Variational Autoencoder for Image Generation

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Preliminary: Distance between Two Probability Distributions

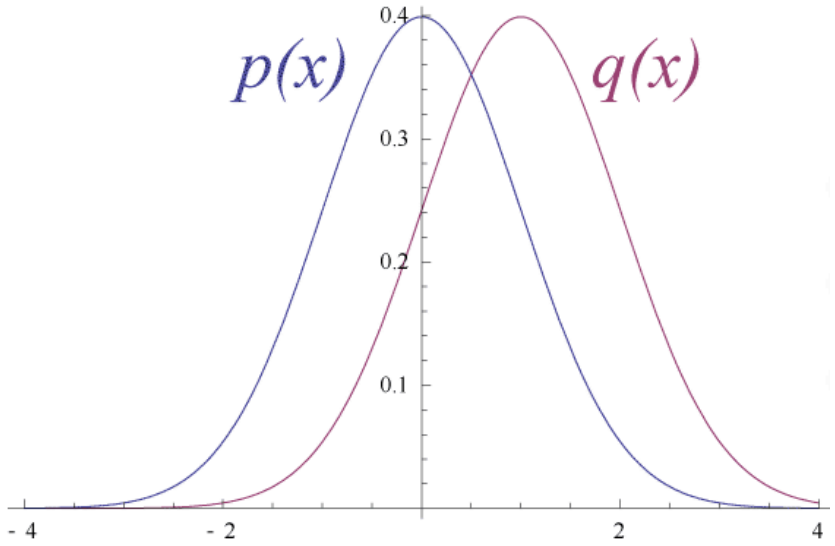
Distance between Two Vectors

- Distance between two vectors is measured by vector norms.
- Examples:
  - ℓ_1 distance: $\left|\left|\mathbf{a}-\mathbf{b}\right|\right|_1 = \sum_j \left|a_j - b_j\right|$.
  - ℓ_2 distance: $\left|\left|\mathbf{a}-\mathbf{b}\right|\right|_2 = \sqrt{\sum_j \left(a_j - b_j\right)^2}$.
  - ℓ_∞ distance: $\left|\left|\mathbf{a}-\mathbf{b}\right|\right|_\infty = \max_j \left|a_j - b_j\right|$.
  - ℓ_p distance: $\left|\left|\mathbf{a}-\mathbf{b}\right|\right|_p = \left[\sum_j \left(a_j - b_j\right)^p\right]^{1/p}$.

Distance between Two Probability Distributions

Question: What is the distance between $p(x)$ and $q(x)$?

- Let $p(x)$ and $q(x)$ be two Probability Density Functions (PDFs).
- E.g., the PDF of a Gaussian distribution is $p(x|\mu,\sigma) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$.



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Definition: The Kullback–Leibler (KL) divergence $D_{\mathrm{KL}}(p||q)$.

- For discrete probability distributions, the KL divergence is

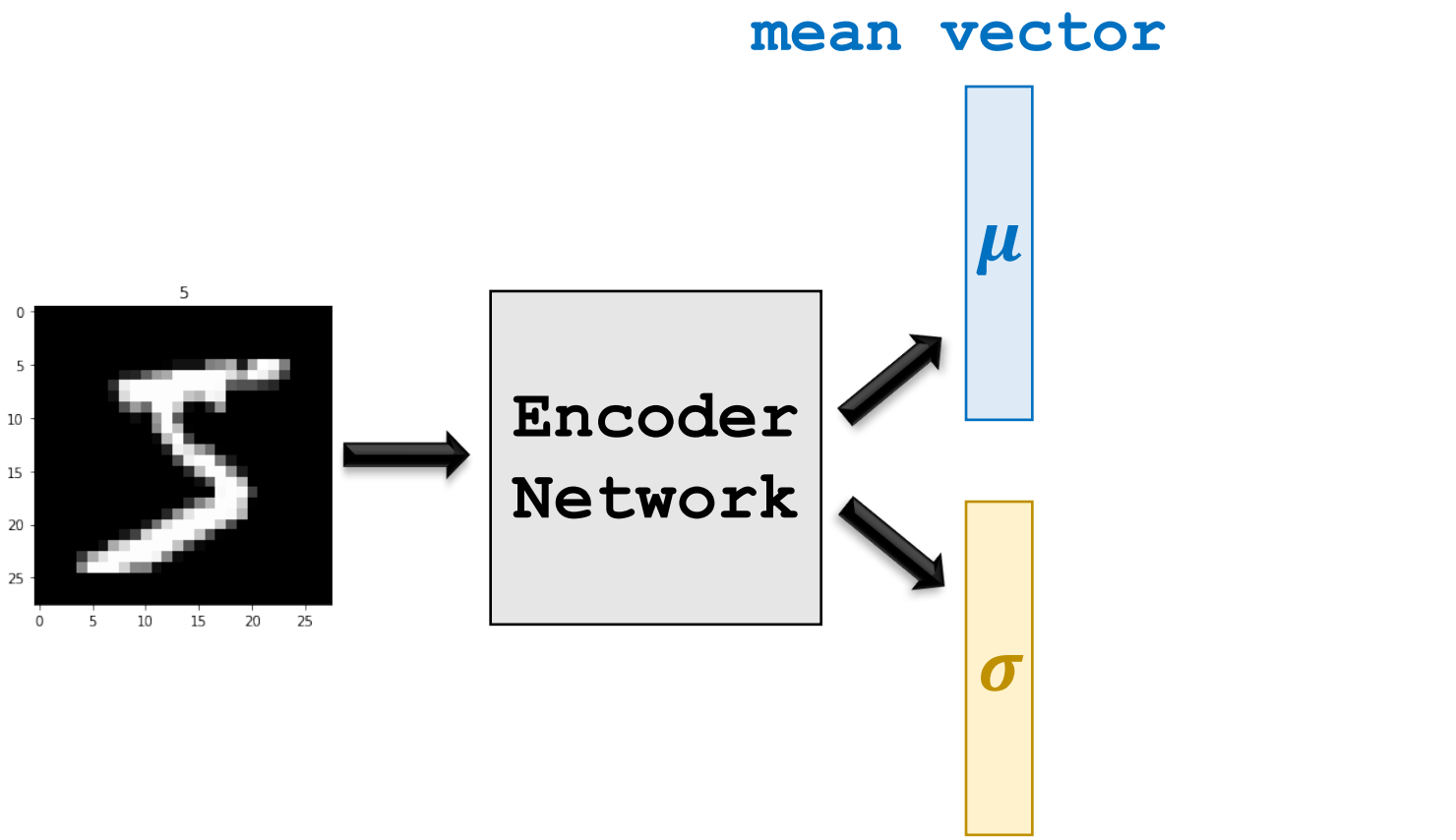
$$D_{\mathrm{KL}}(p||q) = -\sum_i p(i) \log \frac{q(i)}{p(i)}.$$

- For continuous probability distributions, the KL divergence is

$$D_{\mathrm{KL}}(p||q) = -\int_{-\infty}^{+\infty} p(x) \log \frac{q(x)}{p(x)}\, dx.$$

Variational Autoencoder

Variational Autoencoder (VAE)



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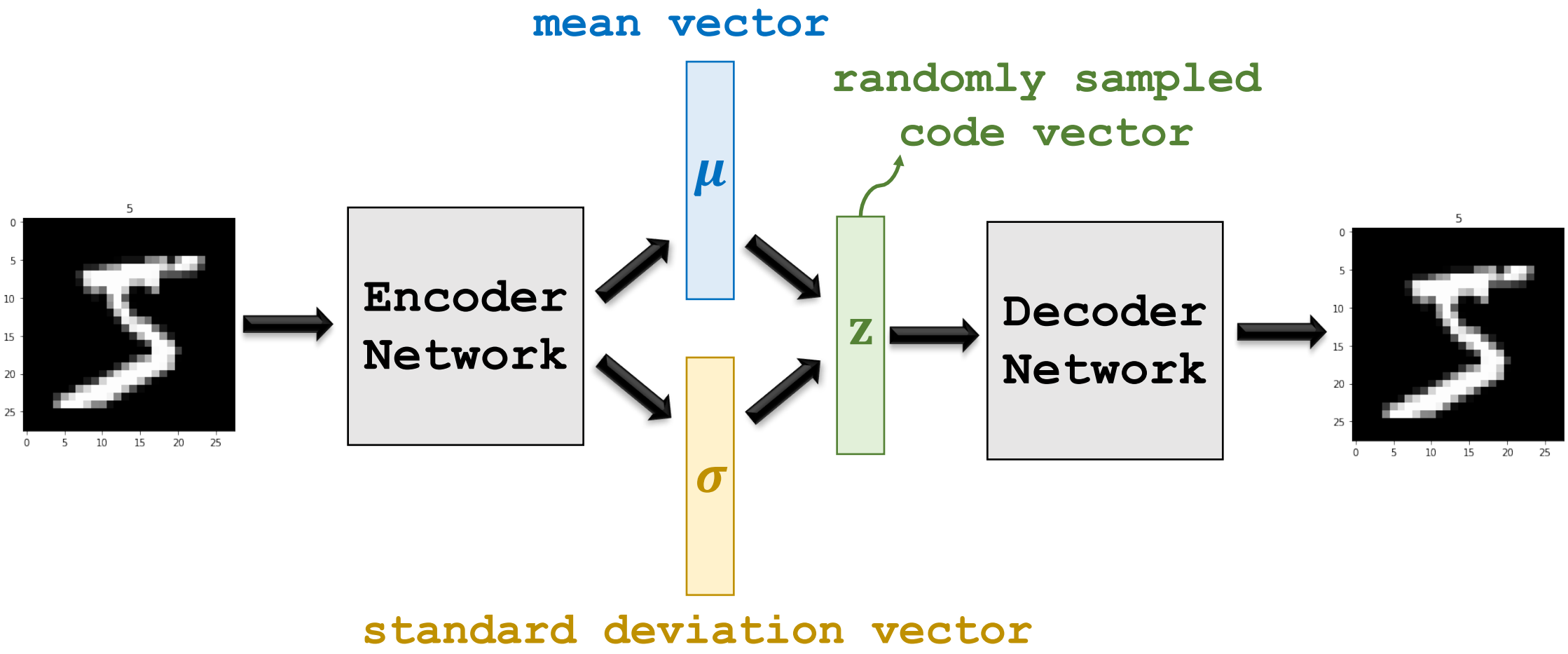
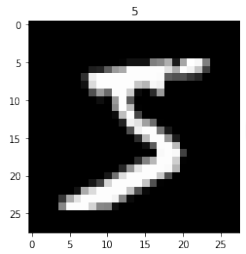


VAE Sampling

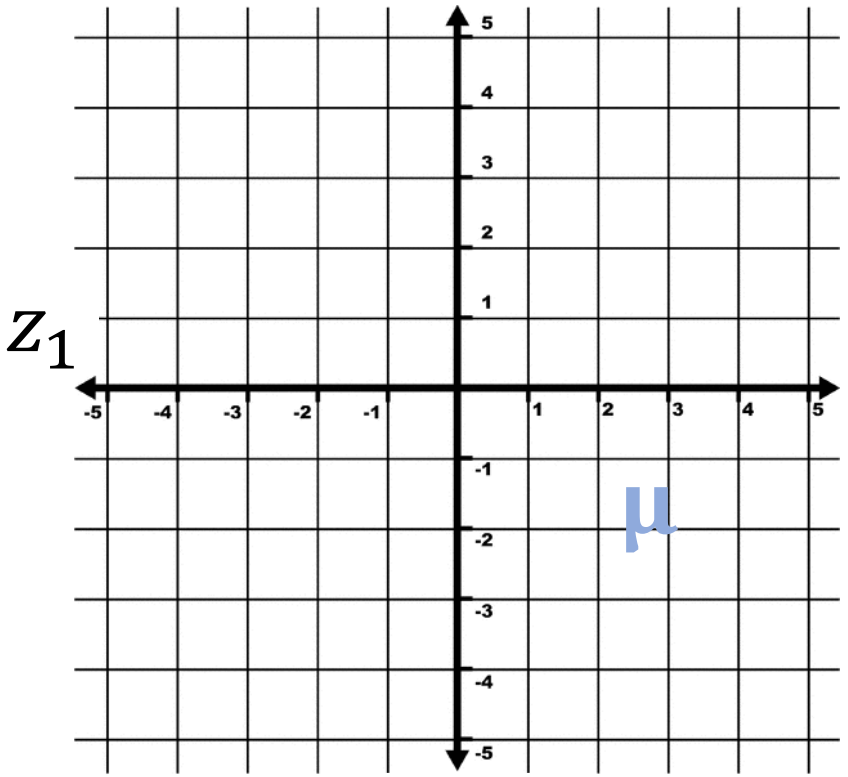


Encoder Network

mean vector

μ

Code vectors

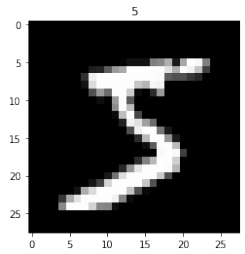


z_1

z_2

VAE Sampling

Code vectors



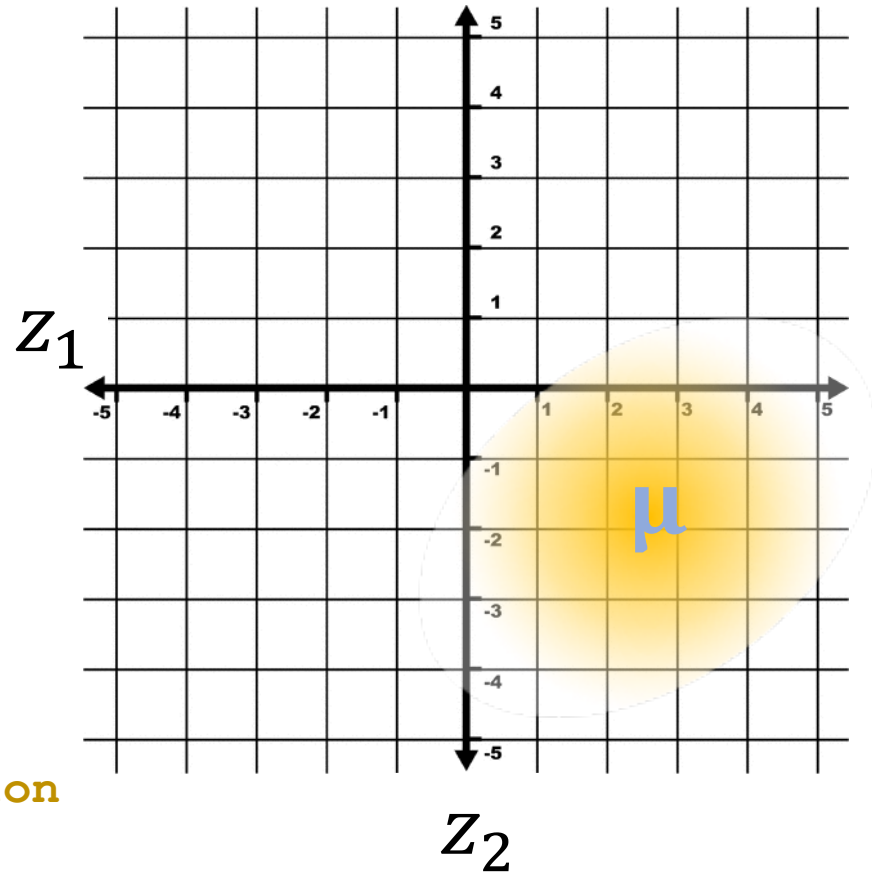
Encoder Network

mean vector

μ

σ

standard deviation vector



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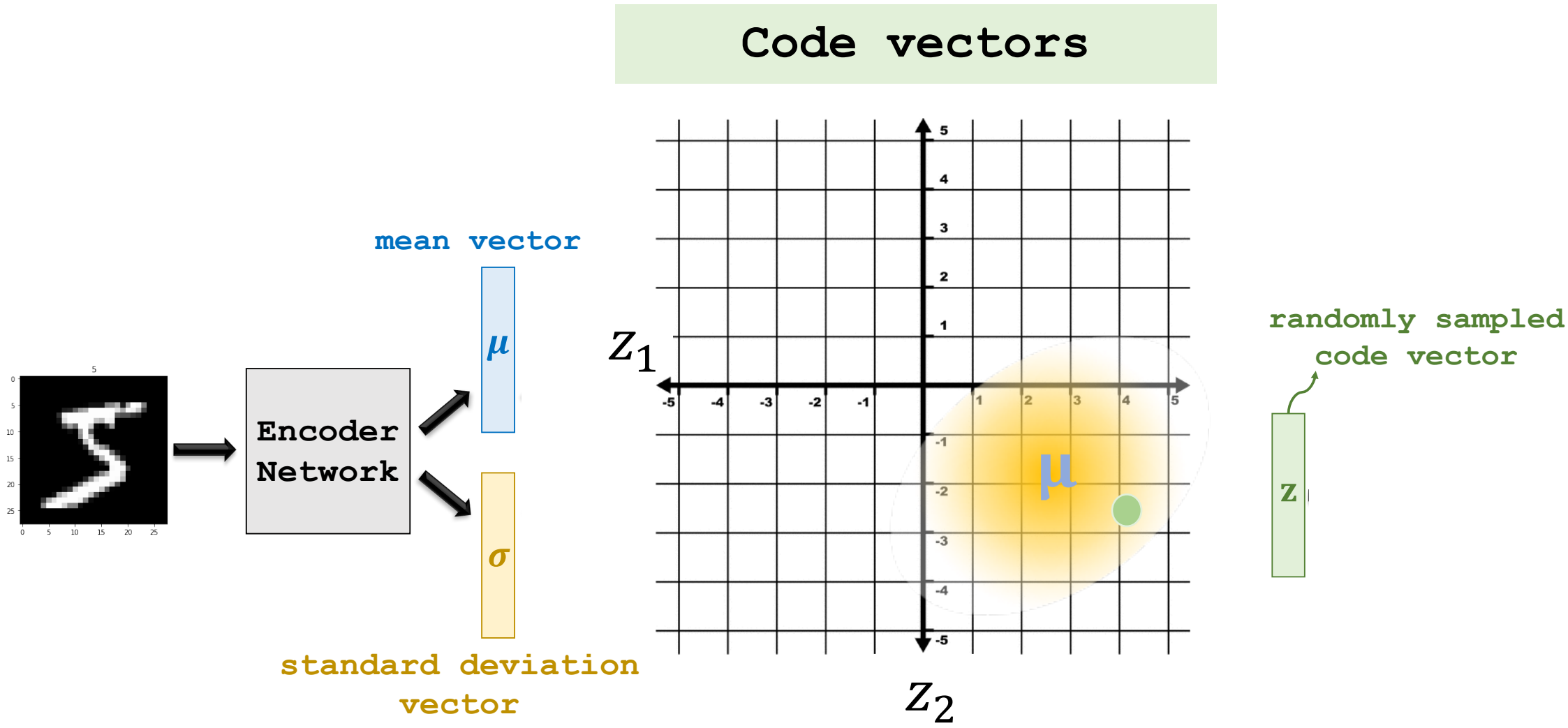

