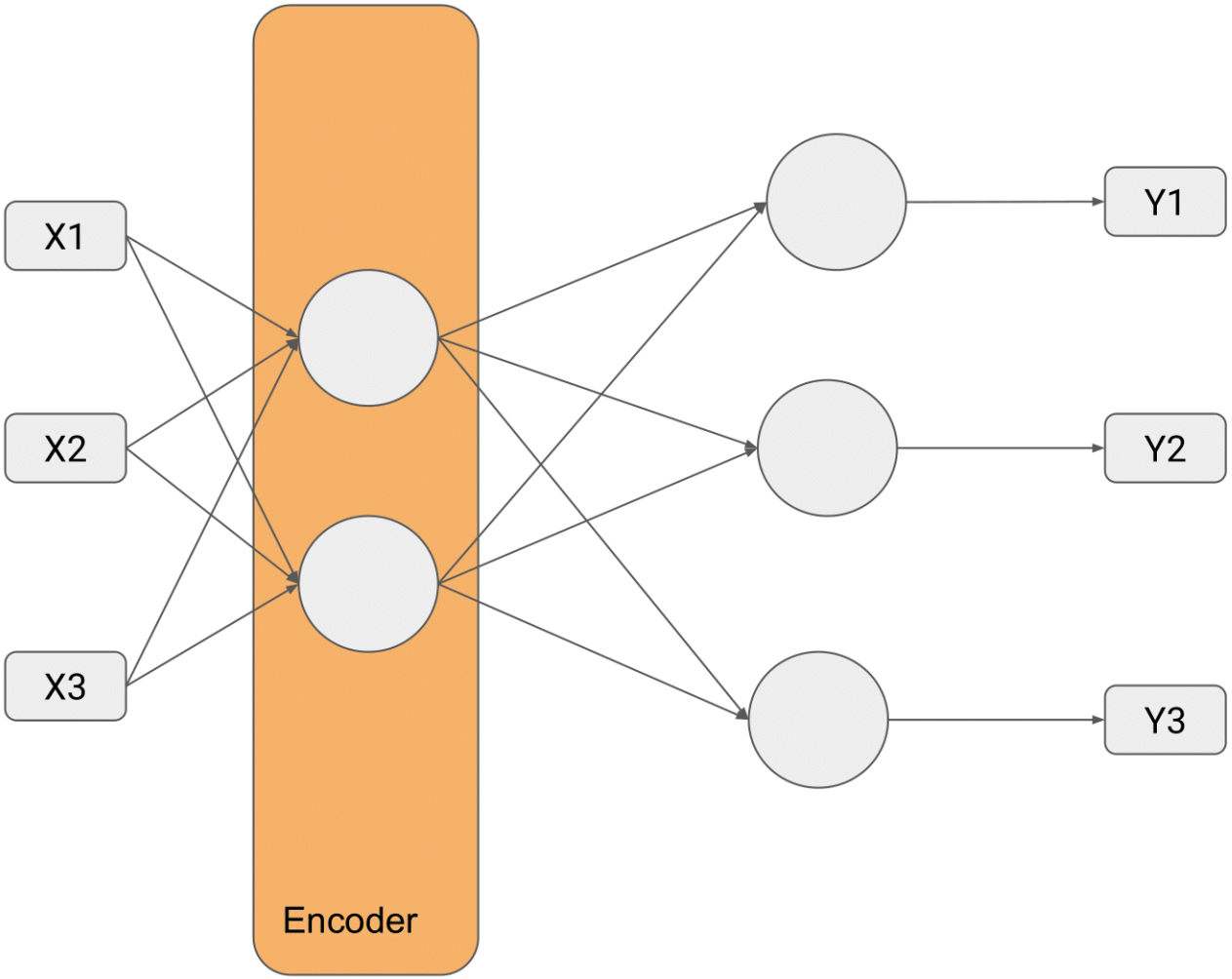
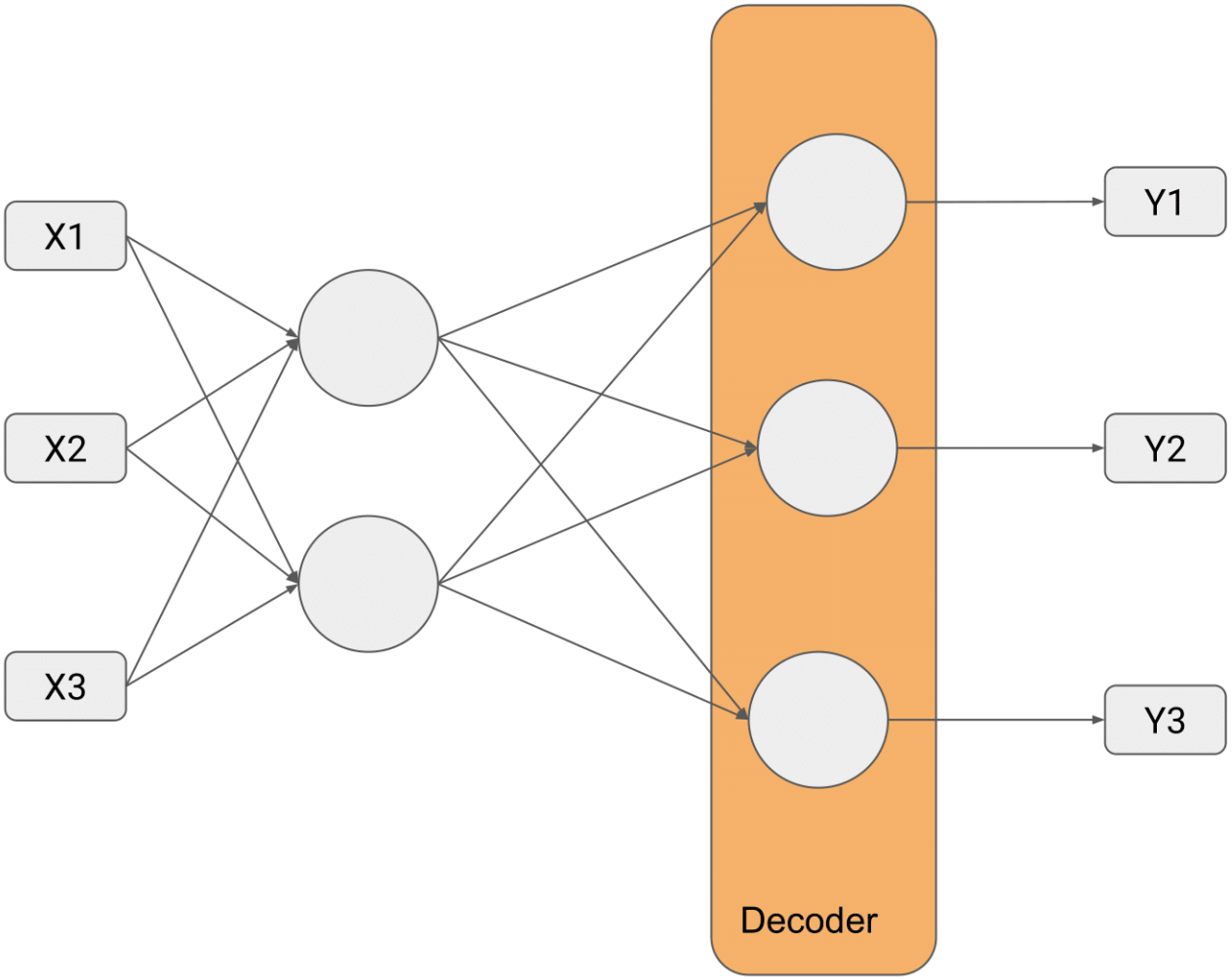
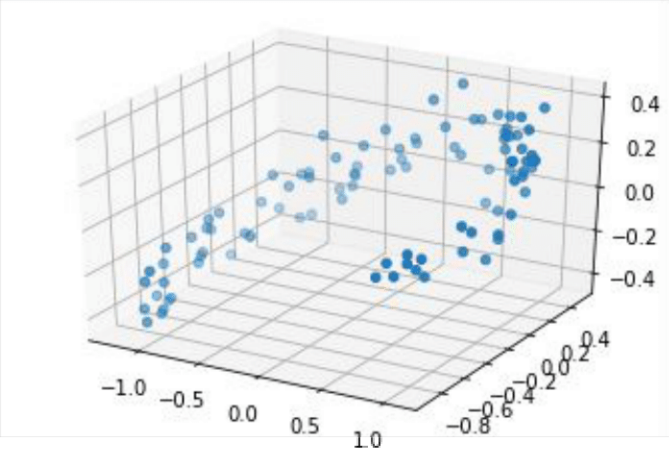
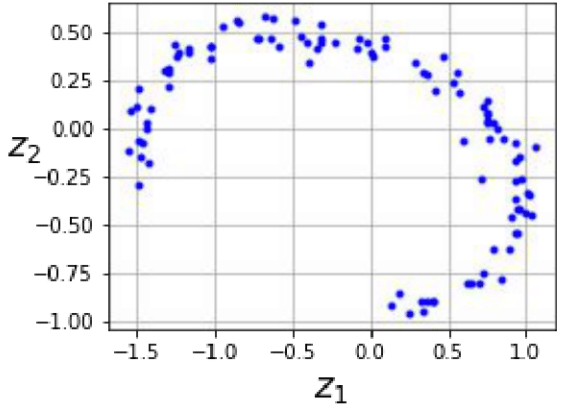
What are AutoEncoders?

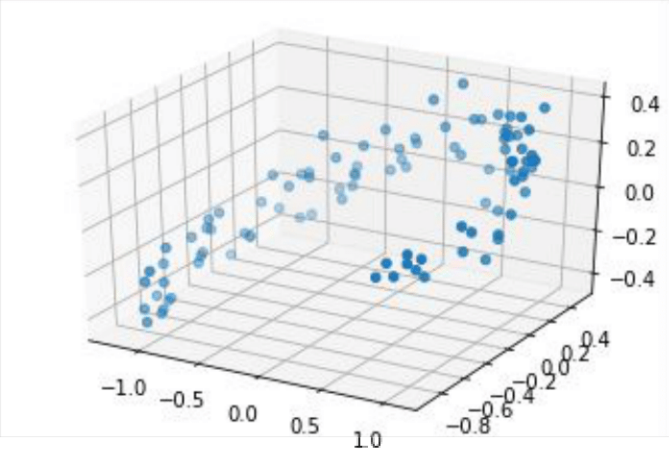
- Neural networks capable of learning dense representations of input data without supervision
  - Training data is not labelled
- Useful for dimensionality reduction and for visualization
- Can be used to generate new data that resembles input data
- In practice they
  - Copy input to output
  - They learn efficient ways to represent data

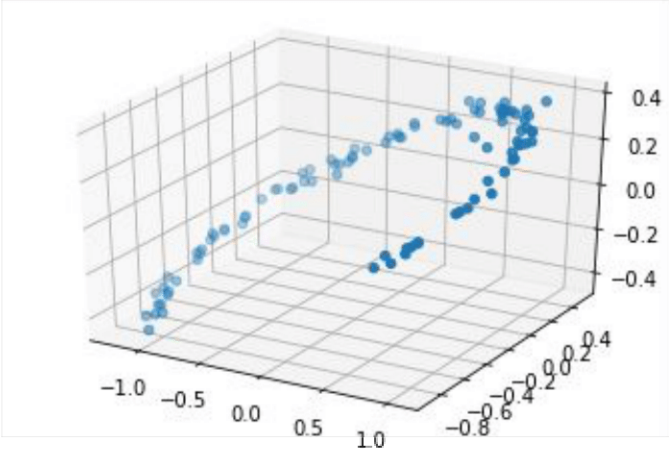

X1
X2
X3
Encoder
Y1
Y2
Y3


X1
X2
X3
Y1
Y2
Y3
Decoder


0.4
0.2
0.0
−0.2
−0.4
−1.0
−0.5
0.0
0.5
1.0
0.4
0.2
0.0
−0.2
−0.4
−0.6
−0.8


0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
z_2
−1.5
−1.0
−0.5
0.0
0.5
1.0
z_1


