

# Deep Learning

## Week 9: Variational autoencoder

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### Introduction

In the last week of the module we saw how normalising flow probabilistic deep learning models can be used to model data distributions. In particular, you learned about the NICE, RealNVP and Glow models, and saw how these flows can be built and trained using custom layers in Keras.

In this week of the module, we will look at another important deep learning algorithm: the variational autoencoder, or VAE. The VAE is an algorithm for inference and learning in a latent variable generative model. It has been successfully applied in a variety of application domains, such as neuroimaging ([Benou et al 2016](#)), drug discovery ([Jin et al 2018](#)), anomaly detection ([Xu et al 2018](#)), image generation ([Vahdat & Kautz 2020](#)) and music generation ([Dhariwal et al 2020](#)).

In its simplest form, the VAE is an unsupervised learning algorithm, and like normalising flows, the generative model can be used to create new examples similar to the dataset. However, unlike normalising flows, the generative model is not invertible, and so it's not as straightforward to train the model using maximum likelihood.

The VAE uses the principle of variational inference to approximate the posterior distribution, by defining a parameterised family of distributions conditioned on a data example, and then maximising a lower bound on the marginal likelihood. This is the evidence lower bound, or ELBO.

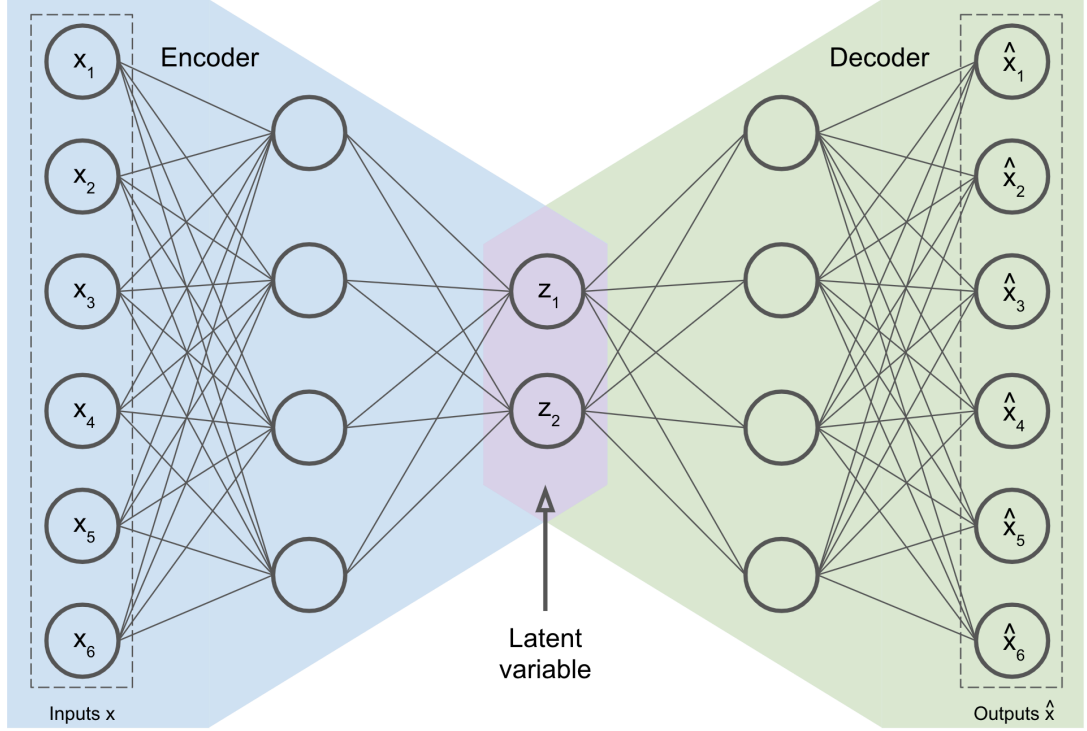
In this week, we'll build up the pieces we need to implement a variational autoencoder with Keras, starting with looking at building regular autoencoder architectures.

### Autoencoders

In this section, we'll look at how to implement a standard autoencoder architecture.

An autoencoder can be viewed as a compression algorithm, similar to a VAE, although it's not a probabilistic model, and it is not a model of the underlying data distribution.

The aim of an autoencoder is to learn an efficient data encoding. The network is normally trained in an unsupervised manner, and the task of the network is to reproduce its input as its output.



An autoencoder network architecture, with bottleneck latent variable  $\mathbf{z}$

The autoencoder has a bottleneck architecture as in the above figure, and can be broken into two parts: the **encoder** network and the **decoder** network. In the middle of the bottleneck is the latent variable  $\mathbf{z}$ , which captures the encoding of the data. The dimensionality of  $\mathbf{z}$  is typically much lower than the data  $\mathbf{x}$ , and so the network is trained to perform nonlinear dimension reduction (Kramer 1991). The job of the encoder is to learn an efficient representation of the data in a much lower dimensional encoding space, whilst the decoder is required to decompress the latent code to reconstruct the data input  $\mathbf{x}$ .

For an autoencoder network  $f_\theta$ , the model is trained to minimise the loss

$$L(\theta; \mathcal{D}_{train}) = \frac{1}{|\mathcal{D}_{train}|} \sum_{x_i \in \mathcal{D}_{train}} l(x_i, f_\theta(x_i)),$$

where  $l : \mathbb{R}^D \times \mathbb{R}^D \mapsto \mathbb{R}$  is a suitable loss function, such as mean squared error. In practice, the model is trained using minibatches of data as usual.

There are several variants of the autoencoder model, one notable example being the **denoising autoencoder** (Vincent & Larochelle 2010). In this model, the input  $\mathbf{x}$  is corrupted with noise to produce the input  $\tilde{\mathbf{x}}$ , and the model is trained to minimise the loss

$$L(\theta; \mathcal{D}_{train}) = \frac{1}{|\mathcal{D}_{train}|} \sum_{x_i \in \mathcal{D}_{train}} l(x_i, f_\theta(\tilde{x}_i)).$$

In other words, the model is tasked to clean the corrupted input by encoding it into a suitable representation. Intuitively, this is motivated by the idea that good representations should be robust to the corruption of the input  $\mathbf{x}$ , and that to denoise the input successfully, the model needs to extract features that capture useful structure in the distribution of the input, and ignore features in the data that are unimportant.

The noise is typically injected stochastically during the training run, according to a prescribed distribution  $q(\tilde{\mathbf{x}} \mid \mathbf{x})$ , so that the noise is different on each epoch.

## CNN autoencoder example

In this section, we will implement a CNN autoencoder for the Fashion-MNIST dataset, and examine the learned encodings.

```
In [2]: import keras
        from keras import ops
```

The Fashion-MNIST dataset can be loaded with the Keras API.

```
In [3]: # Load the dataset

import numpy as np

(x_train, y_train), (x_test, y_test) = keras.datasets.fashion_mnist.load_data()
x_train = (x_train / 255.).astype(np.float32)
x_test = (x_test / 255.).astype(np.float32)
```

```
In [4]: # Store the class names

class_names = np.array(['T-shirt/top', 'Trouser/pants', 'Pullover shirt', 'Dress',
                        'Coat', 'Sandal', 'Shirt', 'Sneaker', 'Bag', 'Ankle boot'])
```

```
In [5]: # Display a few examples

import matplotlib.pyplot as plt

n_rows, n_cols = 3, 5
fig, axes = plt.subplots(n_rows, n_cols, figsize=(14, 8))
inx = np.random.choice(x_train.shape[0], n_rows*n_cols, replace=False)
fig.subplots_adjust(hspace=0.3, wspace=0.1)

for n, (image, label) in enumerate(zip(x_train[inx], y_train[inx])):
    row = n // n_cols
    col = n % n_cols
    axes[row, col].imshow(image, cmap='binary')
    axes[row, col].get_xaxis().set_visible(False)
    axes[row, col].get_yaxis().set_visible(False)
    axes[row, col].text(10., -2.5, f'{class_names[label]}')
plt.show()
```



## Build the CNN autoencoder model

We define the encoder and decoder networks separately.

```
In [7]: # Build a CNN encoder

from keras.models import Sequential
from keras.layers import Input, Conv2D, MaxPool2D, Flatten, Dense

encoded_dim = 2

cnn_encoder = Sequential([
    Input(shape=(28, 28, 1)),
    Conv2D(16, 5, activation='relu'),
    MaxPool2D(2),
    Conv2D(8, 5, activation='relu'),
    Flatten(),
    Dense(64, activation='relu'),
    Dense(encoded_dim)
])
cnn_encoder.summary()
```

Model: "sequential\_1"

Layer (type)	Output Shape	Param #
conv2d_2 (Conv2D)	(None, 24, 24, 16)	416
max_pooling2d_1 (MaxPooling2D)	(None, 12, 12, 16)	0
conv2d_3 (Conv2D)	(None, 8, 8, 8)	3,208
flatten_1 (Flatten)	(None, 512)	0
dense_2 (Dense)	(None, 64)	32,832
dense_3 (Dense)	(None, 2)	130

Total params: 36,586 (142.91 KB)

Trainable params: 36,586 (142.91 KB)

