function creates a numpy array for an image of the contour plot for a given set of density values Z. Feel free to choose your own options for the contour plots.
- Display a sample of 20 images from your generated dataset in a figure.

```
In [13]: # Helper function to compute transformed distribution densities
         X, Y = np.meshgrid(np.linspace(-1, 1, 100), np.linspace(-1, 1, 100))
         inputs = np.transpose(np.stack((X, Y)), [1, 2, 0])
         def get_densities(transformed_distribution):
             11 11 11
             This function takes a (batched) Distribution object as an argument, and returns a
             array Z of shape (batch_shape, 100, 100) of density values, that can be used to m
             contour plot with:
             plt.contourf(X, Y, Z[b, ...], cmap='hot', levels=100)
             where b is an index into the batch shape.
             batch_shape = transformed_distribution.batch_shape
             Z = transformed_distribution.prob(np.expand_dims(inputs, 2))
             Z = np.transpose(Z, list(range(2, 2+len(batch_shape))) + [0, 1])
             return Z
In [14]: # Helper function to convert contour plots to numpy arrays
         import numpy as np
         from matplotlib.backends.backend_agg import FigureCanvasAgg as FigureCanvas
         from matplotlib.figure import Figure
         def get_image_array_from_density_values(Z):
             This function takes a numpy array Z of density values of shape (100, 100)
             and returns an integer numpy array of shape (36, 36, 3) of pixel values for an im
             assert Z.shape == (100, 100)
             fig = Figure(figsize=(0.5, 0.5))
             canvas = FigureCanvas(fig)
             ax = fig.gca()
             ax.contourf(X, Y, Z, cmap='hot', levels=100)
             ax.axis('off')
             fig.tight_layout(pad=0)
             ax.margins(0)
             fig.canvas.draw()
```

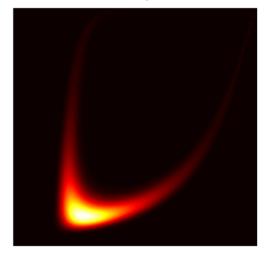
```
image_from_plot = np.frombuffer(fig.canvas.tostring_rgb(), dtype=np.uint8)
    image_from_plot = image_from_plot.reshape(fig.canvas.get_width_height()[::-1] + (
        return image_from_plot

In [15]: plt.figure(figsize = (8, 8))
    for i in range(4):
        theta = theta_dist.sample(1).numpy()[0]
        a = a_dist.sample(1).numpy()[0]

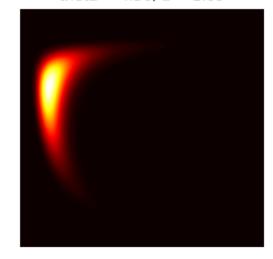
    flow = get_transformed_distribution(base_distribution, a, theta)
        flow = tfd.BatchReshape(flow, [1])

    plt.subplot(2, 2, i+1)
    plt.contourf(X, Y, get_densities(flow).squeeze(), cmap='hot', levels=100)
    plt.title("theta = {:.2f}, a = {:.2f}".format(theta, a))
    plt.axis('off')
    plt.show()
```

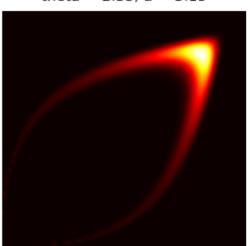
theta = 5.85, a = 2.62



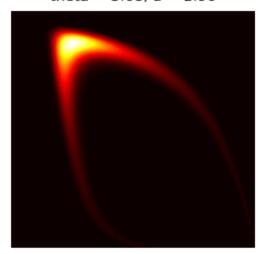
theta = 4.36, a = 1.09



theta = 2.35, a = 3.15



theta = 3.68, a = 2.96



```
In [16]: images = []
    N = 2000

for _ in range(N):
    theta = theta_dist.sample(1).numpy()[0]
    a = a_dist.sample(1).numpy()[0]

flow = get_transformed_distribution(base_distribution, a, theta)
    flow = tfd.BatchReshape(flow, [1])

Z = get_densities(flow).squeeze()

images.append(get_image_array_from_density_values(Z))
```

```
images = np.array(images)
In [17]: plt.figure(figsize=(8, 10))
         for i in range(20):
             plt.subplot(4, 5, i+1)
             idx = np.random.randint(0, N)
             plt.imshow(images[idx])
             plt.axis("off")
         plt.show()
```