0.4
0.2
0.0
−0.2
−0.4
−1.0
−0.5
0.0
0.5
1.0
0.4
0.2
0.0
−0.2
−0.4
−0.6
−0.8

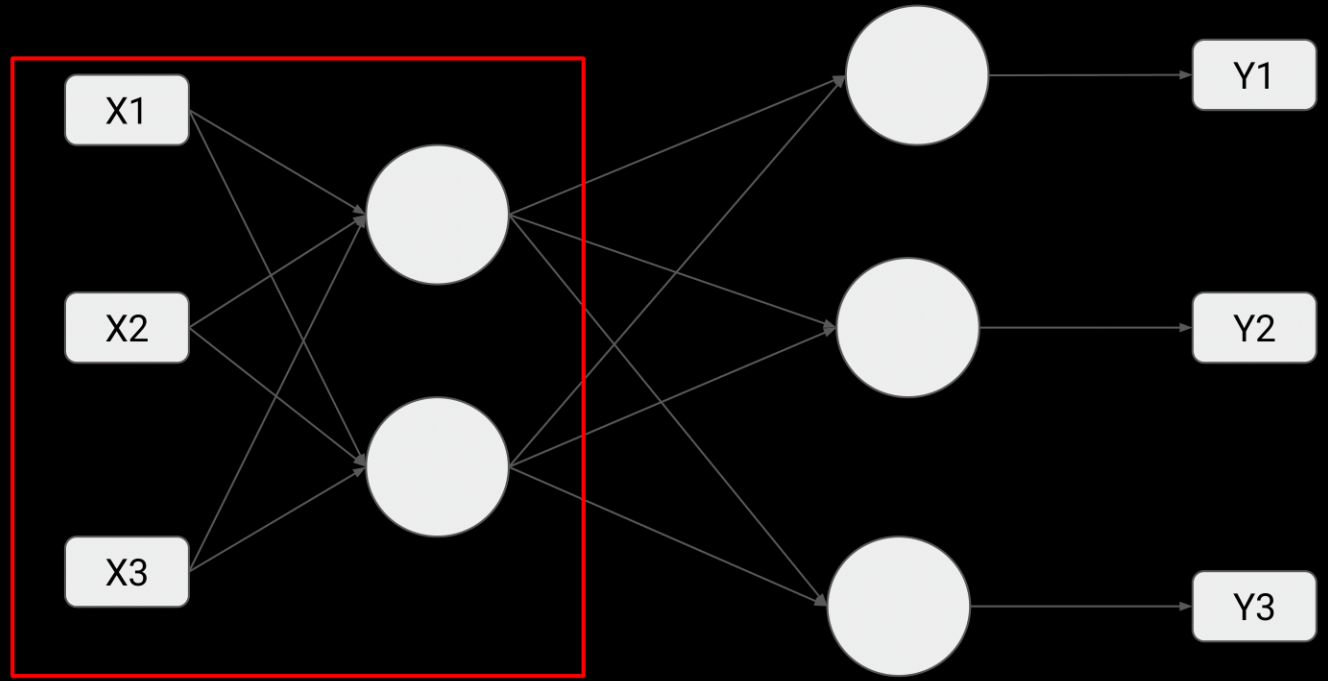

0.4
0.2
0.0
−0.2
−0.4
−1.0
−0.5
0.0
0.5
1.0
0.4
0.2
0.0
−0.2
−0.4
−0.6
−0.8

```
encoder = keras.models.Sequential([keras.layers.Dense(2, input_shape=[3])])

decoder = keras.models.Sequential([keras.layers.Dense(3, input_shape=[2])])

autoencoder = keras.models.Sequential([encoder, decoder])

autoencoder.compile(loss="mse", optimizer=keras.optimizers.SGD(lr=1.5))
```



```
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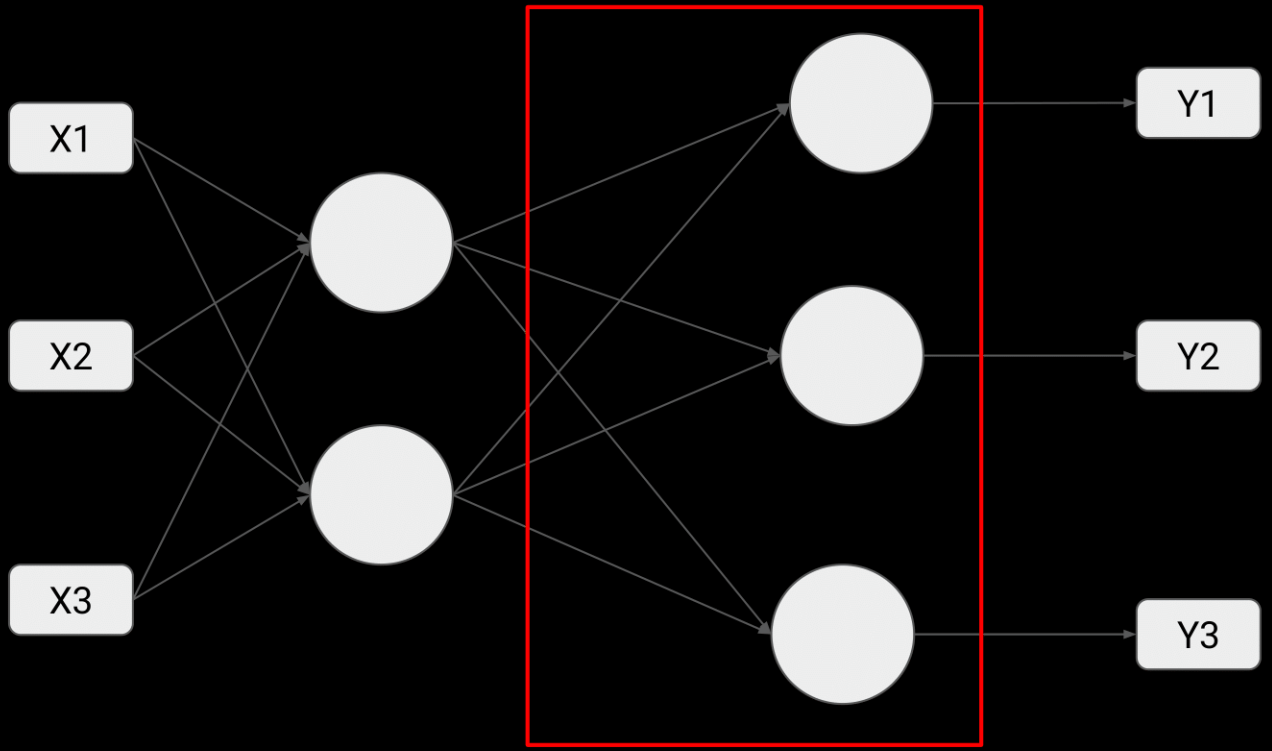
decoder = keras.models.Sequential([keras.layers.Dense(3, input_shape=[2])])
autoencoder = keras.models.Sequential([encoder, decoder])
autoencoder.compile(loss="mse", optimizer=keras.optimizers.SGD(lr=1.5))
```



```
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decoder = keras.models.Sequential([keras.layers.Dense(3, input_shape=[2])])

autoencoder = keras.models.Sequential([encoder, decoder])

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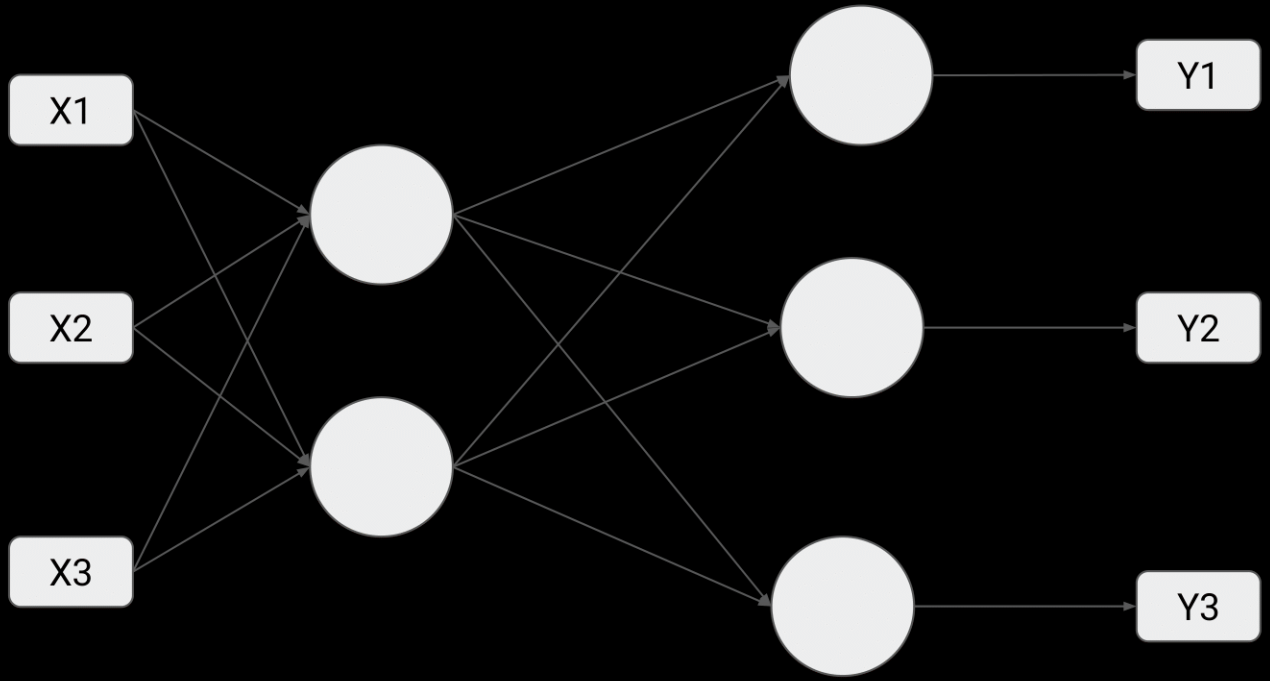
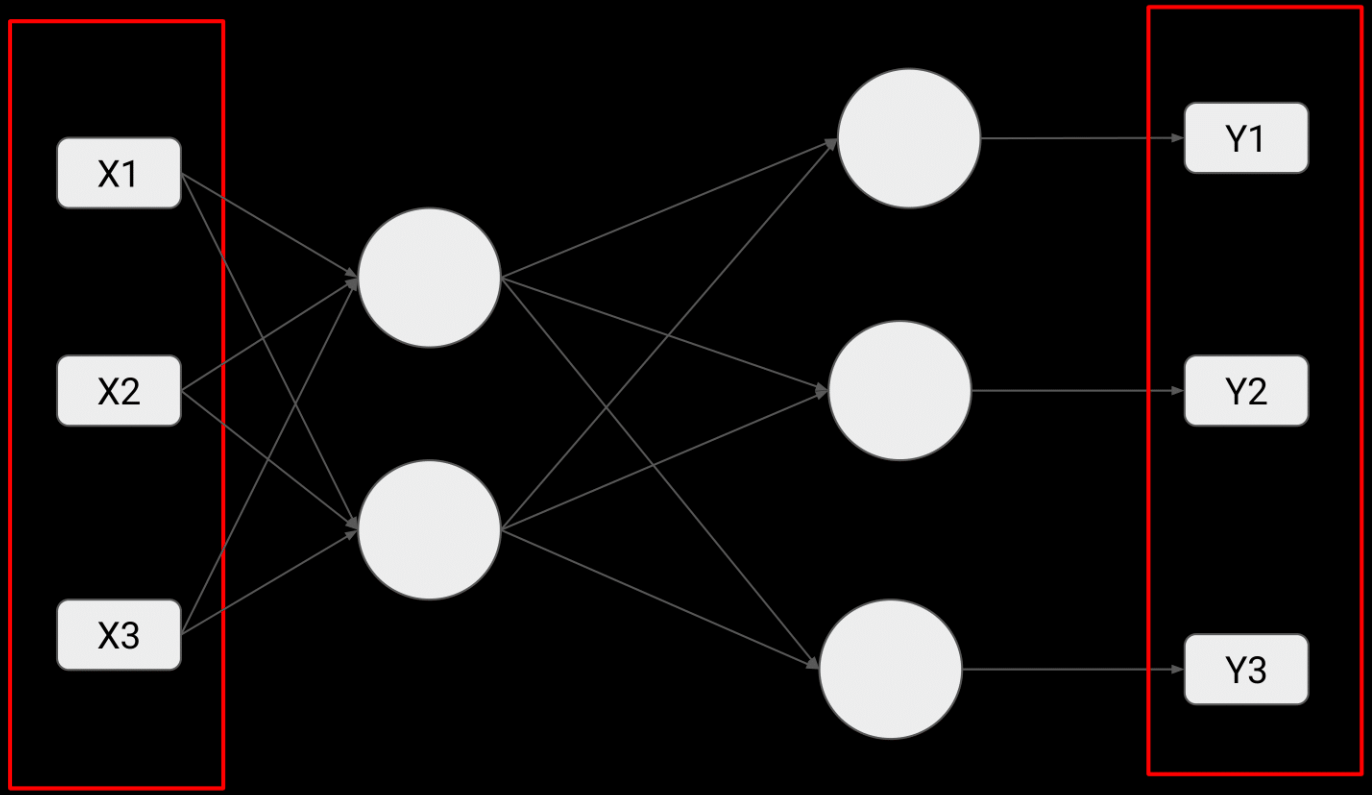
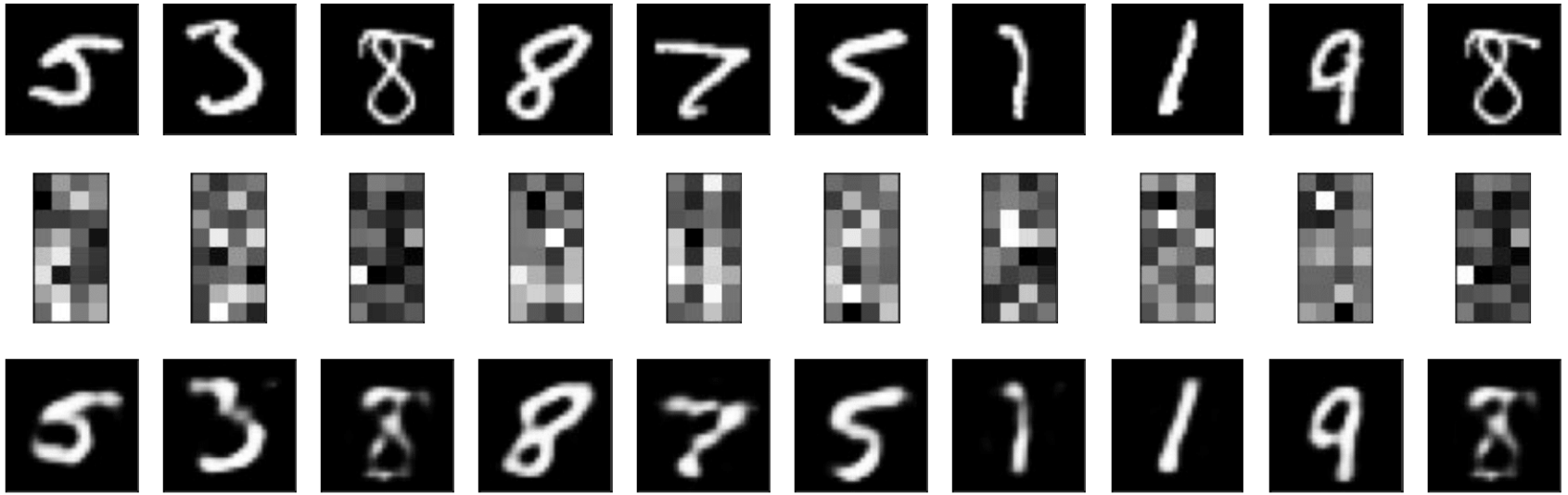


```
history = autoencoder.fit(X_train, X_train, epochs=200)
```



```
codings = encoder.predict(data)
```

```
decodings = decoder.predict(codings)
```



```
inputs =  tf.keras.layers.Input(shape=(784,))

def simple_autoencoder():
    encoder = tf.keras.layers.Dense(units=32, activation='relu')(inputs)
    decoder = tf.keras.layers.Dense(units=784, activation='sigmoid')(encoder)
    return encoder, decoder

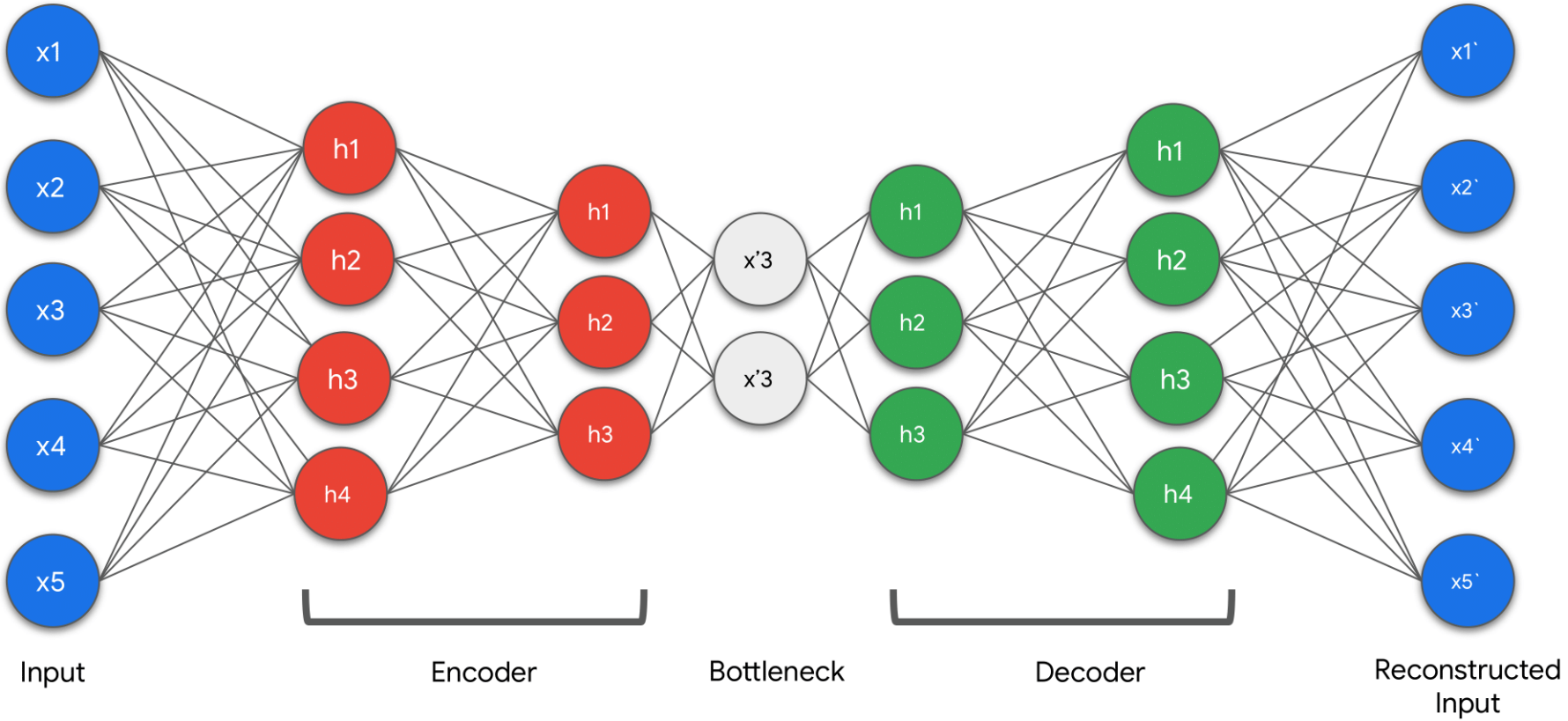
encoder_output, decoder_output = simple_autoencoder()

encoder_model = tf.keras.Model(inputs=inputs, outputs=encoder_output)

autoencoder_model = tf.keras.Model(inputs=inputs, outputs=decoder_output)
```

```
autoencoder_model.compile(
        optimizer=tf.keras.optimizers.Adam(),
        loss='binary_crossentropy')
```

Stacked Auto-Encoders