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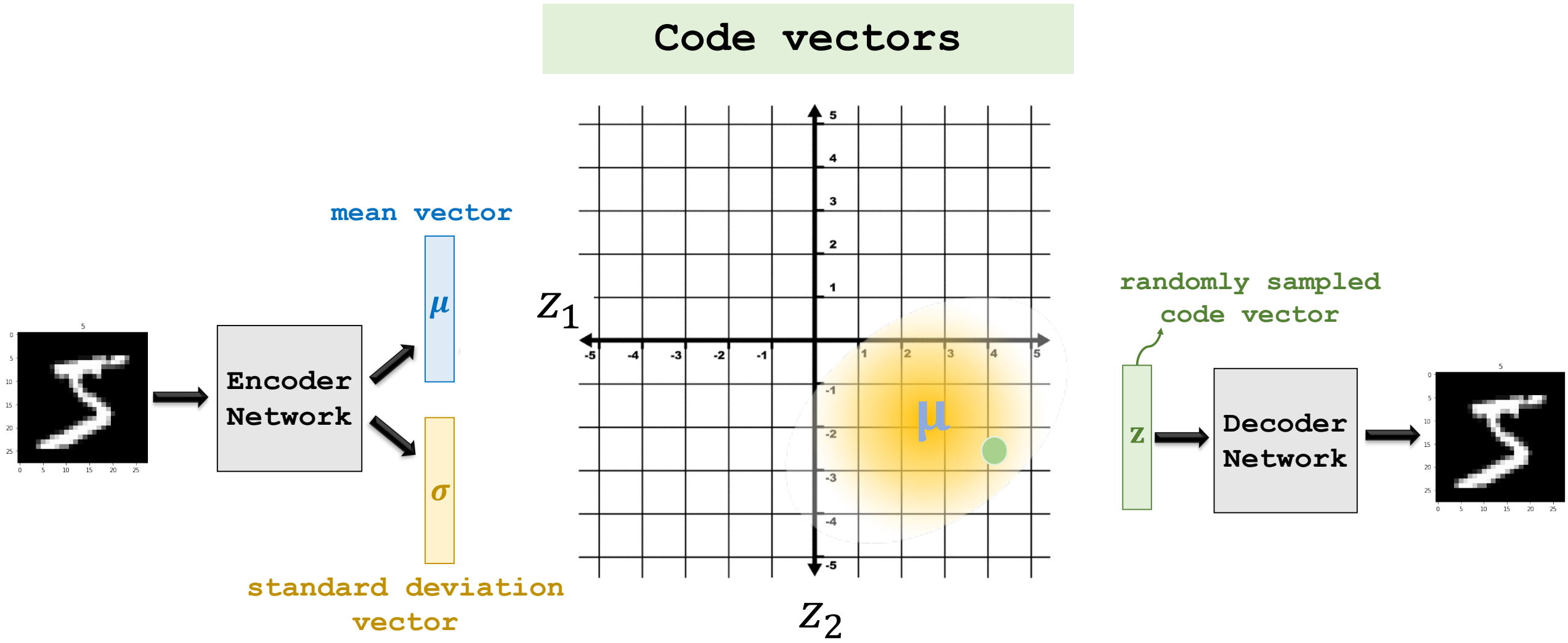
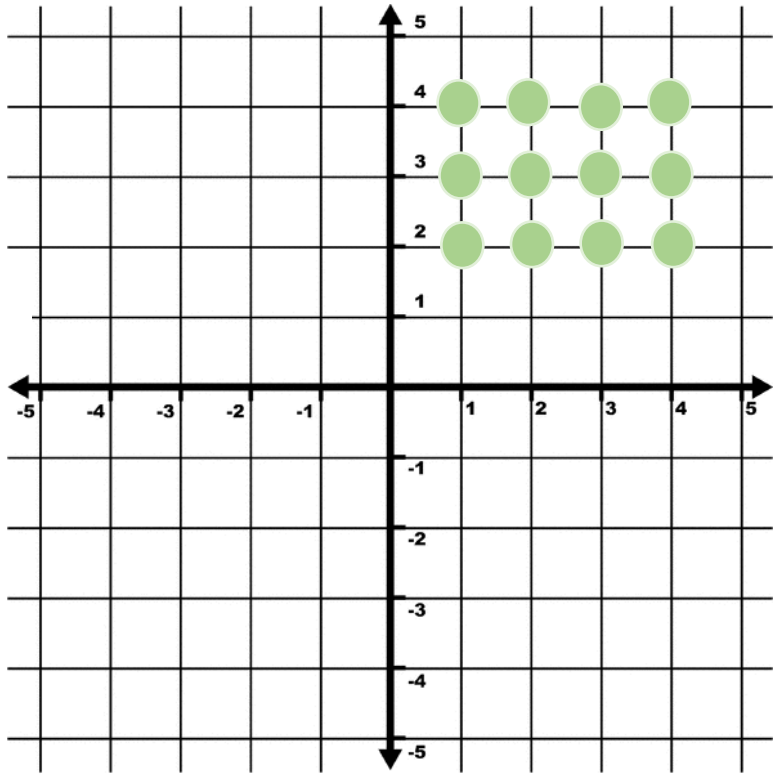


Visualize Code Vectors

Visualize code vectors.

Code vectors

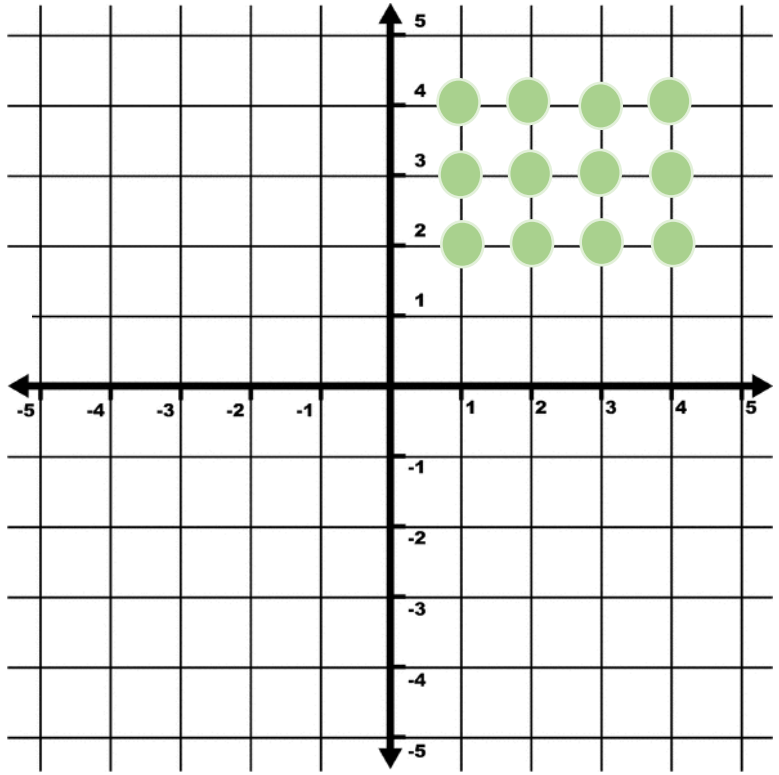


- Get a set of code vectors from the grid:

$$\mathbf{z}_1, \mathbf{z}_2, \mathbf{z}_3, \mathbf{z}_4, \mathbf{z}_5, \cdots$$

Visualize code vectors.

Code vectors



- Get a set of code vectors from the grid:

$$\mathbf{z}_1, \mathbf{z}_2, \mathbf{z}_3, \mathbf{z}_4, \mathbf{z}_5, \cdots$$

- For every code vector $\mathbf{z}_i$, map it to an image using the decoder:

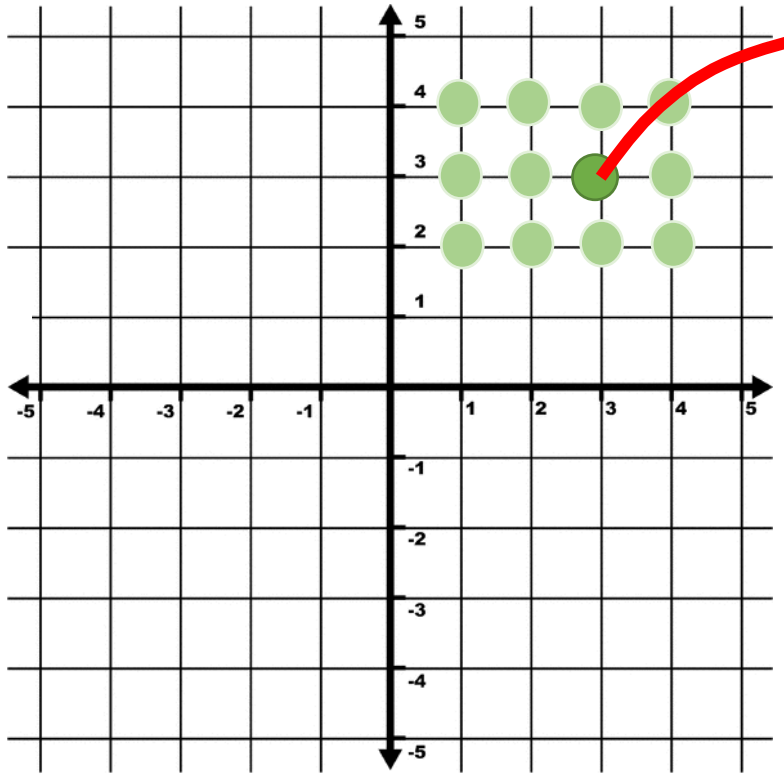
$$\text{image}_i = \text{Decoder}(\mathbf{z}_i).$$

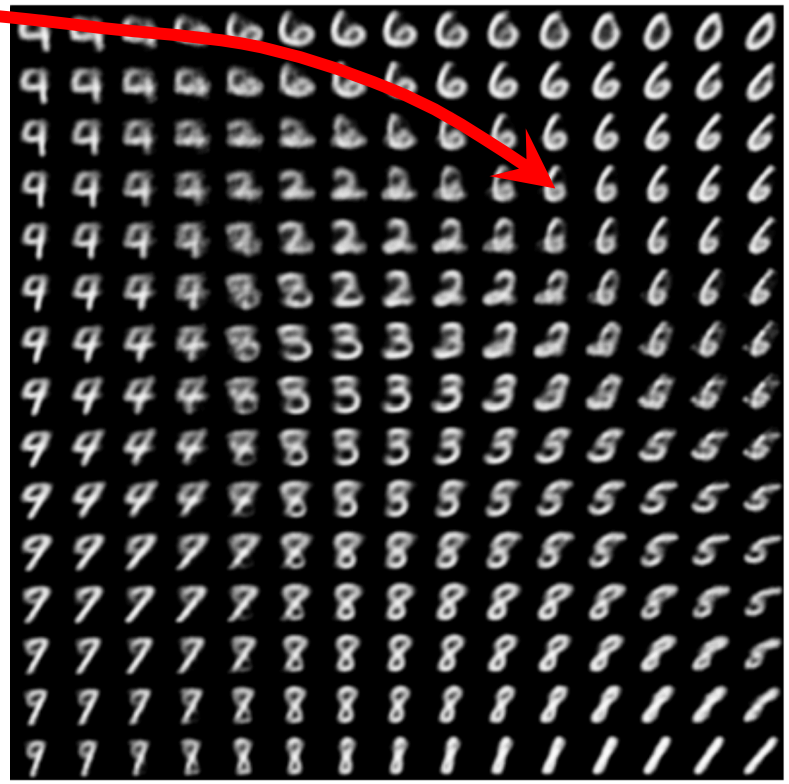
Visualize code vectors.

Code vectors

Images

Decoder





The decoder behaves like a continuous function.

- Function f is continuous if a small change in z (input) results in a small change in $f(z)$ (function value).

- The decoder network is trained to be (almost) continuous.
- If the code vectors $\mathbf{z}$ and $\mathbf{z}'$ are similar, then the images

$$\mathrm{Decoder}(\mathbf{z}) \quad \text{and} \quad \mathrm{Decoder}(\mathbf{z}')$$

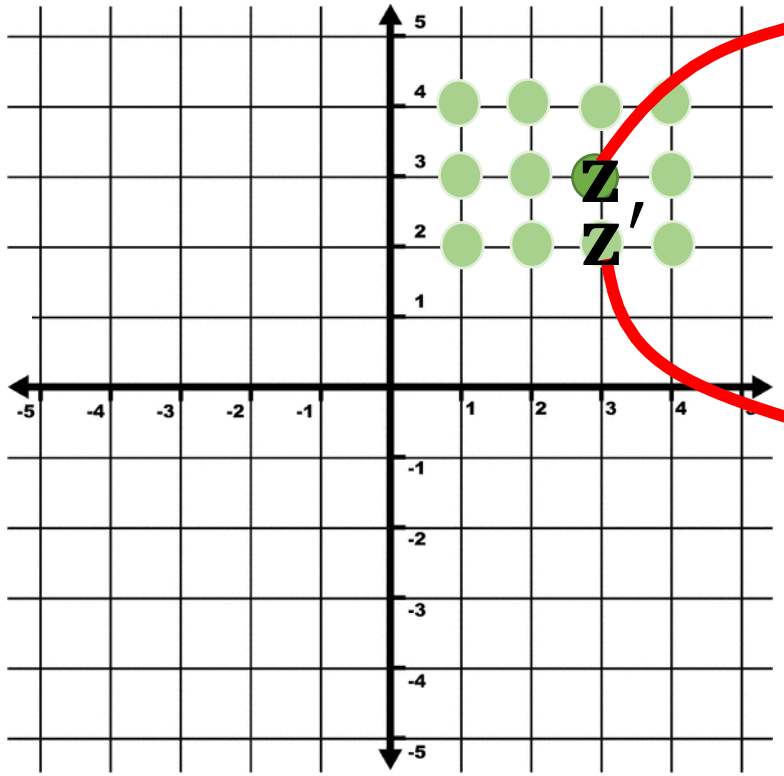
  are similar as well.

The decoder behaves like a continuous function.

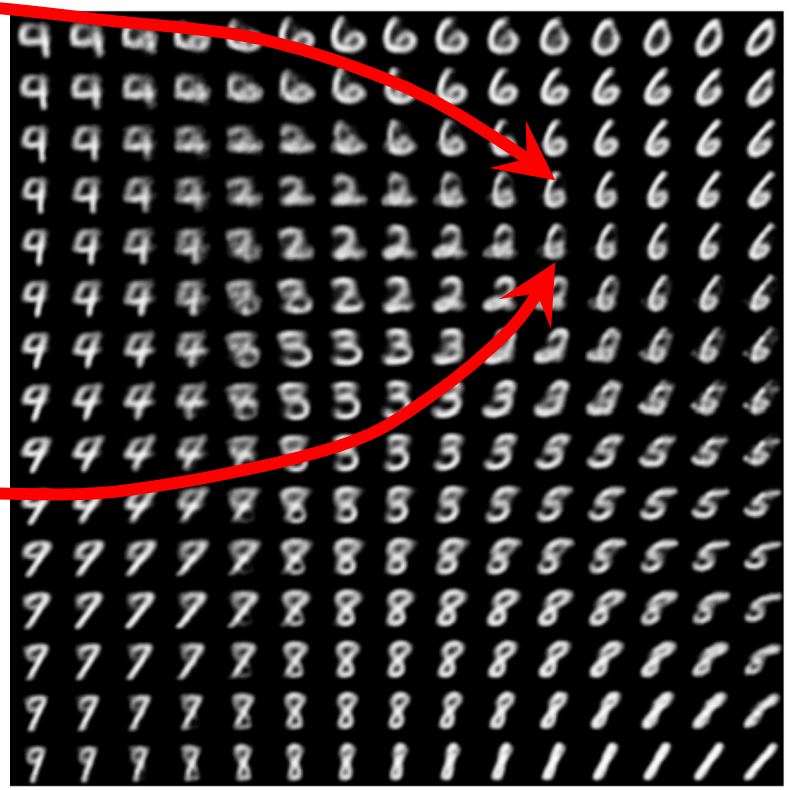
Code vectors

Images

Decoder



Decoder



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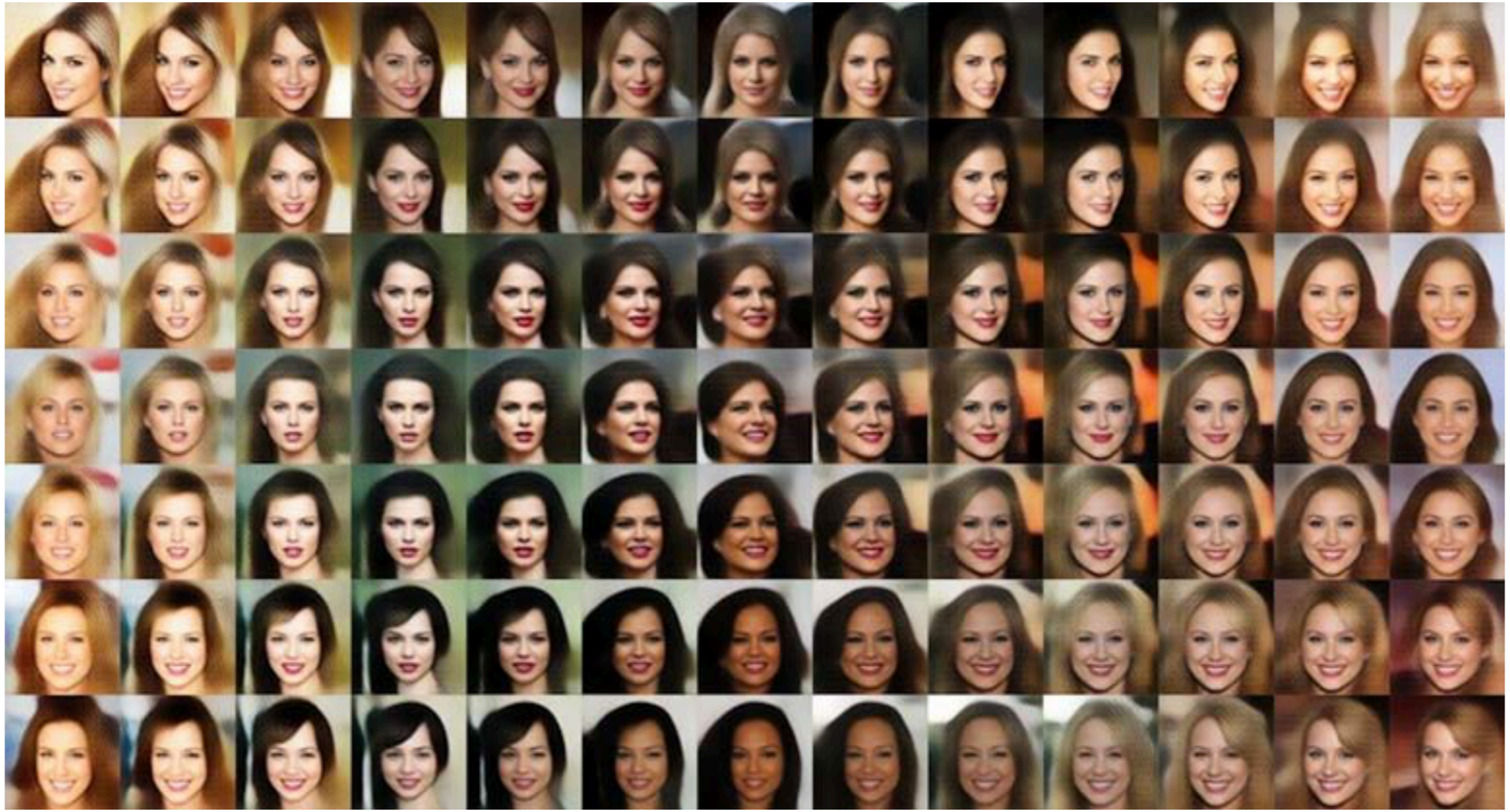
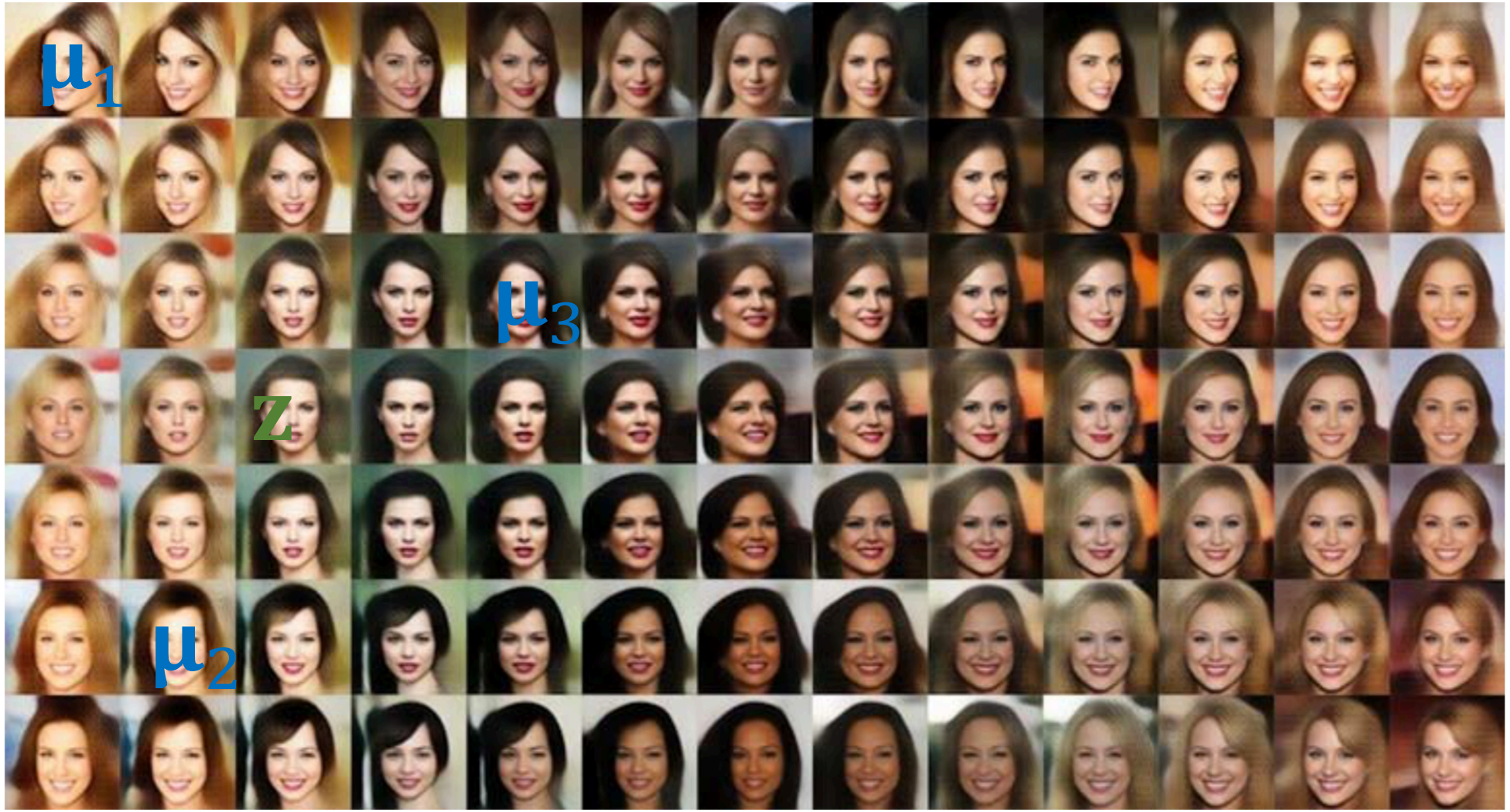