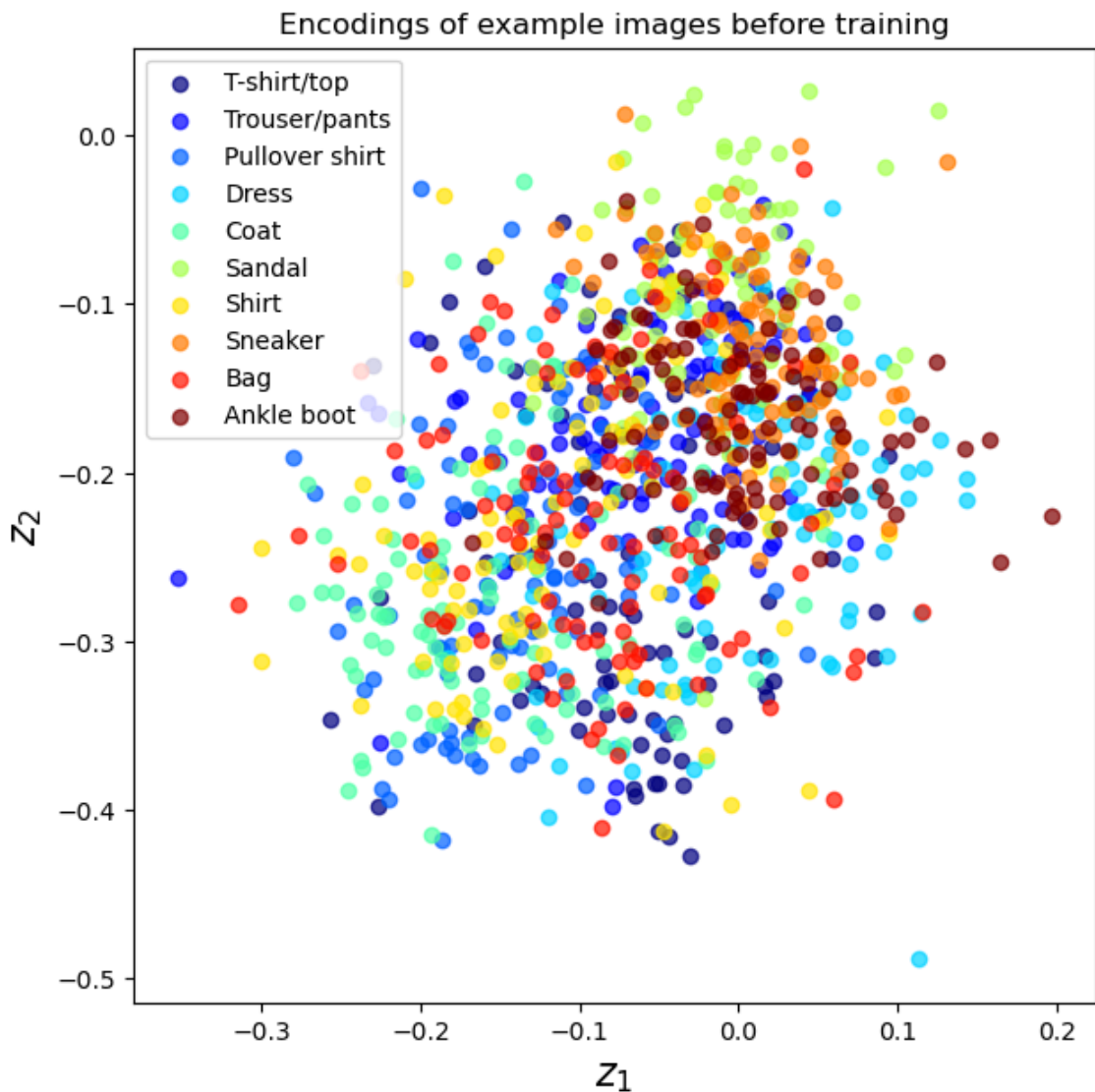
Non-trainable params: 0 (0.00 B)

```
In [9]: # Compute encodings before training
```

```
inx = np.random.choice(x_test.shape[0], 1000, replace=False)
untrained_encodings = ops.convert_to_numpy(cnn_encoder(x_test[inx]))
untrained_encoding_labels = y_test[inx]
```

```
In [10]: # Plot untrained encodings
```

```
plt.figure(figsize=(7, 7))
cmap = plt.get_cmap('jet', 10)
for i, class_label in enumerate(class_names):
    inx = np.where(untrained_encoding_labels == i)[0]
    plt.scatter(untrained_encodings[inx, 0], untrained_encodings[inx, 1],
                color=cmap(i), label=class_label, alpha=0.7)
plt.xlabel('$z_1$', fontsize=16)
plt.ylabel('$z_2$', fontsize=16)
plt.title('Encodings of example images before training')
plt.legend()
plt.show()
```



```
In [11]: # Build a CNN decoder
```

```
from keras.layers import Reshape, UpSampling2D, Conv2DTranspose

cnn_decoder = Sequential([
    Input(shape=(encoded_dim,)),
```

```

Dense(64, activation='relu'),
Dense(512, activation='relu'),
Reshape((8, 8, 8)),
Conv2DTranspose(16, 5, activation='relu'),
UpSampling2D((2, 2)),
Conv2DTranspose(1, 5, activation='sigmoid')
])
cnn_decoder.summary()

```

Model: "sequential\_2"

Layer (type)	Output Shape	Param #
dense_4 (Dense)	(None, 64)	192
dense_5 (Dense)	(None, 512)	33,280
reshape (Reshape)	(None, 8, 8, 8)	0
conv2d_transpose (Conv2DTranspose)	(None, 12, 12, 16)	3,216
up_sampling2d (UpSampling2D)	(None, 24, 24, 16)	0
conv2d_transpose_1 (Conv2DTranspose)	(None, 28, 28, 1)	401

**Total params:** 37,089 (144.88 KB)

**Trainable params:** 37,089 (144.88 KB)

**Non-trainable params:** 0 (0.00 B)

```

In [16]: # Define the autoencoder

from keras.models import Model

cnn_autoencoder = Model(inputs=cnn_encoder.inputs,
                        outputs=cnn_decoder(cnn_encoder.outputs))

```

## Make train and test Datasets

```

In [17]: # Create Dataset objects for train and test sets

import tensorflow as tf

train_dataset = tf.data.Dataset.from_tensor_slices((x_train, x_train))
test_dataset = tf.data.Dataset.from_tensor_slices((x_test, x_test))

```

```

In [18]: # Process the datasets

train_dataset = train_dataset.shuffle(1000)

train_dataset = train_dataset.batch(64).prefetch(tf.data.AUTOTUNE)
test_dataset = test_dataset.batch(64).prefetch(tf.data.AUTOTUNE)

```

```

In [19]: # Compile and fit the model

cnn_autoencoder.compile(loss='binary_crossentropy')
cnn_autoencoder.fit(train_dataset, epochs=10)

```

```

Epoch 1/10
938/938 ————— 5s 3ms/step - loss: 0.3352
Epoch 2/10
938/938 ————— 2s 2ms/step - loss: 0.3331
Epoch 3/10
938/938 ————— 2s 2ms/step - loss: 0.3315
Epoch 4/10
938/938 ————— 2s 2ms/step - loss: 0.3302
Epoch 5/10
938/938 ————— 2s 2ms/step - loss: 0.3296
Epoch 6/10
938/938 ————— 2s 2ms/step - loss: 0.3289
Epoch 7/10
938/938 ————— 2s 2ms/step - loss: 0.3283
Epoch 8/10
938/938 ————— 2s 2ms/step - loss: 0.3276
Epoch 9/10
938/938 ————— 2s 2ms/step - loss: 0.3273
Epoch 10/10
938/938 ————— 2s 2ms/step - loss: 0.3268

```

Out[19]: <keras.src.callbacks.history.History at 0x704e27faeb90>

In [20]: *# Compute encodings after training*

```

inx = np.random.choice(x_test.shape[0], 1000, replace=False)
trained_encodings = ops.convert_to_numpy(cnn_encoder(x_test[inx]))
trained_encoding_labels = y_test[inx]

```

In [21]: *# Plot untrained and trained encodings*

```

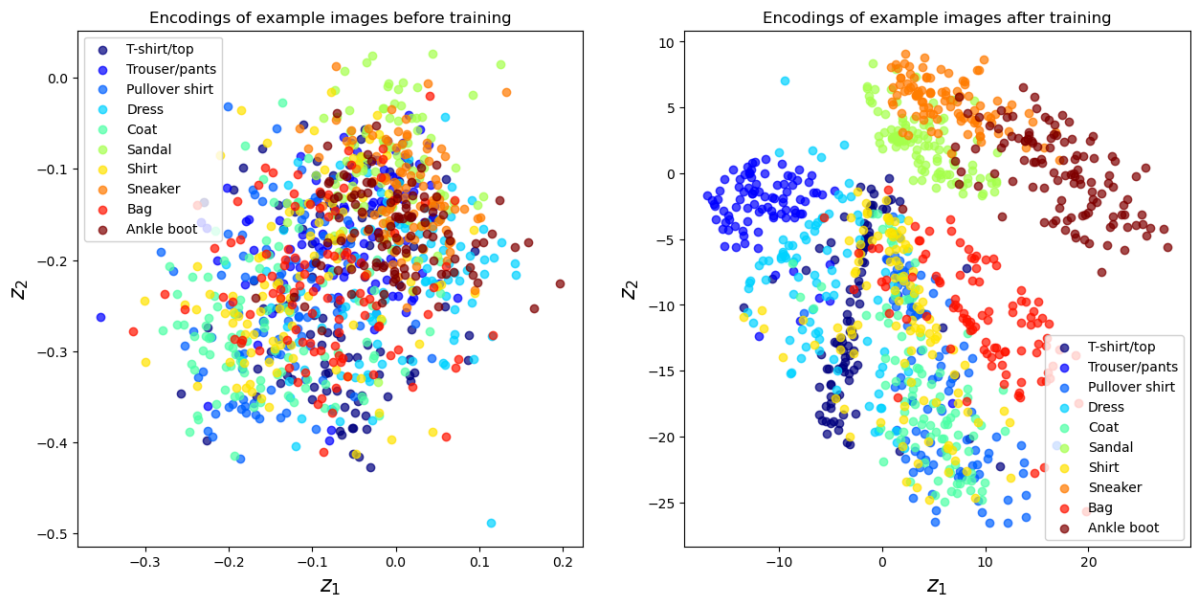
plt.figure(figsize=(15, 7))
cmap = plt.get_cmap('jet', 10)

plt.subplot(1, 2, 1)
for i, class_label in enumerate(class_names):
    inx = np.where(untrained_encoding_labels == i)[0]
    plt.scatter(untrained_encodings[inx, 0], untrained_encodings[inx, 1],
                color=cmap(i), label=class_label, alpha=0.7)
plt.xlabel('$z_1$', fontsize=16)
plt.ylabel('$z_2$', fontsize=16)
plt.title('Encodings of example images before training')
plt.legend()

plt.subplot(1, 2, 2)
for i, class_label in enumerate(class_names):
    inx = np.where(trained_encoding_labels == i)[0]
    plt.scatter(trained_encodings[inx, 0], trained_encodings[inx, 1],
                color=cmap(i), label=class_label, alpha=0.7)
plt.xlabel('$z_1$', fontsize=16)
plt.ylabel('$z_2$', fontsize=16)
plt.title('Encodings of example images after training')
plt.legend()

plt.show()

```

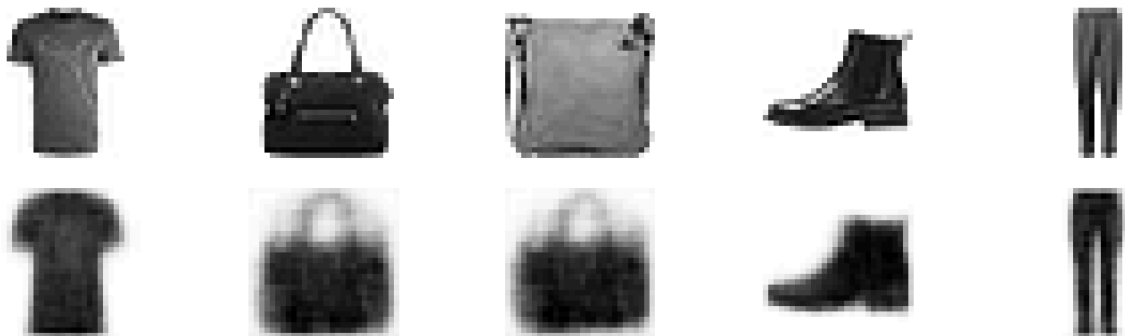


```
In [23]: # Compute the autoencoder's reconstructions

inx = np.random.choice(x_test.shape[0], 5, replace=False)
reconstructed_example_images = ops.convert_to_numpy(cnn_autoencoder(x_test[inx]))
```

```
In [24]: # Evaluate the autoencoder's reconstructions

f, axs = plt.subplots(2, 5, figsize=(15, 4))
for j in range(5):
    axs[0, j].imshow(x_test[inx][j], cmap='binary')
    axs[1, j].imshow(reconstructed_example_images[j].squeeze(), cmap='binary')
    axs[0, j].axis('off')
    axs[1, j].axis('off')
```



*Exercise.* Redesign the CNN autoencoder above using strides  $\geq 2$  for the encoder, and design the decoder to be the reverse architecture.