```
inputs =  tf.keras.layers.Input(shape=(784,))

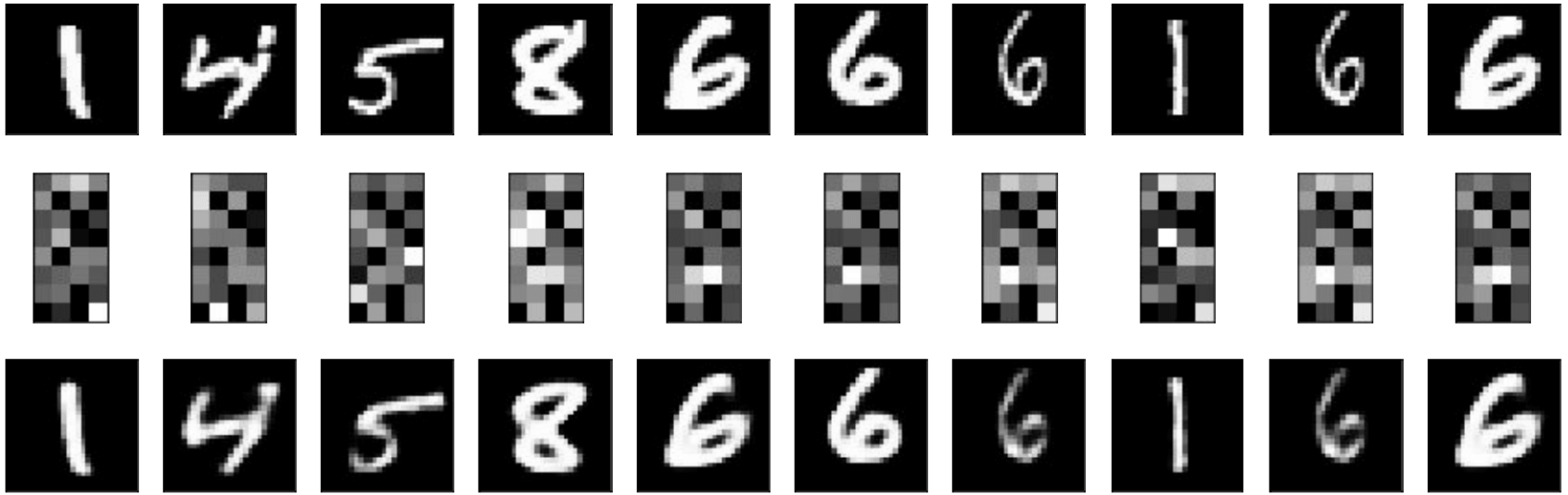
def deep_autoencoder():
 encoder = tf.keras.layers.Dense(units=128, activation='relu')(inputs)
 encoder = tf.keras.layers.Dense(units=64, activation='relu')(encoder)
 encoder = tf.keras.layers.Dense(units=32, activation='relu')(encoder)

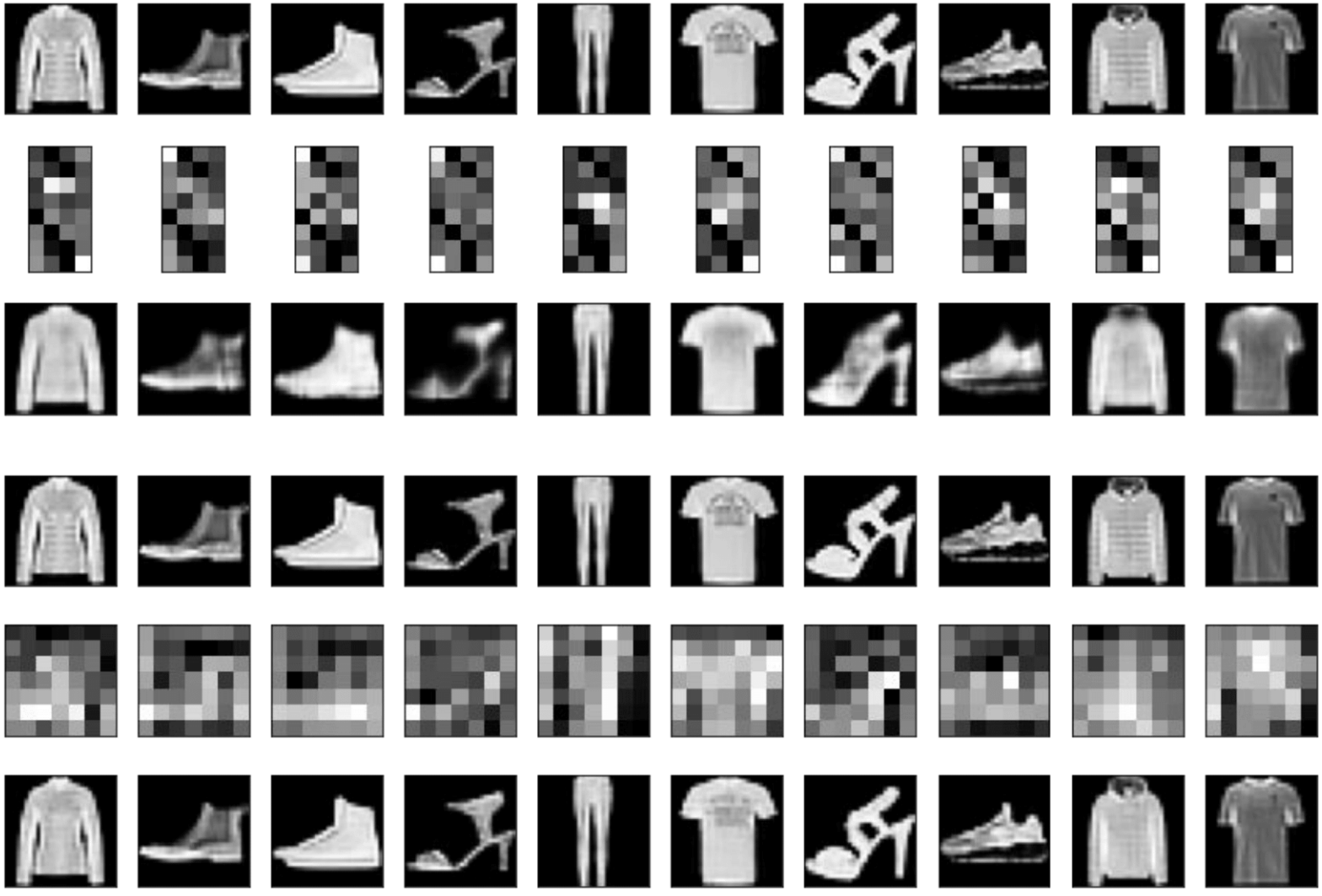
 decoder = tf.keras.layers.Dense(units=64, activation='relu')(encoder)
 decoder = tf.keras.layers.Dense(units=128, activation='relu')(decoder)
 decoder = tf.keras.layers.Dense(units=784, activation='sigmoid')(decoder)

 return encoder, decoder

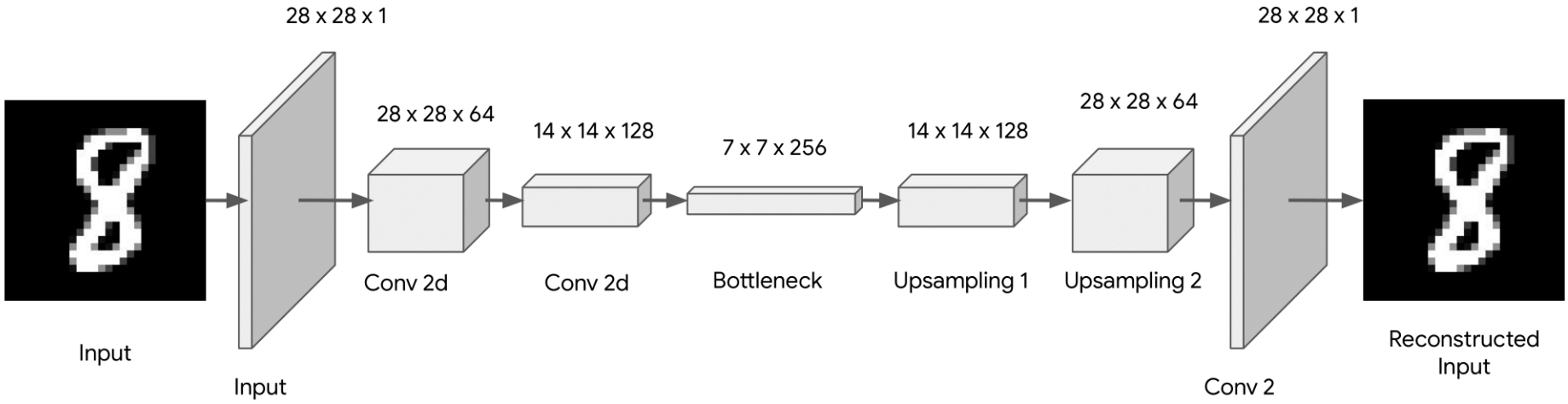
deep_encoder_output, deep_autoencoder_output = deep_autoencoder()

deep_encoder_model = tf.keras.Model(inputs=inputs, outputs=deep_encoder_output)
deep_autoencoder_model = tf.keras.Model(inputs=inputs, outputs=deep_autoencoder_output)
```





Convolutional Auto-Encoders



```
def encoder(inputs):
  conv_1 = tf.keras.layers.Conv2D(filters=64, kernel_size=(3,3),
                                  activation='relu', padding='same')(inputs)

  max_pool_1 = tf.keras.layers.MaxPooling2D(pool_size=(2,2))(conv_1)

  conv_2 = tf.keras.layers.Conv2D(filters=128, kernel_size=(3,3),
                                  activation='relu', padding='same')(max_pool_1)

  max_pool_2 = tf.keras.layers.MaxPooling2D(pool_size=(2,2))(conv_2)

  return max_pool_2
```

```
def bottle_neck(inputs):
  bottle_neck = tf.keras.layers.Conv2D(filters=256, kernel_size=(3,3),
                                       activation='relu', padding='same')(inputs)



  encoder_visualization = tf.keras.layers.Conv2D(filters=1, kernel_size=(3,3),
                                                 activation='sigmoid',
                                                 padding='same')(bottle_neck)

  return bottle_neck, encoder_visualization
```

```
def decoder(inputs):
  conv_1 = tf.keras.layers.Conv2D(filters=128, kernel_size=(3,3),
                                  activation='relu', padding='same')(inputs)
  up_sample_1 = tf.keras.layers.UpSampling2D(size=(2,2))(conv_1)

  conv_2 = tf.keras.layers.Conv2D(filters=64, kernel_size=(3,3),
                                  activation='relu', padding='same')(up_sample_1)
  up_sample_2 = tf.keras.layers.UpSampling2D(size=(2,2))(conv_2)

  conv_3 = tf.keras.layers.Conv2D(filters=1, kernel_size=(3,3),
                                  activation='sigmoid',
                                  padding='same')(up_sample_2)

  return conv_3
```

```
def convolutional_auto_encoder():
  inputs = tf.keras.layers.Input(shape=(28, 28, 1,))

  encoder_output = encoder(inputs)

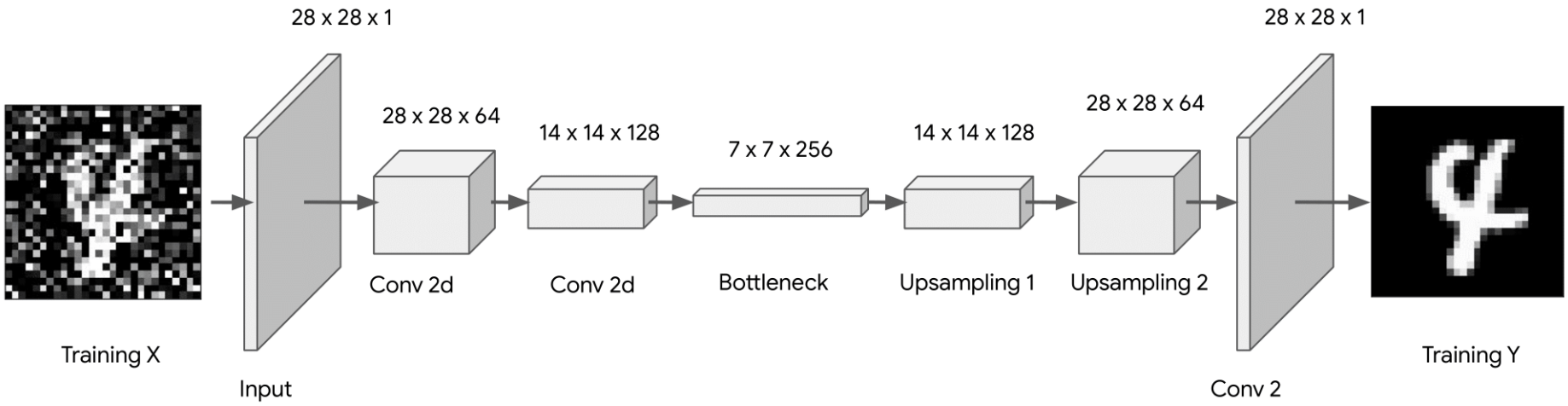
  bottleneck_output, encoder_visualization = bottle_neck(encoder_output)