Visualization of the generated faces (by Tom White)

Averaging images via averaging code vectors



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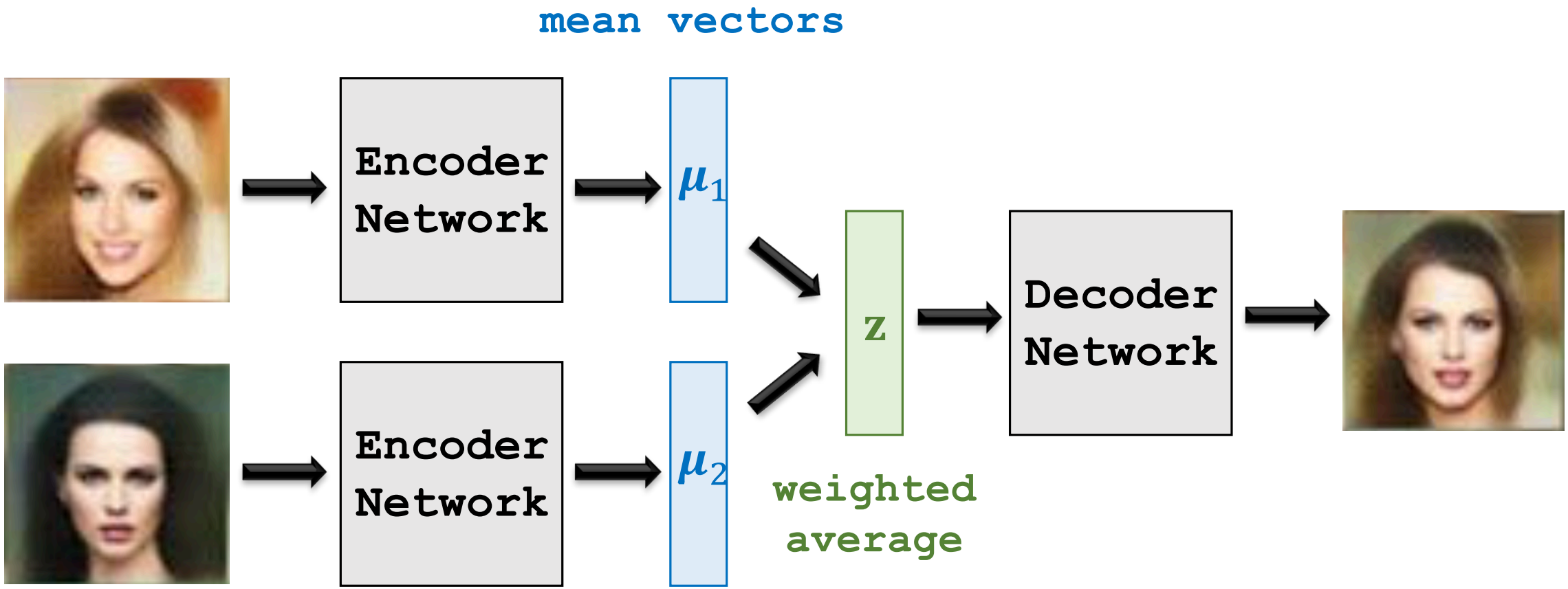
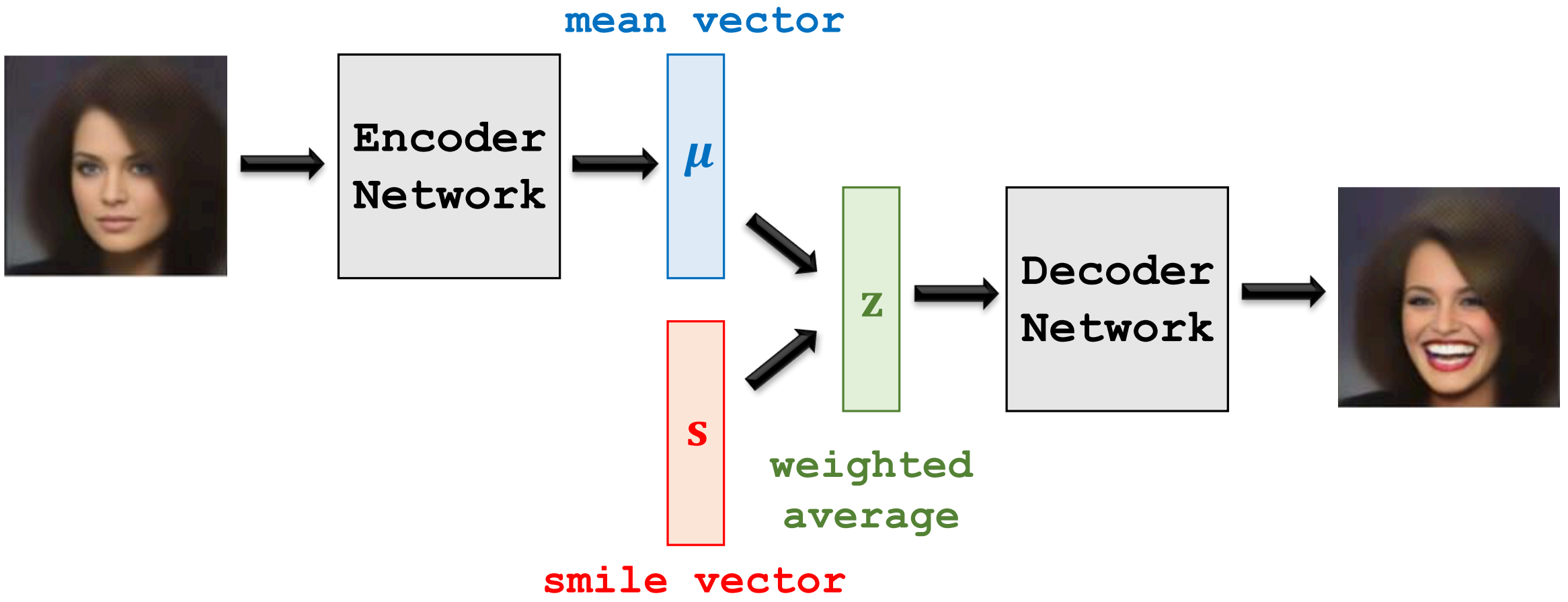
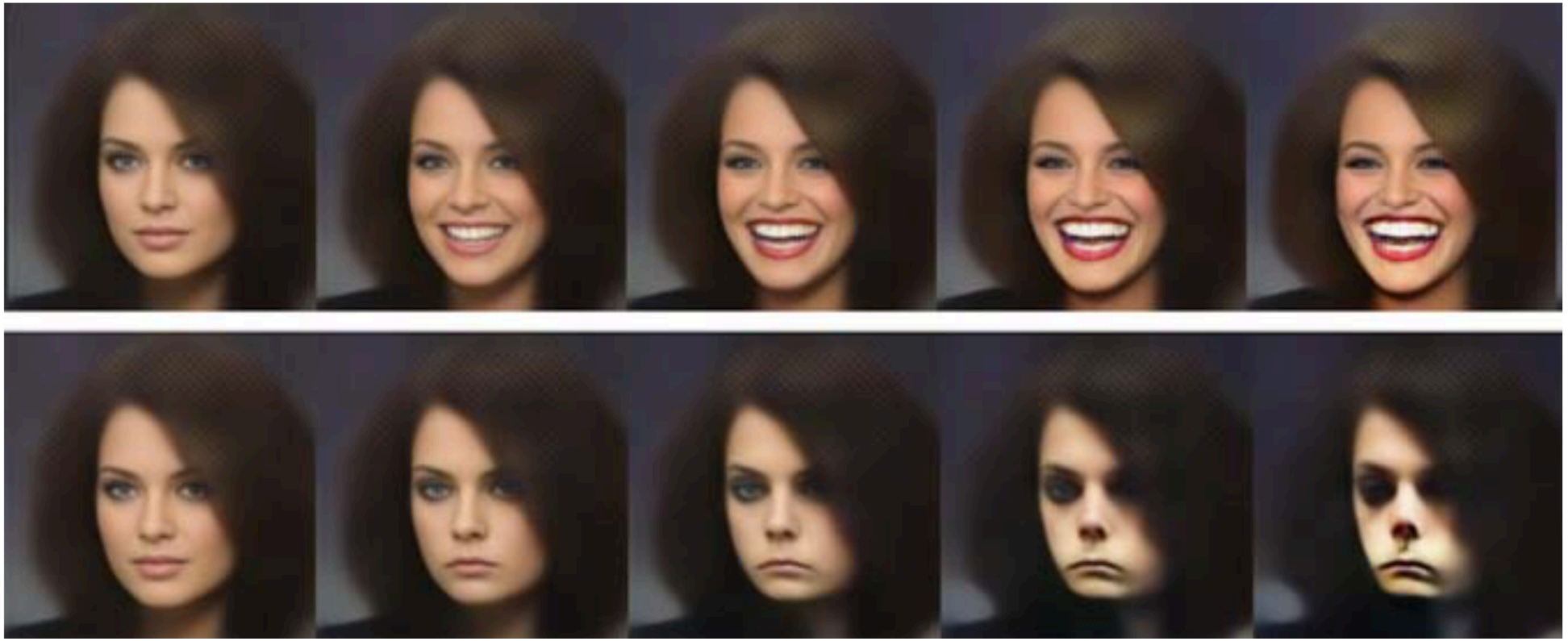


Editing images via editing code vectors



Editing images via editing code vectors

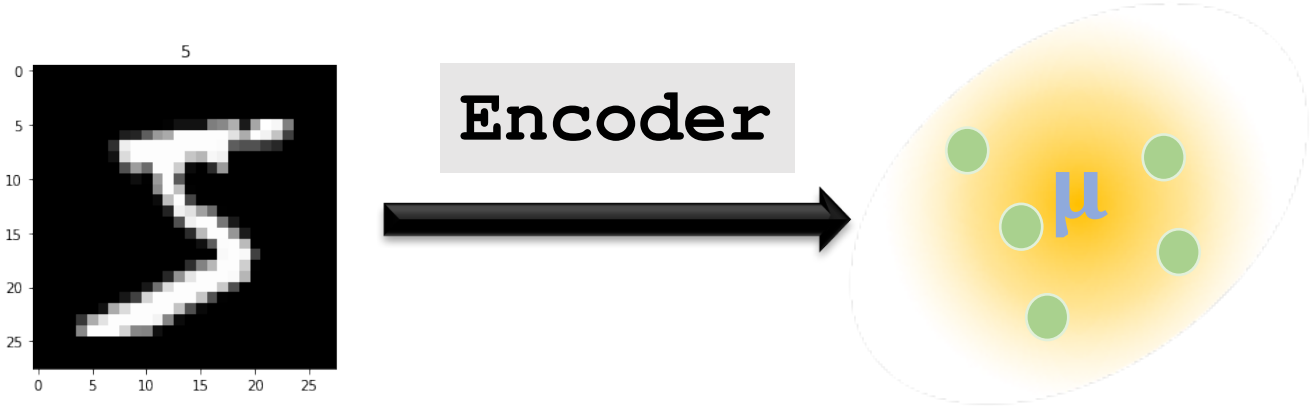
μ $\mu + s$ $\mu + 2s$ $\mu + 3s$ $\mu + 4s$



μ $\mu - s$ $\mu - 2s$ $\mu - 3s$ $\mu - 4s$

What makes the decoder continuous?

- Given $\boldsymbol{\mu}$ and $\boldsymbol{\sigma}$, sample $\mathbf{z}_i \sim \mathcal{N}\left(\boldsymbol{\mu}, \mathrm{diag}\left(\boldsymbol{\sigma}^2\right)\right)$, for $i = 1, 2, 3, \cdots$.



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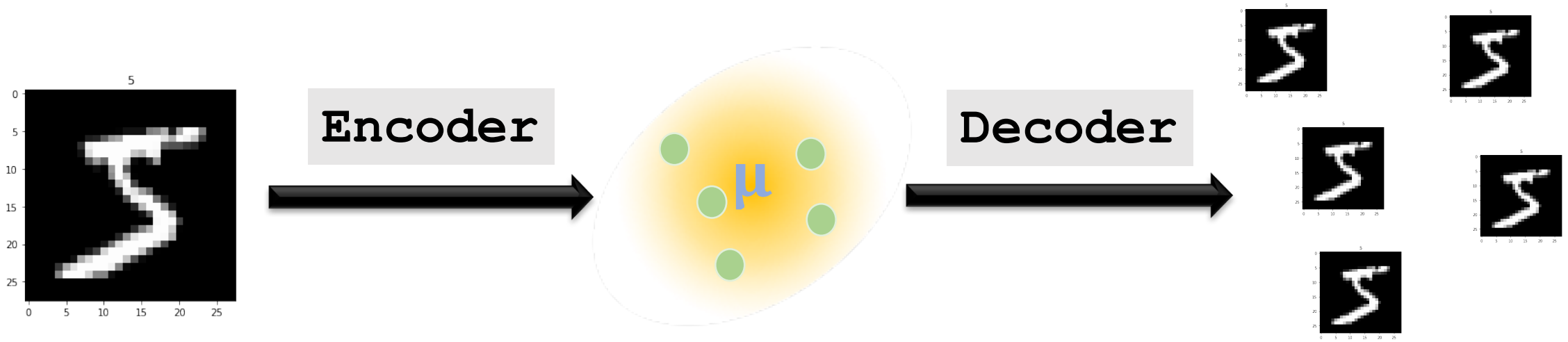
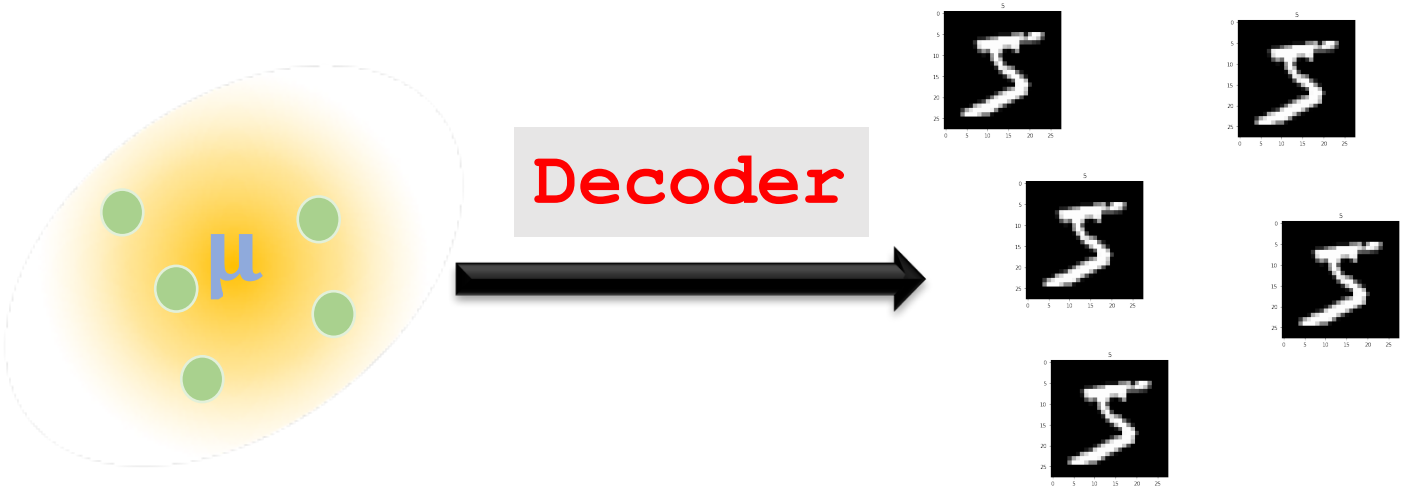
- Given $\boldsymbol{\mu}$ and $\boldsymbol{\sigma}$, sample $\mathbf{z}_i \sim \mathcal{N}\left(\boldsymbol{\mu}, \mathrm{diag}\left(\boldsymbol{\sigma}^2\right)\right)$, for $i = 1, 2, 3, \cdots$.
- Generate images, $\mathrm{Decoder}(\mathbf{z}_1), \mathrm{Decoder}(\mathbf{z}_2), \mathrm{Decoder}(\mathbf{z}_3), \cdots$, have the same target (which is the original image).



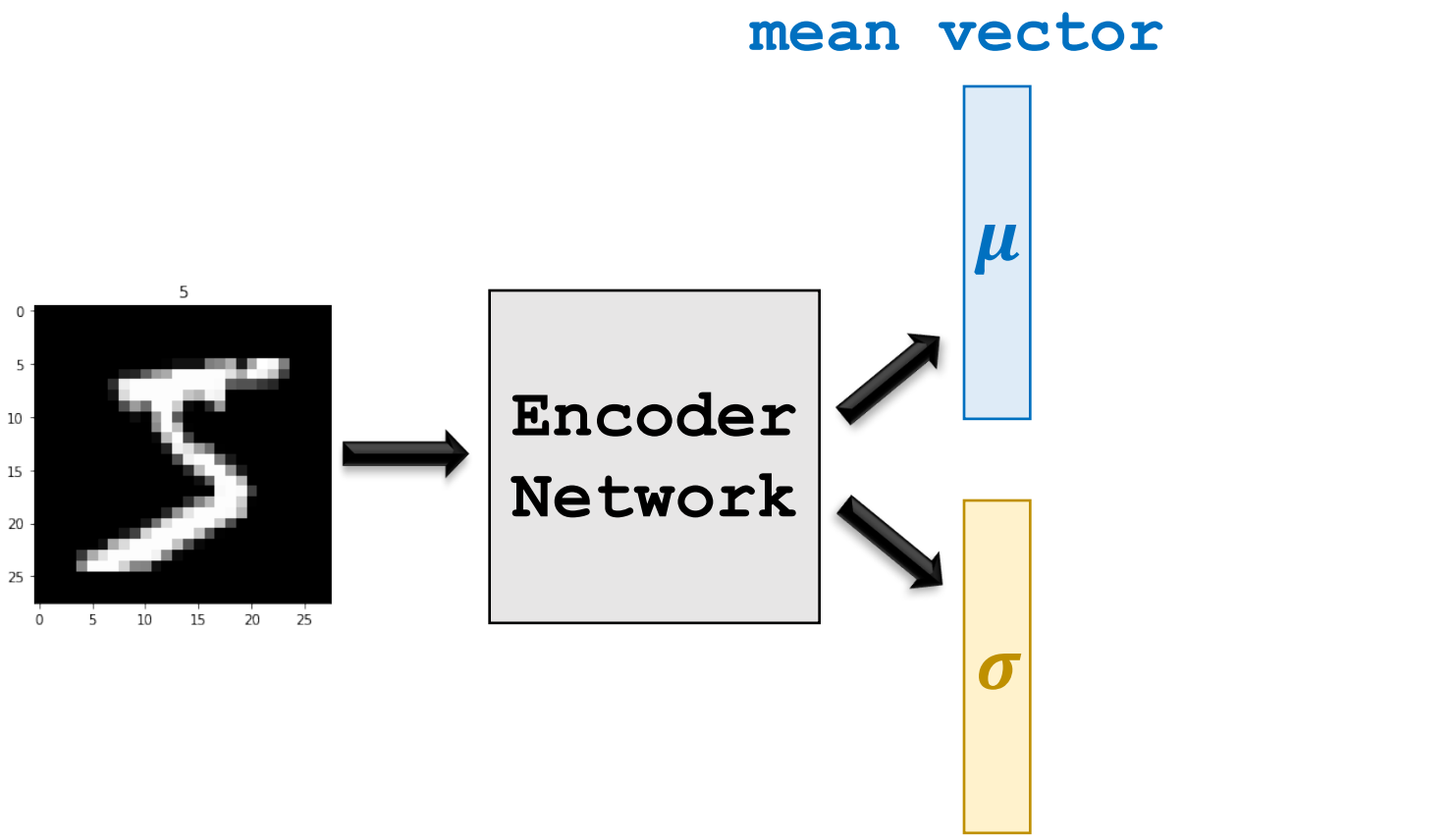
What makes the decoder continuous?