## The variational autoencoder

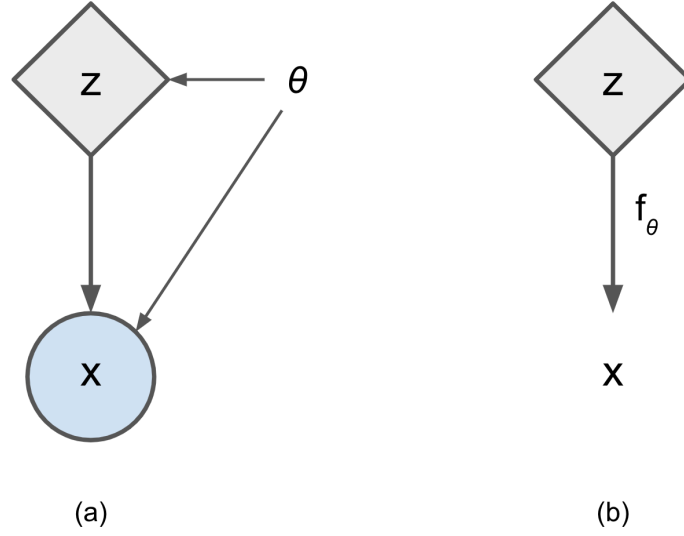
We will now review the variational autoencoder (VAE) algorithm, its derivation from applying the principle of variational inference to a prescribed generative model, and its connection to standard autoencoders. The VAE was developed independently by [Kingma & Welling 2014](#) and [Rezende et al 2014](#) at about the same time. For a general reference on variational inference, see [Blei et al 2017](#).

First, we describe the generative model behind the variational autoencoder. This is a **latent variable generative model**, where we introduce a latent (unobserved) random variable that is intended to capture hidden causes or explanations of the data.



Furthermore, it is a **prescribed model** in the sense that we prescribe a noise model for the observations. Given a latent variable  $z \in \mathbb{R}^l$ , this determines a distribution over possible observations  $p_\theta(x | z)$ , with  $x \in \mathbb{R}^D$ . This class of generative model is also called a **likelihood-based model**, since the observations have an associated likelihood function.

This is in contrast to an **implicit model**, where there is no likelihood function on the observations, and instead a realisation of the latent variable  $z$  implicitly defines the observation  $x$  (note that this is the case with normalising flows, although there we have the additional special structure that the generative model is invertible, and so the observation likelihood can still be explicitly computed). This is illustrated in the following figure.



Latent variable directed graphical models; (a) a prescribed generative model that defines a likelihood for each observation, and (b) an implicit generative model. The VAE is based on the prescribed model

The generative model under consideration can be written as  $p_\theta(z)p_\theta(x | z)$ , where the conditional distribution  $p_\theta(x | z)$  is defined by a neural network. The **marginal likelihood** (or **model evidence**) of an individual datapoint  $x \in \mathbb{R}^D$  is given by

$$p_\theta(x) = \int p_\theta(z)p_\theta(x | z)dz, \quad (1)$$

where  $\theta$  are the model parameters.

Note that under the usual i.i.d. assumption of our dataset  $\mathbf{x} = (x_i)_{i=1}^N$ , the full data log-likelihood is given by

$$\log p_\theta(\mathbf{x}) = \sum_{i=1}^N \log p_\theta(x_i).$$

In the following we will continue to consider the likelihood of a single datapoint  $x_i$ , and drop the subscript  $i$  for notational convenience.

Now, we would like to choose the parameters  $\theta$  that maximise the marginal likelihood. Unfortunately, the integral above is intractable in general (as is the true posterior  $p(z | x)$ ), so we need to approximate it.

The approximation that we will use is the **evidence lower bound** (ELBO), or **variational free energy**, which is a lower bound on the true marginal log-likelihood:

$$\log p_\theta(x) \geq \mathbb{E}_{q_\phi(z|x)} [\log p_\theta(x | z)] - D_{KL} (q_\phi(z | x) || p_\theta(z)) \quad (2)$$

$$=: \mathcal{L}(\theta, \phi; x), \quad (1)$$

where  $q_\phi(z | x)$  is a parameterised distribution of our choosing, and  $D_{KL}$  denotes the Kullback-Leibler divergence, given by

$$D_{KL} (q_\phi(z | x) || p_\theta(z)) = \int q_\phi(z | x) \log \left( \frac{q_\phi(z | x)}{p_\theta(z)} \right) dz.$$

The two terms in (2) are often interpreted as a reconstruction loss term and a regularisation term:

$$\mathcal{L}(\theta, \phi; x) = \underbrace{\mathbb{E}_{q_\phi(z|x)} [\log p_\theta(x | z)]}_{\text{reconstruction loss}} - \underbrace{D_{KL} (q_\phi(z | x) || p_\theta(z))}_{\text{regulariser}}.$$

This decomposition shows the connection to autoencoders: if  $q_\phi(z | x)$  is a parameterised neural network, then we can view this as the encoder and  $p_\theta(x | z)$  as the decoder. Then the reconstruction loss is the probabilistic version of the autoencoder reconstruction loss (where we could consider  $q_\phi(z | x)$  as a delta distribution). The second term regularises the encoder, and ensures it doesn't stray too far from the prior distribution  $p_\theta(z)$ .

The ELBO is also sometimes written as  $\mathcal{L}(\theta, \phi; x) = \mathbb{E}_{q_\phi(z|x)} [-\log q_\phi(z | x) + \log p_\theta(x, z)]$ .

## Derivation of the ELBO

We will derive the evidence lower bound in two different ways. The first is a simple derivation using Jensen's inequality, and the second will help to shed some light on the optimal choice for the distribution  $q_\phi(z | x)$ .

*Derivation 1.* The marginal log-likelihood is given by (cf. (1))

$$\log p_\theta(x) = \log \int p_\theta(x | z) p_\theta(z) dz \quad (2)$$

$$= \log \int p_\theta(x | z) \frac{p_\theta(z)}{q_\phi(z | x)} q_\phi(z | x) dz \quad (3)$$

$$\geq \int \log \left( p_\theta(x | z) \frac{p_\theta(z)}{q_\phi(z | x)} \right) q_\phi(z | x) dz \quad (4)$$

$$= \int q_\phi(z | x) \log p_\theta(x | z) dz - \int q_\phi(z | x) \log \left( \frac{q_\phi(z | x)}{p_\theta(z)} \right) dz \quad (5)$$

$$= \mathcal{L}(\theta, \phi; x), \quad (6)$$

where the third line in the above uses Jensen's inequality.

*Derivation 2.* Let  $q_\phi(z | x)$  be a parameterised family of distributions that we use to approximate the true posterior  $p_\theta(z | x)$ . We define the objective function that we wish to minimise as the KL-divergence  $D_{KL}(q_\phi(z | x) || p_\theta(z | x))$ . Then we have

$$D_{KL}(q_\phi(z | x) || p_\theta(z | x)) = \int q_\phi(z | x) \log \left( \frac{q_\phi(z | x)}{p_\theta(z | x)} \right) dz \quad (7)$$

$$= \int q_\phi(z | x) \log \left( \frac{q_\phi(z | x) p_\theta(x)}{p_\theta(x | z) p_\theta(z)} \right) dz \quad (8)$$

$$= \int q_\phi(z | x) \log p_\theta(x) dz - \int q_\phi(z | x) \log p_\theta(x | z) dz \quad (9)$$

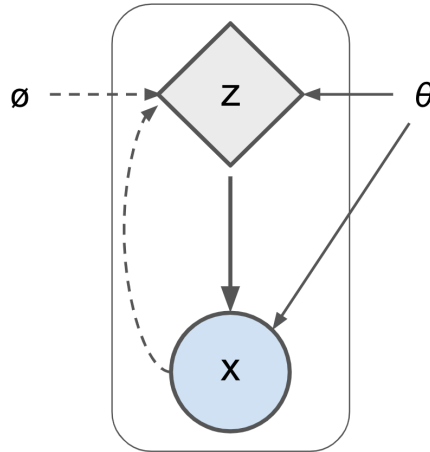
$$+ \int q_\phi(z | x) \log \left( \frac{q_\phi(z | x)}{p_\theta(z)} \right) dz \quad (10)$$

$$= \log p_\theta(x) - \mathcal{L}(\theta, \phi; x) \quad (11)$$

Since the KL-divergence is always non-negative, the above shows that  $\mathcal{L}(\theta, \phi; x)$  is indeed a lower bound on the marginal log-likelihood  $\log p_\theta(x)$ . Furthermore, it shows that the gap in the bound is given by  $D_{KL}(q_\phi(z | x) || p_\theta(z | x))$ .

We see that to maximise the ELBO, the distribution  $q_\phi(z | x)$  should approximate the true posterior  $p_\theta(z | x)$ . And the better the approximation, the tighter the bound.

The following figure illustrates that the variational autoencoder adds the variational approximation  $q_\phi(z | x)$  to the intractable true posterior  $p_\theta(z | x)$ .



The prescribed generative model underlying the variational autoencoder, and the variational approximation  $q_\phi(z | x)$  with variational parameters  $\phi$  depicted with dashed lines

Note that the generative model parameters  $\theta$  and the variational parameters  $\phi$  are **global variables**, whereas the latent random variable  $z$  is a **local variable**. The variational parameters  $\phi$  are shared across all data points, and are not specific to individual data points, in contrast to traditional mean-field variational inference. This strategy is known as **amortized inference** (Hoffman et al 2013).

## The reparameterization trick

We have now defined our ELBO objective function that we wish to maximise, which is a lower bound on the marginal log-likelihood:

$$\mathcal{L}(\theta, \phi; x) = \mathbb{E}_{q_\phi(z|x)} [\log p_\theta(x | z)] - D_{KL}(q_\phi(z | x) || p_\theta(z))$$

Note that we are able to evaluate the densities  $q_\phi(z | x)$ ,  $p_\theta(x | z)$ ,  $p_\theta(z)$  as well as sample from the approximating distribution  $q_\phi(z | x)$ , so the ELBO can be evaluated using Monte Carlo samples  $\{z^{(j)}\}_{j=1}^L$ , with  $z^{(j)}$  sampled from  $q_\phi(z | x)$

$$\mathcal{L}(\theta, \phi; x) \approx \frac{1}{L} \sum_{j=1}^L \log p_\theta(x | z^{(j)}) + \log p_\theta(z^{(j)}) - \log q_\phi(z^{(j)} | x)$$

The question remains how to optimise the ELBO with respect to the parameters  $\theta$  and  $\phi$ . Note that taking gradients with respect to  $\phi$  is not straightforward, as the  $z^{(j)}$  are samples.

A typical **score-function estimator** (Glynn 1990, Kleijnen & Rubinstein 1996) for the general type of problem of taking a gradient of an expectation of some function  $f(z)$  is given by

$$\nabla_\phi \mathbb{E}_{q_\phi(z)} [f(z)] = \mathbb{E}_{q_\phi(z)} [f(z) \nabla_\phi \log q_\phi(z)] \quad (12)$$

$$\approx \frac{1}{L} \sum_{j=1}^L [f(z^{(j)}) \nabla_\phi \log q_\phi(z^{(j)})]. \quad (13)$$

This estimator is also used in reinforcement learning for policy gradients, where it is often referred to as the REINFORCE algorithm (Williams 1992). However, this estimator typically has high variance (Blei et al 2012), and in our case we can do better, in particular since our function  $f(z)$  ( $= \log p_\theta(x, z^{(j)}) - \log q_\phi(z^{(j)} | x)$ ) is differentiable.