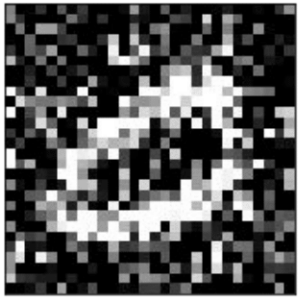
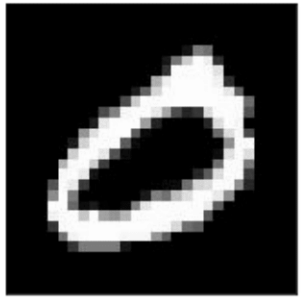
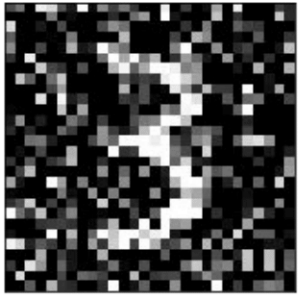
  decoder_output = decoder(bottleneck_output)

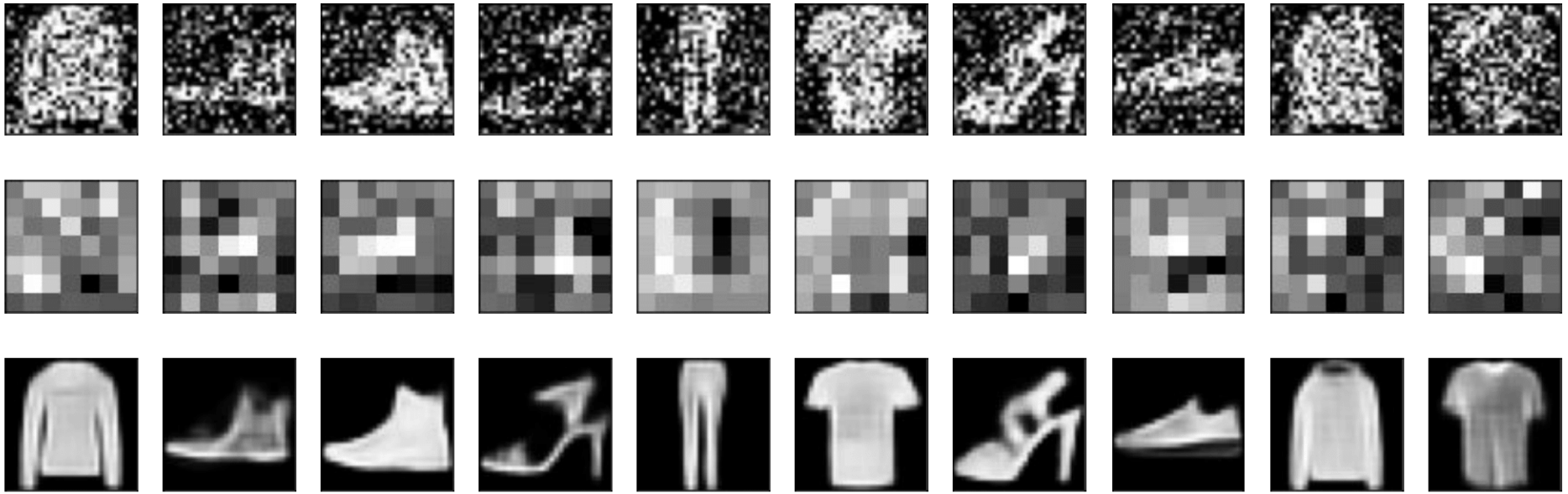
  model = tf.keras.Model(inputs =inputs, outputs=decoder_output)
  encoder_model = tf.keras.Model(inputs=inputs, outputs=encoder_visualization)

  return model, encoder_model
```

Convolutional Auto-Encoders



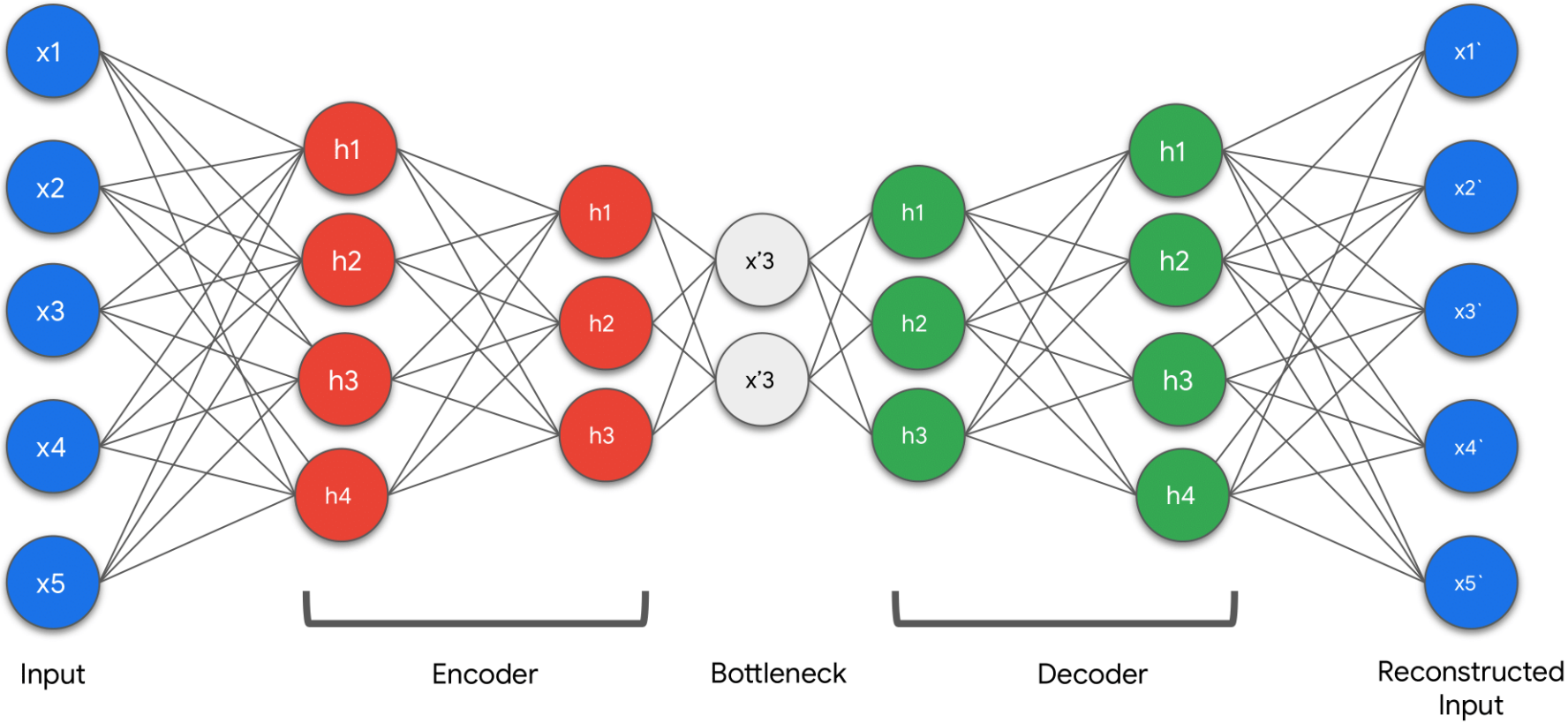




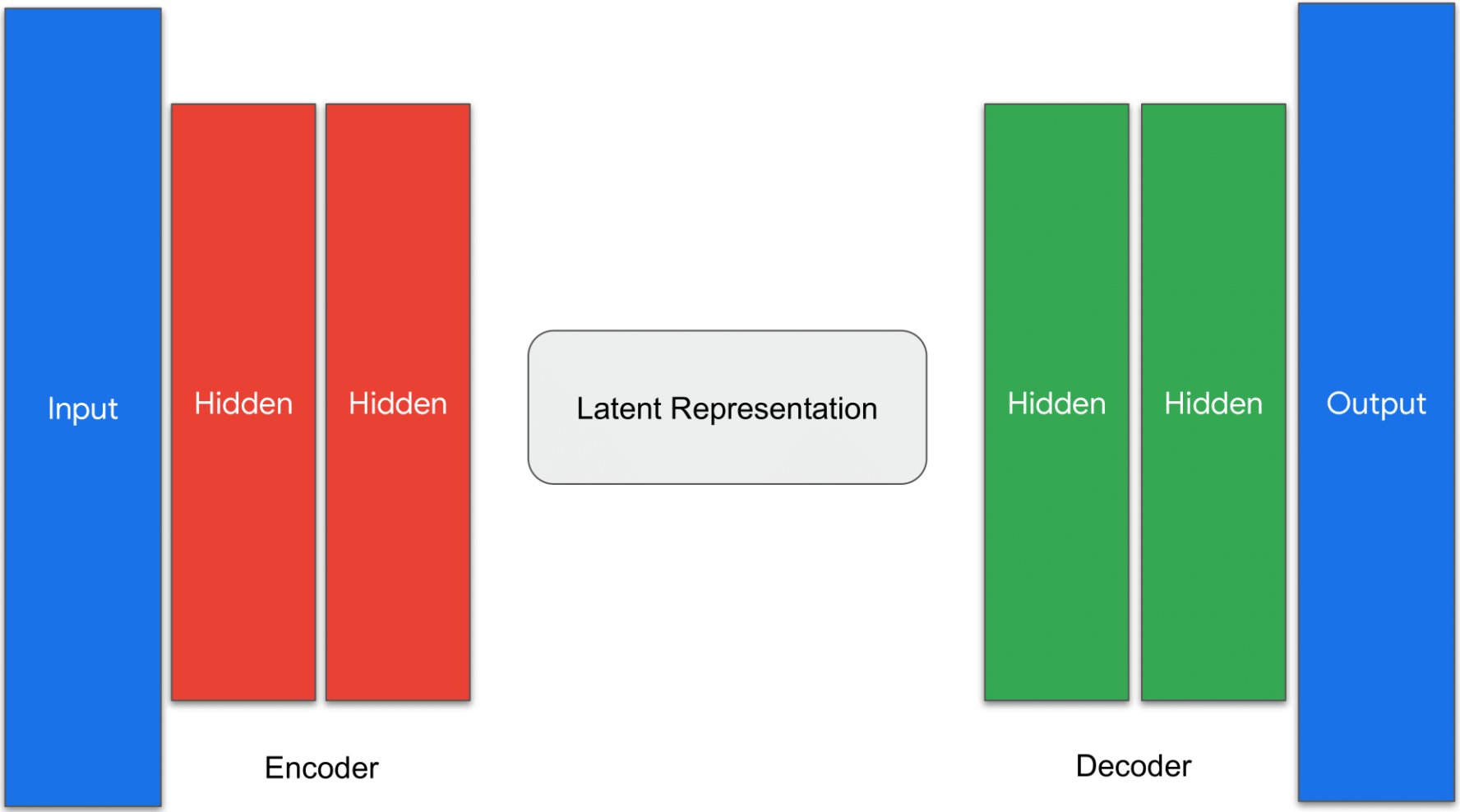



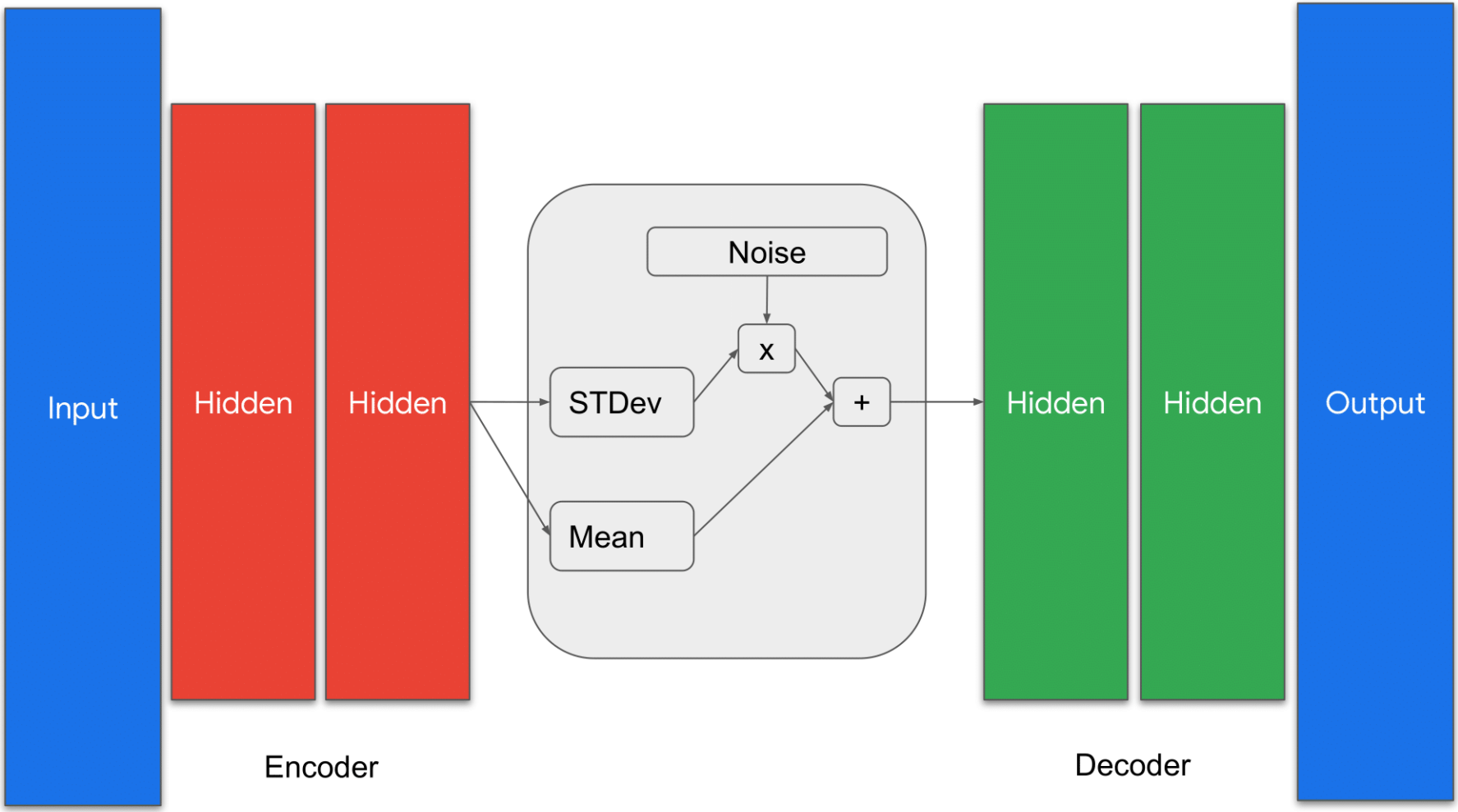
```
def map_image_with_noise(image, label):
  noise_factor = 0.5
  image = tf.cast(image, dtype=tf.float32)
  image = image / 255.0

