## **Capstone Project**

### **Probabilistic generative models**

#### 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.

#### 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.

#### 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.

```
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 p
import math as m
from sklearn.model_selection import train_test_split
from matplotlib import gridspec
%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  $\Sigma=\sigma^2I_2$ , with  $\sigma=0.3$ .
- This normalising flow uses bijectors that are parameterised by the following random variables:
  - $\theta \sim U \tilde{c}$   $a \sim N(3.1)$

The complete normalising flow is given by the following chain of transformations:

- $f_1(z) = (z_1, z_2 2)$ ,
- $f_2(z) = \left(z_1, \frac{z_2}{2}\right)$ ,
- $f_3(z) = (z_1, z_2 + a z_1^2),$
- $f_4(z) = Rz$ , 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  $x = f_5(f_4(f_2(f_1(z))))$ .

- 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].

```
theta_dist = tfd.Uniform(low = 0, high = 2*np.pi)
a_dist = tfd.Normal(loc = 3, scale = 1)

mu, sigma = 0, 0.3
base_dist = tfd.MultivariateNormalDiag(loc = [mu, mu], scale_diag = [sigma, sigma])

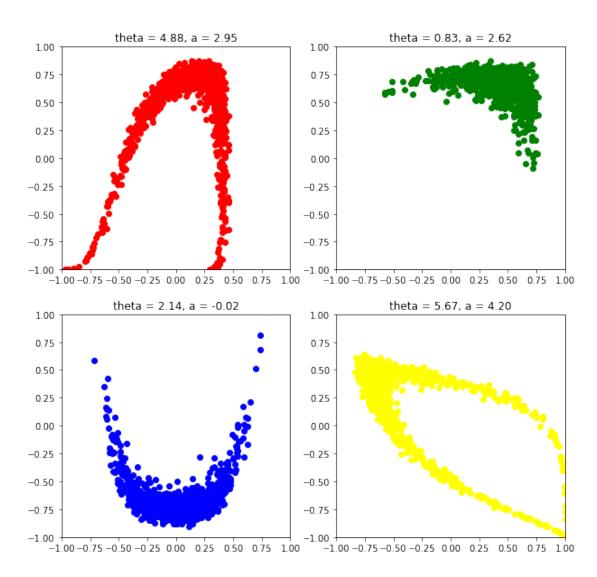
def getBaseDist():
    sigma = 0.3
    mvn = tfd.MultivariateNormalDiag(loc=[0., 0.],
```

```
scale diag=[sigma, sigma])
  return mvn
n = 1000
mvn = getBaseDist()
z = mvn.sample(n).numpy().squeeze()
p.figure()
p.scatter(z[:, 0], z[:, 1])
p.title("Base Distribution")
p.show()
                              Base Distribution
    1.00
    0.75
    0.50
    0.25
    0.00
   -0.25
   -0.50
   -0.75
   -1.00
              -1.0
                          -0.5
                                      0.0
                                                  0.5
                                                              1.0
class Polynomial(tfb.Bijector):
    def __init__(self, a, name="Polynomial", **kwargs):
    super(Polynomial, self).__init__(forward_min_event_ndims=1,
                                               name=name,
                                               is constant jacobian=True,
                                               validate_args=False,
                                               **kwargs)
         self.a = tf.cast(a, dtype=tf.float32)
    def _forward(self, x):
         \overline{x} = tf.cast(x, dtype=tf.float32)
         return tf.concat([x[..., 0:1],
                              x[..., 1:] + self.a * tf.square(x[...,
0:1])], axis=-1)
```

def \_inverse(self, y):