- Inputs (code vectors) are similar. (Because they are in a small neighborhood around μ.)
- Outputs (generated images) are encouraged to be similar. (Because they have the same target.)
- ➔ The decoder is trained to behave like a continuous function.



Build the Networks

1. The Encoder Network



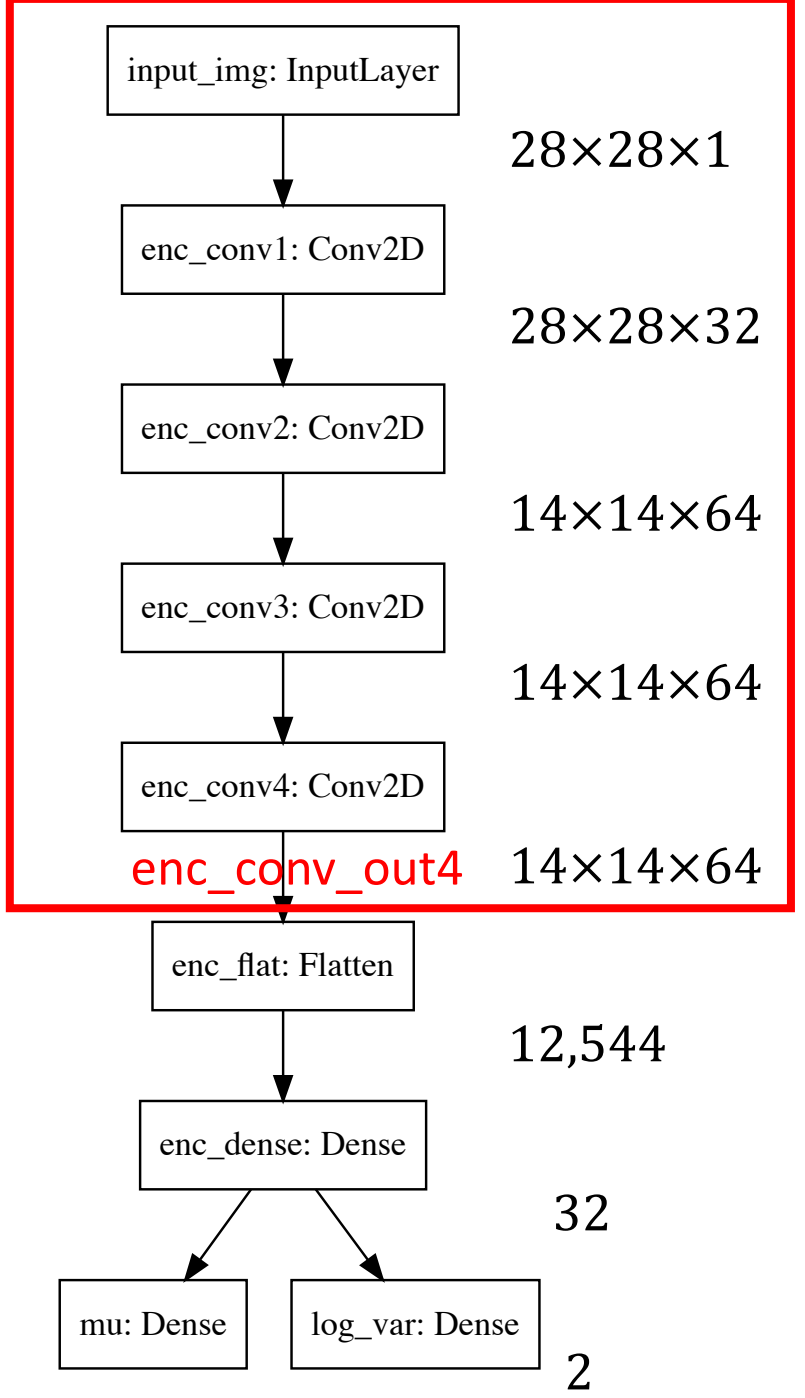
1. The Encoder Network

```
from keras.layers import Input, Conv2D, Flatten, Dense
from keras import models

shape_z = 2

# define convolutional layers
enc_conv1 = Conv2D(32, 3, padding='same',
                   activation='relu', name='enc_conv1')
enc_conv2 = Conv2D(64, 3, padding='same', activation='relu',
                      strides=(2, 2), name='enc_conv2')
enc_conv3 = Conv2D(64, 3, padding='same',
                   activation='relu', name='enc_conv3')
enc_conv4 = Conv2D(64, 3, padding='same',
                   activation='relu', name='enc_conv4')

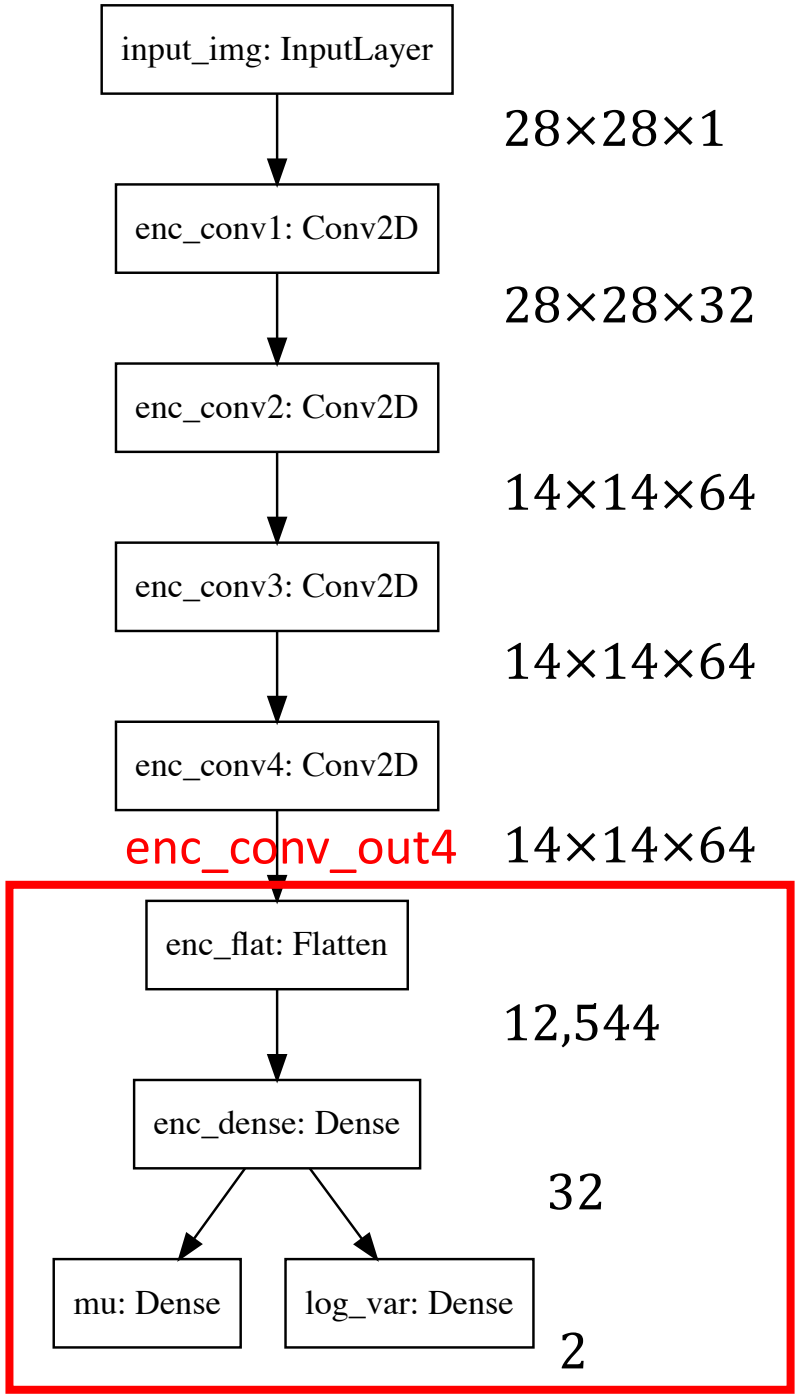
input_img = Input(shape=(28, 28, 1), name='input_img')
enc_conv_out1 = enc_conv1(input_img)
enc_conv_out2 = enc_conv2(enc_conv_out1)
enc_conv_out3 = enc_conv3(enc_conv_out2)
enc_conv_out4 = enc_conv4(enc_conv_out2)
```



1. The Encoder Network

```
# define flatten and dense layers
enc_flat = Flatten(name='enc_flat')
enc_dense = Dense(32, activation='relu',
                  name='enc_dense')
enc_mu = Dense(shape_z, name='mu')
enc_log_var = Dense(shape_z, name='log_var')

enc_flat_out = enc_flat(enc_conv_out4)
enc_dense_out = enc_dense(enc_flat_out)
mu = enc_mu(enc_dense_out)
log_var = enc_log_var(enc_dense_out)
```



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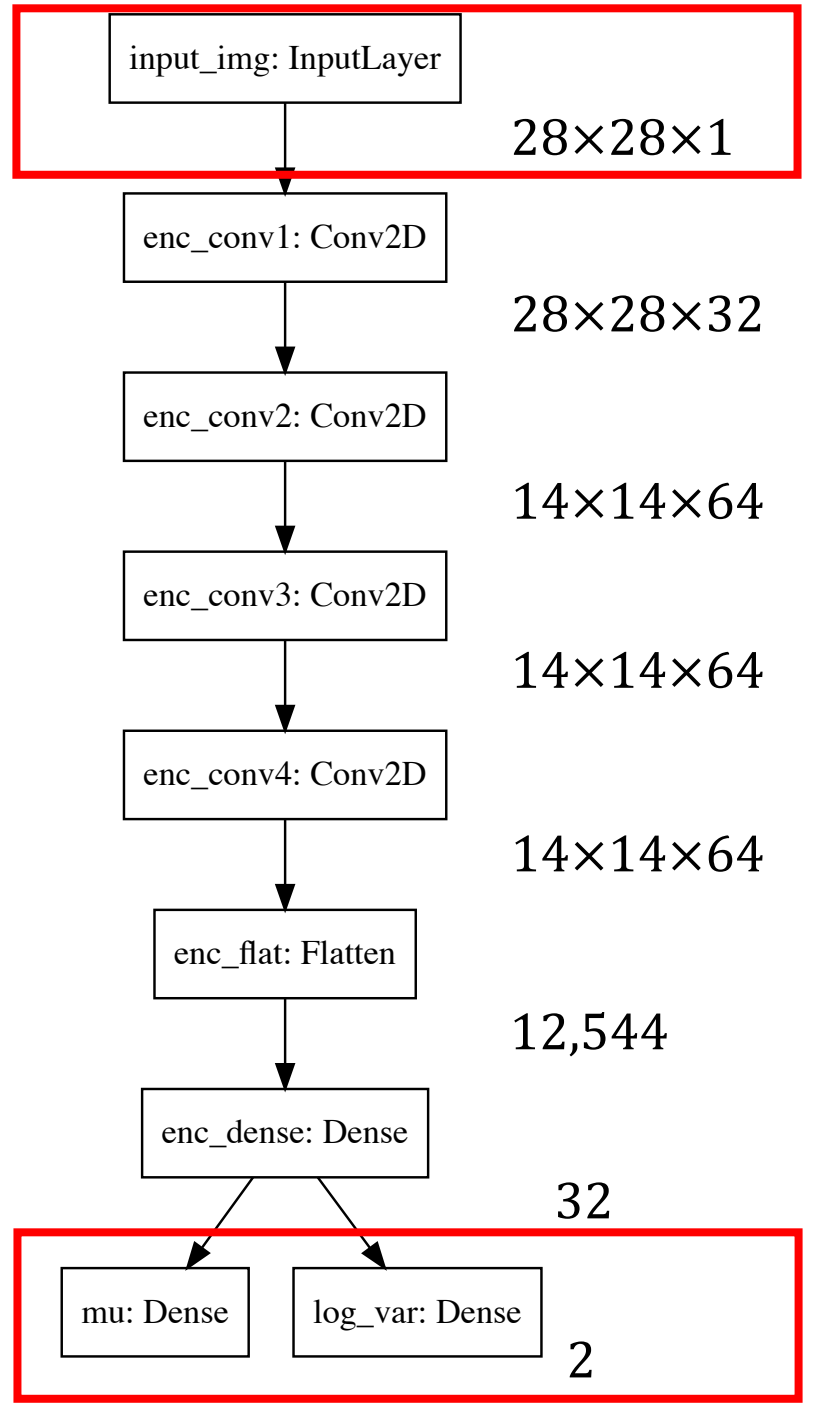
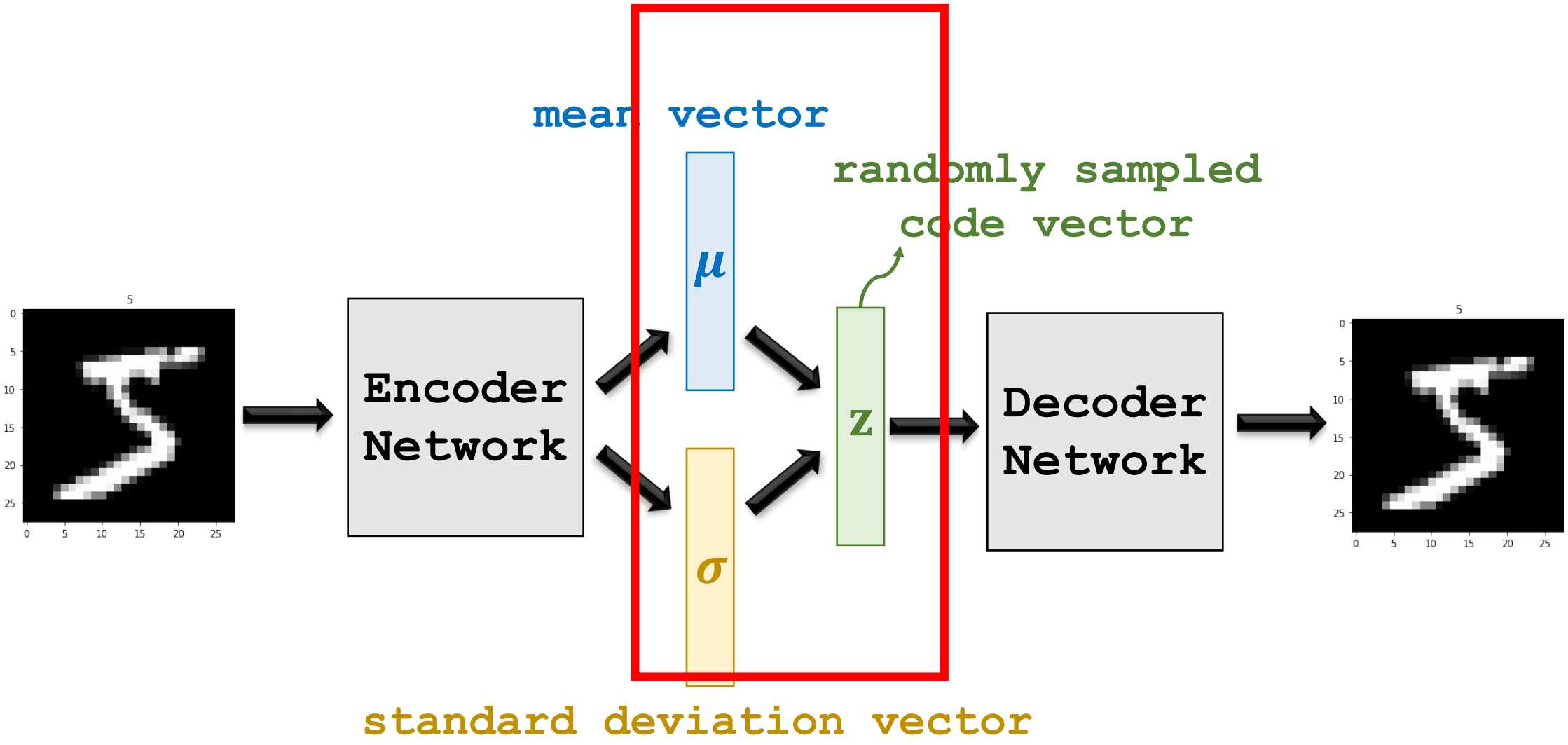
enc_dense_out = enc_dense(enc_flat_out)
mu = enc_mu(enc_dense_out)
log_var = enc_log_var(enc_dense_out)

# model
encoder = models.Model(inputs=input_img,
                       outputs=[mu, log_var],
                       name='encoder')
```



2. The Sampling Network

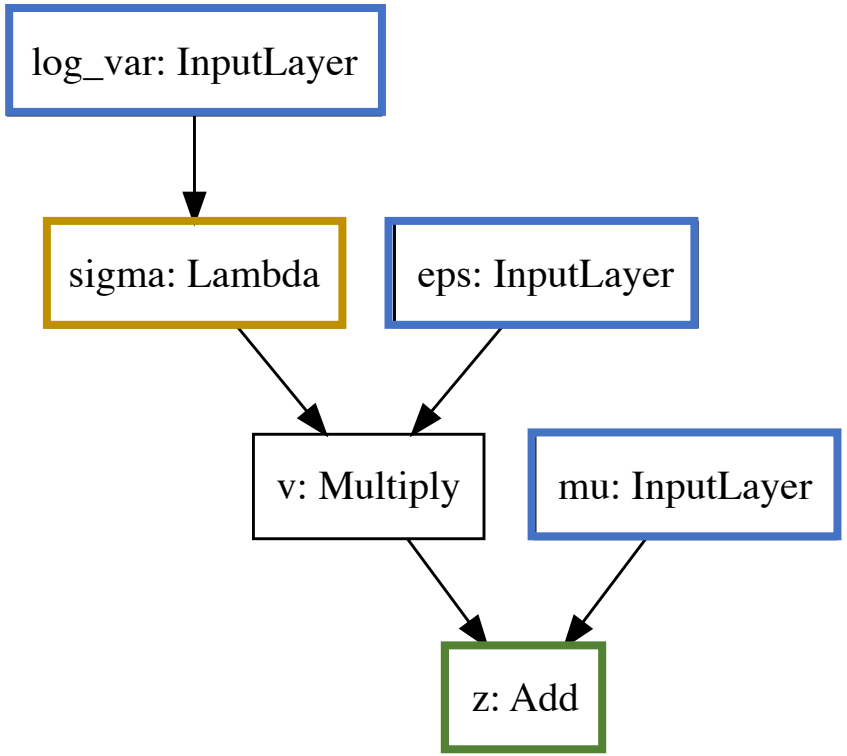


2. The Sampling Network

- The i-th entry of $\mathbf{z}$ (denote z_i) is randomly sampled from $\mathcal{N}\left(\mu_i, \sigma_i^2\right)$.
- Equivalently,
  - Randomly sample scalar variable ϵ_i from $\mathcal{N}(0,1)$.
  - Let $v_i = \sigma_i \cdot \epsilon_i$. (Equivalently, v_i is sampled from $\mathcal{N}\left(0, \sigma_i^2\right)$.)
  - $z_i = \mu_i + v_i$.

2. The Sampling Network

- Shape of $\mathbf{z}$: k ($= 2$ in our implementation).
- Input of the sampling network.
  - Log variance: $\boldsymbol{\eta}$ (k-dim vector).
  - Mean: $\boldsymbol{\mu}$ (k-dim vector).
  - $\boldsymbol{\epsilon}$: randomly sampled from $\mathcal{N}(\mathbf{0}, \mathbf{I}_k)$.
- The sampling network:
  - $\boldsymbol{\sigma} = e^{0.5\boldsymbol{\eta}}$ (k-dim vector).
  - $\mathbf{v} = \boldsymbol{\sigma} \circ \boldsymbol{\epsilon}$ (k-dim vector).
  - $\mathbf{z} = \boldsymbol{\mu} + \mathbf{v}$ (k-dim vector).
  - Output $\mathbf{z}$.



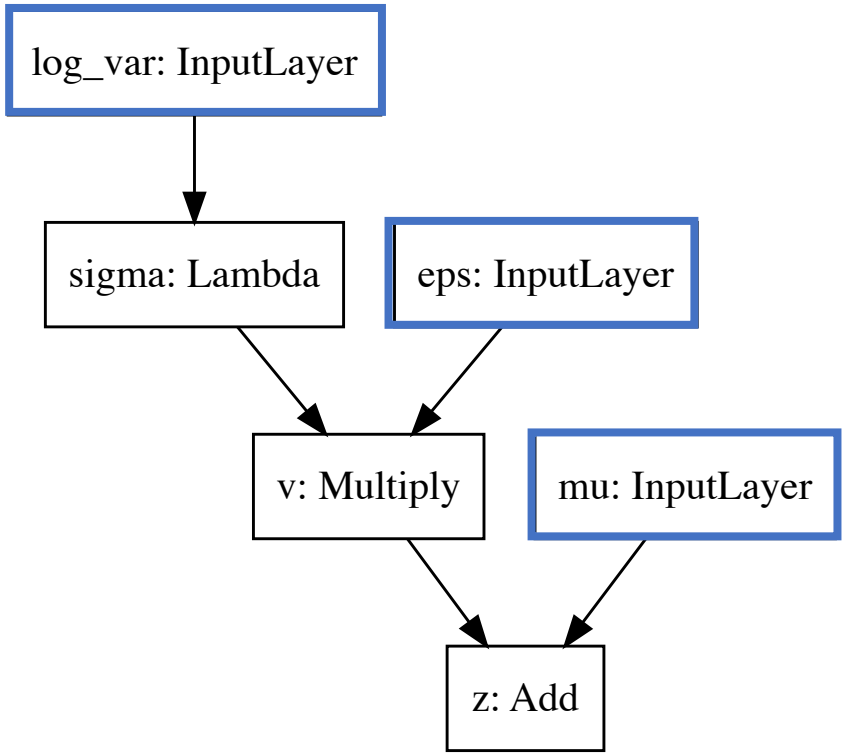
2. The Sampling Network