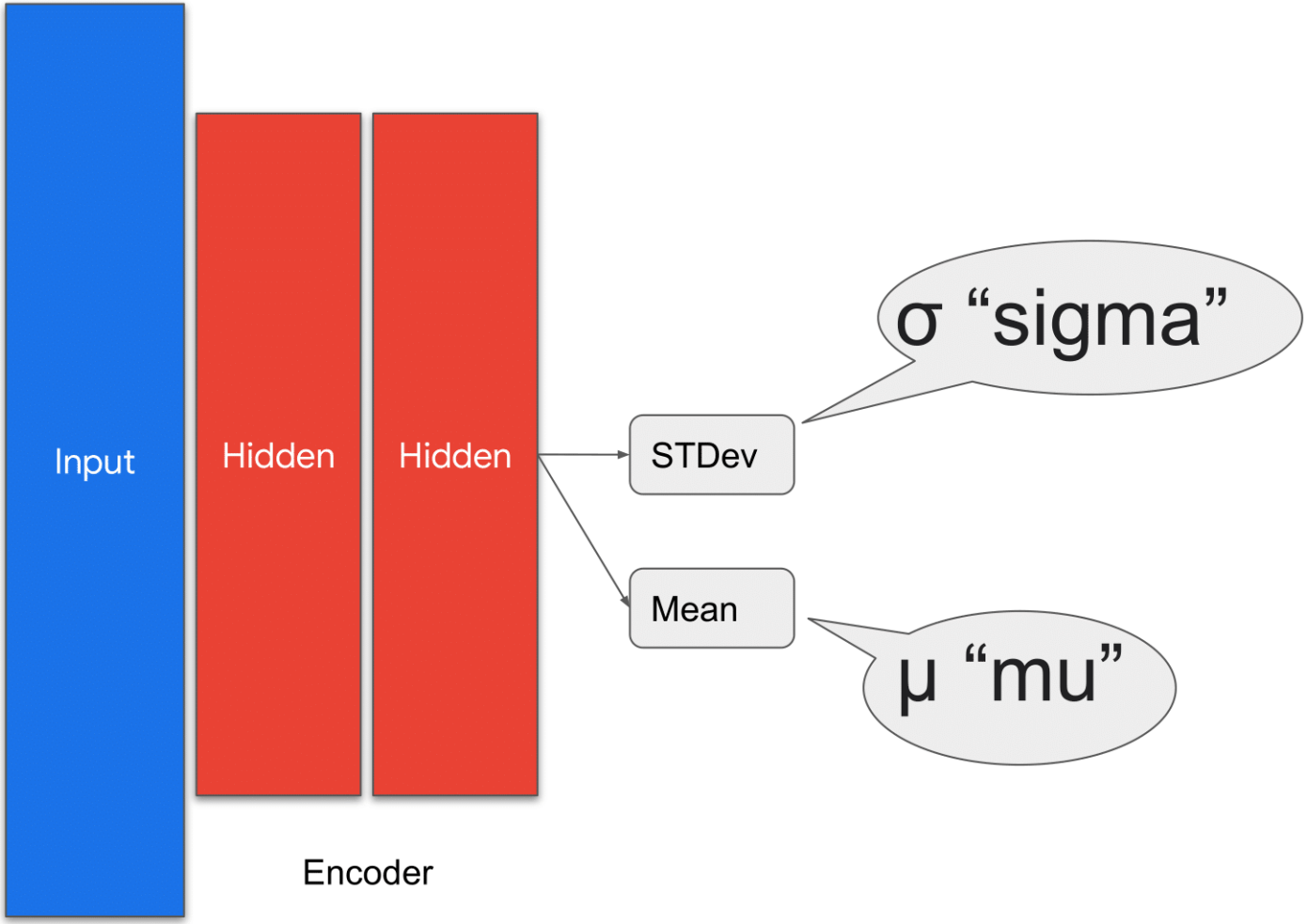
  factor = noise_factor * tf.random.normal(shape=image.shape)
  image_noisy = image + factor
  image_noisy = tf.clip_by_value(image_noisy, 0.0, 1.0)