The 'reparameterization trick' simply reparameterises the random latent variable  $z \sim q_\phi(z | x)$  using a differentiable transformation  $g_\phi(\epsilon, x)$  of an auxiliary noise variable  $\epsilon \sim p(\epsilon)$ :

$$\begin{aligned} z &\sim q_\phi(z | x) \\ z &= g_\phi(\epsilon, x), \quad \epsilon \sim p(\epsilon) \end{aligned}$$

An example is if  $q_\phi(z | x)$  a multivariate Gaussian distribution  $N(\mu_\phi(x), \Sigma_\phi(x))$ . Then we could reparameterise the distribution as

$$p(\epsilon) = N(\mathbf{0}, \mathbf{I}), \quad g_\phi(\epsilon, x) = \mu_\phi(x) + L_\phi(x)\epsilon, \quad \text{where } L_\phi(x)L_\phi(x)^T = \Sigma_\phi(x).$$

The encoder network would then output the distribution parameters  $\mu_\phi(x)$  and  $L_\phi(x)$ , which are both fully differentiable with respect to  $\phi$ . Note that the noise variable distribution does not depend on any parameters.

If the transformation  $g_\phi(\cdot, x) : \mathbb{R}^d \mapsto \mathbb{R}^l$  is invertible, this is nothing more than a change of variables, so the change of variables formula applies to give

$$q_\phi(z | x) = |\det J_{g_\phi}(\epsilon)|^{-1} \cdot p(\epsilon) \quad (14)$$

$$= \left| \frac{d\epsilon}{dz} \right| \cdot p(\epsilon) \quad (15)$$

This leads to the **pathwise estimator** (Devroye 1996), which for a general function  $f(z)$  and reparameterization  $g_\phi(\epsilon)$  is given by

$$\nabla_\phi \mathbb{E}_{q_\phi(z)} [f(z)] = \nabla_\phi \int q_\phi(z) f(z) dz \quad (16)$$

$$= \nabla_\phi \int \left| \frac{d\epsilon}{dz} \right| \cdot p(\epsilon) f(g_\phi(\epsilon)) \left| \frac{dz}{d\epsilon} \right| d\epsilon \quad (17)$$

$$= \nabla_\phi \mathbb{E}_{p(\epsilon)} [f(g_\phi(\epsilon))] \quad (18)$$

$$= \mathbb{E}_{p(\epsilon)} [\nabla_\phi f(g_\phi(\epsilon))] \quad (19)$$

In our case, the reparameterization  $g_\phi(\epsilon, x)$  and noise variable  $\epsilon \sim p(\epsilon)$  leads to the **Stochastic Gradient Variational Bayes** (SGVB) estimator  $\hat{\mathcal{L}}^A(\theta, \phi; x) \approx \mathcal{L}(\theta, \phi; x)$ :

$$\hat{\mathcal{L}}^A(\theta, \phi; x) := \frac{1}{L} \sum_{j=1}^L \log p_\theta(x, z^{(j)}) - \log q_\phi(z^{(j)} | x) \quad (3)$$

$$\text{where } z^{(j)} = g_\phi(\epsilon^{(j)}, x) \quad \text{and} \quad \epsilon^{(j)} \sim p(\epsilon)$$

We can now use this estimator to approximate the ELBO objective, and take its gradients with respect to the parameters  $(\theta, \phi)$  on minibatches of data to optimise them:

$$\mathbb{E}_{x \sim p_{\text{data}}} [\log p_\theta(x)] \approx \frac{1}{|\mathcal{D}_{\text{train}}|} \sum_{i \in \mathcal{D}_{\text{train}}} \log p_\theta(x_i) \quad (20)$$

$$\geq \frac{1}{|\mathcal{D}_{\text{train}}|} \sum_{i \in \mathcal{D}_{\text{train}}} \mathcal{L}(\theta, \phi; x_i) \quad (21)$$

$$\approx \frac{1}{|\mathcal{D}_{\text{train}}|} \sum_{i \in \mathcal{D}_{\text{train}}} \hat{\mathcal{L}}^A(\theta, \phi; x) \quad (22)$$

$$\approx \frac{1}{M} \sum_{i \in \mathcal{D}_m} \hat{\mathcal{L}}^A(\theta, \phi; x), \quad (23)$$

where as usual  $\mathcal{D}_m$  is a randomly sampled minibatch of training data points, and  $M = |\mathcal{D}_m|$ .

Note that we wish to maximise the above objective, so in practice we will take the negative of the quantity above to minimise.

Finally, depending on the choice of prior  $p_\theta(z)$  and variational posterior  $q_\phi(z | x)$ , it may be possible to analytically evaluate the KL-divergence term  $D_{KL}(q_\phi(z | x) || p_\theta(z))$ . This is true, for example, in the case where both distributions are Gaussian. In this case, there is no need to approximate this term in the ELBO with Monte Carlo samples, and we can instead use the alternate version of the SGVB estimator:

$$\hat{\mathcal{L}}^B(\theta, \phi; x) := \frac{1}{L} \sum_{j=1}^L \log p_\theta(x | z^{(j)}) - D_{KL}(q_\phi(z | x) || p_\theta(z)), \quad (4)$$

where as before  $z^{(j)} = g_\phi(\epsilon^{(j)}, x)$  and  $\epsilon^{(j)} \sim p(\epsilon)$ .

It is worth noting that it is common in practice to take a single Monte Carlo sample ( $L = 1$ ) in the SGVB estimator (3) or (4), particularly for larger minibatch sizes.

We summarise the Auto-Encoding Variational Bayes (variational autoencoder) algorithm as follows. The algorithm inputs are the encoder and decoder networks  $q_\phi(z | x)$ ,  $p_\theta(x | z)$ , prior distribution  $p_\theta(z)$ , minibatch size  $M$  and number of Monte Carlo samples  $L$ .

Initialise  $\phi, \theta$  randomly

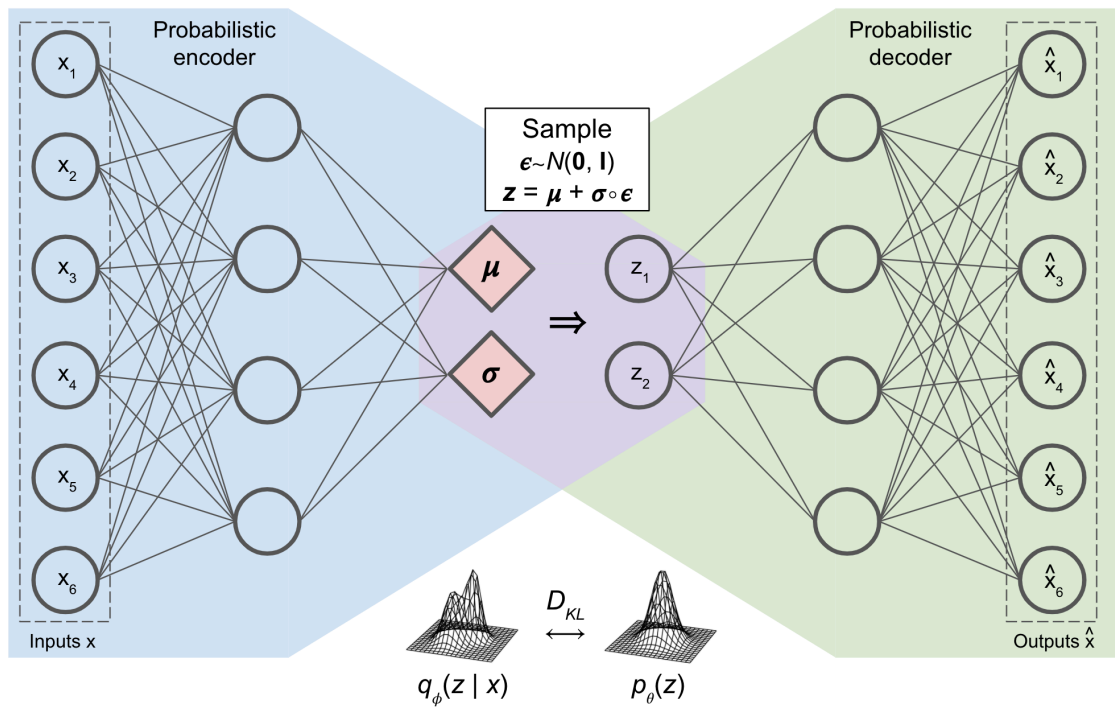
**while** not converged:

sample minibatch  $\mathcal{D}_m$  of  $M$  data examples

sample  $M \times L$  noise variables  $\epsilon^{(i,j)}$  for each  $x_i \in \mathcal{D}_m$  and  $j = 1, \dots, L$

compute gradient  $\frac{1}{M} \sum_{x_i \in \mathcal{D}_m} \nabla_{\phi, \theta} \hat{\mathcal{L}}(\theta, \phi; x_i)$ , where  $\hat{\mathcal{L}}$  is  $\hat{\mathcal{L}}^A$  or  $\hat{\mathcal{L}}^B$

update parameters by applying gradient with a NN optimiser (e.g. SGD, Adam)



The variational encoder. The encoder/inference network defines the latent variable distribution via the reparameterization trick, the decoder/generative network reconstructs the original input by defining a likelihood  $p_{\theta}(x | z)$ . The variational posterior  $q_{\phi}(z | x)$  is penalised for varying too much from the prior  $p_{\theta}(z)$

## VAE implementation

In this section we will develop a full implementation of the variational autoencoder. This implementation will involve model subclassing, which is a fully flexible way to build models in Keras.

```
In [2]: import keras
        from keras import ops
```

### Load the Frey Face dataset

We will use the [Frey Face](#) dataset to demonstrate the VAE, as in the original paper by [Kingma & Welling](#).

```
In [3]: # Load the data

import numpy as np

faces_data = np.load('./data/frey_faces.npy')
faces_data.shape
```

```
Out[3]: (1965, 28, 20)
```

```
In [4]: # Split data into train and validation sets

from sklearn.model_selection import train_test_split

x_train, x_val = train_test_split(faces_data, test_size=0.1)
x_train.shape
```

```
Out[4]: (1768, 28, 20)
```

```
In [5]: # View a sample of the data
```

```
import matplotlib.pyplot as plt

n_rows, n_cols = 4, 10
fig, axes = plt.subplots(n_rows, n_cols, figsize=(14, 8))
inx = np.random.choice(x_train.shape[0], n_rows*n_cols, replace=False)
fig.subplots_adjust(hspace=0., wspace=0.)

for n, image in enumerate(x_train[inx]):
    row = n // n_cols
    col = n % n_cols
    axes[row, col].imshow(image, cmap='gray')
    axes[row, col].get_xaxis().set_visible(False)
    axes[row, col].get_yaxis().set_visible(False)
plt.show()
```



```
In [6]: # Load the data into DataLoaders
```

[illegible]

## Generative model

Recall that the generative model  $p_\theta(z)p_\theta(x | z)$  is defined by the prior  $p_\theta(z)$  and decoder  $p_\theta(x | z)$ . We will choose a standard isotropic Gaussian distribution for the prior.

For the decoder, we follow [Kingma & Welling](#) and use a Gaussian likelihood, but constrain the mean to  $[0, 1]$ .