## 1.3 3. Make tf.data.Dataset objects

- You should now split your dataset to create tf.data.Dataset objects for training and validation data.
- Using the map method, normalise the pixel values so that they lie between 0 and 1.
- These Datasets will be used to train a variational autoencoder (VAE). Use the map method to return a tuple of input and output Tensors where the image is duplicated as both input and output.
- Randomly shuffle the training Dataset.
- Batch both datasets with a batch size of 20, setting drop\_remainder=True.
- Print the element\_spec property for one of the Dataset objects.

```
In [18]: def get_tf_dataset(data, batch_size, shuffle=False):
             dataset = tf.data.Dataset.from_tensor_slices(data)
             dataset = dataset.map(lambda x: x/255.0)
             dataset = dataset.map(lambda x: (x, x))
             dataset = dataset.batch(batch_size, drop_remainder=True)
             if shuffle:
                 dataset = dataset.shuffle(data.shape[0])
             return dataset
In [19]: train_fraction = 0.8
         train_len = int(train_fraction * images.shape[0])
         train_data = images[0:train_len]
         test_data = images[train_len:]
         train_dataset = get_tf_dataset(train_data.astype(np.float32), 20, shuffle=True)
         test_dataset = get_tf_dataset(test_data.astype(np.float32), 20)
In [20]: print(train_dataset.element_spec)
(TensorSpec(shape=(20, 36, 36, 3), dtype=tf.float32, name=None), TensorSpec(shape=(20, 36, 36,
```

### 1.4 4. Build the encoder and decoder networks

- You should now create the encoder and decoder for the variational autoencoder algorithm.
- You should design these networks yourself, subject to the following constraints:
  - The encoder and decoder networks should be built using the Sequential class.
  - The encoder and decoder networks should use probabilistic layers where necessary to represent distributions.
  - The prior distribution should be a zero-mean, isotropic Gaussian (identity covariance matrix).
  - The encoder network should add the KL divergence loss to the model.
- Print the model summary for the encoder and decoder networks.

```
In [22]: latent_dim = 2
        event_shape = images.shape[1:]
In [23]: def get_prior(latent_dim):
           return tfd.MultivariateNormalDiag(loc=tf.Variable(tf.zeros(latent_dim)),
                                           scale_diag=tfp.util.TransformedVariable(tf.ones
                                                                         bijector=tfb.Se
                                           )
        prior = get_prior(latent_dim)
In [24]: def get_encoder(latent_dim, prior):
           return Sequential([
                   Conv2D(32, (4,4), activation='relu', strides=(1,1), padding='same', input
                   BatchNormalization(),
                   Conv2D(64, (4,4), activation='relu', strides=(2,2), padding='same'),
                   BatchNormalization(),
                   Conv2D(128, (4,4), activation='relu', strides=(2,2), padding='same'),
                   BatchNormalization(),
                   Conv2D(256, (4,4), activation='relu', strides=(2,2), padding='same'),
                   BatchNormalization(),
                   Flatten(),
                   Dense(units=tfpl.MultivariateNormalTriL.params_size(latent_dim)),
                   tfpl.MultivariateNormalTriL(event_size=latent_dim),
                   tfpl.KLDivergenceAddLoss(prior,
                                         use_exact_kl = False,
                                         test_points_fn = lambda q:q.sample(3),
                                         test_points_reduce_axis=(0,1))
           ])
In [25]: encoder = get_encoder(latent_dim, prior)
        encoder.summary()
Model: "sequential"
Layer (type)
                   Output Shape
                                                 Param #
______
                          (None, 36, 36, 32)
conv2d (Conv2D)
batch_normalization (BatchNo (None, 36, 36, 32) 128
conv2d_1 (Conv2D) (None, 18, 18, 64) 32832
batch_normalization_1 (Batch (None, 18, 18, 64) 256
conv2d_2 (Conv2D) (None, 9, 9, 128) 131200
batch_normalization_2 (Batch (None, 9, 9, 128)
                        (None, 5, 5, 256)
conv2d_3 (Conv2D)
                                                524544
```

```
batch_normalization_3 (Batch (None, 5, 5, 256)
                                        1024
flatten (Flatten) (None, 6400)
                    (None, 5)
dense (Dense)
                                        32005
_____
multivariate_normal_tri_l (M multiple
kl_divergence_add_loss (KLDi multiple
_____
Total params: 724,073
Trainable params: 723,113
Non-trainable params: 960
In [26]: def get_decoder(latent_dim):
         return Sequential([
               Dense(6400, activation='relu', input_shape=(latent_dim,)),
               Reshape ((5, 5, 256)),
               UpSampling2D((2,2)),
               Conv2D(128, (3,3), activation='relu', padding='same'),
               UpSampling2D((2,2)),
               Conv2D(64, (3,3), activation='relu', padding='same'),
               UpSampling2D((2,2)),
               Conv2D(32, (3,3), activation='relu', padding='valid'),
               # UpSampling2D((2,2)),
               # Conv2D(128, (3,3), activation='relu', padding='same'),
               Conv2D(3, (3,3), padding='valid'),
               Flatten(),
               tfpl.IndependentBernoulli(event_shape=event_shape)
         ])
In [27]: decoder = get_decoder(latent_dim)
      decoder.summary()
Model: "sequential_1"
 -----
Layer (type) Output Shape Param #
 .....
dense 1 (Dense)
                     (None, 6400)
_____
               (None, 5, 5, 256)
reshape (Reshape)
up_sampling2d (UpSampling2D) (None, 10, 10, 256) 0
conv2d_4 (Conv2D) (None, 10, 10, 128) 295040
```