```
from keras.layers import Lambda, Multiply, Add
from keras import backend as K

# inputs
mu = Input(shape=(shape_z,), name='mu')
log_var = Input(shape=(shape_z,), name='log_var')
eps = Input(shape=(shape_z,), name='eps')

# layers
sigma = Lambda(lambda t: K.exp(.5*t), name='sigma')(log_var)
v = Multiply(name='v')([sigma, eps])
z = Add(name='z')([mu, v])

# model
sampling = models.Model(inputs=[mu, log_var, eps],
                        outputs=z,
                        name='sampling')
```



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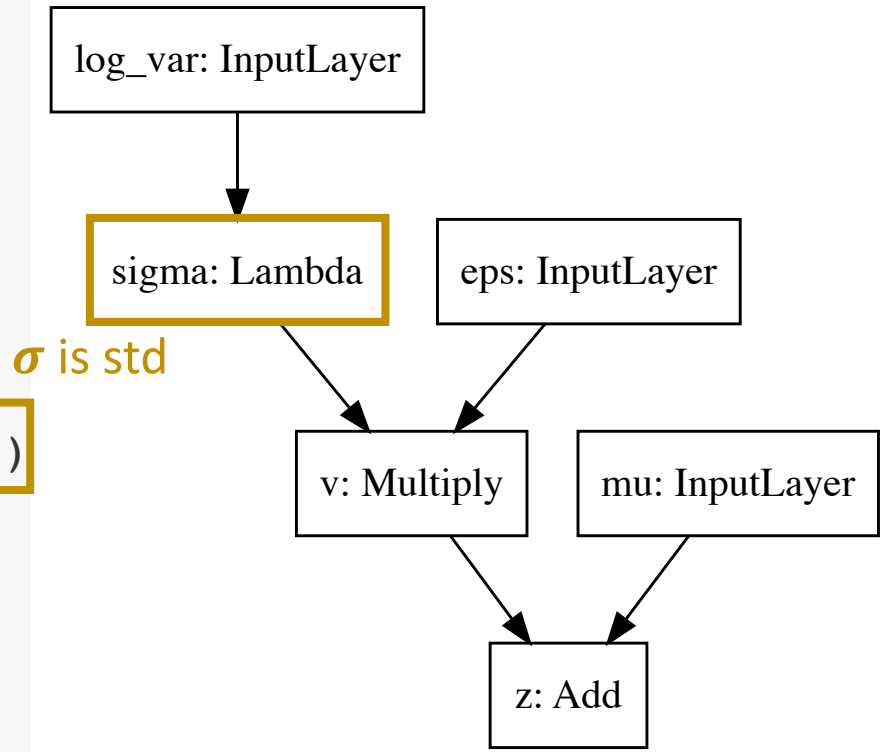

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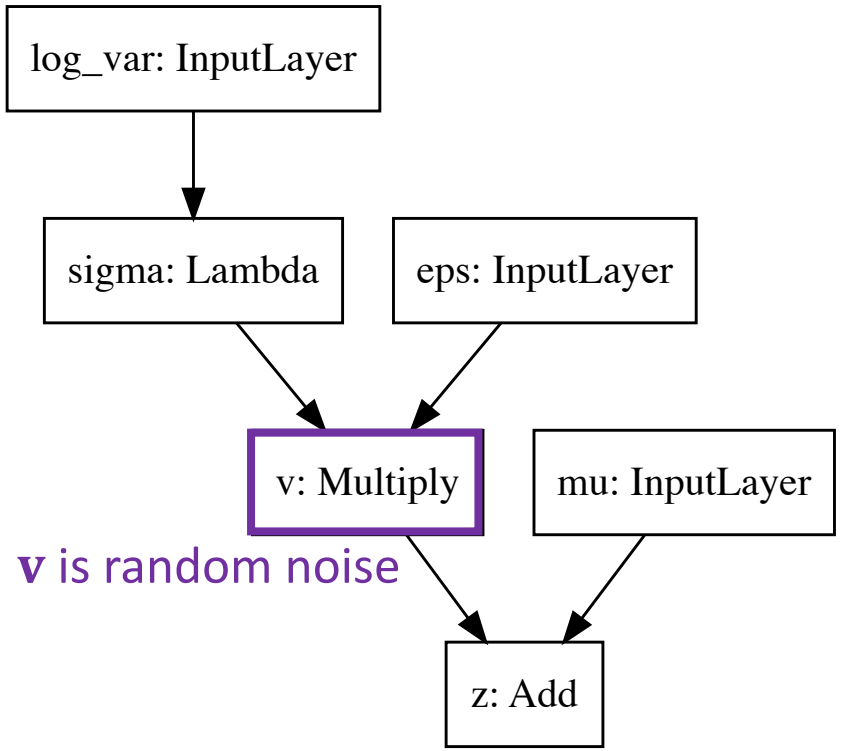

v is random noise

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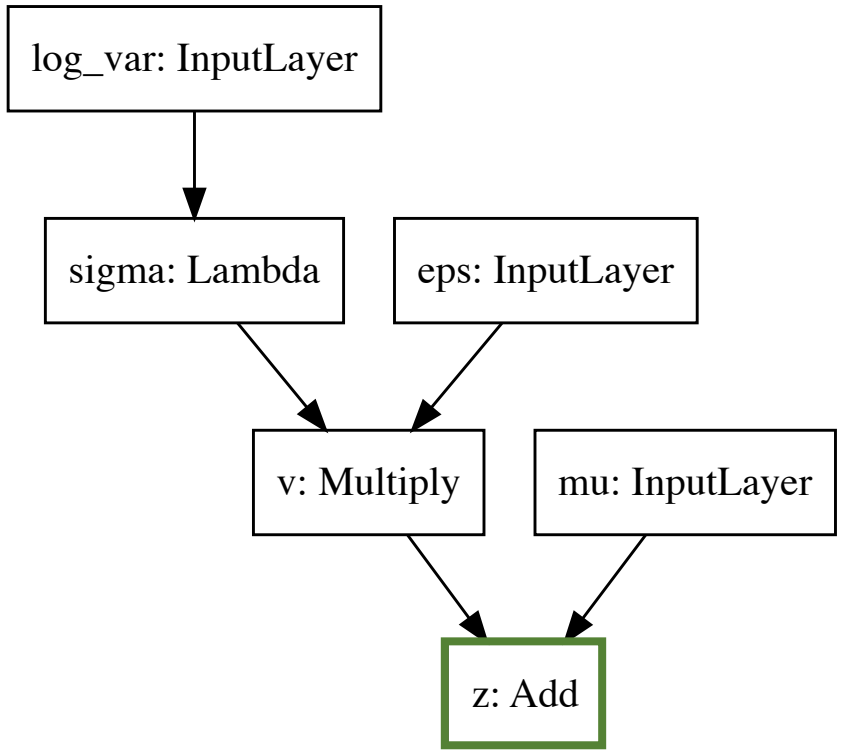
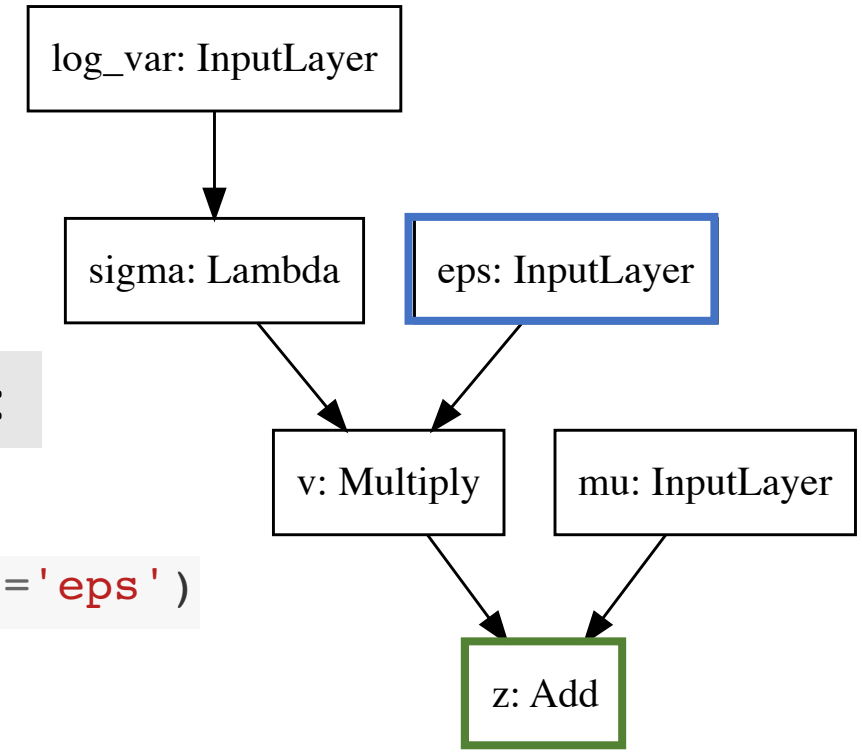
                        name='sampling')
```



z is the sampled latent vector

2. The Sampling Network

Question: Where is the random sampling $\epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I}_k)$?

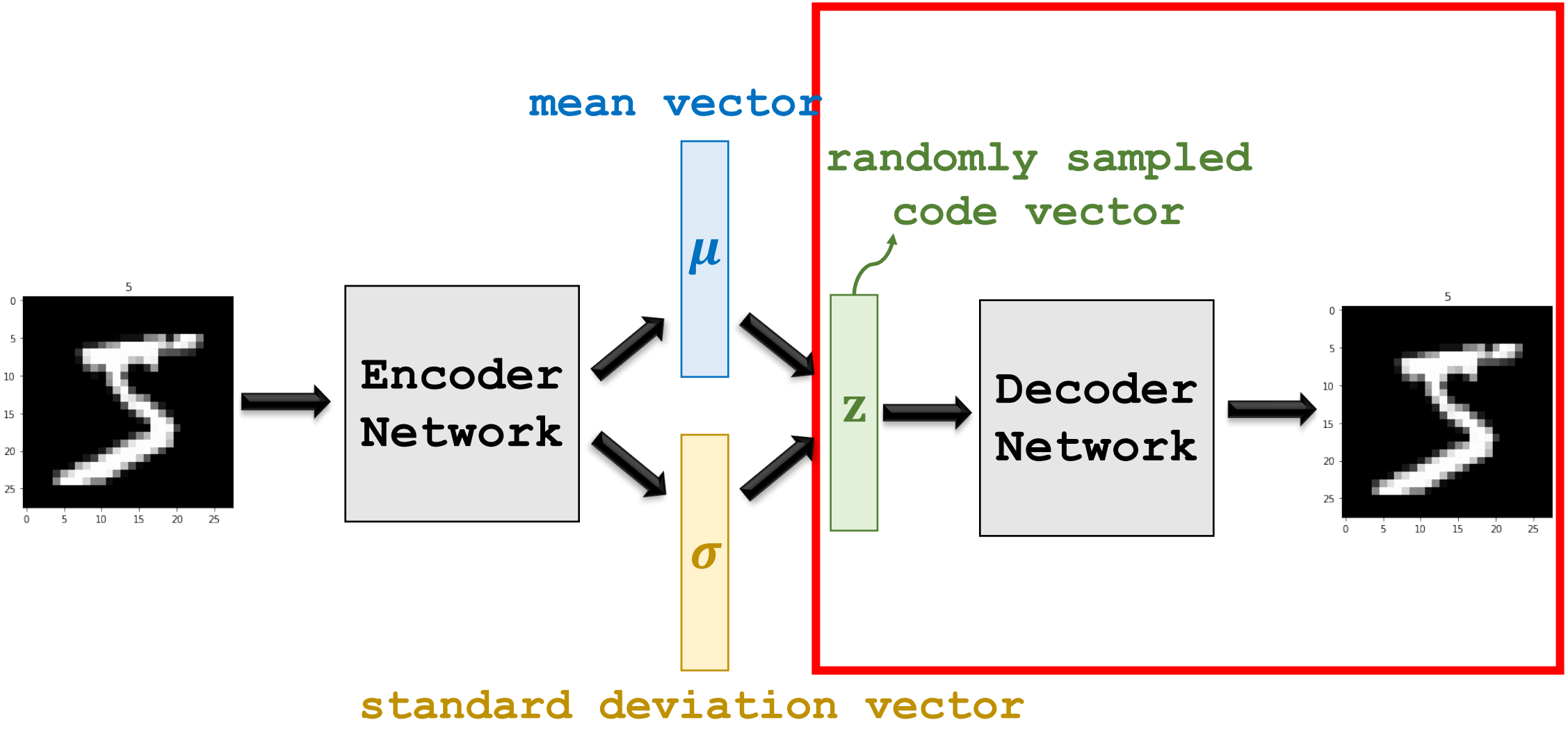


During training, set the input layer "eps" to the following code:

```
eps = Input(tensor=K.random_normal(shape=(n, shape_z)), name='eps')
```

z is the sampled latent vector

3. The Decoder Network



3. The Decoder Network

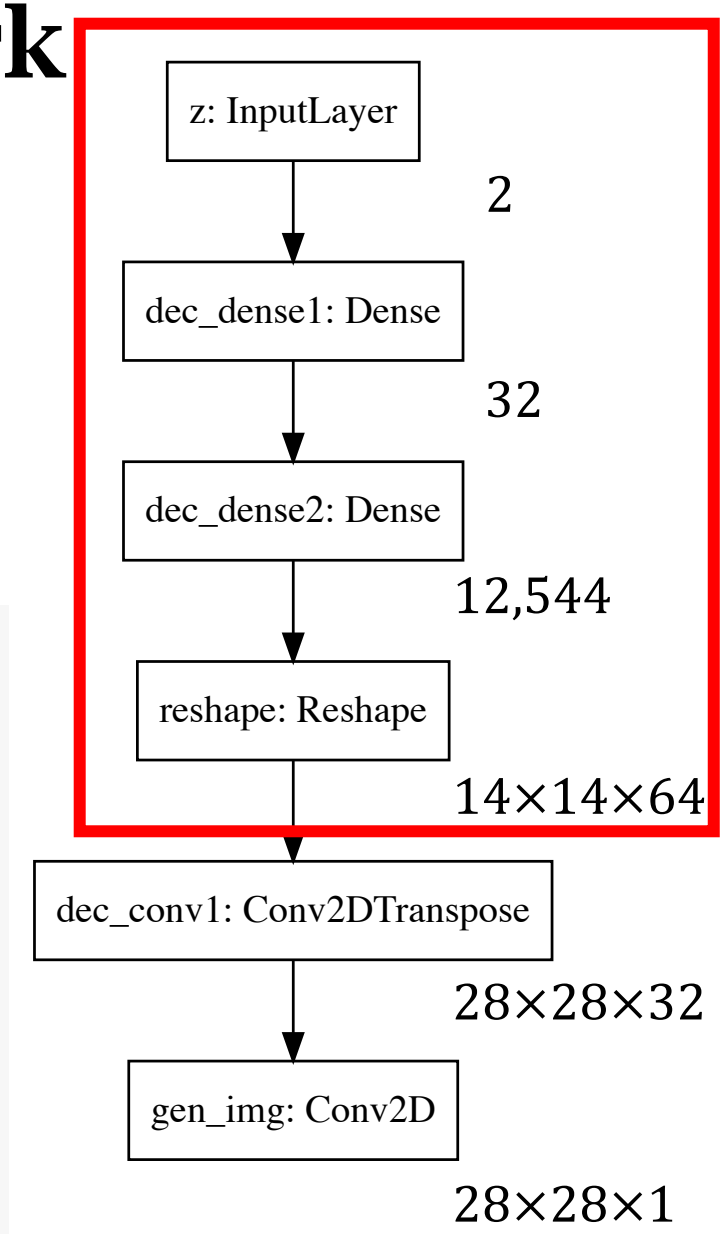
```
from keras import backend as K
import numpy

shape_before_flattening = K.int_shape(enc_conv_out4)[1:]
shape_after_flattening = numpy.prod(shape_before_flattening)
```

```
from keras.layers import Dense, Reshape, Conv2D, Conv2DTranspose

dec_dense1 = Dense(32, activation='relu', name='dec_dense1')
dec_dense2 = Dense(shape_after_flattening,
                   activation='relu', name='dec_dense2')
dec_reshape = Reshape(shape_before_flattening, name='reshape')

z = Input(shape=(shape_z,), name='z')
dec_dense_out1 = dec_dense1(z)
dec_dense_out2 = dec_dense2(dec_dense_out1)
dec_reshape_out = dec_reshape(dec_dense_out2)
```