```
y = tf.cast(y, dtype=tf.float32)
        return tf.concat([y[..., 0:1],
                          y[..., 1:] - self.a * tf.square(y[...,
0:1])], axis=-1)
    def _forward_log_det_jacobian(self, x):
        return tf.constant(0., dtype=x.dtype)
class Rotation(tfb.Bijector):
    def init (self, theta, name="Rotation", **kwargs):
        super(Rotation, self). init (name=name,
                                       forward min event ndims=1,
                                       validate args=False,
                                       **kwargs)
        self.rot_matrix = tf.convert_to_tensor([[tf.cos(theta), -
tf.sin(theta)],
                                                 [tf.sin(theta),
tf.cos(theta)]], dtype=tf.float32)
    def forward(self, x):
        x = tf.cast(x, dtype=tf.float32)
        return tf.linalg.matvec(self.rot matrix, x)
    def inverse(self, v):
        y = tf.cast(y, dtype=tf.float32)
        return tf.linalg.matvec(tf.transpose(self.rot_matrix), y)
    def forward log det jacobian(self, x):
        return tf.constant(0., dtype=x.dtype)
def createFlow(a, theta):
  f1 = tfb.Shift([0, -2])
  f2 = tfb.Scale([1, 0.5])
  f3 = Polynomial(a)
  f4 = Rotation(theta)
 f5 = tfb.Tanh()
  return tfb.Chain([f5, f4, f3, f2, f1])
def createTransformedDist(theta, a, base dist):
  return tfd.TransformedDistribution(distribution=base dist,
                                     bijector=createFlow(theta, a))
p.figure(figsize = (10, 10))
base dist = getBaseDist()
```

```
colors = ['red', 'green', 'blue', 'yellow']
for i, col in enumerate(colors):
   theta = theta_dist.sample(1).numpy()[0]
   a = a_dist.sample(1).numpy()[0]
   transformed_dist = createTransformedDist(theta, a, base_dist)
   p.subplot(2, 2, i+1)
   samples = transformed_dist.sample(1000).numpy().squeeze()
   p.scatter(samples[:,0], samples[:, 1], color=col)
   p.title("theta = {:.2f}, a = {:.2f}".format(theta, a))
   p.xlim([-1,1])
   p.ylim([-1,1])
```



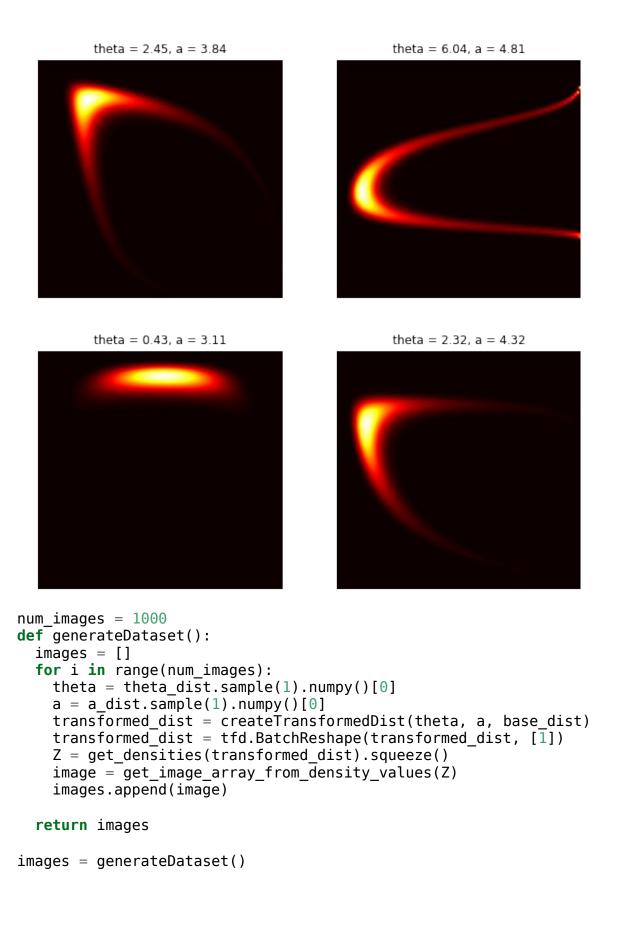
## 2. Create the image dataset

 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 distribution 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. # 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): This function takes a (batched) Distribution object as an argument, and returns a numpy array Z of shape (batch shape, 100, 100) of density values, that can be used to make a 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 # 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 image.
    assert Z.shape == (100, 100)
    fig = Figure(figsize=(0.5, 0.5))
    canvas = FigureCanvas(fig)
    ax = fiq.qca()
    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] + (3,))
    return image from plot
p.figure(figsize = (10, 10))
for i in range (4):
  theta = theta dist.sample(1).numpy()[0]
  a = a dist.sample(1).numpy()[0]
  transformed dist = createTransformedDist(theta, a, base dist)
  transformed dist = tfd.BatchReshape(transformed dist, [1])
  p.subplot(2, 2, i+1)
  p.contourf(X, Y, get densities(transformed dist).squeeze(),
cmap='hot', levels=\overline{100})
  p.title("theta = {:..2f}, a = {:..2f}".format(theta, a))
  p.xlim([-1,1])
  p.ylim([-1,1])
  p.axis('off')
p.show()
```



```
images = np.array(images)
print(images.shape)
(1000, 36, 36, 3)
p.figure(figsize = (15, 15))
for i in range(20):
  idx = np.random.randint(0, 1000)
  p.subplot(5, 4, i+1)
  image = images[i, ...]
  p.axis('off')
  p.imshow(image)
p.show()
```