  return image_noisy, image
```


x1
x2
x3
x4
x5
h1
h2
h3
h4
h1
h2
h3
x'3
x'3
h1
h2
h3
h1
h2
h3
h4
x1`
x2`
x3`
x4`
x5`
Input
Encoder
Bottleneck
Decoder
Reconstructed Input


Input
Hidden
Hidden
Latent Representation
Hidden
Hidden
Output
Encoder
Decoder


Input
Hidden
Hidden
Noise
x
STDev
+
Mean
Hidden
Hidden
Output
Encoder
Decoder


Input
Hidden
Hidden
STDev
Mean
σ “sigma”
μ “mu”
Encoder

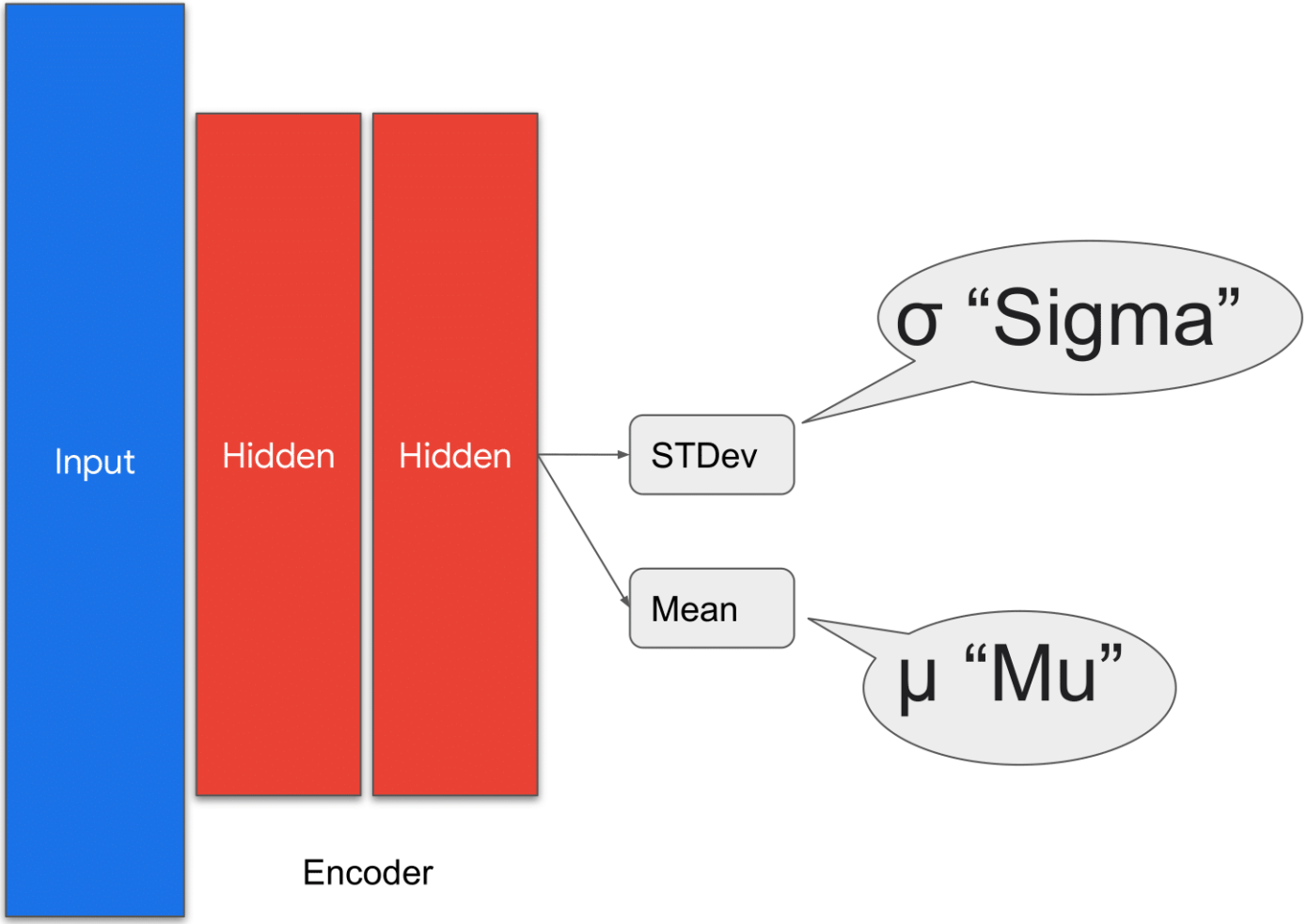
Probability Distribution

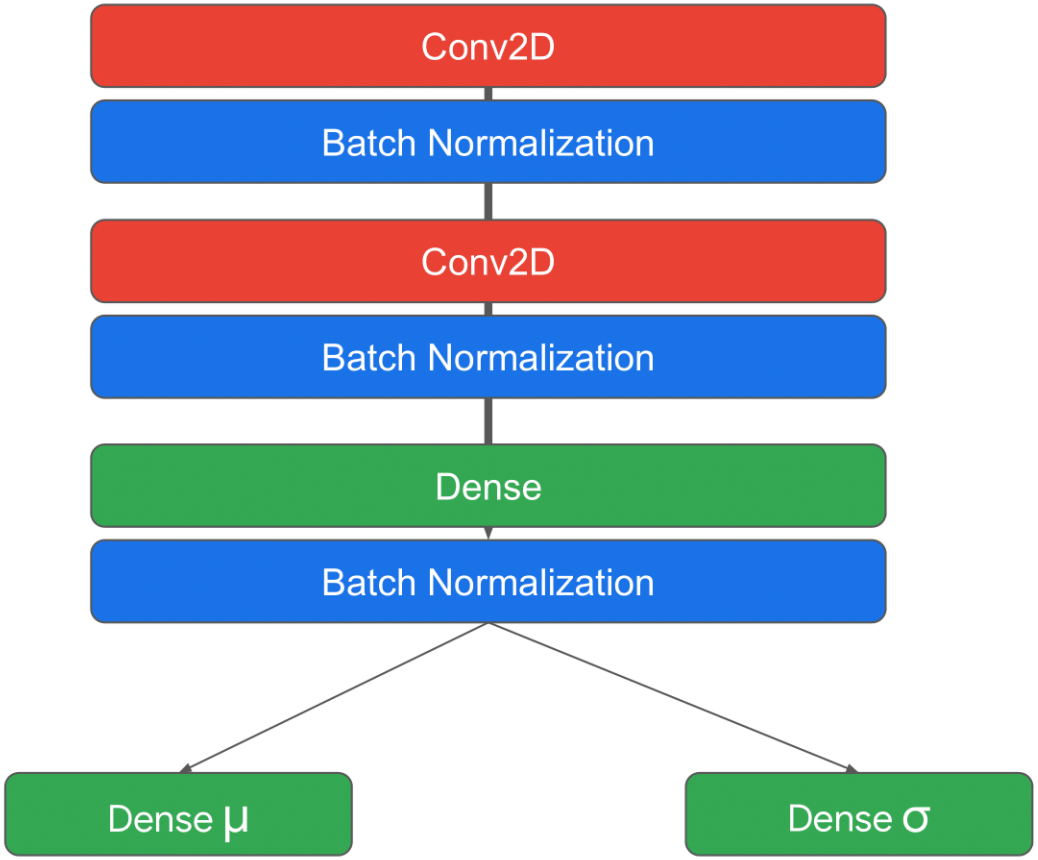
Gaussian probability density function or **Normal Distribution.**

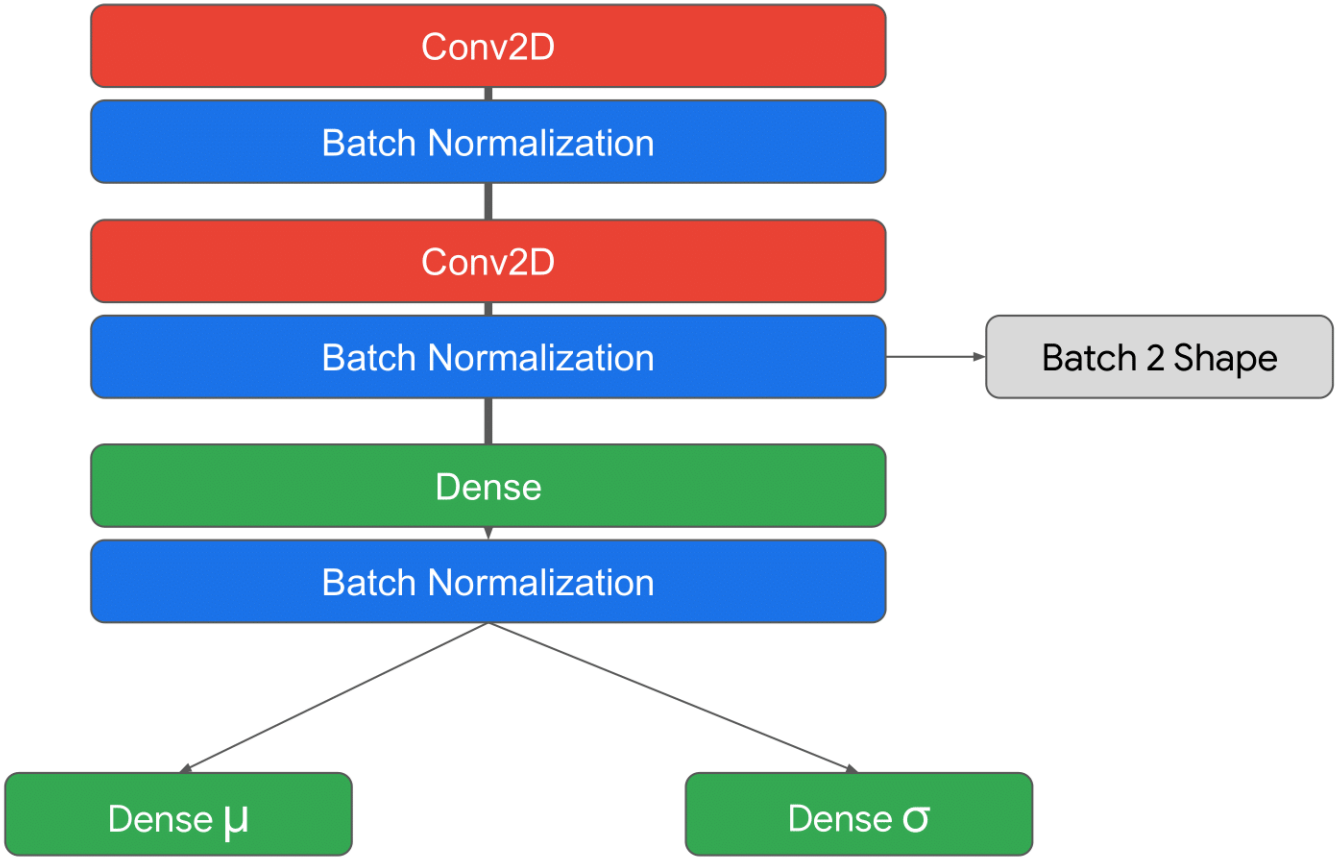
Normal Distribution is controlled by:

- **μ “mean”**
- **σ “standard deviation”**

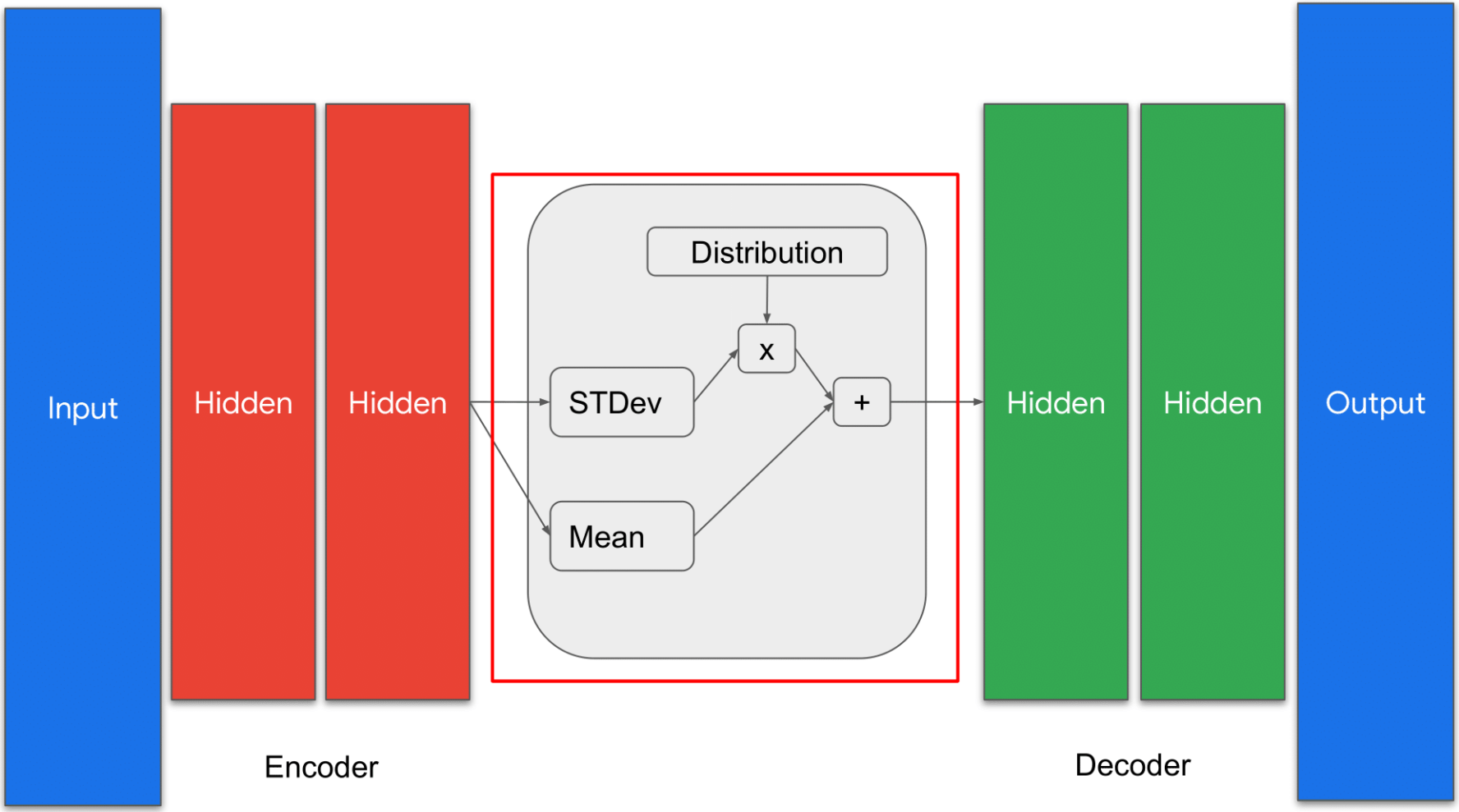
$$N(\mu, \sigma)$$

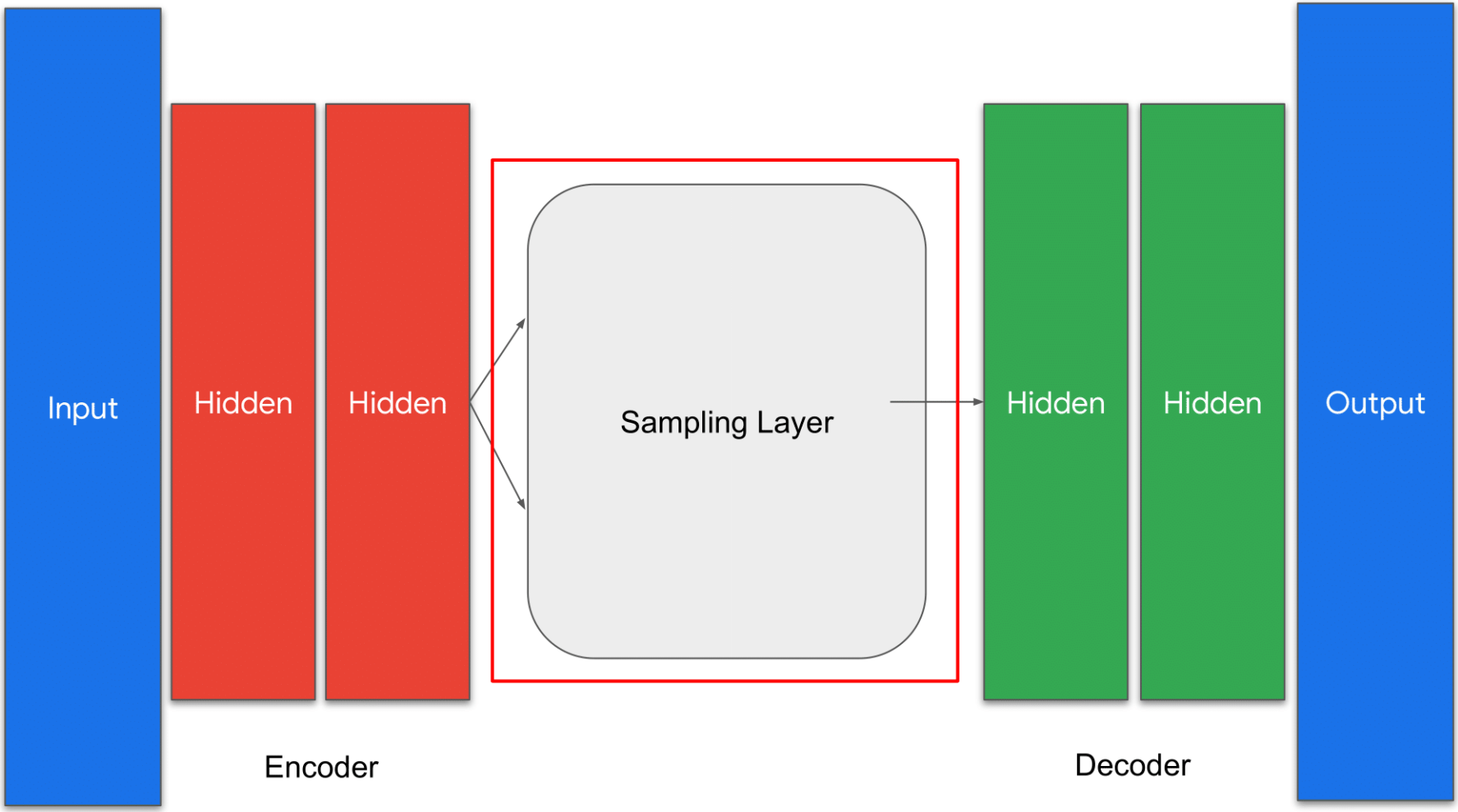

Input
Hidden
Hidden
STDev
Mean
σ “Sigma”
μ “Mu”
Encoder


Conv2D
Batch Normalization
Conv2D
Batch Normalization
Dense
Batch Normalization
Dense μ
Dense σ

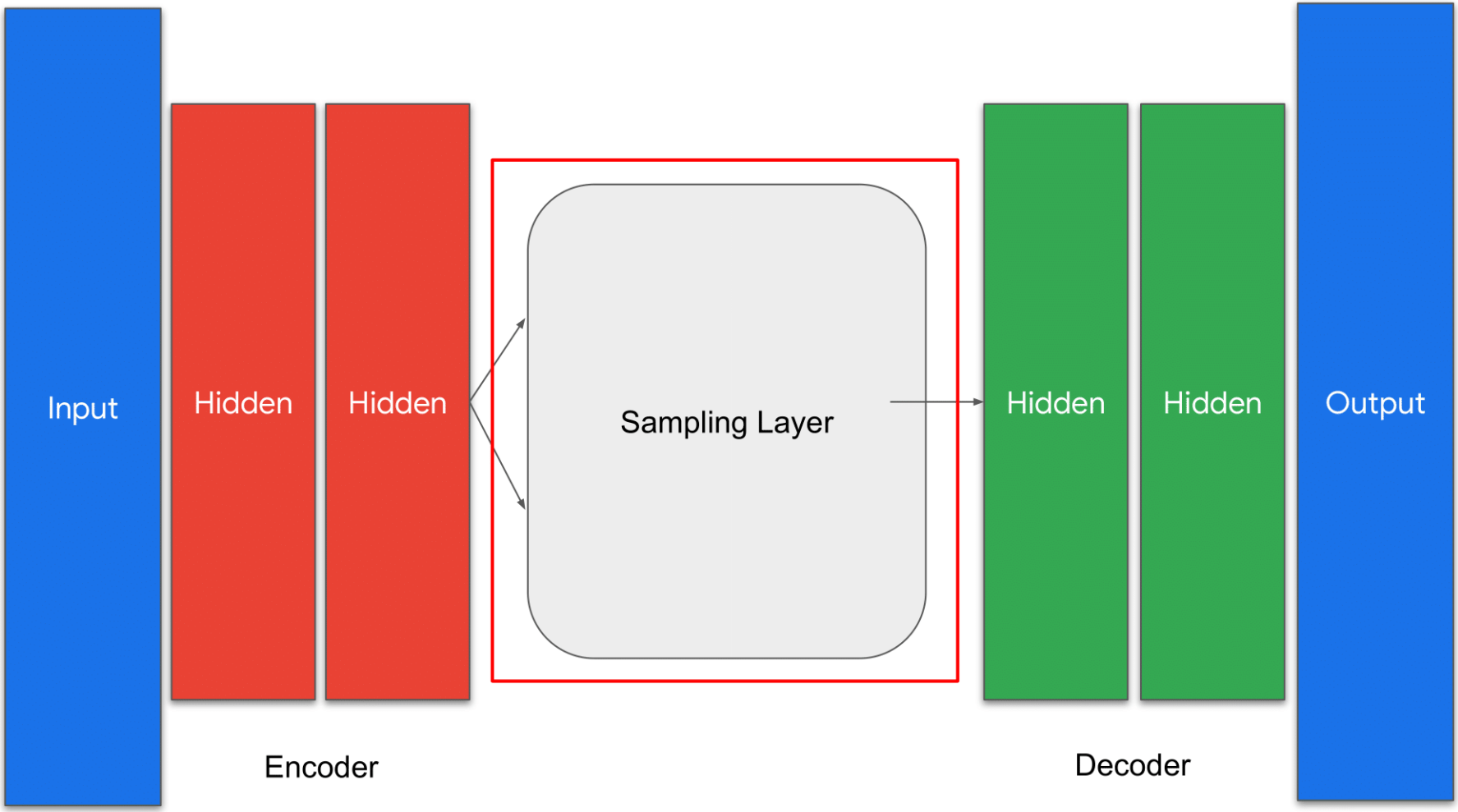

Conv2D
Batch Normalization
Conv2D
Batch Normalization
Batch 2 Shape
Dense
Batch Normalization
Dense μ
Dense σ

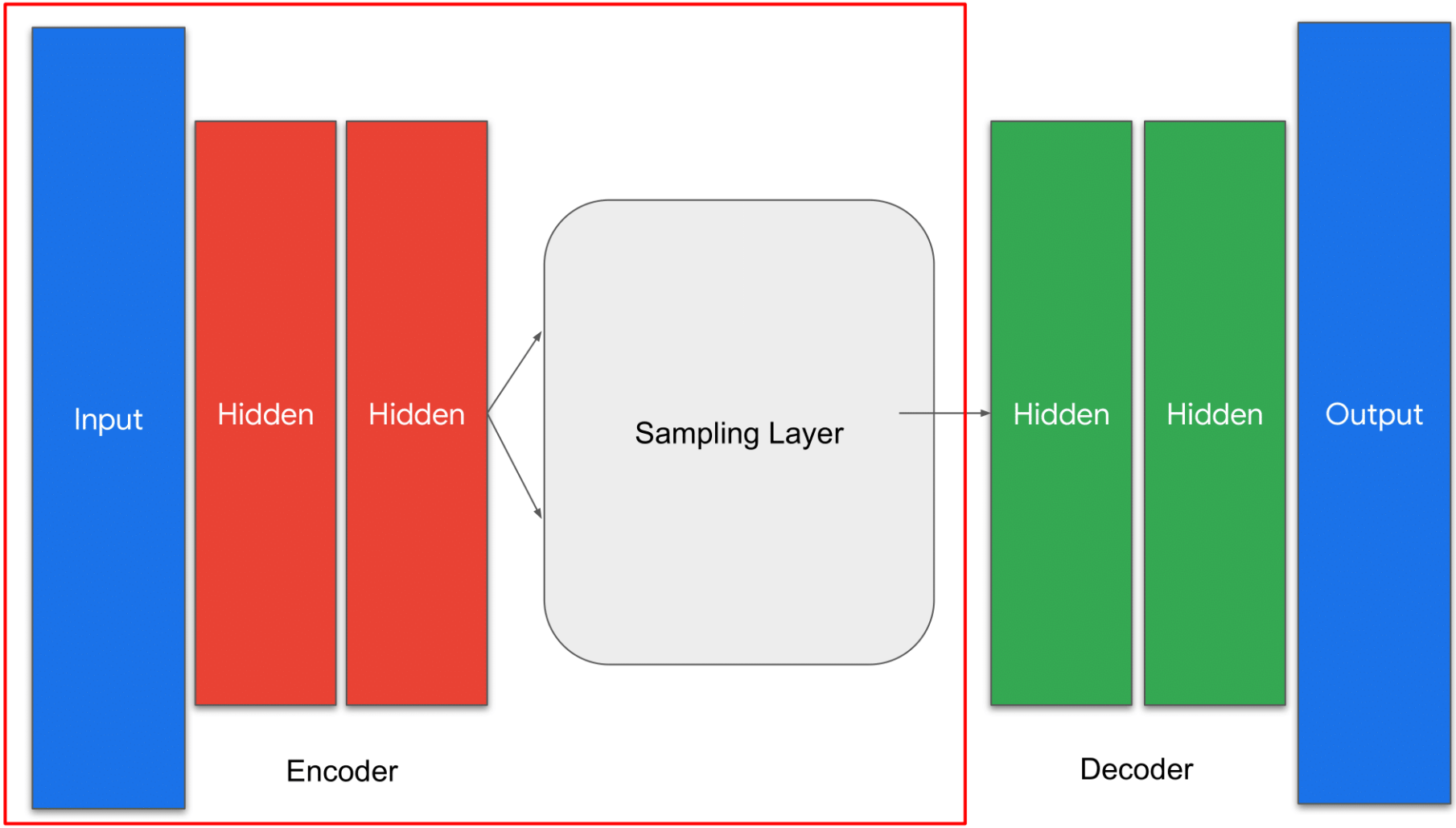
```python
# This function defines the encoder's layers
def encoder_layers(inputs, latent_dim):
  x = tf.keras.layers.Conv2D(filters=32, kernel_size=3, strides=2,
                             padding="same", activation='relu',
                             name="encode_conv1")(inputs)
  x = tf.keras.layers.BatchNormalization()(x)

  x = tf.keras.layers.Conv2D(filters=64, kernel_size=3, strides=2,
                             padding='same', activation='relu',
                             name="encode_conv2")(x)
  batch_2 = tf.keras.layers.BatchNormalization()(x)

  x = tf.keras.layers.Flatten(name="encode_flatten")(batch_2)
  x = tf.keras.layers.Dense(20, activation='relu', name="encode_dense")(x)
  x = tf.keras.layers.BatchNormalization()(x)