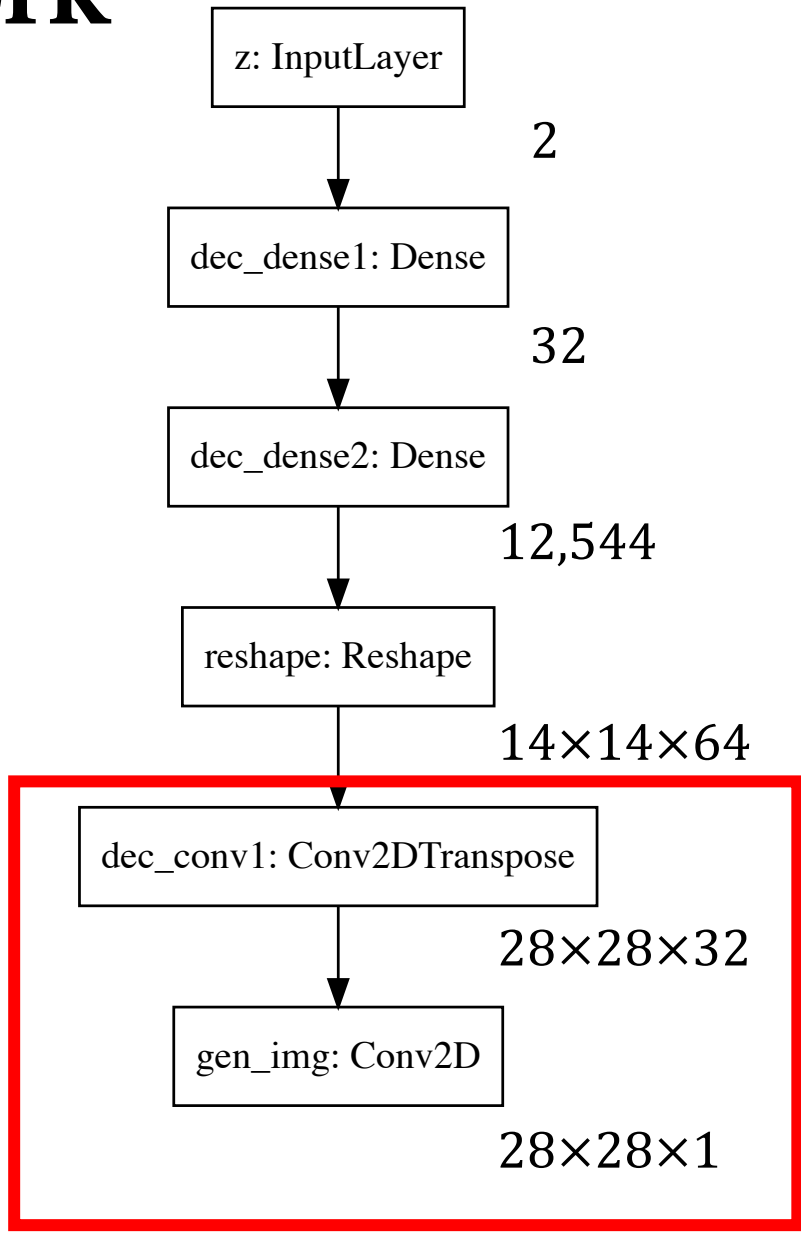


3. The Decoder Network

```
dec_conv1 = Conv2DTranspose(32, 3, padding='same',
                            activation='relu',
                            strides=(2, 2),
                            name='dec_conv1')
dec_conv2 = Conv2D(1, 3, padding='same',
                   activation='relu',
                   name='gen_img')

dec_conv_out1 = dec_conv1(dec_reshape_out)
gen_img = dec_conv2(dec_conv_out1)
```

```
decoder = models.Model(inputs=z,
                       outputs=gen_img,
                       name='decoder')
```



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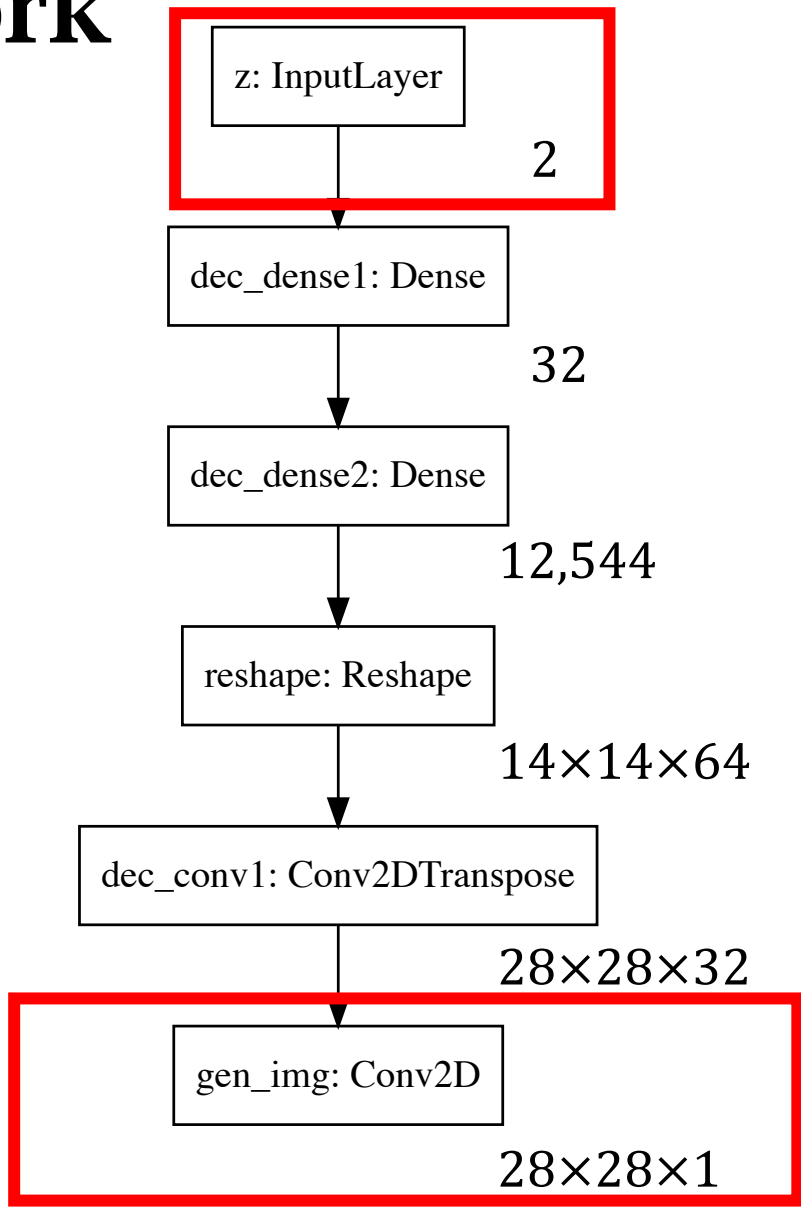
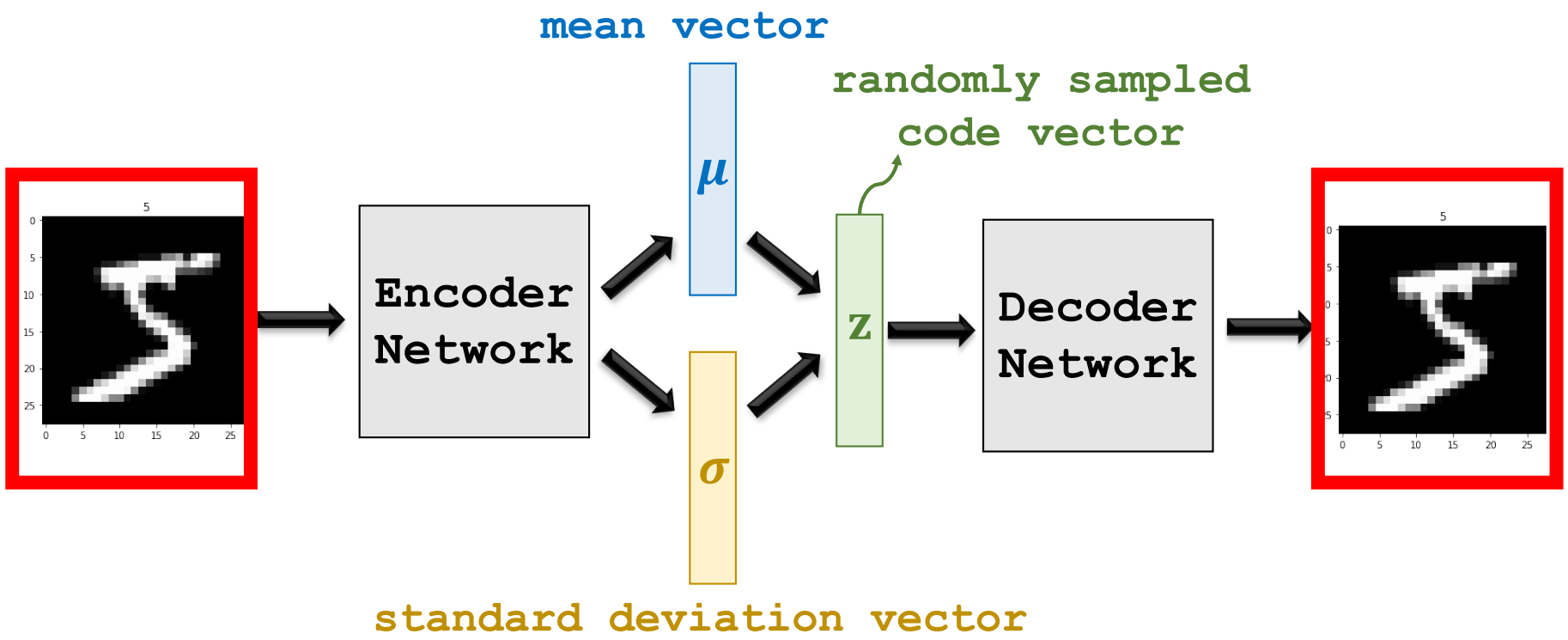


Loss Functions

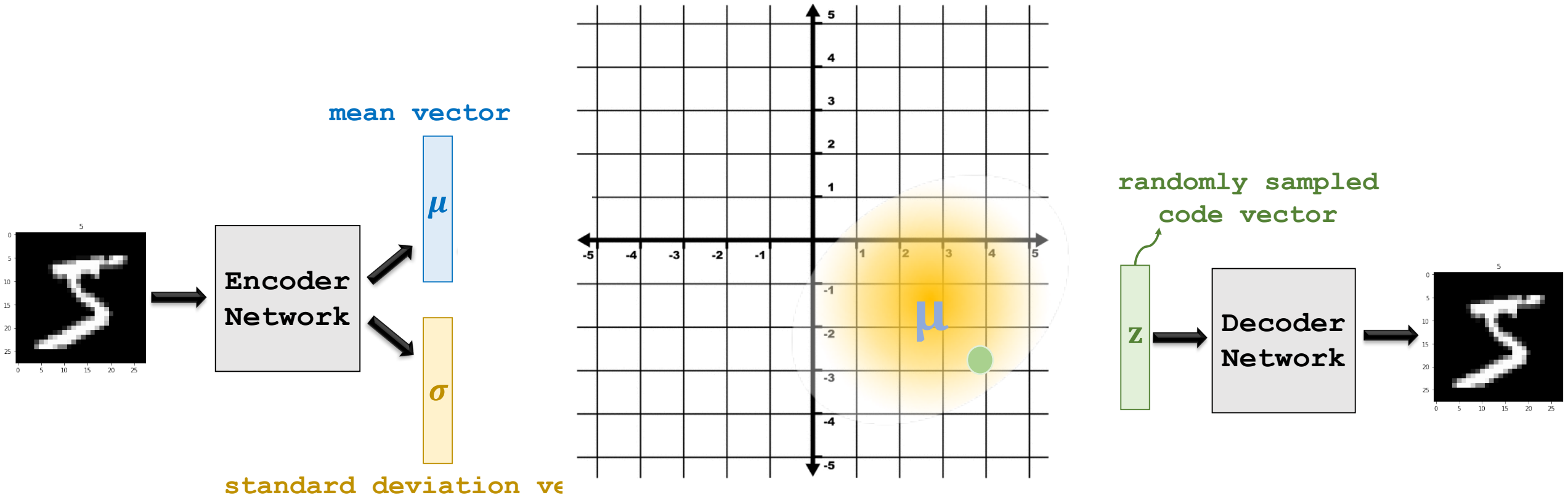
Generation Loss

- `GenLoss = dist(input_img, generated_img)`.
- E.g., the ℓ_2 distance, the cross-entropy, etc.



A problem with generation loss

Difficulty: The encoder network will learn an std vector $\sigma \to 0$.



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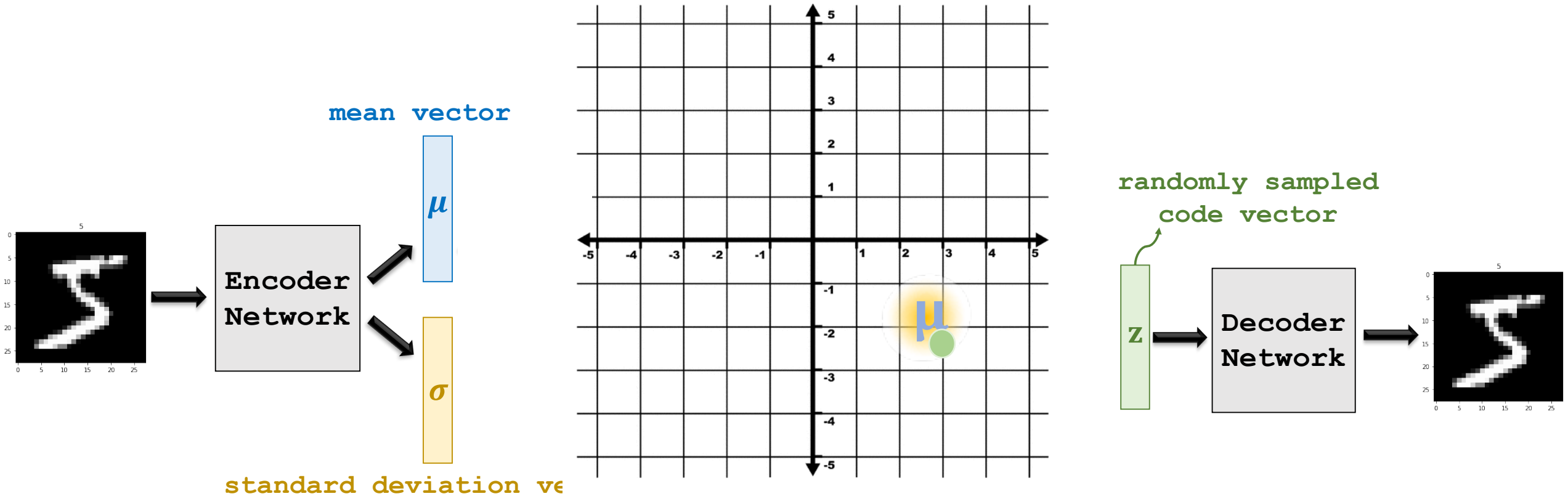
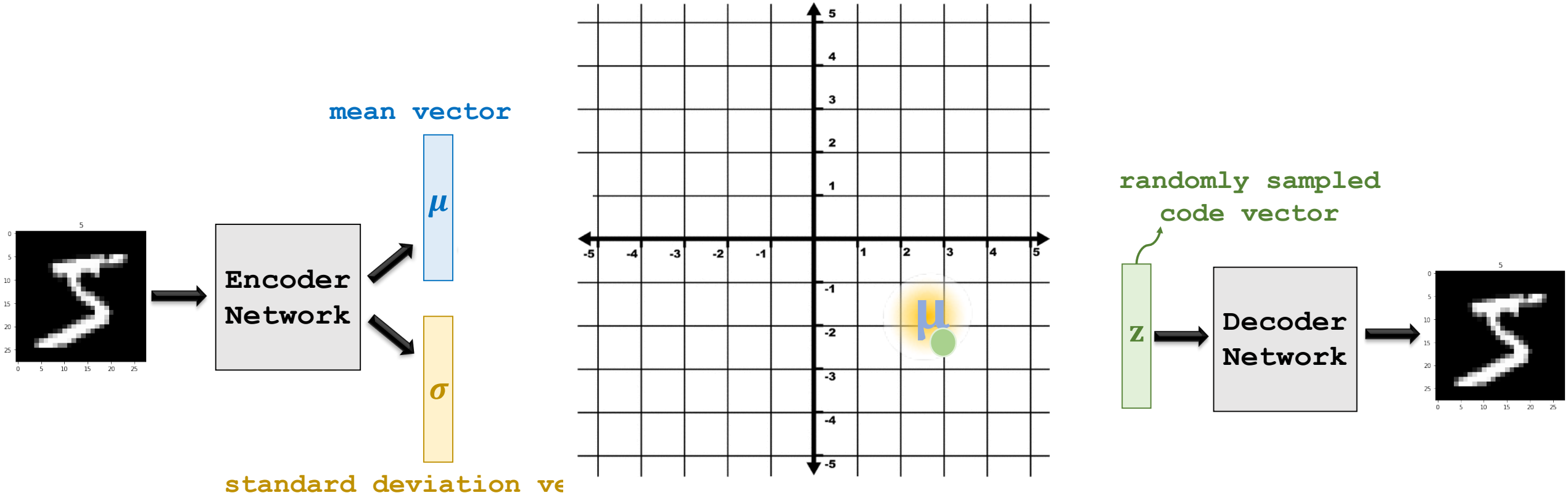


A problem with generation loss

Difficulty: The encoder network will learn an std vector $\sigma \to 0$. (Why?)

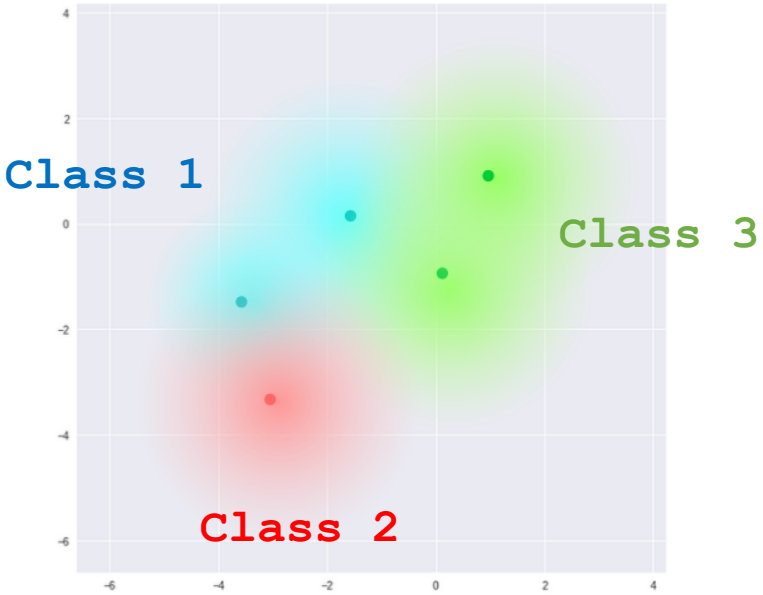
- Minimize `GenLoss` ➔ encourage z close to μ ➔ encourage small σ.
- VAE degrades to the standard AE (VAE with $\sigma = 0$ is exactly AE).



A problem with generation loss

Difficulty: By minimizing generation loss, VAE becomes standard AE.

Dots are code vectors ($\boldsymbol{\mu}$); shadows illustrate std ($\boldsymbol{\sigma}$).



What we hope to learn.

What we actually learn by minimizing `GenLoss`.