up_sampling2d_1 (UpSampling2	(None, 20, 20, 128)	0
conv2d_5 (Conv2D)	(None, 20, 20, 64)	73792
up_sampling2d_2 (UpSampling2	(None, 40, 40, 64)	0
conv2d_6 (Conv2D)	(None, 38, 38, 32)	18464
conv2d_7 (Conv2D)	(None, 36, 36, 3)	867
flatten_1 (Flatten)	(None, 3888)	0
independent_bernoulli (Indep	multiple	0
Total params: 407,363 Trainable params: 407,363		

Non-trainable params: 0

## 1.5 5. Train the variational autoencoder

- You should now train the variational autoencoder. Build the VAE using the Model class and the encoder and decoder models. Print the model summary.
- Compile the VAE with the negative log likelihood loss and train with the fit method, using the training and validation Datasets.
- Plot the learning curves for loss vs epoch for both training and validation sets.

In [28]: vae = Model(inputs=encoder.inputs, outputs=decoder(encoder.outputs))

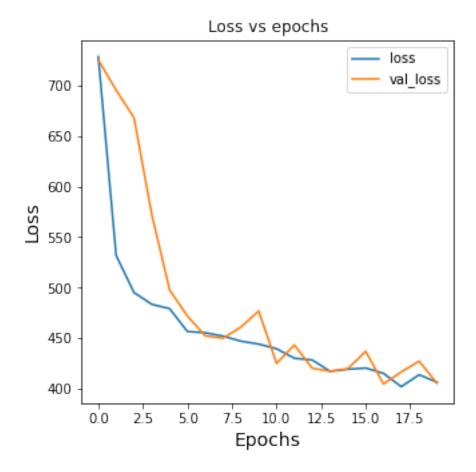
In [39]: vae.summary()

Model: "model"

Layer (type)	Output Shape	Param #
conv2d_input (InputLayer)	[(None, 36, 36, 3)]	0
conv2d (Conv2D)	(None, 36, 36, 32)	1568
batch_normalization (BatchNo	(None, 36, 36, 32)	128
conv2d_1 (Conv2D)	(None, 18, 18, 64)	32832
batch_normalization_1 (Batch	(None, 18, 18, 64)	256
conv2d_2 (Conv2D)	(None, 9, 9, 128)	131200

```
batch_normalization_2 (Batch (None, 9, 9, 128)
                       512
_____
conv2d_3 (Conv2D)
           (None, 5, 5, 256)
                       524544
batch_normalization_3 (Batch (None, 5, 5, 256)
                       1024
flatten (Flatten)
           (None, 6400)
-----
dense (Dense)
            (None, 5)
                       32005
_____
multivariate_normal_tri_l (M multiple
kl_divergence_add_loss (KLDi multiple
sequential_1 (Sequential) multiple
______
Total params: 1,131,436
Trainable params: 1,130,476
Non-trainable params: 960
 -----
In [29]: def reconstruction_loss(batch_of_images, decoding_dist):
     return -tf.reduce_mean(decoding_dist.log_prob(batch_of_images))
In [31]: optimizer = tf.keras.optimizers.Adam(learning_rate=0.001)
   vae.compile(optimizer=optimizer, loss=reconstruction_loss)
In [32]: history = vae.fit(train_dataset, validation_data=test_dataset, epochs=20)
Epoch 1/20
Epoch 2/20
Epoch 3/20
Epoch 4/20
Epoch 5/20
Epoch 6/20
Epoch 7/20
Epoch 8/20
Epoch 9/20
Epoch 10/20
```

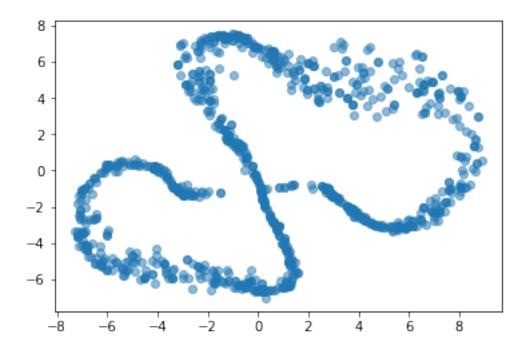
```
Epoch 11/20
Epoch 12/20
Epoch 13/20
Epoch 14/20
Epoch 15/20
Epoch 16/20
Epoch 17/20
Epoch 18/20
Epoch 19/20
Epoch 20/20
In [43]: import matplotlib.pyplot as plt
   fig, axes = plt.subplots(1, 1, figsize=(5, 5))
   train_loss = history.history['loss']
   val_loss = history.history['val_loss']
   axes.set_xlabel("Epochs", fontsize=14)
   axes.set_ylabel("Loss", fontsize=14)
   axes.set_title('Loss vs epochs')
   axes.plot(train_loss, label='loss')
   axes.plot(val_loss, label='val_loss')
   axes.legend()
Out[43]: <matplotlib.legend.Legend at 0x7fe60e12c390>
```