It is worth mentioning that it is also common practice to use an independent Bernoulli likelihood per pixel in the decoder for similar image datasets ([Kingma & Welling](#) uses this for MNIST), despite this being incorrect as the data is not binary.

```
In [7]: # Define the decoder

from keras.models import Model
from keras.layers import Input, Dense, Reshape

img_h, img_w = 28, 20
latent_dim = 2

inputs = Input(shape=(latent_dim,))
h = Dense(200, activation='relu')(inputs)
h = Dense(img_h * img_w * 2)(h)
h = Reshape((img_h, img_w, 2))(h)
h1, h2 = ops.unstack(h, axis=-1)
x_mean = ops.sigmoid(h1)
x_log_std = h2

decoder = Model(inputs=inputs, outputs=[x_mean, x_log_std], name='decoder')
decoder.summary()
```

Model: "decoder"

Layer (type)	Output Shape	Param #
input_layer (InputLayer)	(None, 2)	0
dense (Dense)	(None, 200)	600
dense_1 (Dense)	(None, 1120)	225,120
reshape (Reshape)	(None, 28, 20, 2)	0
unstack (Unstack)	[ (None, 28, 20), (None, 28, 20) ]	0
sigmoid (Sigmoid)	(None, 28, 20)	0

Total params: 225,720 (881.72 KB)

Trainable params: 225,720 (881.72 KB)

Non-trainable params: 0 (0.00 B)

## Inference model

We now define the encoder, or inference model  $q_\phi(z | x)$ . We will use a diagonal Gaussian for the approximate posterior, where the mean and diagonal covariance matrix are predicted by the encoder.

```
In [8]: # Define the encoder

from keras.layers import Flatten
```



```

inputs = Input(shape=(img_h, img_w))
h = Flatten()(inputs)
h = Dense(200, activation='relu')(h)
h = Dense(2 * latent_dim)(h)
z_mean, z_log_var = ops.split(h, 2, axis=-1)

encoder = Model(inputs=inputs, outputs=[z_mean, z_log_var], name='encoder')
encoder.summary()

```

Model: "encoder"

Layer (type)	Output Shape	Param #
input_layer_1 (InputLayer)	(None, 28, 20)	0
flatten (Flatten)	(None, 560)	0
dense_2 (Dense)	(None, 200)	112,200
dense_3 (Dense)	(None, 4)	804
split (Split)	[ (None, 2), (None, 2) ]	0

Total params: 113,004 (441.42 KB)

Trainable params: 113,004 (441.42 KB)

Non-trainable params: 0 (0.00 B)

## Training the encoder and decoder

We now compile and fit the encoder and decoder networks. Recall the ELBO objective

$$\mathcal{L}(\theta, \phi; x) = \mathbb{E}_{q_{\phi}(z|x)} [\log p_{\theta}(x | z)] - D_{KL}(q_{\phi}(z | x) || p_{\theta}(z)).$$

Since the prior and approximate posterior are both Gaussian, we will use the second form of the SGVB estimator (we will set  $L = 1$ ):

$$\hat{\mathcal{L}}^B(\theta, \phi; x) := \frac{1}{L} \sum_{j=1}^L \log p_{\theta}(x | z^{(j)}) - D_{KL}(q_{\phi}(z | x) || p_{\theta}(z)),$$

We have chosen the prior  $p_{\theta}(z)$  to be  $N(\mathbf{0}, \mathbf{I})$ , and the approximate posterior can be written as  $N(\mu_q, \text{diag}(\sigma_q))$ . In this case, we can write the KL divergence as

$$D_{KL}(q_{\phi}(z | x) || p_{\theta}(z)) = \frac{1}{2} \left[ \mu_q^T \mu_q + \sum_{i=1}^l (\sigma_q)_i - l - \log \prod_{i=1}^l (\sigma_q)_i \right], \quad (24)$$

where  $l$  is the dimension of the latent space.

To implement the VAE, we will use [model subclassing](#) to override the in-built `train_step` method (see the [TensorFlow](#) and [PyTorch](#) guides). This gives us control over what happens when we call the `.fit()` method.

```

In [9]: # Build the VAE Model object

from keras.metrics import Mean
import tensorflow as tf

class VAE(Model):

    def __init__(self, encoder, decoder, **kwargs):
        super().__init__(**kwargs)

```

```

self.encoder = encoder
self.decoder = decoder
self.loss_metric = Mean(name='loss')
self.nll_metric = Mean(name='nll')
self.kl_metric = Mean(name='kl')
self.pi = ops.array(np.pi)

def _get_losses(self, data):
    z_mean, z_log_var = self.encoder(data[0])
    kl_loss = 0.5 * ops.sum((ops.square(z_mean)
                             + ops.exp(z_log_var) - 1 - z_log_var), axis=-1)
    kl_loss = ops.mean(kl_loss)

    epsilon = keras.random.normal(ops.shape(z_mean))
    z_std = ops.exp(0.5 * z_log_var)
    z_sample = z_mean + (z_std * epsilon)

    x_mean, x_log_std = self.decoder(z_sample) # (B, 28, 20)
    log_Z = 0.5 * ops.log(2 * self.pi)
    nll_loss = 0.5 * ops.square((data - x_mean) / ops.exp(x_log_std))
    + x_log_std + log_Z
    nll_loss = ops.mean(ops.sum(nll_loss, axis=[-1, -2]))

    loss = kl_loss + nll_loss
    return loss, kl_loss, nll_loss

def call(self, inputs):
    z_mean, z_log_var = self.encoder(inputs)
    epsilon = keras.random.normal(ops.shape(z_mean))
    z_std = ops.exp(0.5 * z_log_var)
    z_sample = z_mean + (z_std * epsilon)
    return self.decoder(z_sample)

def train_step(self, data):
    backend = keras.config.backend()
    if backend == 'tensorflow':
        with tf.GradientTape() as tape:
            loss, kl_loss, nll_loss = self._get_losses(data)
            grads = tape.gradient(loss, self.trainable_weights)
            self.optimizer.apply_gradients(zip(grads, self.trainable_weights))
    elif backend == 'torch':
        self.zero_grad()
        loss, kl_loss, nll_loss = self._get_losses(data)

        loss.backward()

        gradients = [v.value.grad for v in self.trainable_weights]
        with torch.no_grad():
            self.optimizer.apply(gradients, self.trainable_weights)
    else:
        raise NotImplementedError(f"Unsupported backend: {backend}")

    self.loss_metric.update_state(loss)
    self.nll_metric.update_state(nll_loss)
    self.kl_metric.update_state(kl_loss)
    return {m.name: m.result() for m in self.metrics}

def test_step(self, data):
    loss, kl_loss, nll_loss = self._get_losses(data)
    self.loss_metric.update_state(loss)
    self.nll_metric.update_state(nll_loss)
    self.kl_metric.update_state(kl_loss)
    return {m.name: m.result() for m in self.metrics}

```

@property

```
def metrics(self):  
    return [self.loss_metric, self.nll_metric, self.kl_metric]
```

In [10]: *# Instantiate the Model*

```
vae = VAE(encoder, decoder, name='vae')
```

In [ ]: *# Compile and fit the Model*

```
from keras.callbacks import EarlyStopping  
  
early_stopping = EarlyStopping(patience=10)  
  
vae.compile(optimizer='adam')  
history = vae.fit(train_dataloader, validation_data=val_dataloader,  
                  epochs=200, callbacks=[early_stopping])
```

Epoch 1/200  
18/18 ————— 2s 27ms/step - kl: 54.5660 - loss: 295.6676 - nll: 241.10  
16 - val\_kl: 92.9325 - val\_loss: -392.6727 - val\_nll: -485.6052  
Epoch 2/200  
18/18 ————— 0s 18ms/step - kl: 77.1622 - loss: -447.5816 - nll: -524.  
7438 - val\_kl: 46.5437 - val\_loss: -533.4911 - val\_nll: -580.0348  
Epoch 3/200  
18/18 ————— 1s 29ms/step - kl: 42.6011 - loss: -551.5690 - nll: -594.  
1702 - val\_kl: 33.3567 - val\_loss: -571.9655 - val\_nll: -605.3221  
Epoch 4/200  
18/18 ————— 0s 27ms/step - kl: 32.0961 - loss: -591.4537 - nll: -623.  
5499 - val\_kl: 27.2290 - val\_loss: -584.3499 - val\_nll: -611.5788  
Epoch 5/200  
18/18 ————— 1s 28ms/step - kl: 26.5386 - loss: -598.4175 - nll: -624.  
9561 - val\_kl: 25.3625 - val\_loss: -577.7645 - val\_nll: -603.1269  
Epoch 6/200  
18/18 ————— 1s 28ms/step - kl: 23.1810 - loss: -584.0470 - nll: -607.  
2280 - val\_kl: 20.9089 - val\_loss: -588.4152 - val\_nll: -609.3241  
Epoch 7/200  
18/18 ————— 1s 28ms/step - kl: 21.7657 - loss: -607.1662 - nll: -628.  
9319 - val\_kl: 19.8475 - val\_loss: -600.1986 - val\_nll: -620.0461  
Epoch 8/200  
18/18 ————— 1s 28ms/step - kl: 20.4701 - loss: -622.4835 - nll: -642.  
9536 - val\_kl: 19.0233 - val\_loss: -612.3876 - val\_nll: -631.4109  
Epoch 9/200  
18/18 ————— 1s 27ms/step - kl: 19.5551 - loss: -630.3776 - nll: -649.  
9327 - val\_kl: 20.3582 - val\_loss: -621.5499 - val\_nll: -641.9083  
Epoch 10/200  
18/18 ————— 0s 22ms/step - kl: 19.3845 - loss: -647.2494 - nll: -666.  
6339 - val\_kl: 18.8008 - val\_loss: -649.7042 - val\_nll: -668.5049  
Epoch 11/200  
18/18 ————— 1s 32ms/step - kl: 18.5915 - loss: -665.9258 - nll: -684.  
5173 - val\_kl: 17.8761 - val\_loss: -662.1248 - val\_nll: -680.0010  
Epoch 12/200  
18/18 ————— 0s 20ms/step - kl: 17.7757 - loss: -676.2123 - nll: -693.  
9880 - val\_kl: 18.1330 - val\_loss: -656.0035 - val\_nll: -674.1366  
Epoch 13/200  
18/18 ————— 0s 12ms/step - kl: 17.1271 - loss: -676.8470 - nll: -693.  
9741 - val\_kl: 17.2919 - val\_loss: -668.1827 - val\_nll: -685.4745  
Epoch 14/200  
18/18 ————— 0s 20ms/step - kl: 16.6053 - loss: -691.6306 - nll: -708.  
2359 - val\_kl: 16.9079 - val\_loss: -676.5692 - val\_nll: -693.4771  
Epoch 15/200  
18/18 ————— 0s 24ms/step - kl: 16.3898 - loss: -701.5421 - nll: -717.  
9319 - val\_kl: 15.3904 - val\_loss: -691.3827 - val\_nll: -706.7731  
Epoch 16/200  
18/18 ————— 0s 23ms/step - kl: 15.8592 - loss: -719.2132 - nll: -735.  
0724 - val\_kl: 15.2328 - val\_loss: -698.7263 - val\_nll: -713.9592  
Epoch 17/200  
18/18 ————— 0s 27ms/step - kl: 15.3298 - loss: -725.6563 - nll: -740.  
9860 - val\_kl: 14.2831 - val\_loss: -702.2245 - val\_nll: -716.5076  
Epoch 18/200  
18/18 ————— 1s 28ms/step - kl: 14.7039 - loss: -717.1664 - nll: -731.  
8704 - val\_kl: 14.7673 - val\_loss: -707.3248 - val\_nll: -722.0922  
Epoch 19/200  
18/18 ————— 1s 27ms/step - kl: 14.5581 - loss: -726.3088 - nll: -740.  
8670 - val\_kl: 14.5427 - val\_loss: -702.0098 - val\_nll: -716.5525  
Epoch 20/200  
18/18 ————— 1s 28ms/step - kl: 13.8592 - loss: -716.1331 - nll: -729.  
9923 - val\_kl: 13.8332 - val\_loss: -703.8502 - val\_nll: -717.6834  
Epoch 21/200  
18/18 ————— 1s 26ms/step - kl: 13.9117 - loss: -724.3967 - nll: -738.  
3083 - val\_kl: 13.4566 - val\_loss: -718.3166 - val\_nll: -731.7732  
Epoch 22/200  
18/18 ————— 0s 24ms/step - kl: 13.5363 - loss: -732.7628 - nll: -746.  
2991 - val\_kl: 13.3069 - val\_loss: -722.5202 - val\_nll: -735.8270  
Epoch 23/200