#### 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.

```
data = images.astype(dtype=np.float32)
batch_size = 20
train, test = train_test_split(data, train_size=0.8, test_size=0.2)

ds_train = tf.data.Dataset.from_tensor_slices(train)
ds_train = ds_train.map(lambda t: t/255.0)
ds_train = ds_train.map(lambda x: (x, x))
ds_train = ds_train.batch(batch_size, drop_remainder=True)
ds_train = ds_train.shuffle(buffer_size=1001)

ds_test = tf.data.Dataset.from_tensor_slices(test)
ds_test = ds_test.map(lambda t: t/255.0)
ds_test = ds_test.map(lambda x: (x, x))
ds_test = ds_test.batch(batch_size, drop_remainder=True)

print(ds_train.element_spec)
(TensorSpec(shape=(20, 36, 36, 3), dtype=tf.float32, name=None),
TensorSpec(shape=(20, 36, 36, 3), dtype=tf.float32, name=None))
```

#### 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.

```
from tensorflow.keras import Sequential, Model
from tensorflow.keras.layers import (Dense, Flatten, Reshape,
Concatenate, Conv2D,
                                     UpSampling2D, BatchNormalization)
tfd = tfp.distributions
tfb = tfp.bijectors
tfpl = tfp.layers
def get prior(latent dim):
    prior = tfd.MultivariateNormalDiag(loc =
tf.Variable(tf.zeros(latent dim), dtype=tf.float32),
                                       scale diag =
tfp.util.TransformedVariable(initial value = tf.ones(latent_dim,
dtype=tf.float32),
bijector = tfb.Softplus(),
dtype = tf.float32)
                                       )
    return prior
def get encoder(latent_dim):
    encoder = Sequential([
        Conv2D(32, 4, activation='relu', strides=2, padding='SAME',
input shape=(36, 36, 3),
        BatchNormalization(),
        Conv2D(64, 4, activation='relu', strides=2, padding='SAME'),
        BatchNormalization(),
        Conv2D(128, 4, activation='relu', strides=2, padding='SAME'),
        BatchNormalization(),
        Conv2D(256, 4, activation='relu', strides=2, padding='SAME'),
        BatchNormalization(),
        Flatten(),
        Dense(tfpl.MultivariateNormalTriL.params size(latent dim)),
        tfpl.MultivariateNormalTriL(latent dim),
        tfpl.KLDivergenceAddLoss(get prior(latent dim),
                                 use exact kl = False,
                                 test points fn = lambda
q:q.sample(5),
                                 test points reduce axis=(0,1)
    ])
```

#### return encoder

latent\_dim = 2
encoder = get\_encoder(latent\_dim)

encoder.summary()

Model: "sequential"

-	Layer (type)	Output Shape	Param #
	conv2d (Conv2D)	(None, 18, 18, 32)	1568
	<pre>batch_normalization (BatchN ormalization)</pre>	(None, 18, 18, 32)	128
	conv2d_1 (Conv2D)	(None, 9, 9, 64)	32832
	<pre>batch_normalization_1 (Batc hNormalization)</pre>	(None, 9, 9, 64)	256
	conv2d_2 (Conv2D)	(None, 5, 5, 128)	131200
	<pre>batch_normalization_2 (Batc hNormalization)</pre>	(None, 5, 5, 128)	512
	conv2d_3 (Conv2D)	(None, 3, 3, 256)	524544
	<pre>batch_normalization_3 (Batc hNormalization)</pre>	(None, 3, 3, 256)	1024
	flatten (Flatten)	(None, 2304)	0
	dense (Dense)	(None, 5)	11525
	<pre>multivariate_normal_tri_l ( MultivariateNormalTriL)</pre>		0
	<pre>kl_divergence_add_loss (KLD ivergenceAddLoss)</pre>	(None, 2)	4

\_\_\_\_\_\_

Total params: 703,593 Trainable params: 702,633 Non-trainable params: 960

This function should build a CNN decoder model according to the above specification.