  mu = tf.keras.layers.Dense(latent_dim, name='latent_mu')(x)
  sigma = tf.keras.layers.Dense(latent_dim, name ='latent_sigma')(x)


  return mu, sigma, batch_2.shape
```


Input
Hidden
Hidden
Distribution
x
STDev
+
Mean
Hidden
Hidden
Output
Encoder
Decoder

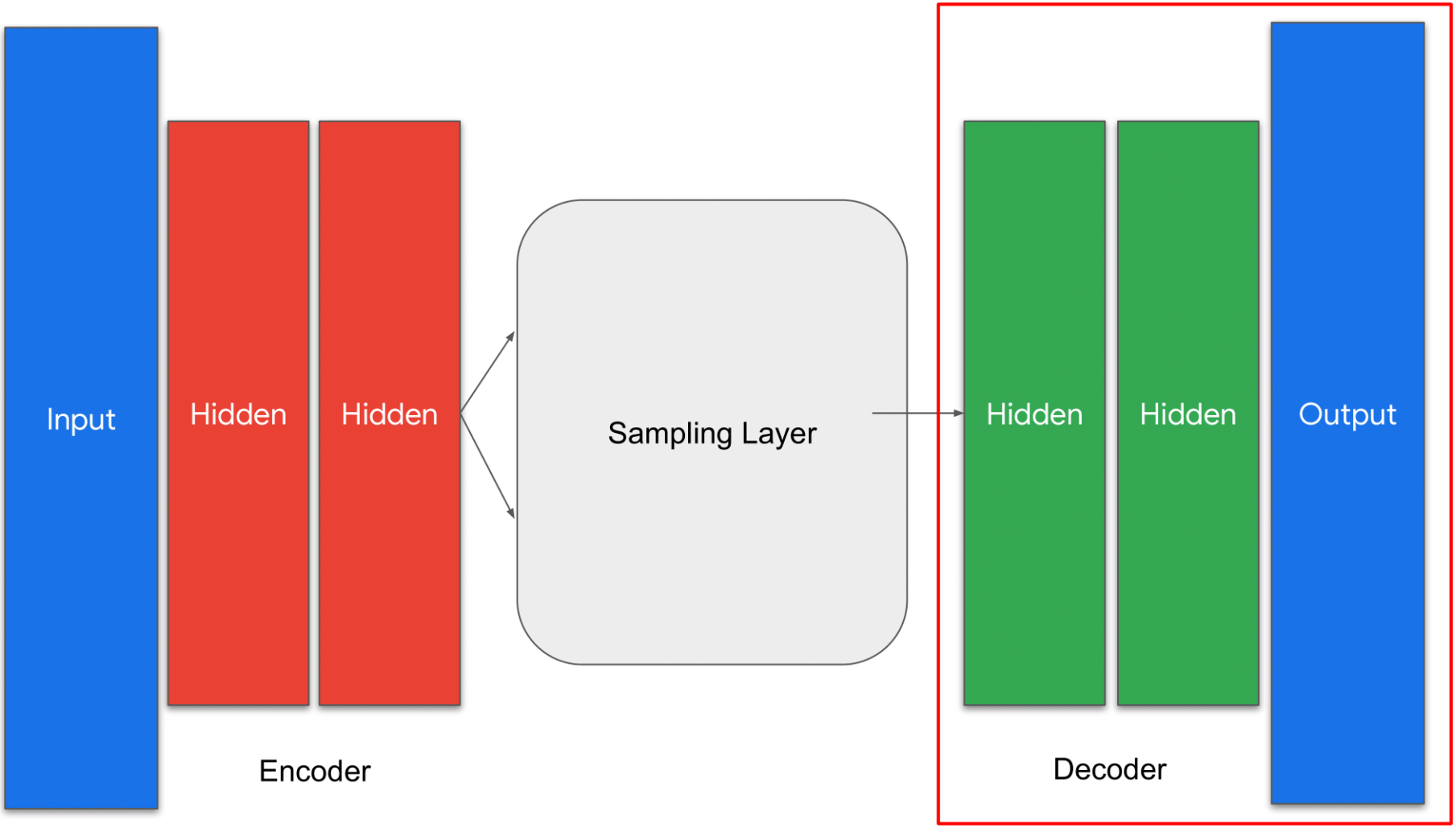

Input
Hidden
Hidden
Sampling Layer
Hidden
Hidden
Output
Encoder
Decoder

```python
class Sampling(tf.keras.layers.Layer):
  def call(self, inputs):
    mu, sigma = inputs
    batch = tf.shape(mu)[0]
    dim = tf.shape(mu)[1]
    epsilon = tf.keras.backend.random_normal(shape=(batch, dim))
    return mu + tf.exp(0.5 * sigma) * epsilon
```


Input
Hidden
Hidden
Sampling Layer
Hidden
Hidden
Output
Encoder
Decoder

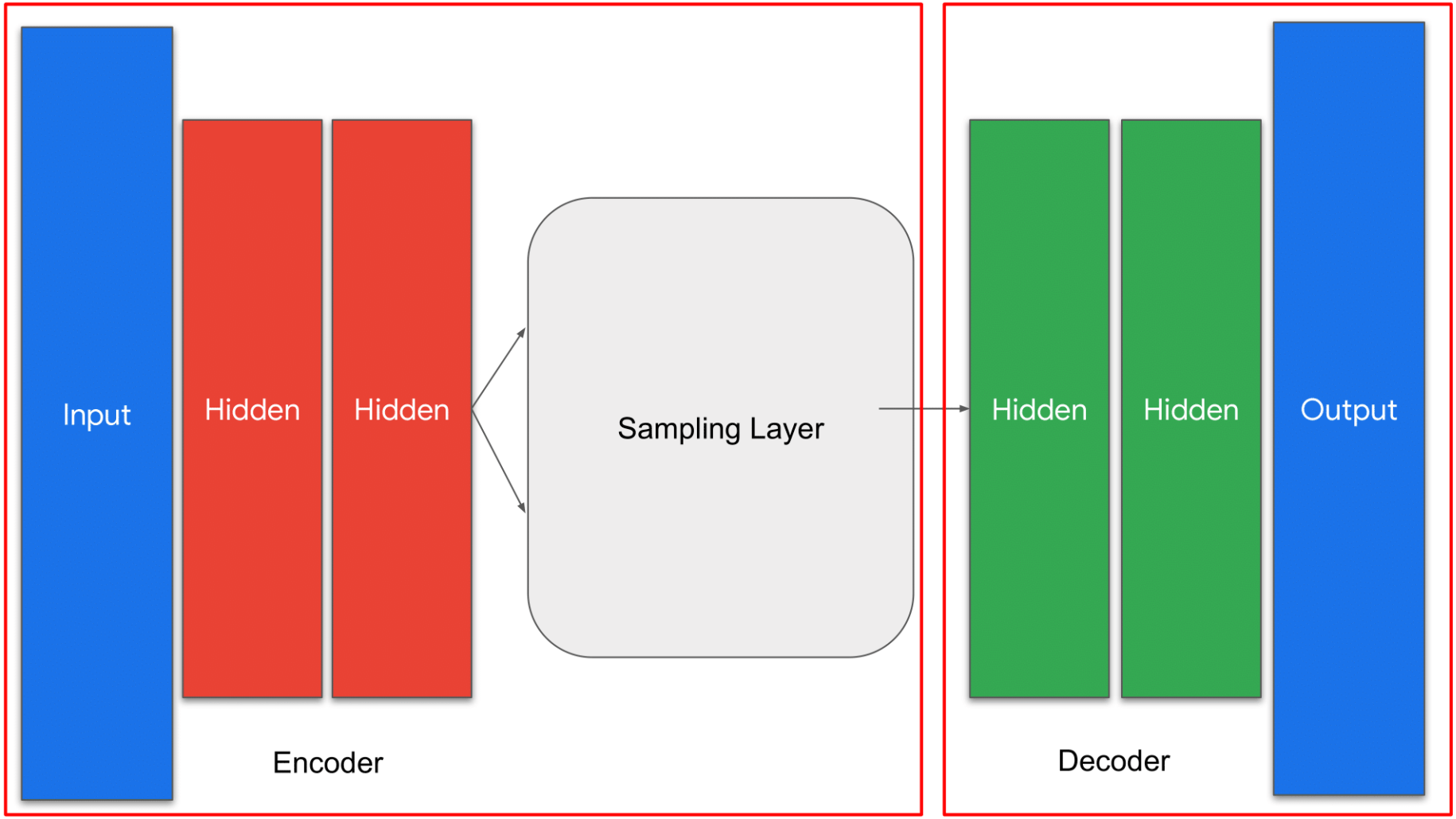

Input
Hidden
Hidden
Sampling Layer
Hidden
Hidden
Output
Encoder
Decoder

```
def encoder_model(LATENT_DIM, input_shape):
  inputs = tf.keras.layers.Input(shape=input_shape)
  mu, sigma, conv_shape = encoder_layers(inputs, latent_dim=LATENT_DIM)
  z = Sampling()((mu, sigma))
  model = tf.keras.Model(inputs, outputs=[mu, sigma, z])
  return model, conv_shape
```


Input
Hidden
Hidden
Sampling Layer
Hidden
Hidden
Output
Encoder
Decoder

```
def decoder_layers(inputs, conv_shape):
  units = conv_shape[1] * conv_shape[2] * conv_shape[3]
  x = tf.keras.layers.Dense(units, activation = 'relu',
                            name="decode_dense1")(inputs)
  x = tf.keras.layers.BatchNormalization()(x)

  x = tf.keras.layers.Reshape((conv_shape[1], conv_shape[2], conv_shape[3]),
                              name="decode_reshape")(x)
  x = tf.keras.layers.Conv2DTranspose(filters=64, kernel_size=3, strides=2,
                                      padding='same', activation='relu',
                                      name="decode_conv2d_2")(x)
  x = tf.keras.layers.BatchNormalization()(x)

  x = tf.keras.layers.Conv2DTranspose(filters=32, kernel_size=3, strides=2,
                                      padding='same', activation='relu',
                                      name="decode_conv2d3")(x)
  x = tf.keras.layers.BatchNormalization()(x)

  x = tf.keras.layers.Conv2DTranspose(filters=1, kernel_size=3, strides=1, padding='same',
                                      activation='sigmoid', name="decode_final")(x)

  return x
```

```
def decoder_model(latent_dim, conv_shape):
  inputs = tf.keras.layers.Input(shape=(latent_dim,))
  outputs = decoder_layers(inputs, conv_shape)
  model = tf.keras.Model(inputs, outputs)
  return model
```

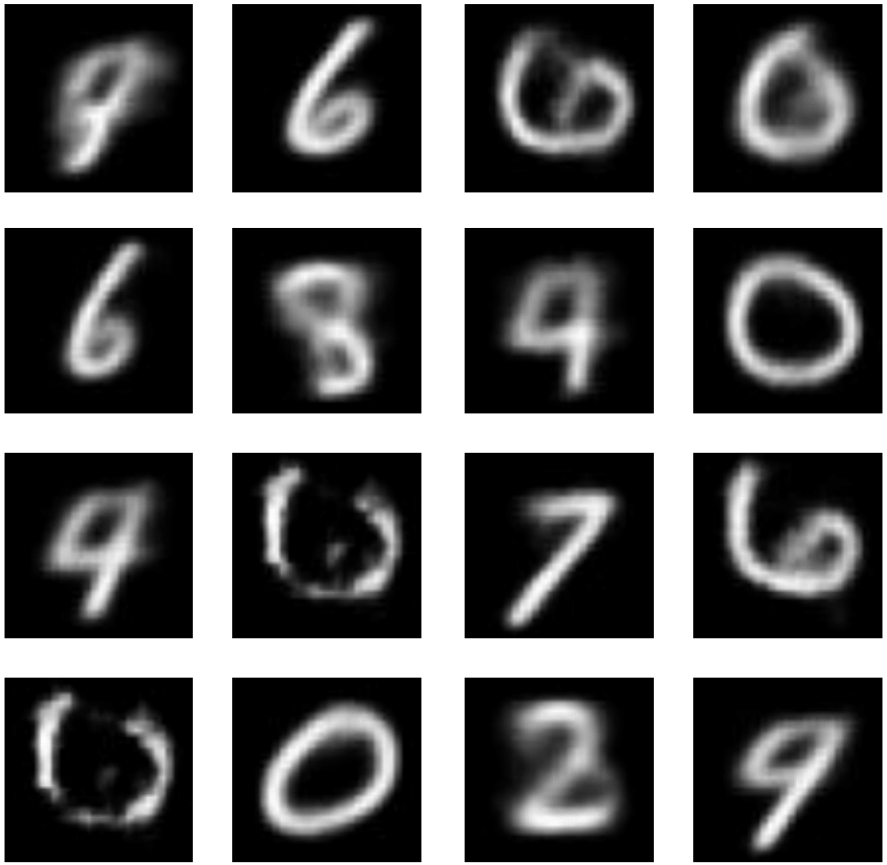

Input
Hidden
Hidden
Sampling Layer
Hidden
Hidden
Output
Encoder
Decoder

```python
# Define a kl reconstruction loss function
def kl_reconstruction_loss(inputs, outputs, mu, sigma):
  kl_loss = 1 + sigma - tf.square(mu) - tf.math.exp(sigma)
  return tf.reduce_mean(kl_loss) * -0.5
```

```
def vae_model(encoder, decoder, input_shape):
  inputs = tf.keras.layers.Input(shape=input_shape)
  mu = encoder(inputs)[0]
  sigma = encoder(inputs)[1]
  z = encoder(inputs)[2]
  reconstructed = decoder(z)
  model = tf.keras.Model(inputs=inputs, outputs=reconstructed)
  loss = kl_reconstruction_loss(inputs, z, mu, sigma)
  model.add_loss(loss)
  return model
```