18/18 ————— 0s 26ms/step - kl: 13.5034 - loss: -737.2853 - nll: -750.7888 - val\_kl: 12.8192 - val\_loss: -724.6711 - val\_nll: -737.4904  
Epoch 24/200

18/18 ————— 1s 27ms/step - kl: 13.1229 - loss: -735.1896 - nll: -748.3124 - val\_kl: 12.7345 - val\_loss: -724.5156 - val\_nll: -737.2502  
Epoch 25/200

18/18 ————— 0s 16ms/step - kl: 12.8833 - loss: -738.8208 - nll: -751.7041 - val\_kl: 12.2381 - val\_loss: -727.9149 - val\_nll: -740.1531  
Epoch 26/200

18/18 ————— 1s 27ms/step - kl: 12.5965 - loss: -744.9024 - nll: -757.4990 - val\_kl: 12.2817 - val\_loss: -730.6133 - val\_nll: -742.8951  
Epoch 27/200

18/18 ————— 0s 21ms/step - kl: 12.4851 - loss: -746.4224 - nll: -758.9075 - val\_kl: 12.3861 - val\_loss: -734.6251 - val\_nll: -747.0112  
Epoch 28/200

18/18 ————— 0s 12ms/step - kl: 12.5243 - loss: -753.2223 - nll: -765.7465 - val\_kl: 12.6983 - val\_loss: -719.9800 - val\_nll: -732.6783  
Epoch 29/200

18/18 ————— 1s 29ms/step - kl: 12.3299 - loss: -748.8930 - nll: -761.2230 - val\_kl: 11.6475 - val\_loss: -729.3101 - val\_nll: -740.9576  
Epoch 30/200

18/18 ————— 0s 23ms/step - kl: 12.0809 - loss: -751.4343 - nll: -763.5153 - val\_kl: 12.4502 - val\_loss: -720.9672 - val\_nll: -733.4172  
Epoch 31/200

18/18 ————— 0s 27ms/step - kl: 12.0861 - loss: -746.5848 - nll: -758.6709 - val\_kl: 11.6610 - val\_loss: -737.7368 - val\_nll: -749.3978  
Epoch 32/200

18/18 ————— 1s 26ms/step - kl: 12.0127 - loss: -756.8195 - nll: -768.8322 - val\_kl: 11.7769 - val\_loss: -741.7223 - val\_nll: -753.4991  
Epoch 33/200

18/18 ————— 1s 24ms/step - kl: 11.9954 - loss: -765.7440 - nll: -777.7393 - val\_kl: 11.6515 - val\_loss: -743.1998 - val\_nll: -754.8513  
Epoch 34/200

18/18 ————— 0s 25ms/step - kl: 11.8301 - loss: -758.6342 - nll: -770.4644 - val\_kl: 11.5139 - val\_loss: -738.7375 - val\_nll: -750.2513  
Epoch 35/200

18/18 ————— 0s 20ms/step - kl: 11.7782 - loss: -760.4554 - nll: -772.2335 - val\_kl: 11.4057 - val\_loss: -745.9750 - val\_nll: -757.3807  
Epoch 36/200

18/18 ————— 1s 25ms/step - kl: 11.6614 - loss: -768.4497 - nll: -780.1112 - val\_kl: 11.3183 - val\_loss: -747.2803 - val\_nll: -758.5986  
Epoch 37/200

18/18 ————— 1s 27ms/step - kl: 11.5143 - loss: -768.8934 - nll: -780.4077 - val\_kl: 11.1536 - val\_loss: -741.8081 - val\_nll: -752.9617  
Epoch 38/200

18/18 ————— 0s 18ms/step - kl: 11.4459 - loss: -767.6762 - nll: -779.1221 - val\_kl: 11.2587 - val\_loss: -729.6229 - val\_nll: -740.8816  
Epoch 39/200

18/18 ————— 0s 20ms/step - kl: 11.5458 - loss: -764.6865 - nll: -776.2323 - val\_kl: 11.4317 - val\_loss: -739.2997 - val\_nll: -750.7313  
Epoch 40/200

18/18 ————— 0s 22ms/step - kl: 11.3954 - loss: -765.4913 - nll: -776.8867 - val\_kl: 11.1125 - val\_loss: -752.6779 - val\_nll: -763.7904  
Epoch 41/200






















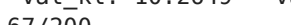
18/18 ————— 0s 24ms/step - kl: 11.2509 - loss: -764.4271 - nll: -775.6780 - val\_kl: 10.8315 - val\_loss: -751.3973 - val\_nll: -762.2288  
Epoch 42/200

18/18 ————— 0s 16ms/step - kl: 11.0681 - loss: -778.8685 - nll: -789.9366 - val\_kl: 11.0474 - val\_loss: -751.0557 - val\_nll: -762.1031  
Epoch 43/200

18/18 ————— 0s 22ms/step - kl: 11.1320 - loss: -781.8817 - nll: -793.0137 - val\_kl: 10.7007 - val\_loss: -749.0486 - val\_nll: -759.7493  
Epoch 44/200

18/18 ————— 0s 15ms/step - kl: 11.1345 - loss: -777.4308 - nll: -788.5653 - val\_kl: 10.7763 - val\_loss: -752.3547 - val\_nll: -763.1311  
Epoch 45/200

18/18 ————— 1s 26ms/step - kl: 10.9617 - loss: -778.2737 - nll: -789.

2354 - val\_kl: 10.8709 - val\_loss: -758.5714 - val\_nll: -769.4422  
Epoch 46/200  
18/18  1s 25ms/step - kl: 10.8848 - loss: -781.4102 - nll: -792.2949 - val\_kl: 10.4668 - val\_loss: -757.9376 - val\_nll: -768.4043  
Epoch 47/200  
18/18  0s 26ms/step - kl: 10.8193 - loss: -784.1684 - nll: -794.9877 - val\_kl: 10.1987 - val\_loss: -747.6705 - val\_nll: -757.8691  
Epoch 48/200  
18/18  0s 20ms/step - kl: 10.5925 - loss: -775.3235 - nll: -785.9160 - val\_kl: 10.3628 - val\_loss: -757.1893 - val\_nll: -767.5521  
Epoch 49/200  
18/18  0s 13ms/step - kl: 10.7023 - loss: -780.2882 - nll: -790.9905 - val\_kl: 10.3819 - val\_loss: -758.8394 - val\_nll: -769.2212  
Epoch 50/200  
18/18  1s 28ms/step - kl: 10.6878 - loss: -779.8488 - nll: -790.5367 - val\_kl: 10.7772 - val\_loss: -759.6715 - val\_nll: -770.4486  
Epoch 51/200  
18/18  0s 22ms/step - kl: 10.6500 - loss: -778.7781 - nll: -789.4282 - val\_kl: 10.6284 - val\_loss: -760.3243 - val\_nll: -770.9527  
Epoch 52/200  
18/18  0s 25ms/step - kl: 10.5825 - loss: -782.9460 - nll: -793.5285 - val\_kl: 10.7892 - val\_loss: -756.4574 - val\_nll: -767.2465  
Epoch 53/200  
18/18  0s 21ms/step - kl: 10.6430 - loss: -779.3554 - nll: -789.9983 - val\_kl: 10.1091 - val\_loss: -756.4230 - val\_nll: -766.5321  
Epoch 54/200  
18/18  1s 27ms/step - kl: 10.5684 - loss: -773.9346 - nll: -784.5030 - val\_kl: 10.5815 - val\_loss: -767.6227 - val\_nll: -778.2041  
Epoch 55/200  
18/18  0s 21ms/step - kl: 10.6393 - loss: -793.1954 - nll: -803.8348 - val\_kl: 10.6673 - val\_loss: -766.2513 - val\_nll: -776.9186  
Epoch 56/200  
18/18  0s 20ms/step - kl: 10.6701 - loss: -788.6266 - nll: -799.2966 - val\_kl: 10.3836 - val\_loss: -769.7987 - val\_nll: -780.1823  
Epoch 57/200  
18/18  1s 28ms/step - kl: 10.5720 - loss: -788.7788 - nll: -799.3507 - val\_kl: 10.4613 - val\_loss: -772.5193 - val\_nll: -782.9805  
Epoch 58/200  
18/18  1s 27ms/step - kl: 10.5870 - loss: -795.3962 - nll: -805.9832 - val\_kl: 10.2609 - val\_loss: -771.6398 - val\_nll: -781.9007  
Epoch 59/200  
18/18  0s 20ms/step - kl: 10.3914 - loss: -792.1815 - nll: -802.5728 - val\_kl: 10.3098 - val\_loss: -761.8081 - val\_nll: -772.1179  
Epoch 60/200  
18/18  0s 25ms/step - kl: 10.1931 - loss: -780.7876 - nll: -790.9807 - val\_kl: 9.9375 - val\_loss: -773.2677 - val\_nll: -783.2052  
Epoch 61/200  
18/18  0s 21ms/step - kl: 10.0782 - loss: -780.8503 - nll: -790.9285 - val\_kl: 9.6190 - val\_loss: -751.7928 - val\_nll: -761.4119  
Epoch 62/200  
18/18  0s 25ms/step - kl: 10.1235 - loss: -762.9006 - nll: -773.0240 - val\_kl: 10.3801 - val\_loss: -772.2001 - val\_nll: -782.5802  
Epoch 63/200  
18/18  1s 26ms/step - kl: 10.4697 - loss: -803.1576 - nll: -813.6273 - val\_kl: 10.1986 - val\_loss: -770.2116 - val\_nll: -780.4103  
Epoch 64/200  
18/18  0s 20ms/step - kl: 10.2120 - loss: -803.8167 - nll: -814.0287 - val\_kl: 9.8290 - val\_loss: -773.8790 - val\_nll: -783.7079  
Epoch 65/200  
18/18  1s 26ms/step - kl: 10.1675 - loss: -797.5135 - nll: -807.6810 - val\_kl: 10.2830 - val\_loss: -776.2853 - val\_nll: -786.5682  
Epoch 66/200  
18/18  0s 16ms/step - kl: 10.3077 - loss: -787.8779 - nll: -798.1855 - val\_kl: 10.2649 - val\_loss: -774.7249 - val\_nll: -784.9899  
Epoch 67/200  
18/18  0s 27ms/step - kl: 10.2700 - loss: -798.0064 - nll: -808.2764 - val\_kl: 10.1084 - val\_loss: -776.2153 - val\_nll: -786.3237