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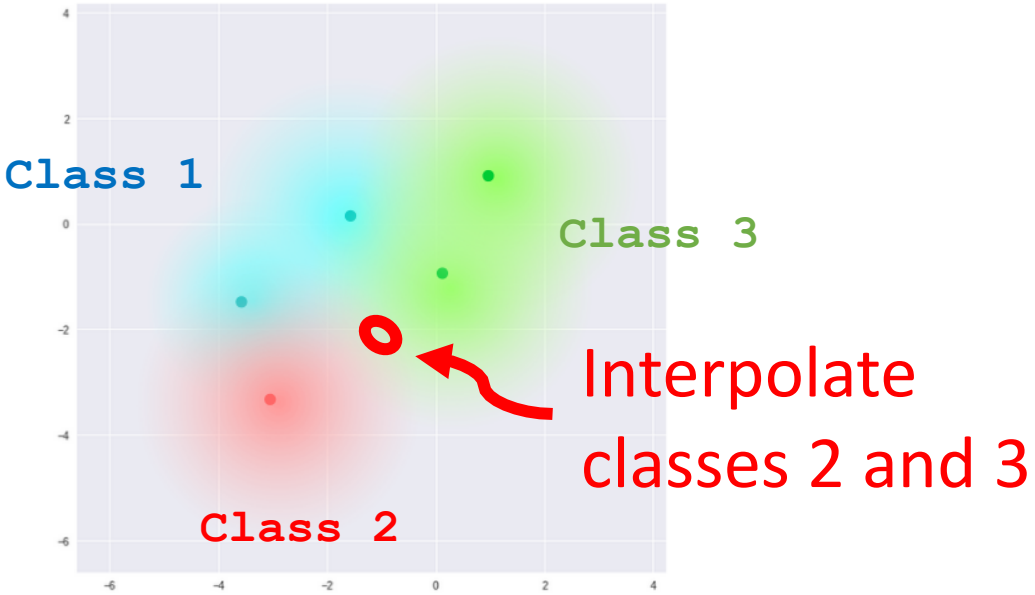

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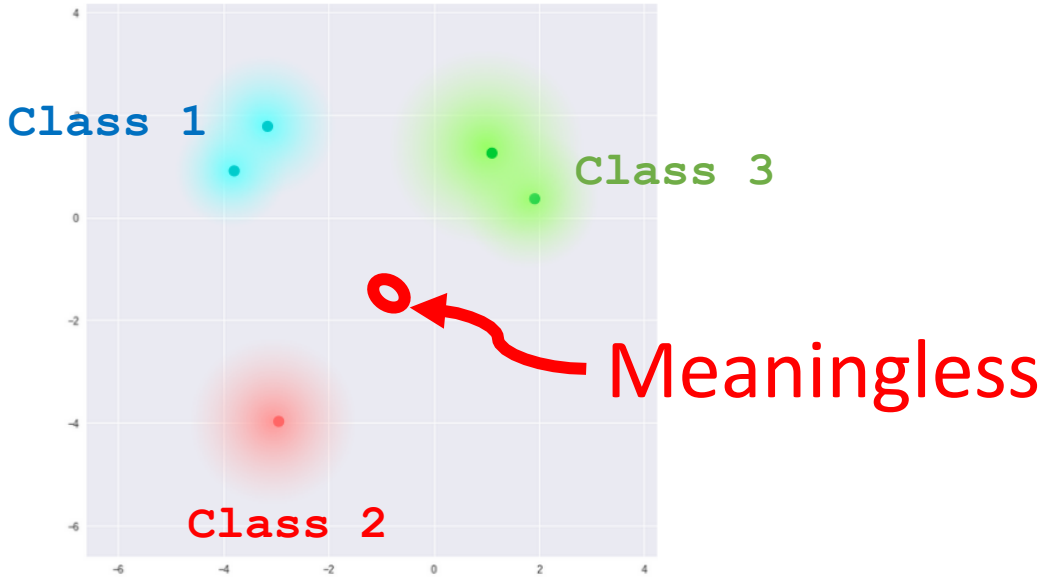

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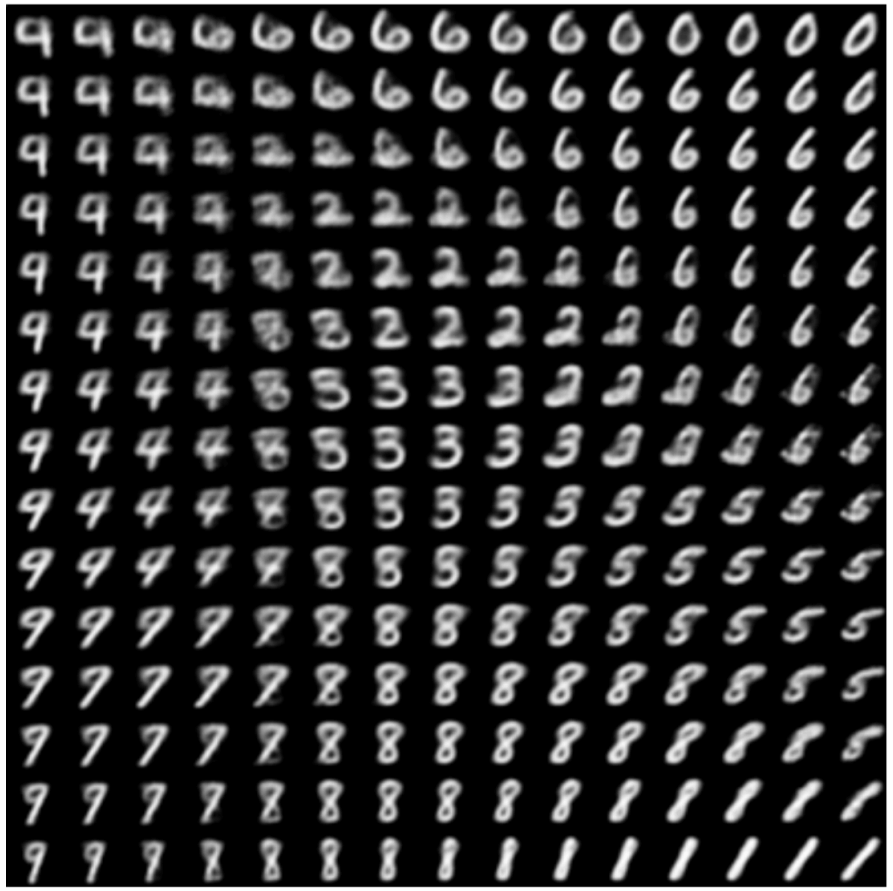

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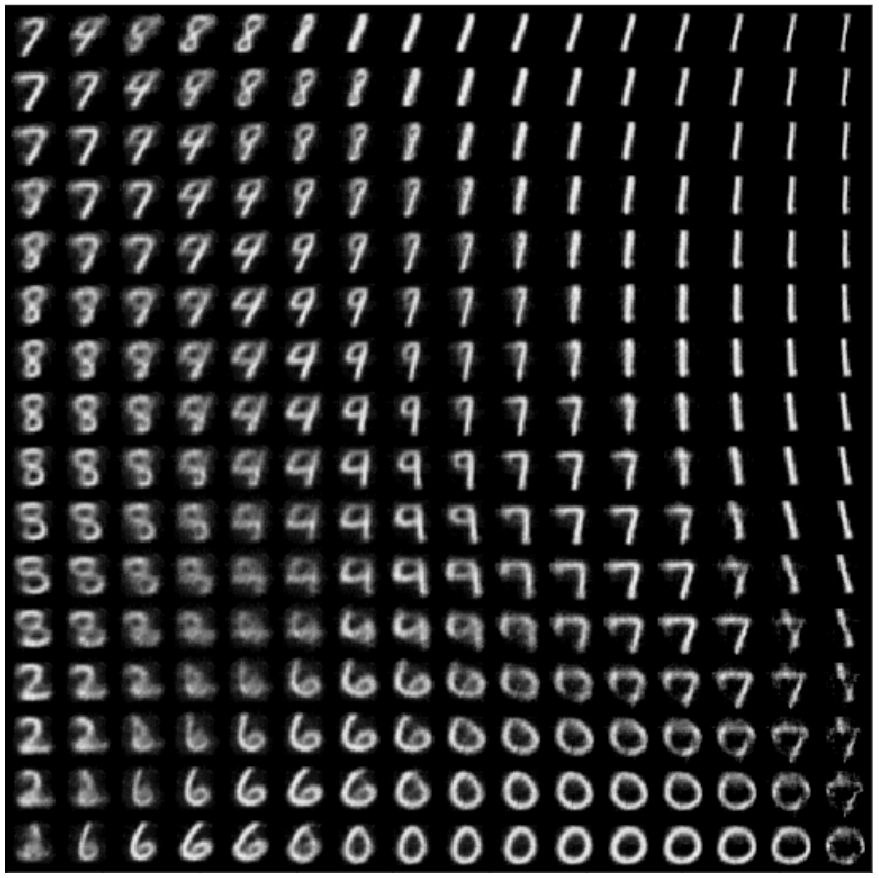

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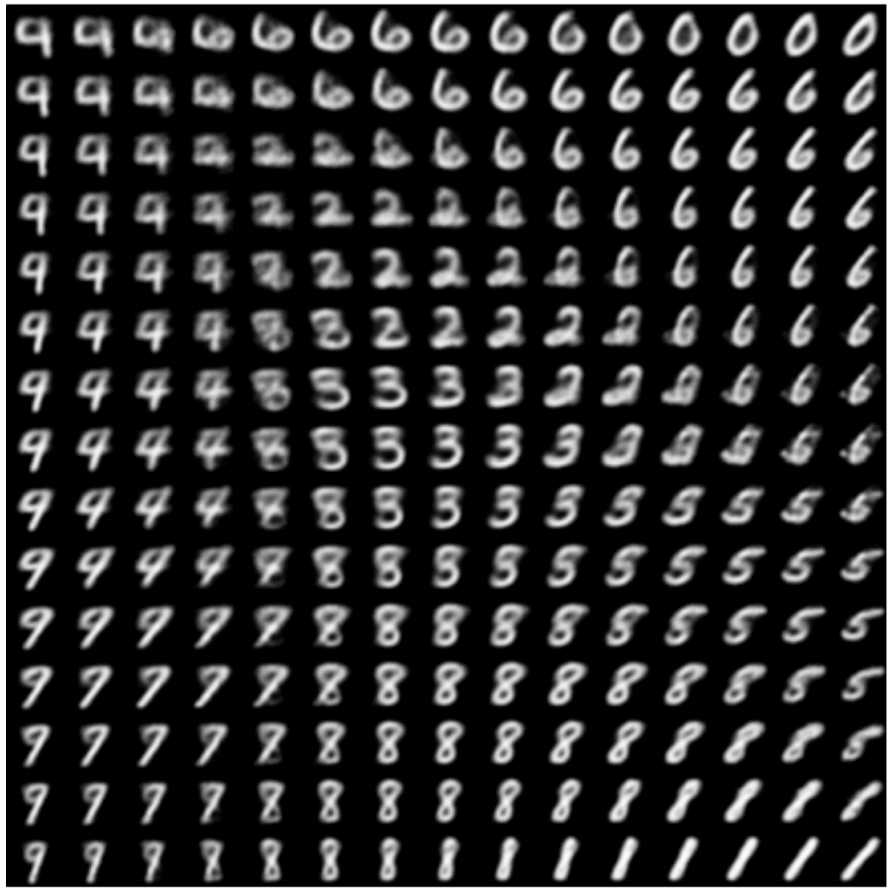

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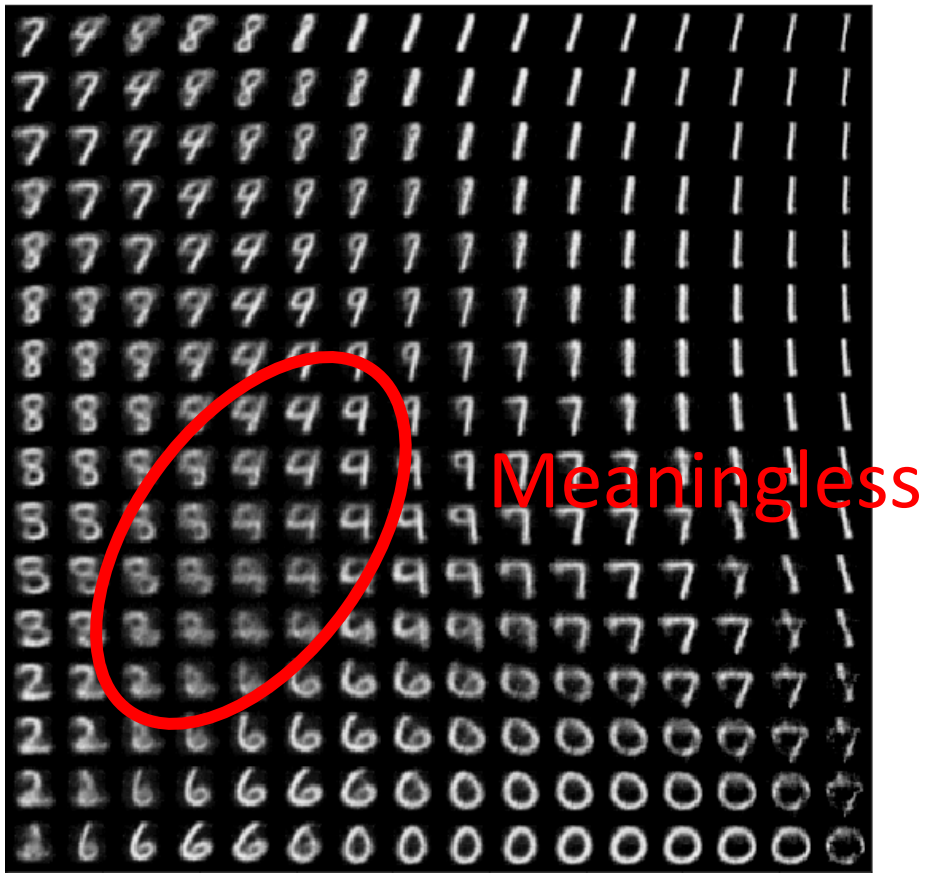
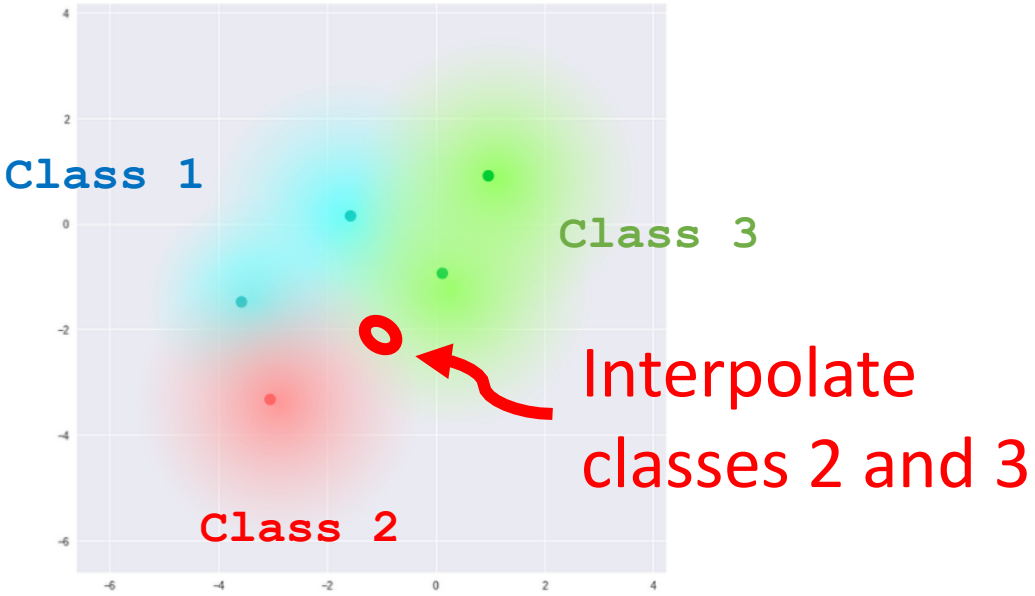


What we actually learn by minimizing `GenLoss`.

KL Loss

Idea: Encourage the distribution of z to be unit Gaussian.

- There will be a probability density everywhere around the origin.
- ➔ No more void.



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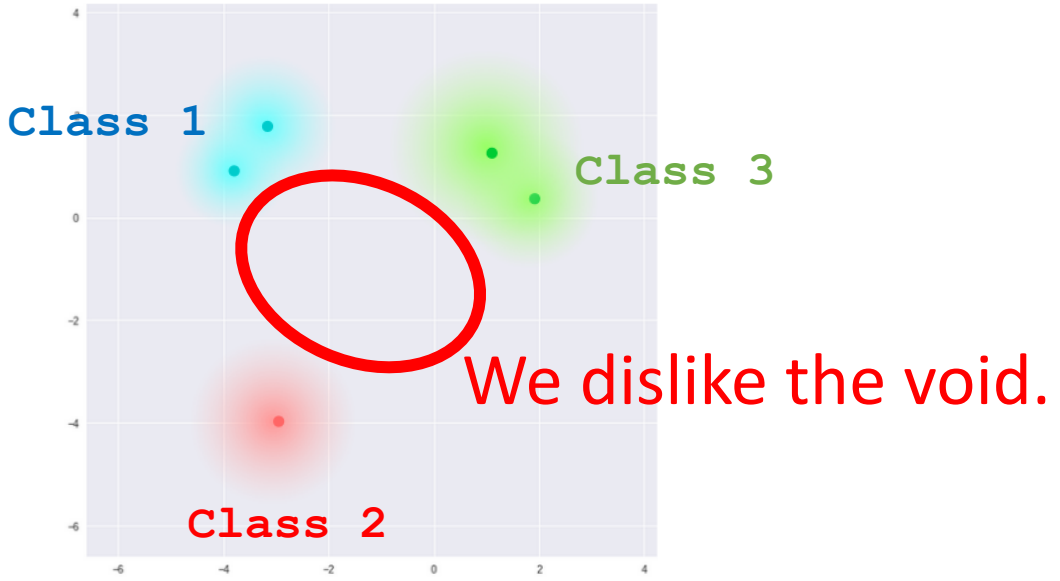

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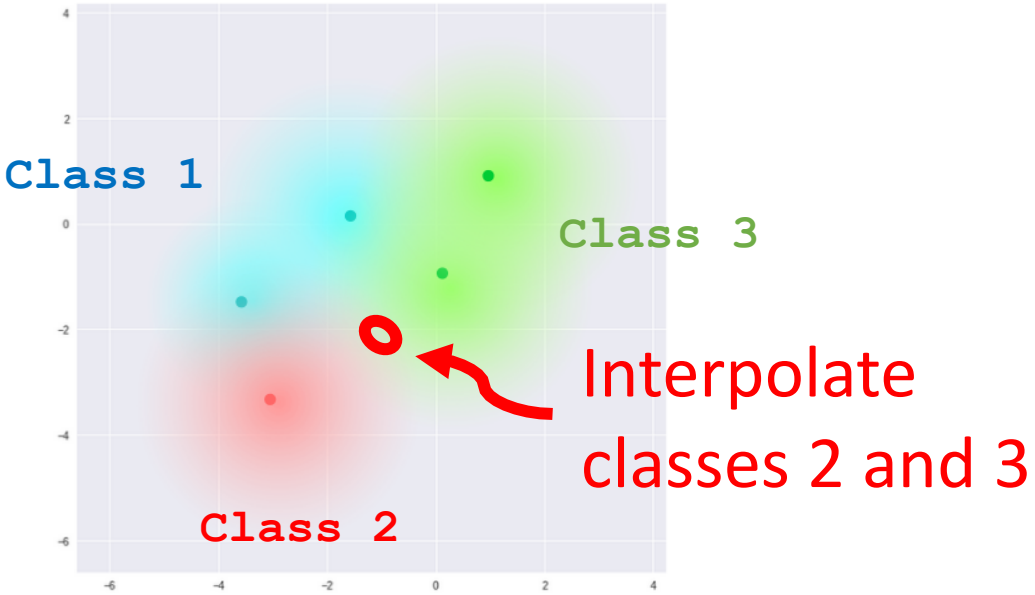
KL Loss

Idea: Encourage the distribution of $\mathbf{z}$ to be unit Gaussian.