```
for epoch in range(epochs):
  for step, x_batch_train in enumerate(train_dataset):
    with tf.GradientTape() as tape:
      reconstructed = vae(x_batch_train)
      flattened_inputs = tf.reshape(x_batch_train, shape=[-1])
      flattened_outputs = tf.reshape(reconstructed, shape=[-1])
      loss = bce_loss(flattened_inputs, flattened_outputs) * 784
      loss += sum(vae.losses)  # Add KLD regularization loss

    grads = tape.gradient(loss, vae.trainable_weights)
    optimizer.apply_gradients(zip(grads, vae.trainable_weights))
```

epoch: 99, step: 400



Variational Autoencoders

by Paul Hand
Northeastern University

Outline:

- Generative Models and Autoencoders
- Variational Lower Bound (VLB)
- Optimizing VLB + Variational Autoencoders

Resource: Kingma and Welling 2019, Chapter 2, "Introduction to Variational Autoencoders"

Generative Models

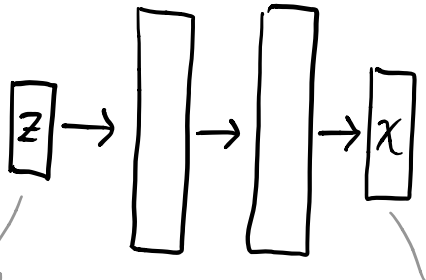
A model that can sample from a learned distribution

(a) 2-D latent space

(Kingma and Welling, 2014)

(Razavi et al. 2019)

In some generative models, samples are generated by a net applied to a random latent code



latent code

typically $Z \sim N(0, I)$

typically low-dimensional

sample/image

high dimensional

$$x = G_\theta(z)$$

random

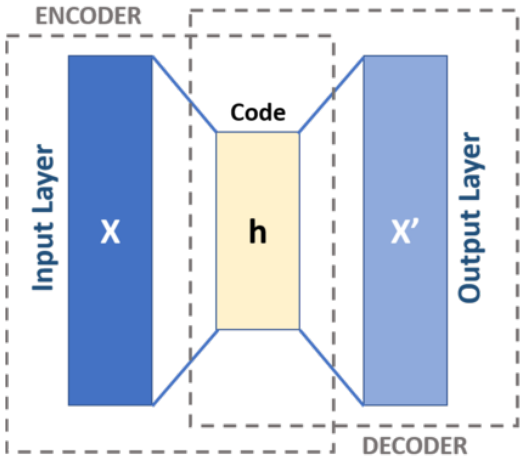
deterministic

induced random variable

Autoencoders

Autoencoders attempt to reconstruct input signals/images by learning mappings to and from a code

Want: $x' = D_\theta(E_\phi(x)) \approx x$



$$\min_{\theta,\phi} \sum_{i=1}^{n} \| D_\theta(E_\phi(x_i)) - x_i \|^2 \quad \text{w/} \quad \{x_i\}_{i=1\cdots n} \text{ is dataset}$$

A (plain) autoencoder is not a generative model as it does not define a distribution

Training a low latent-dimensional generative model by likelihood

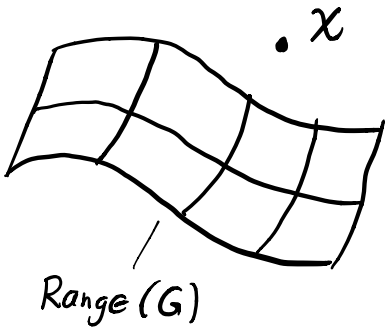
Given data $\{x_i\}_{i=1\cdots n}$, train a gen. model to maximize the likelihood of the observed data

If gen. model

$G_\theta : \mathbb{R}^k \to \mathbb{R}^d$ w/ $k < d$,

$z \mapsto x$

then $p(x) = 0$ almost everywhere



So, can't directly optimize likelihood

To have nonzero likelihood everywhere,

define noisy observation model

$$P_\theta(x \mid z) = \mathcal{N}(x;\, G_\theta(z), \eta I)$$

Under a simple prior $p(z)$, this induces

a joint distribution $p_\theta(x, z)$

Now $p(x) = \int p(z)\, p(x|z)\, dz$

intractable to evaluate at each iteration

optimize a lower bound instead

Variational Lower Bound

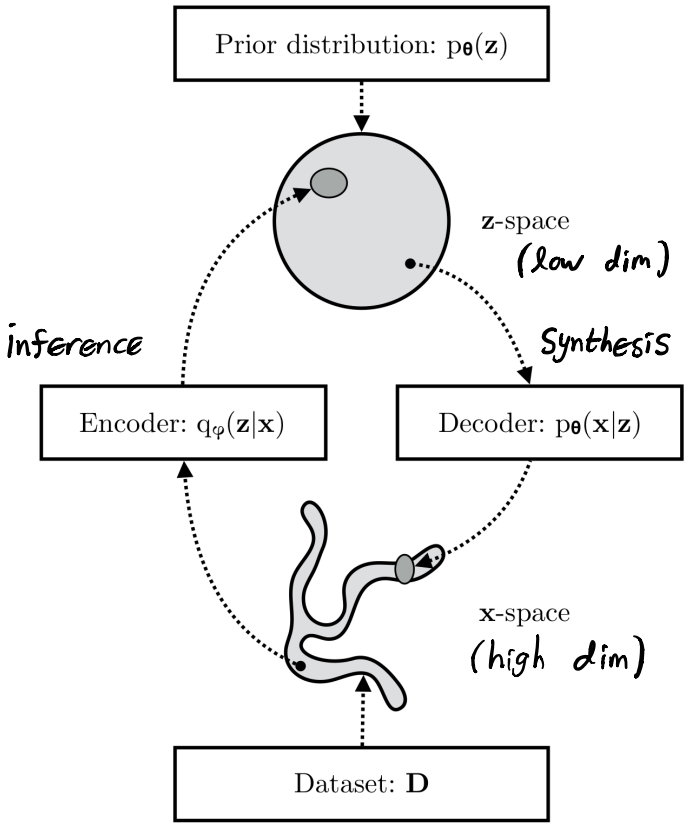
Setup:

Data generated by

$z \sim p(z)$ prior

$x \sim p_\theta(x|z)$

Use $q_\phi(z|x)$ as proxy for $p_\theta(z|x)$



(Kingma and Welling 2019)

Find a lower bound to $p_\theta(x)$

$$\log p_\theta(x) = \mathop{\mathbb{E}}_{z\sim q_\phi(z|x)} \log p_\theta(x) = \mathop{\mathbb{E}}_{z\sim q_\phi(z|x)} \log \frac{p_\theta(x,z)}{p_\theta(z|x)}$$

$$= \mathop{\mathbb{E}}_{z\sim q_\phi(z|x)} \log \left(\frac{p_\theta(x,z)}{q_\phi(z|x)} \cdot \frac{q_\phi(z|x)}{p_\theta(z|x)} \right)$$

$$= \underbrace{\mathop{\mathbb{E}}_{z\sim q_\phi(z|x)} \log \frac{p_\theta(x,z)}{q_\phi(z|x)}}_{\mathcal{L}_{\theta,\phi}(x)} + \underbrace{\mathop{\mathbb{E}}_{z\sim q_\phi(z|x)} \log \frac{q_\phi(z|x)}{p_\theta(z|x)}}_{D_{KL}(q_\phi(z|x) \,\|\, p_\theta(z|x))}$$

Variational Lower Bound (VLB)
Evidence lower bound (ELBO)

Define: $D_{KL}(q\|p) = \mathop{\mathbb{E}}_{z\sim q} \log \frac{q(z)}{p(z)}$

Note:
- $D_{KL}(q\|p) \neq D_{KL}(p\|q)$
- Measure of how far p is from q
- $D_{KL}(q\|p) \geq 0$ (and is 0 iff $p=q$)

So, $\log p_\theta(x) \geq \mathop{\mathbb{E}}_{z\sim q_\phi(z|x)} \log \frac{p_\theta(x,z)}{q_\phi(z|x)} = \mathcal{L}_{\theta,\phi}(x)$

Interpretation of VLB

$$\mathcal{L}_{\theta,\varphi}(x) = \mathop{\mathbb{E}}_{z\sim q_\varphi(z|x)} \log \frac{p_\theta(x,z)}{q_\varphi(z|x)} = \mathop{\mathbb{E}}_{z\sim q_\varphi(z|x)} \log p_\theta(x|z)\, \frac{p(z)}{q_\varphi(z|x)}$$

$$= \underbrace{\mathop{\mathbb{E}}_{z\sim q_\varphi(z|x)} \log p_\theta(x|z)}_{\text{reconstruction error}} + \underbrace{\mathop{\mathbb{E}}_{z\sim q_\varphi(z|x)} \log \frac{p(z)}{q_\varphi(z|x)}}_{\text{regularization}}$$

First term: $p_\theta(x|z) = \mathcal{N}(x;\, G_\theta(z), \eta I)$

$\Rightarrow \log p_\theta(x|z) = -\frac{1}{2\eta}\|x - G_\theta(z)\|^2 + \text{constant}$

So $\mathop{\mathbb{E}}_{z\sim q_\varphi} \log p_\theta(x|z)$ is expected l_2 reconstruction error under the encoder model

Maximizing VLB encourages q_φ to be point mass

Second term: $\mathop{\mathbb{E}}_{z\sim q_\varphi(z|x)} \log \frac{p(z)}{q_\varphi(z|x)} = -D_{KL}(q_\varphi(z|x) \,\|\, p(z))$

So maximizing VLB $\mathcal{L}_{\theta,\varphi}$ pushes $q_\varphi(z|x)$ toward $p(z)$. Prevents q_φ from being a point mass.

Makes $q_\varphi(z|x)$ more like standard normal

Maximizing VLB $\mathcal{L}_{\theta,\varphi}$:

- Roughly maximizes $P(x)$
- Minimizes KL divergence of $q_\varphi(z|x)$ and $p_\theta(z|x)$, making q_φ better

Main Idea: Instead of optimizing $\sum_{i=1}^{n} \log p_\theta(x_i)$,

optimize $\sum_{i=1}^{n} \mathcal{L}_{\theta,\varphi}(x_i)$

w/ $\mathcal{L}_{\theta,\varphi}(x) = \mathbb{E}_{z\sim q_\varphi(z|x)} \log \frac{p_\theta(x,z)}{q_\varphi(z|x)}$

Optimizing Variational Lower Bound

$$\max_{\theta,\varphi} \sum_{i=1}^{n} \mathcal{L}_{\theta,\varphi}(x_i)$$

One possibility:

for each x_i, find best $q_\varphi(z|x_i)$ by multiple gradient steps in φ. Then gradient ascend in θ.

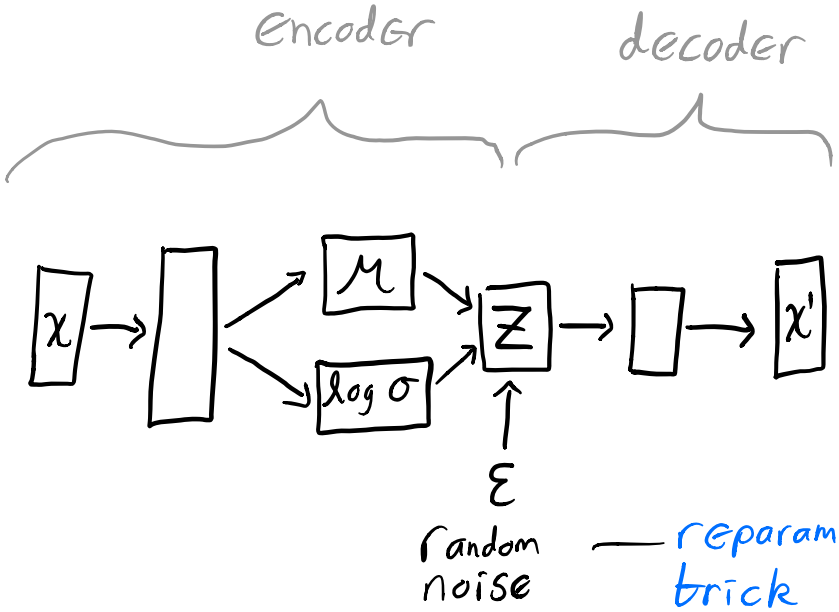
Expensive inference updates

Instead:

amortize the inference costs
by learning an inference net
$x \mapsto (\mu, \Sigma)$ w/ $q_\phi(z|x) = \mathcal{N}(z; \mu(x), \Sigma(x))$
or $\sigma(x) I$

Parameters of inference model
are shared between data points

Variational Autoencoder architecture



reparameterization trick
- separate random source from diff'able quantities

Stochastic Gradient Optimization of VLB

Dataset $D = \{x_i\}_{i=1\dots n}$

Solve $\max_{\theta,\varphi} \sum_{x_i \in D} \mathcal{L}_{\theta,\varphi}(x_i)$

w/ $\mathcal{L}_{\theta,\varphi}(x) = \mathbb{E}_{z\sim q_\varphi(z|x)} \log \frac{p_\theta(x,z)}{q_\varphi(z|x)}$

Computing $\nabla_{\theta,\varphi} \mathcal{L}_{\theta,\varphi}(x_i)$ is intractable, but there are unbiased estimators

Easy to get unbiased $\nabla_\theta \mathcal{L}_{\theta,\varphi}$:

$$\nabla_\theta \mathcal{L}_{\theta,\varphi}(x) = \nabla_\theta \mathop{\mathbb{E}}_{z\sim q_\varphi(z|x)} \left[\log p_\theta(x,z) - \log q_\varphi(z|x)\right]$$

$$= \mathop{\mathbb{E}}_{z\sim q_\varphi} \nabla_\theta \log p_\theta(x,z)$$

$$\simeq \nabla_\theta \log p_\theta(x,z) \quad \text{w/ } z\sim q_\varphi(z|x)$$

unbiased estimate

Not as easy to get unbiased $\nabla_\varphi \mathcal{L}_{\theta,\varphi}$:

$$\nabla_\varphi \mathcal{L}_{\theta,\varphi}(x) = \nabla_\varphi \mathop{\mathbb{E}}_{z\sim q_\varphi(z|x)} \left[\log p_\theta(x,z) - \log q_\varphi(z|x)\right]$$

$$\neq \mathop{\mathbb{E}}_{z\sim q_\varphi} \nabla_\varphi \left(\log p_\theta(x,z) - \log q_\varphi(z|x)\right)$$

Recall, $q_\varphi(z|x) = N(z; \mu(x), \sigma(x)I)$

$$= \mu(x) + \sigma(x)\cdot \varepsilon, \quad \text{w/ } \varepsilon \sim N(0,I)$$

$$\mathcal{L}_{\theta,\varphi}(x) = \mathop{\mathbb{E}}_{z\sim q_\varphi(z|x)} \left(\log p_\theta(x,z) - \log q_\varphi(z|x)\right)$$

$$= \mathop{\mathbb{E}}_{\varepsilon\sim p(\varepsilon)} \left(\log p_\theta(x,z) - \log q_\varphi(z|x)\right)$$

Form estimator of $\mathcal{L}_{\theta,\varphi}(x)$ as $\widetilde{\mathcal{L}}_{\theta,\varphi}(x)$ by:

$$\varepsilon \sim p(\varepsilon)$$
$$z = \mu_\varphi(x) + \sigma_\varphi(x)\varepsilon = g(\varphi, x, \varepsilon)$$
$$\widetilde{\mathcal{L}}_{\theta,\varphi}(x) = \log p_\theta(x,z) - \log q_\varphi(z|x)$$

Unbiased estimate of $\nabla_\varphi \mathcal{L}_{\theta,\varphi}(x)$:

$$\nabla_\varphi \tilde{\mathcal{L}}_{\theta,\varphi}(x)$$

Note: $\mathop{\mathbb{E}}_{\varepsilon\sim p(\varepsilon)} \tilde{\mathcal{L}}_{\theta,\varphi}(x) = \mathcal{L}_{\theta,\varphi}(x)$

So $\mathop{\mathbb{E}}_{\varepsilon\sim p(\varepsilon)} \nabla_\varphi \tilde{\mathcal{L}}_{\theta,\varphi}(x) = \nabla_\varphi \mathop{\mathbb{E}}_{\varepsilon\sim p(\varepsilon)} \tilde{\mathcal{L}}_{\theta,\varphi} = \nabla_\varphi \mathcal{L}_{\theta,\varphi}$

Optimize VAE parameters w/ stochastic gradients.

Can extend models to be more sophisticated, eg $\Sigma(x)$ vs $\sigma I(x)$ as inference model.

Key points:

- optimize a lower bound to likelihood
- lower bound has terms for reconstruction and for regularization
- maintain an inference model for $z|x$ in place of intractable true distribution

- reparameterization trick allows back propagating on mean and variance of inference model
- VAEs have been trained with photorealistic outputs