Epoch 68/200  
18/18 ————— 0s 22ms/step - kl: 10.3277 - loss: -799.6561 - nll: -809.9838 - val\_kl: 9.8556 - val\_loss: -767.0026 - val\_nll: -776.8582  
Epoch 69/200  
18/18 ————— 1s 26ms/step - kl: 10.1793 - loss: -802.3119 - nll: -812.4911 - val\_kl: 10.0749 - val\_loss: -780.1770 - val\_nll: -790.2520  
Epoch 70/200  
18/18 ————— 0s 19ms/step - kl: 10.2012 - loss: -808.7274 - nll: -818.9285 - val\_kl: 9.9825 - val\_loss: -783.3392 - val\_nll: -793.3217  
Epoch 71/200  
18/18 ————— 0s 23ms/step - kl: 10.0680 - loss: -808.9020 - nll: -818.9700 - val\_kl: 10.0016 - val\_loss: -778.4155 - val\_nll: -788.4172  
Epoch 72/200  
18/18 ————— 0s 22ms/step - kl: 9.9695 - loss: -806.8411 - nll: -816.8105 - val\_kl: 9.7090 - val\_loss: -780.6629 - val\_nll: -790.3719  
Epoch 73/200  
18/18 ————— 1s 26ms/step - kl: 9.9707 - loss: -790.8351 - nll: -800.8057 - val\_kl: 9.9377 - val\_loss: -780.3218 - val\_nll: -790.2596  
Epoch 74/200  
18/18 ————— 0s 19ms/step - kl: 10.0911 - loss: -800.9391 - nll: -811.0303 - val\_kl: 9.7348 - val\_loss: -784.8478 - val\_nll: -794.5825  
Epoch 75/200  
18/18 ————— 0s 25ms/step - kl: 9.8420 - loss: -800.1721 - nll: -810.0140 - val\_kl: 9.3694 - val\_loss: -768.0602 - val\_nll: -777.4296  
Epoch 76/200  
18/18 ————— 1s 26ms/step - kl: 9.6625 - loss: -787.0721 - nll: -796.7347 - val\_kl: 9.3039 - val\_loss: -768.4344 - val\_nll: -777.7383  
Epoch 77/200  
18/18 ————— 0s 16ms/step - kl: 9.5776 - loss: -796.4427 - nll: -806.0203 - val\_kl: 9.5101 - val\_loss: -784.4468 - val\_nll: -793.9569  
Epoch 78/200  
18/18 ————— 1s 28ms/step - kl: 9.8602 - loss: -811.1672 - nll: -821.0274 - val\_kl: 10.0442 - val\_loss: -781.6166 - val\_nll: -791.6608  
Epoch 79/200  
18/18 ————— 0s 20ms/step - kl: 9.9959 - loss: -812.8063 - nll: -822.8022 - val\_kl: 9.7850 - val\_loss: -772.8030 - val\_nll: -782.5880  
Epoch 80/200  
18/18 ————— 1s 27ms/step - kl: 9.7770 - loss: -806.7320 - nll: -816.5090 - val\_kl: 9.6886 - val\_loss: -789.6354 - val\_nll: -799.3240  
Epoch 81/200  
18/18 ————— 1s 27ms/step - kl: 9.8141 - loss: -811.6374 - nll: -821.4514 - val\_kl: 9.7835 - val\_loss: -788.5890 - val\_nll: -798.3724  
Epoch 82/200  
18/18 ————— 1s 27ms/step - kl: 9.8310 - loss: -810.3112 - nll: -820.1422 - val\_kl: 9.5103 - val\_loss: -792.5886 - val\_nll: -802.0989  
Epoch 83/200  
18/18 ————— 1s 26ms/step - kl: 9.7302 - loss: -816.3682 - nll: -826.0984 - val\_kl: 9.6603 - val\_loss: -788.3881 - val\_nll: -798.0484  
Epoch 84/200  
18/18 ————— 1s 26ms/step - kl: 9.7586 - loss: -817.6969 - nll: -827.4556 - val\_kl: 9.6160 - val\_loss: -791.1253 - val\_nll: -800.7413  
Epoch 85/200  
18/18 ————— 0s 24ms/step - kl: 9.7075 - loss: -815.5018 - nll: -825.2094 - val\_kl: 9.5316 - val\_loss: -792.3756 - val\_nll: -801.9071  
Epoch 86/200  
18/18 ————— 1s 27ms/step - kl: 9.6196 - loss: -805.0212 - nll: -814.6408 - val\_kl: 9.7754 - val\_loss: -782.6927 - val\_nll: -792.4681  
Epoch 87/200  
18/18 ————— 1s 26ms/step - kl: 9.8170 - loss: -812.1644 - nll: -821.9815 - val\_kl: 9.8602 - val\_loss: -786.2432 - val\_nll: -796.1034  
Epoch 88/200  
18/18 ————— 0s 22ms/step - kl: 9.8065 - loss: -814.5376 - nll: -824.3441 - val\_kl: 9.6441 - val\_loss: -797.3018 - val\_nll: -806.9459  
Epoch 89/200  
18/18 ————— 0s 25ms/step - kl: 9.6987 - loss: -821.1002 - nll: -830.7988 - val\_kl: 9.3623 - val\_loss: -796.3478 - val\_nll: -805.7101  
Epoch 90/200



18/18 ————— 1s 27ms/step - kl: 9.5656 - loss: -824.2831 - nll: -833.8  
487 - val\_kl: 9.2619 - val\_loss: -794.2492 - val\_nll: -803.5111  
Epoch 91/200

18/18 ————— 0s 19ms/step - kl: 9.4976 - loss: -812.9114 - nll: -822.4  
091 - val\_kl: 9.3437 - val\_loss: -793.0164 - val\_nll: -802.3600  
Epoch 92/200

18/18 ————— 0s 20ms/step - kl: 9.4857 - loss: -817.8033 - nll: -827.2  
890 - val\_kl: 9.5047 - val\_loss: -799.8885 - val\_nll: -809.3931  
Epoch 93/200

18/18 ————— 0s 19ms/step - kl: 9.6282 - loss: -825.7262 - nll: -835.3  
544 - val\_kl: 9.5272 - val\_loss: -795.5555 - val\_nll: -805.0827  
Epoch 94/200

18/18 ————— 0s 26ms/step - kl: 9.6589 - loss: -823.1824 - nll: -832.8  
413 - val\_kl: 9.4766 - val\_loss: -800.2495 - val\_nll: -809.7262  
Epoch 95/200

18/18 ————— 1s 26ms/step - kl: 9.4960 - loss: -823.5439 - nll: -833.0  
399 - val\_kl: 9.4700 - val\_loss: -798.1188 - val\_nll: -807.5888  
Epoch 96/200

18/18 ————— 0s 19ms/step - kl: 9.4788 - loss: -820.9158 - nll: -830.3  
947 - val\_kl: 9.3604 - val\_loss: -800.3260 - val\_nll: -809.6863  
Epoch 97/200

18/18 ————— 1s 27ms/step - kl: 9.5538 - loss: -827.2442 - nll: -836.7  
980 - val\_kl: 9.6967 - val\_loss: -795.8373 - val\_nll: -805.5339  
Epoch 98/200

18/18 ————— 0s 22ms/step - kl: 9.5708 - loss: -821.3774 - nll: -830.9  
482 - val\_kl: 9.2928 - val\_loss: -803.1716 - val\_nll: -812.4645  
Epoch 99/200

18/18 ————— 0s 17ms/step - kl: 9.4655 - loss: -822.4689 - nll: -831.9  
344 - val\_kl: 9.3770 - val\_loss: -799.6027 - val\_nll: -808.9798  
Epoch 100/200

18/18 ————— 1s 26ms/step - kl: 9.5466 - loss: -828.8375 - nll: -838.3  
840 - val\_kl: 9.3376 - val\_loss: -799.8305 - val\_nll: -809.1681  
Epoch 101/200

18/18 ————— 0s 21ms/step - kl: 9.4045 - loss: -826.8464 - nll: -836.2  
508 - val\_kl: 9.4119 - val\_loss: -799.2919 - val\_nll: -808.7040  
Epoch 102/200

18/18 ————— 0s 25ms/step - kl: 9.3704 - loss: -831.2337 - nll: -840.6  
041 - val\_kl: 9.3567 - val\_loss: -796.8973 - val\_nll: -806.2540  
Epoch 103/200

18/18 ————— 0s 14ms/step - kl: 9.3577 - loss: -821.0459 - nll: -830.4  
037 - val\_kl: 9.2779 - val\_loss: -805.5562 - val\_nll: -814.8340  
Epoch 104/200

18/18 ————— 0s 13ms/step - kl: 9.5228 - loss: -835.5372 - nll: -845.0  
599 - val\_kl: 9.4387 - val\_loss: -804.3253 - val\_nll: -813.7639  
Epoch 105/200

18/18 ————— 0s 20ms/step - kl: 9.4810 - loss: -825.3038 - nll: -834.7  
849 - val\_kl: 9.5230 - val\_loss: -792.9158 - val\_nll: -802.4389  
Epoch 106/200

18/18 ————— 0s 17ms/step - kl: 9.4141 - loss: -827.0316 - nll: -836.4  
457 - val\_kl: 9.5914 - val\_loss: -794.3239 - val\_nll: -803.9152  
Epoch 107/200

18/18 ————— 0s 19ms/step - kl: 9.4433 - loss: -828.2502 - nll: -837.6  
935 - val\_kl: 9.5316 - val\_loss: -803.0966 - val\_nll: -812.6283  
Epoch 108/200

18/18 ————— 0s 25ms/step - kl: 9.4660 - loss: -825.1511 - nll: -834.6  
171 - val\_kl: 9.4126 - val\_loss: -804.9681 - val\_nll: -814.3807  
Epoch 109/200

18/18 ————— 0s 17ms/step - kl: 9.4652 - loss: -823.7717 - nll: -833.2  
369 - val\_kl: 9.0969 - val\_loss: -805.2094 - val\_nll: -814.3063  
Epoch 110/200








18/18 ————— 1s 27ms/step - kl: 9.2710 - loss: -827.3738 - nll: -836.6  
448 - val\_kl: 9.2581 - val\_loss: -806.5124 - val\_nll: -815.7706  
Epoch 111/200

18/18 ————— 0s 24ms/step - kl: 9.3778 - loss: -823.6774 - nll: -833.0  
552 - val\_kl: 9.3647 - val\_loss: -802.4485 - val\_nll: -811.8133  
Epoch 112/200