- $\text{KLLoss} = D_{\text{KL}}\left(p(\mathbf{z}) \;||\; \mathcal{N}(0, \mathbf{I})\right)$



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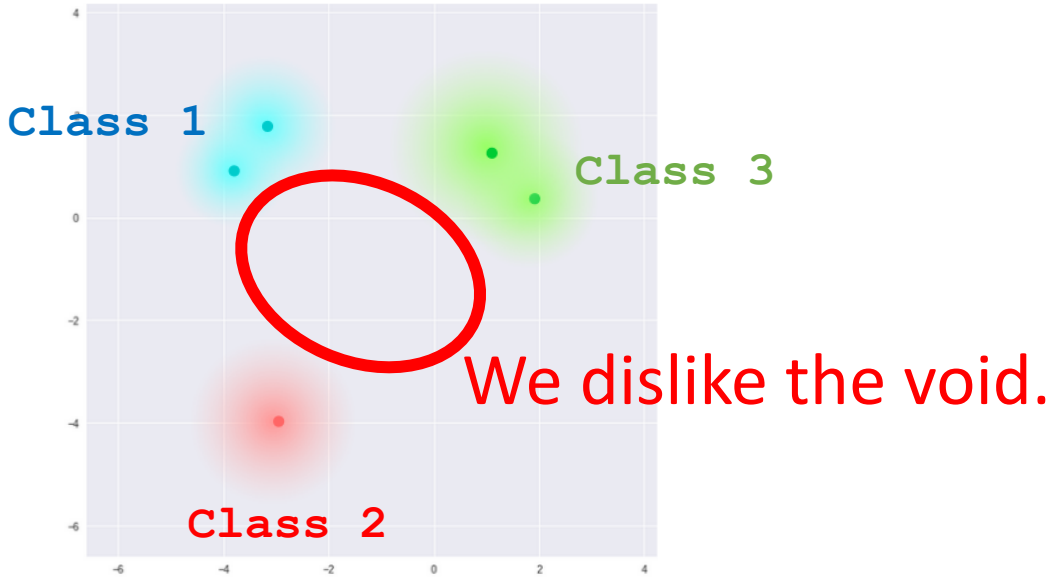

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- $\text{KLLoss} = D_{\text{KL}}\left(p(\mathbf{z}) \;||\; \mathcal{N}(0, \mathbf{I})\right)$

- $\text{Loss} = \text{GenLoss} + \lambda \cdot \text{KLLoss}$

Generation Loss + KL Loss

- Generation loss:

$$\text{GenLoss} = \text{dist}(\text{input\_img}, \text{output\_img}).$$

```
l = keras.metrics.binary_crossentropy(input_img, output_img)
```

Generation Loss + KL Loss

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```

- KL loss:

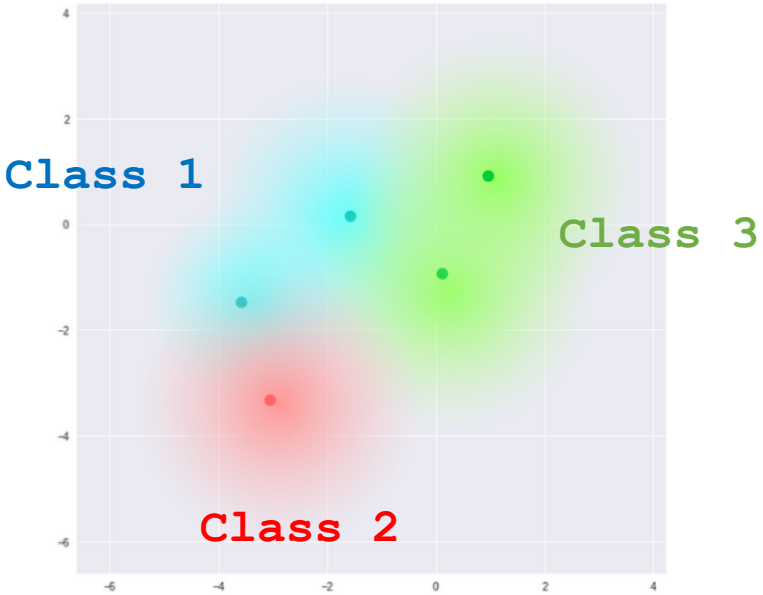
$$\text{KLLoss} = D_{\text{KL}}\left(p(\mathbf{z}) \;||\; \mathcal{N}(0, \mathbf{I})\right)$$

```
l = -0.5 * K.mean(1 + log_var - K.square(mu) - K.exp(log_var), axis=-1)
```

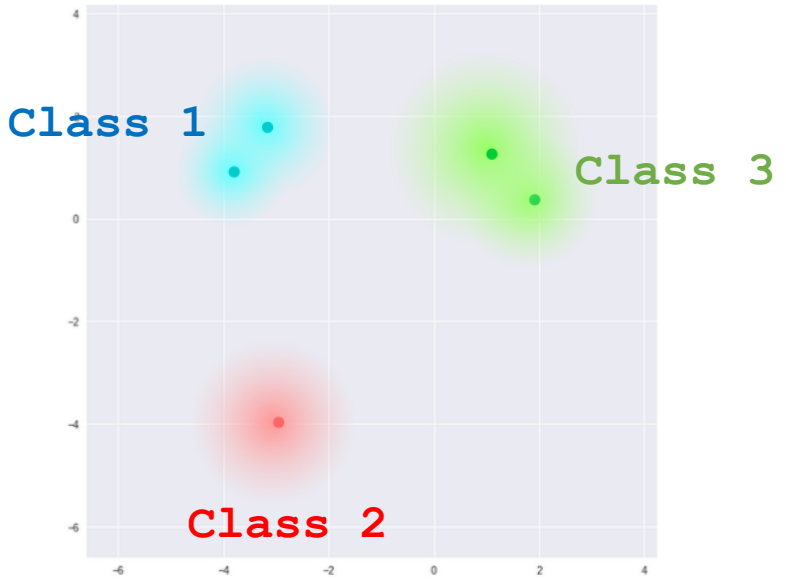
Another interpretation:

- Encourage the variance σ^2 to be big. (Avoid vanishing variance.)
- Pull the mean $\boldsymbol{\mu}$ towards the origin. (Avoid isolated clusters.)

Generation Loss + KL Loss



What we hope to learn.



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```
l = -0.5 * K.mean(1 + log_var - K.square(mu) - K.exp(log_var), axis=-1)
```

- $\text{Loss} = \text{GenLoss} + 10^{-3} \cdot \text{KLLoss}$

Take `input_img` and `output_img` as inputs

tuning hyper-parameter

Take `log_var` and `mu` as inputs

Implement loss function

```
import keras
from keras import backend as K

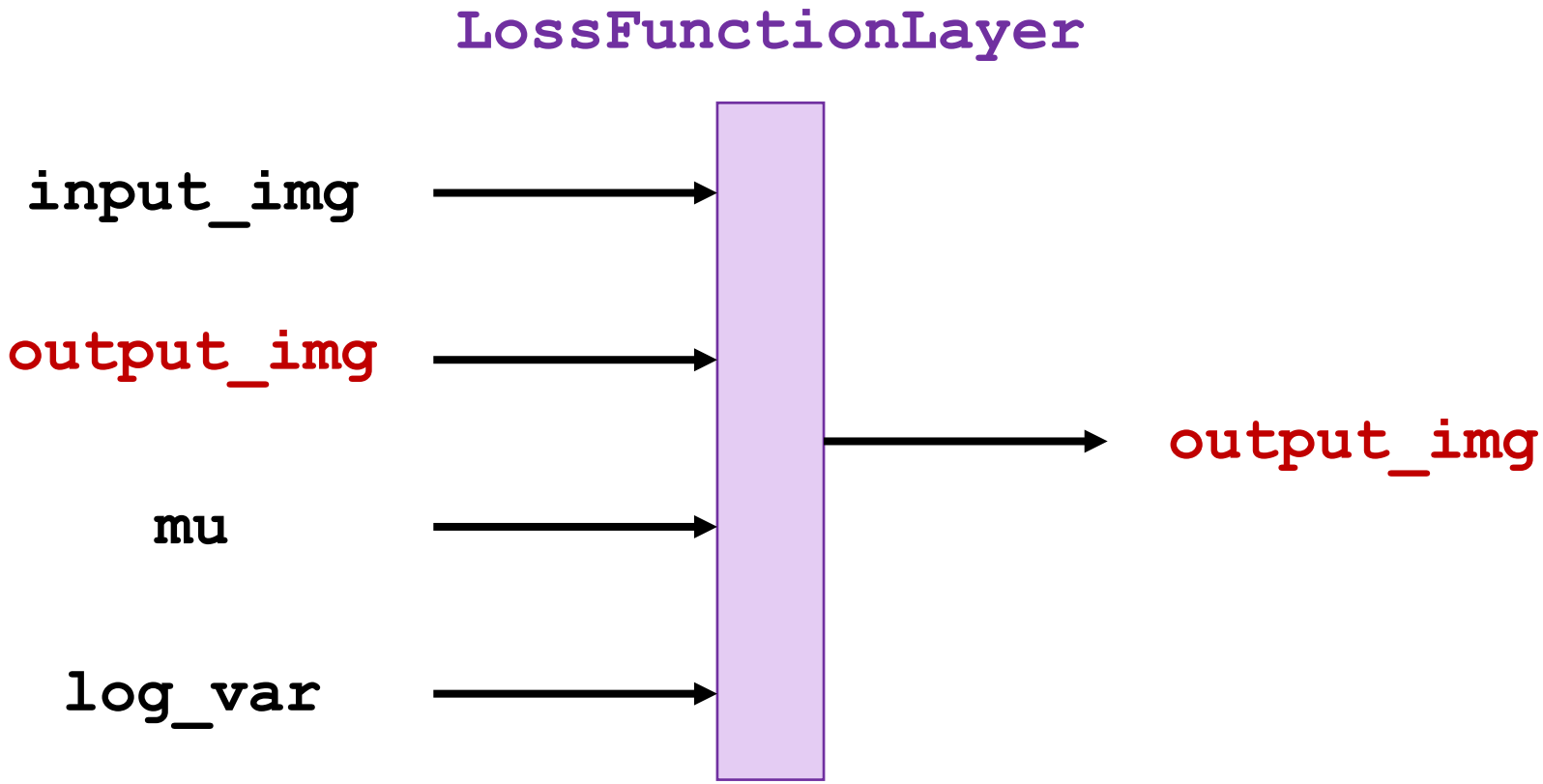
class LossFunctionLayer(keras.layers.Layer):
    param = 1E-3

    def kl_loss(self, mu, log_var):
        l = -0.5 * K.mean(1 + log_var - K.square(mu) - K.exp(log_var), axis=-1)
        return self.param * K.mean(l)

    def gen_loss(self, input_img, output_img):
        l = keras.metrics.binary_crossentropy(input_img, output_img)
        return K.mean(l)

    def call(self, inputs):
        input_img, output_img, mu, log_var = inputs
        loss1 = self.gen_loss(input_img, output_img)
        loss2 = self.kl_loss(mu, log_var)
        self.add_loss(loss1+loss2, inputs=inputs)
        return output_img
```

Implement loss function



Also compute the loss function.

- **input_img** and **output_img** for **GenerationLoss**.
- **mu** and **log_var** for **KLtLoss**.

Training

Connect the modules

We have defined 4 modules:

- **Encoder:** `[input_img]` → `[mu, log_var]`
- **Sampling:** `[mu, log_var, eps]` → `[z]`
- **Decoder:** `[z]` → `[output_img]`
- **LossFunctionLayer:** `[input_img, output_img, mu, log_var]` → `[output_img]`

```
input_img = Input(shape=(28,28,1), name='input_img')
n = K.shape(input_img)[0]
eps = Input(tensor=K.random_normal(shape=(n, shape_z)), name='eps')
```

Connect the modules

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- **Encoder:** [input_img] → [mu, log_var]
- **Sampling:** [mu, log_var, eps] → [z]
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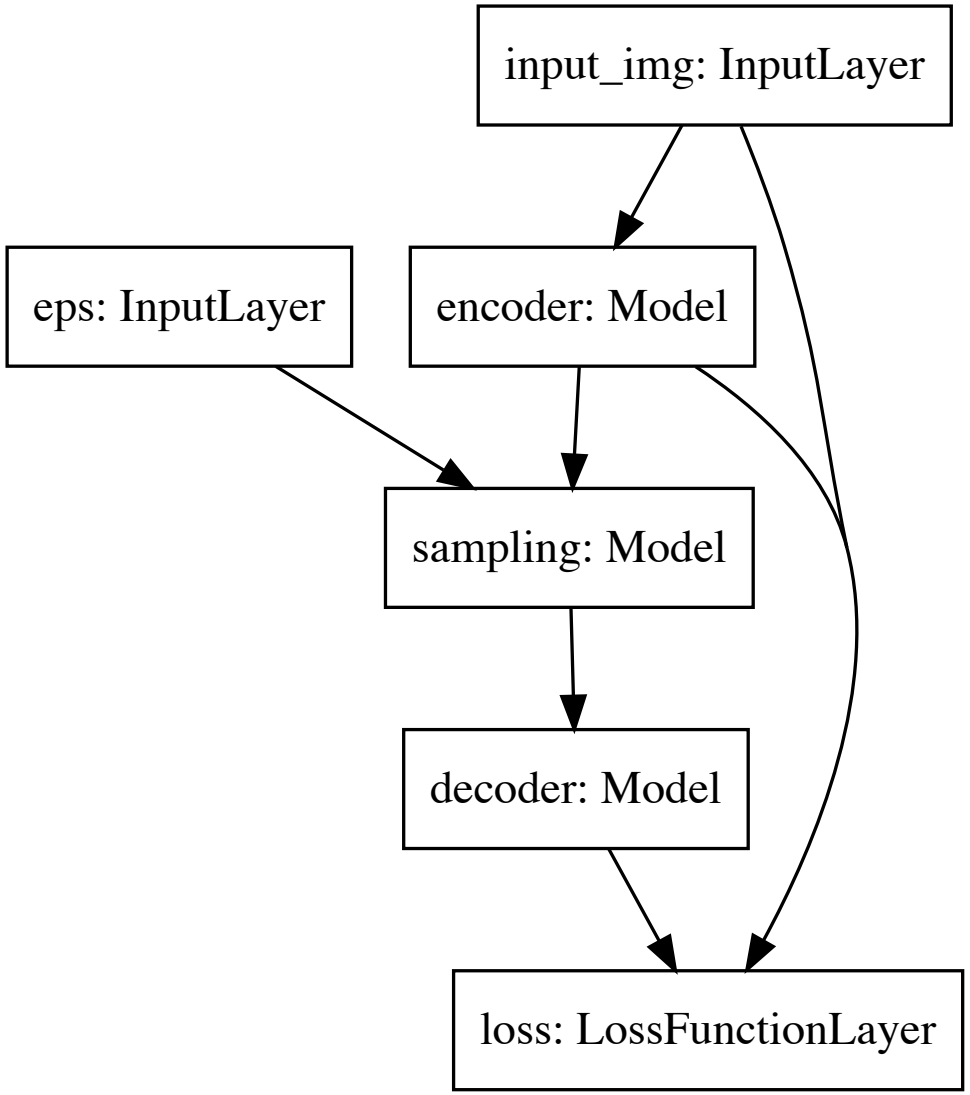
```
input_img = Input(shape=(28,28,1), name='input_img')
n = K.shape(input_img)[0]
eps = Input(tensor=K.random_normal(shape=(n, shape_z)), name='eps')

mu, log_var = encoder(input_img)
z = sampling([mu, log_var, eps])
output_img = decoder(z)
output_img = LossFunctionLayer(name='loss')([input_img, output_img, mu, log_var])
model = models.Model(inputs=[input_img, eps], outputs=output_img)
```

Connect the modules



Train the model on MNIST dataset

```
history = model.fit(
    x_train,
    None,
    shuffle=True,
    epochs=50,
    batch_size=128,
    validation_data=(x_test, None)
)
```

```
Train on 60000 samples, validate on 10000 samples
Epoch 1/50
60000/60000 [==============================] - 231s 4ms/step - loss: 0.6717 - val_loss: 0.2194
Epoch 2/50
60000/60000 [==============================] - 251s 4ms/step - loss: 0.2139 - val_loss: 0.2083
Epoch 3/50
60000/60000 [==============================] - 299s 5ms/step - loss: 0.2066 - val_loss: 0.2096
    ⋮
Epoch 49/50
60000/60000 [==============================] - 240s 4ms/step - loss: 0.1839 - val_loss: 0.1859
Epoch 50/50
60000/60000 [==============================] - 233s 4ms/step - loss: 0.1837 - val_loss: 0.1858
```

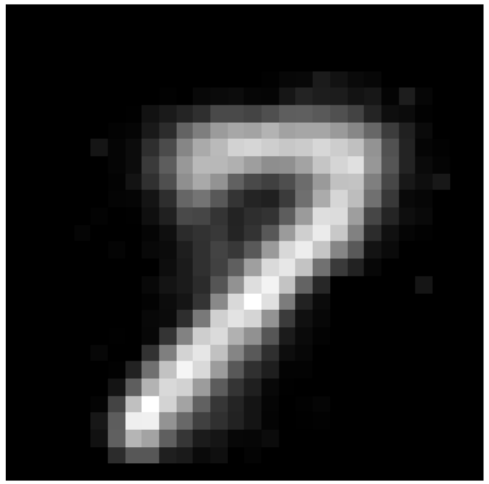
Visualize code vectors

arbitrary 2-dim vector

map the 2-dim vector to a 28×28 image

```
z_sample = np.array([0.1, 0.2]).reshape((1, 2))
x_decoded = decoder.predict(z_sample)[0].reshape((28, 28))

fig = plt.figure(figsize=(6, 6))
plt.imshow(x_decoded, cmap='gray')
plt.axis('off')
plt.show()
```

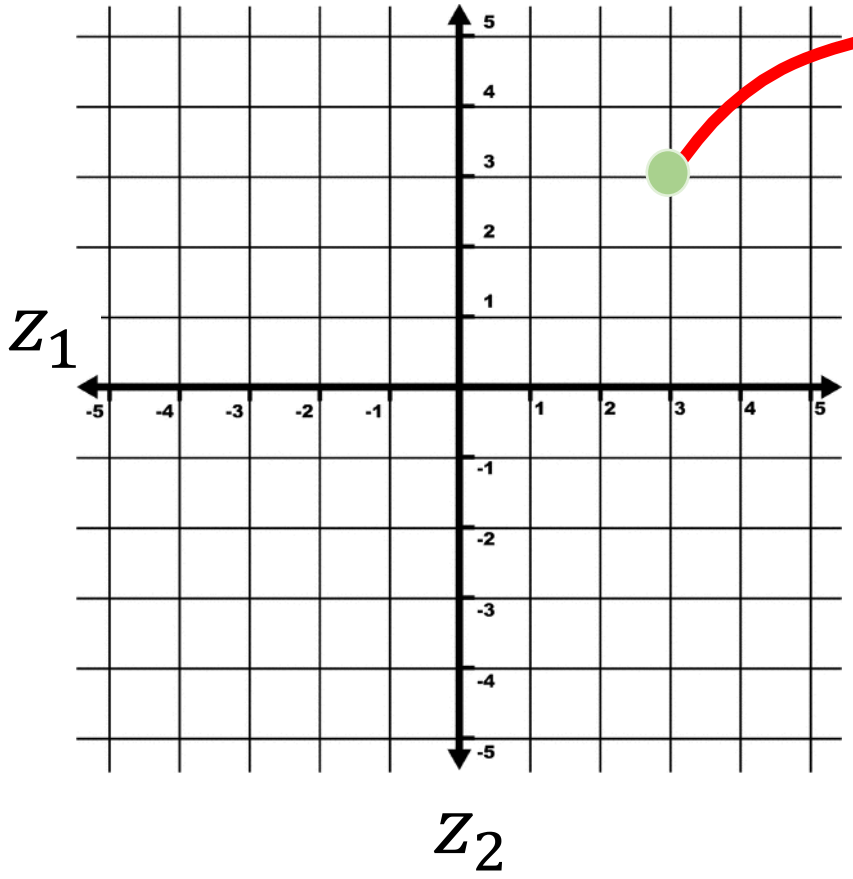


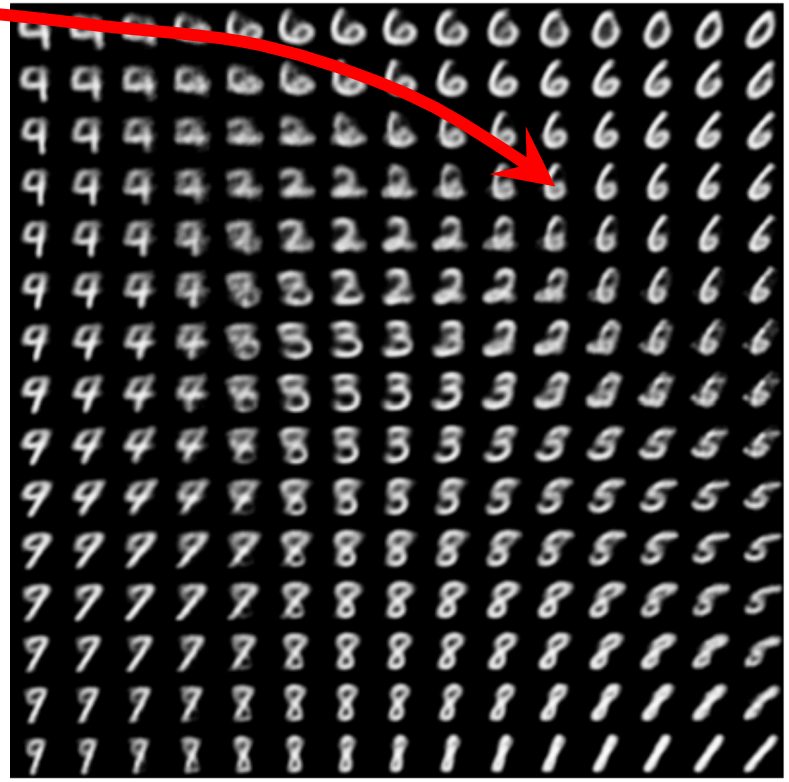
Visualize code vectors

Code vectors

Images

Decoder





Summary

Variational Autoencoder (VAE)

- VAE = AE + probability tricks.
- The decoder network behaves like a continuous function.

Variational Autoencoder (VAE)

- VAE = AE + probability tricks.
- The decoder network behaves like a continuous function.
- Loss = Generation Loss + $\lambda \cdot$ KL Loss.
- Application: edit images via editing code vectors.
  - Average faces.
  - Add smile.