The function takes latent\_dim as an argument, which should be used to define the model.

```
Your function should return the decoder model.
```

```
image dim = (36, 36, 3)
decoder = Sequential([
    Dense(4096, activation='relu', input shape=(latent dim,)),
    Reshape ((4, 4, 256)),
    UpSampling2D(size=(2, 2)),
    Conv2D(128, 3, activation='relu', padding='SAME'),
    UpSampling2D(size=(2, 2)),
    Conv2D(64, 3, activation='relu', padding='SAME'),
    UpSampling2D(size=(2, 2)),
    Conv2D(32, 3, activation='relu', padding='SAME'),
    UpSampling2D(size=(2, 2)),
    Conv2D(128, 3, activation='relu', padding='SAME'),
    Conv2D(3, 3, padding='SAME'),
    Flatten(),
    Dense(tfpl.IndependentBernoulli.params size(image dim)),
    tfpl.IndependentBernoulli(event shape=image dim)
])
```

#### return decoder

decoder = get\_decoder(latent\_dim)

decoder.summary()

Model: "sequential 1"

Layer (type)	Output Shape	Param #
dense_1 (Dense)	(None, 4096)	12288
reshape (Reshape)	(None, 4, 4, 256)	0
<pre>up_sampling2d (UpSampling2D )</pre>	(None, 8, 8, 256)	0
conv2d_4 (Conv2D)	(None, 8, 8, 128)	295040
<pre>up_sampling2d_1 (UpSampling 2D)</pre>	(None, 16, 16, 128)	0
conv2d_5 (Conv2D)	(None, 16, 16, 64)	73792
<pre>up_sampling2d_2 (UpSampling 2D)</pre>	(None, 32, 32, 64)	0

```
conv2d 6 (Conv2D)
                            (None, 32, 32, 32)
                                                       18464
up sampling2d 3 (UpSampling (None, 64, 64, 32)
                                                       0
2D)
conv2d 7 (Conv2D)
                            (None, 64, 64, 128)
                                                       36992
conv2d 8 (Conv2D)
                            (None, 64, 64, 3)
                                                       3459
flatten 1 (Flatten)
                            (None, 12288)
                                                       0
dense 2 (Dense)
                            (None, 3888)
                                                      47779632
independent bernoulli (Inde ((None, 36, 36, 3),
                                                       0
pendentBernoulli)
                             (None, 36, 36, 3))
```

\_\_\_\_\_

Total params: 48,219,667 Trainable params: 48,219,667 Non-trainable params: 0

#### 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.

vae = Model(inputs=encoder.inputs, outputs=decoder(encoder.outputs))

```
def reconstruction_loss(batch_of_images, decoding_dist):
```

This function should compute and return the average expected reconstruction loss,

as defined above.

The function takes batch\_of\_images (Tensor containing a batch of input images to

the encoder) and decoding\_dist (output distribution of decoder after passing the

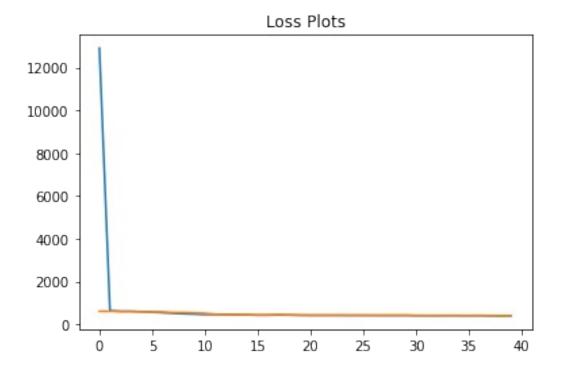
image batch through the encoder and decoder) as arguments.
The function should return the scalar average expected
reconstruction loss.