18/18 ————— 0s 25ms/step - kl: 9.3662 - loss: -821.6652 - nll: -831.0



```

315 - val_kl: 9.1988 - val_loss: -803.9826 - val_nll: -813.1814
Epoch 113/200
18/18  1s 27ms/step - kl: 9.3111 - loss: -828.6627 - nll: -837.9
739 - val_kl: 9.4771 - val_loss: -809.4242 - val_nll: -818.9012
Epoch 114/200
18/18  0s 24ms/step - kl: 9.4746 - loss: -830.7944 - nll: -840.2
689 - val_kl: 9.4643 - val_loss: -799.8790 - val_nll: -809.3434
Epoch 115/200
18/18  0s 24ms/step - kl: 9.3897 - loss: -831.3996 - nll: -840.7
893 - val_kl: 9.2081 - val_loss: -810.4515 - val_nll: -819.6597
Epoch 116/200
18/18  0s 24ms/step - kl: 9.3147 - loss: -837.1895 - nll: -846.5
042 - val_kl: 9.1060 - val_loss: -808.5238 - val_nll: -817.6298
Epoch 117/200
18/18  0s 19ms/step - kl: 9.3753 - loss: -836.0165 - nll: -845.3
918 - val_kl: 9.0375 - val_loss: -798.2362 - val_nll: -807.2737
Epoch 118/200
18/18  1s 26ms/step - kl: 9.4081 - loss: -828.3523 - nll: -837.7
603 - val_kl: 9.3380 - val_loss: -810.4990 - val_nll: -819.8370
Epoch 119/200
18/18  0s 20ms/step - kl: 9.2772 - loss: -842.4493 - nll: -851.7
264 - val_kl: 9.3076 - val_loss: -804.7904 - val_nll: -814.0980
Epoch 120/200
18/18  0s 17ms/step - kl: 9.2532 - loss: -833.3672 - nll: -842.6
204 - val_kl: 9.4805 - val_loss: -808.2543 - val_nll: -817.7349
Epoch 121/200
18/18  1s 26ms/step - kl: 9.4678 - loss: -830.4432 - nll: -839.9
109 - val_kl: 9.4099 - val_loss: -812.4645 - val_nll: -821.8745
Epoch 122/200
18/18  0s 19ms/step - kl: 9.5259 - loss: -843.0267 - nll: -852.5
526 - val_kl: 9.3369 - val_loss: -814.5245 - val_nll: -823.8613
Epoch 123/200
18/18  0s 22ms/step - kl: 9.4729 - loss: -841.4292 - nll: -850.9
021 - val_kl: 9.3514 - val_loss: -806.1848 - val_nll: -815.5361
Epoch 124/200
18/18  0s 18ms/step - kl: 9.2935 - loss: -833.5746 - nll: -842.8
682 - val_kl: 9.1475 - val_loss: -810.0343 - val_nll: -819.1818
Epoch 125/200
18/18  0s 11ms/step - kl: 9.2145 - loss: -819.3718 - nll: -828.5
863 - val_kl: 9.0292 - val_loss: -813.7303 - val_nll: -822.7595
Epoch 126/200
18/18  0s 23ms/step - kl: 9.1484 - loss: -829.1292 - nll: -838.2
775 - val_kl: 9.2539 - val_loss: -810.9033 - val_nll: -820.1572
Epoch 127/200
18/18  0s 10ms/step - kl: 9.3182 - loss: -835.7309 - nll: -845.0
491 - val_kl: 9.1182 - val_loss: -813.3168 - val_nll: -822.4349
Epoch 128/200
18/18  0s 11ms/step - kl: 9.2954 - loss: -831.2030 - nll: -840.4
984 - val_kl: 9.2065 - val_loss: -813.6806 - val_nll: -822.8871
Epoch 129/200
18/18  0s 10ms/step - kl: 9.2659 - loss: -842.8499 - nll: -852.1
158 - val_kl: 9.3582 - val_loss: -813.4840 - val_nll: -822.8423
Epoch 130/200
18/18  0s 12ms/step - kl: 9.4276 - loss: -841.3474 - nll: -850.7
750 - val_kl: 9.2242 - val_loss: -813.4524 - val_nll: -822.6766
Epoch 131/200
18/18  0s 23ms/step - kl: 9.2754 - loss: -842.6168 - nll: -851.8
922 - val_kl: 9.2061 - val_loss: -812.5172 - val_nll: -821.7233
Epoch 132/200
18/18  0s 23ms/step - kl: 9.1347 - loss: -841.4671 - nll: -850.6
017 - val_kl: 9.2920 - val_loss: -800.6252 - val_nll: -809.9171

```

In [12]: `# Plot the learning curves`

```

fig = plt.figure(figsize=(15, 4))
fig.add_subplot(1, 3, 1)
plt.plot(history.history['loss'], label='train')

```

```

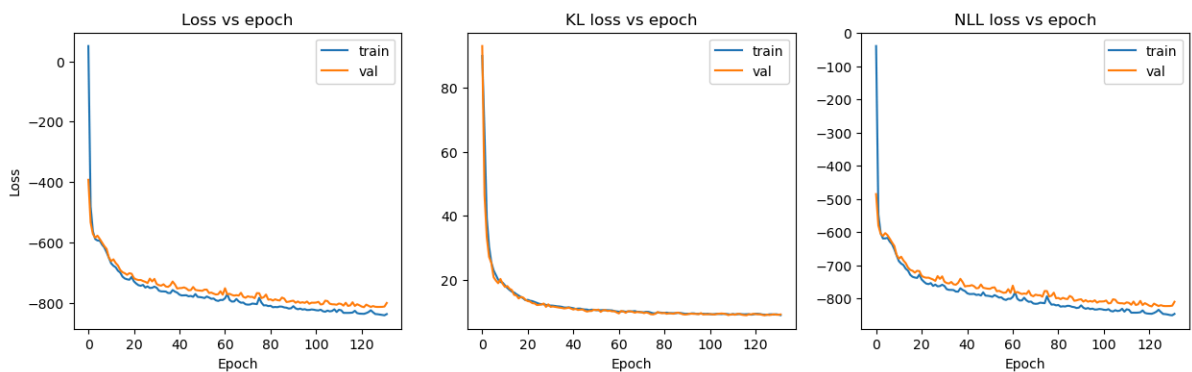
plt.plot(history.history['val_loss'], label='val')
plt.xlabel("Epoch")
plt.ylabel("Loss")
plt.title("Loss vs epoch")
plt.legend()

fig.add_subplot(1, 3, 2)
plt.plot(history.history['kl'], label='train')
plt.plot(history.history['val_kl'], label='val')
plt.xlabel("Epoch")
plt.title("KL loss vs epoch")
plt.legend()

fig.add_subplot(1, 3, 3)
plt.plot(history.history['nll'], label='train')
plt.plot(history.history['val_nll'], label='val')
plt.xlabel("Epoch")
plt.title("NLL loss vs epoch")
plt.legend()

plt.show()

```



In [13]: *# Evaluate performance on the validation set*

```
vae.evaluate(val_data_loader, return_dict=True)
```

10/10 ————— 0s 4ms/step - kl: 9.2344 - loss: -800.0823 - nll: -809.3167

```

Out[13]: {'kl': 9.291972160339355,
          'loss': -798.3985595703125,
          'nll': -807.6905517578125}

```

## View samples and reconstructions

In [14]: *# Sample from the generative model*

```
samples = ops.convert_to_numpy(vae.decoder(keras.random.normal(shape=(40, 2)))[0])
```

In [15]: *# View the samples*

```

n_rows, n_cols = 4, 10
fig, axes = plt.subplots(n_rows, n_cols, figsize=(14, 8))
fig.subplots_adjust(hspace=0., wspace=0.)

for n, image in enumerate(samples):
    row = n // n_cols
    col = n % n_cols
    axes[row, col].imshow(image, cmap='gray')
    axes[row, col].get_xaxis().set_visible(False)
    axes[row, col].get_yaxis().set_visible(False)
plt.show()

```



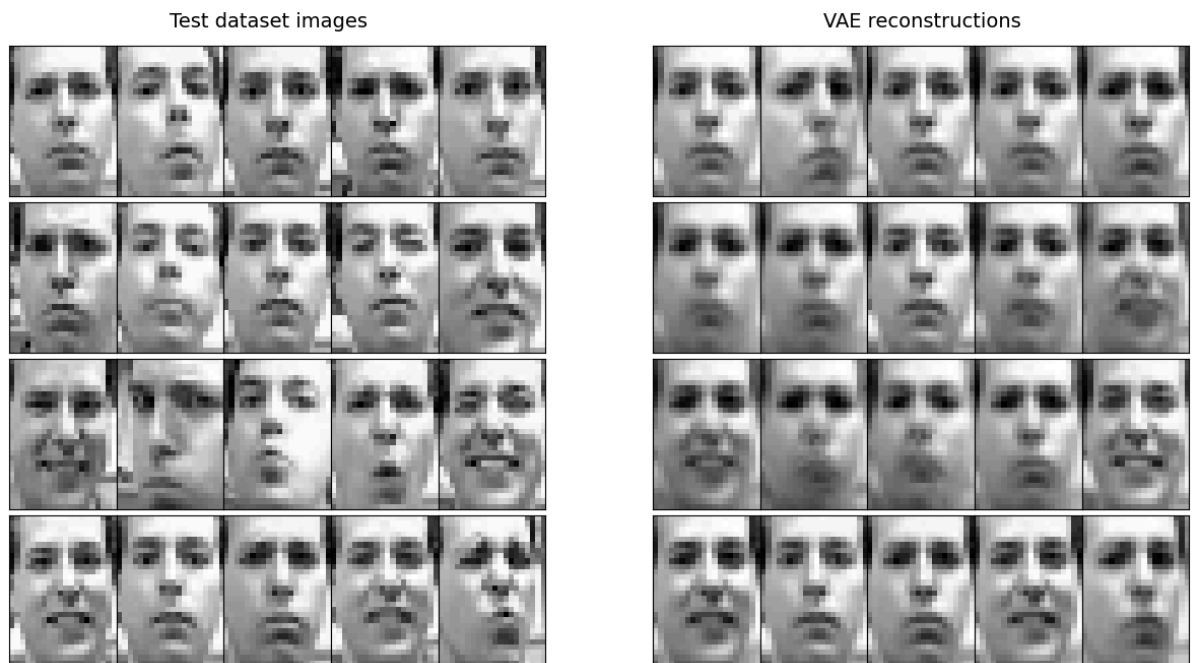
In [16]: *# Compute reconstructions from the validation dataset*

```
images = next(iter(val_dataloader))[0]
reconstructions = ops.convert_to_numpy(vae(images)[0])
```

In [17]: *# Plot some reconstructions from the test dataset*

```
import matplotlib.pyplot as plt
import matplotlib.gridspec as gridspec

fig = plt.figure(figsize=(15, 8))
outer = gridspec.GridSpec(1, 2, hspace=0.2)
n_rows, n_cols = 4, 5
fig.text(0.23, 0.9, "Test dataset images", fontsize=14)
fig.text(0.66, 0.9, "VAE reconstructions", fontsize=14)
for i in range(2):
    inner = gridspec.GridSpecFromSubplotSpec(n_rows, n_cols,
                                              subplot_spec=outer[i], wspace=0., hspace=0.)
    display_images = [images, reconstructions][i]
    for j in range(n_rows * n_cols):
        row = j // n_cols
        col = j % n_cols
        ax = plt.Subplot(fig, inner[j])
        ax.imshow(display_images[j], cmap='gray')
        ax.get_xaxis().set_visible(False)
        ax.get_yaxis().set_visible(False)
        fig.add_subplot(ax)
```



*Exercise.* Rewrite the loss function above so the KL divergence is approximated with Monte Carlo samples, so the SGVB estimator  $\hat{\mathcal{L}}^A(\theta, \phi; x)$  is used instead. Also try modifying the posterior to be a full covariance Gaussian. Does this improve the model performance?

## References

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