## 1.6 6. Use the encoder and decoder networks

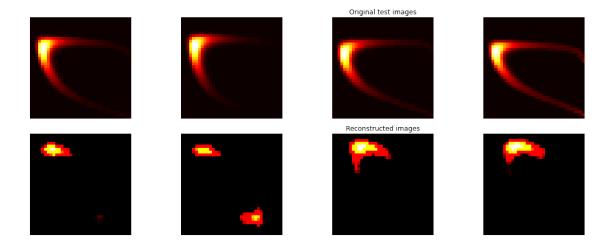
- You can now put your encoder and decoder networks into practice!
- Randomly sample 1000 images from the dataset, and pass them through the encoder. Display the embeddings in a scatter plot (project to 2 dimensions if the latent space has dimension higher than two).
- Randomly sample 4 images from the dataset and for each image, display the original and reconstructed image from the VAE in a figure.
  - Use the mean of the output distribution to display the images.
- Randomly sample 6 latent variable realisations from the prior distribution, and display the images in a figure.
  - Again use the mean of the output distribution to display the images.

```
print(images[embeddings_idx].shape)
    embeddings = encoder(images[embeddings_idx]/255.0).mean()
(1000, 36, 36, 3)
```



```
In [37]: n_reconstructions = 4
    reconstruction_idx = get_random_idx(images.shape[0], n_reconstructions)
    reconstructions = vae(images[reconstruction_idx]).mean().numpy()

f, axs = plt.subplots(2, n_reconstructions, figsize=(16, 6))
    axs[0, n_reconstructions // 2].set_title("Original test images")
    axs[1, n_reconstructions // 2].set_title("Reconstructed images")
    for j in range(n_reconstructions):
        axs[0, j].imshow(images[reconstruction_idx[j]])
        axs[1, j].imshow(reconstructions[j])
        axs[0, j].axis('off')
        axs[1, j].axis('off')
```



```
In [38]: n_latent = 6
    z = prior.sample(n_latent)
    generated_images = decoder(z).mean().numpy()

    f, axs = plt.subplots(1, n_latent, figsize=(16, 6))

    for j in range(n_latent):
        axs[j].imshow(generated_images[j])
        axs[j].axis('off')

    plt.tight_layout();
```

# 1.7 Make a video of latent space interpolation (not assessed)

• Just for fun, you can run the code below to create a video of your decoder's generations, depending on the latent space.

```
In []: # Function to create animation
    import matplotlib.animation as anim
    from IPython.display import HTML
```

```
def get_animation(latent_size, decoder, interpolation_length=500):
            assert latent_size >= 2, "Latent space must be at least 2-dimensional for plotting
            fig = plt.figure(figsize=(9, 4))
            ax1 = fig.add_subplot(1,2,1)
            ax1.set_xlim([-3, 3])
            ax1.set_ylim([-3, 3])
            ax1.set_title("Latent space")
            ax1.axes.get_xaxis().set_visible(False)
            ax1.axes.get_yaxis().set_visible(False)
            ax2 = fig.add_subplot(1,2,2)
            ax2.set_title("Data space")
            ax2.axes.get_xaxis().set_visible(False)
            ax2.axes.get_yaxis().set_visible(False)
            # initializing a line variable
            line, = ax1.plot([], [], marker='o')
            img2 = ax2.imshow(np.zeros((36, 36, 3)))
            freqs = np.random.uniform(low=0.1, high=0.2, size=(latent_size,))
            phases = np.random.randn(latent_size)
            input_points = np.arange(interpolation_length)
            latent_coords = []
            for i in range(latent size):
                latent_coords.append(2 * np.sin((freqs[i]*input_points + phases[i])).astype(np
            def animate(i):
                z = tf.constant([coord[i] for coord in latent_coords])
                img_out = np.squeeze(decoder(z[np.newaxis, ...]).mean().numpy())
                line.set_data(z.numpy()[0], z.numpy()[1])
                img2.set_data(np.clip(img_out, 0, 1))
                return (line, img2)
            return anim.FuncAnimation(fig, animate, frames=interpolation_length,
                                      repeat=False, blit=True, interval=150)
In [ ]: # Create the animation
        a = get_animation(latent_size, decoder, interpolation_length=200)
       HTML(a.to html5 video())
In []:
```