return -

```
tf.reduce sum(decoding dist.log prob(batch of images))/batch of images
.shape[0]
optimizer = tf.keras.optimizers.Adam(learning rate=0.005)
vae.compile(optimizer=optimizer, loss=reconstruction loss)
history = vae.fit(ds train, validation data=ds test, epochs=40)
Epoch 1/40
40/40 [============= ] - 19s 90ms/step - loss:
12912.0527 - val loss: 613.5903
Epoch 2/40
- val loss: 614.3257
Epoch 3/40
- val_loss: 607.0528
Epoch 4/40
- val loss: 608.5170
Epoch 5/40
- val loss: 595.1943
Epoch 6/40
- val loss: 580.5905
Epoch 7/40
- val loss: 582.9617
Epoch 8/40
- val loss: 552.4846
Epoch 9/40
- val loss: 551.5870
Epoch 10/40
- val_loss: 532.7495
Epoch 11/40
- val_loss: 518.2845
Epoch 12/40
- val loss: 476.1368
Epoch 13/40
- val loss: 452.5573
- val_loss: 459.9346
Epoch 15/40
```

```
- val loss: 443.4171
Epoch 16/40
- val loss: 432.9738
Epoch 17/40
- val loss: 437.9270
Epoch 18/40
- val loss: 453.9005
Epoch 19/40
- val loss: 440.6649
Epoch 20/40
- val loss: 429.5184
Epoch 21/40
- val loss: 422.8842
Epoch 22/40
40/40 [============== ] - 3s 74ms/step - loss: 426.7986
- val loss: 420.3523
Epoch 23/40
- val loss: 425.3409
Epoch 24/40
- val loss: 422.0417
Epoch 25/40
- val loss: 420.9660
Epoch 26/40
- val loss: 422.8844
Epoch 27/40
40/40 [============== ] - 3s 72ms/step - loss: 421.9485
- val loss: 417.8807
Epoch 28/40
- val loss: 427.3566
Epoch 29/40
- val loss: 435.4379
Epoch 30/40
- val loss: 421.9115
Epoch 31/40
- val loss: 411.8120
```

```
Epoch 32/40
- val loss: 414.0316
Epoch 33/40
- val_loss: 413.8081
Epoch 34/40
- val loss: 410.1511
Epoch 35/40
40/40 [============== ] - 3s 83ms/step - loss: 410.5901
- val loss: 413.5927
Epoch 36/40
- val loss: 408.7293
Epoch 37/40
- val_loss: 417.9182
Epoch 38/40
- val loss: 402.7227
Epoch 39/40
- val loss: 403.2838
Epoch 40/40
- val_loss: 403.3502
p.plot(history.history["loss"])
p.plot(history.history["val loss"])
p.title("Loss Plots")
p.show()
```



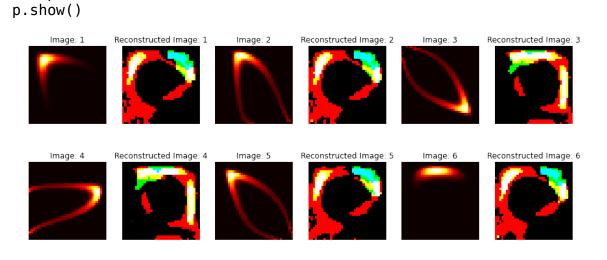
#### 6. Use the encoder and decoder networks

- 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.

```
idx = np.random.choice(np.arange(images.shape[0]), 1000)
embeddings = encoder(images[idx]/255.0).mean()

p.figure()
p.scatter(embeddings[:, 0], embeddings[:, 1])
p.title("Embeddings")
p.show()
```

# **Embeddings** 15 10 5 0 -5 -7.5-5.0-2.5 0.0 2.5 5.0 7.5 10.0 N = 6idx = np.random.choice(np.arange(data.shape[0]), N) reconstructed images = vae(data[idx]).mean().numpy() p.figure(figs $\overline{i}$ ze=(15, 6)) for i in range(N): p.subplot(2, 6, 2\*i+1)p.imshow(data[idx[i]].astype(np.uint8)) p.title("Image: {}".format(i+1)) p.axis("off") p.subplot(2, 6, 2\*i+2) p.imshow(reconstructed images[i]) p.title("Reconstructed Image: {}".format(i+1))



p.axis("off")

```
N = 6
embeddings = np.random.uniform(-2, 2, (N, latent dim))
reconstructed_images = decoder(embeddings).mean()
fig = p.figure(figsize=(14, 6))
gs = gridspec.GridSpec(2, 5)
for i in range(2):
    for j in range(3):
        ax1 = p.subplot(gs[i, 2+j])
        ax1.imshow(reconstructed_images[2*i + j])
        ax1.set_axis_off()
p.show()
```

## 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.

# Function to create animation

import matplotlib.animation as anim

```
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.float32))
    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)
# Create the animation
a = get animation(latent size, decoder, interpolation length=200)
HTML(a.to html5 video())
```