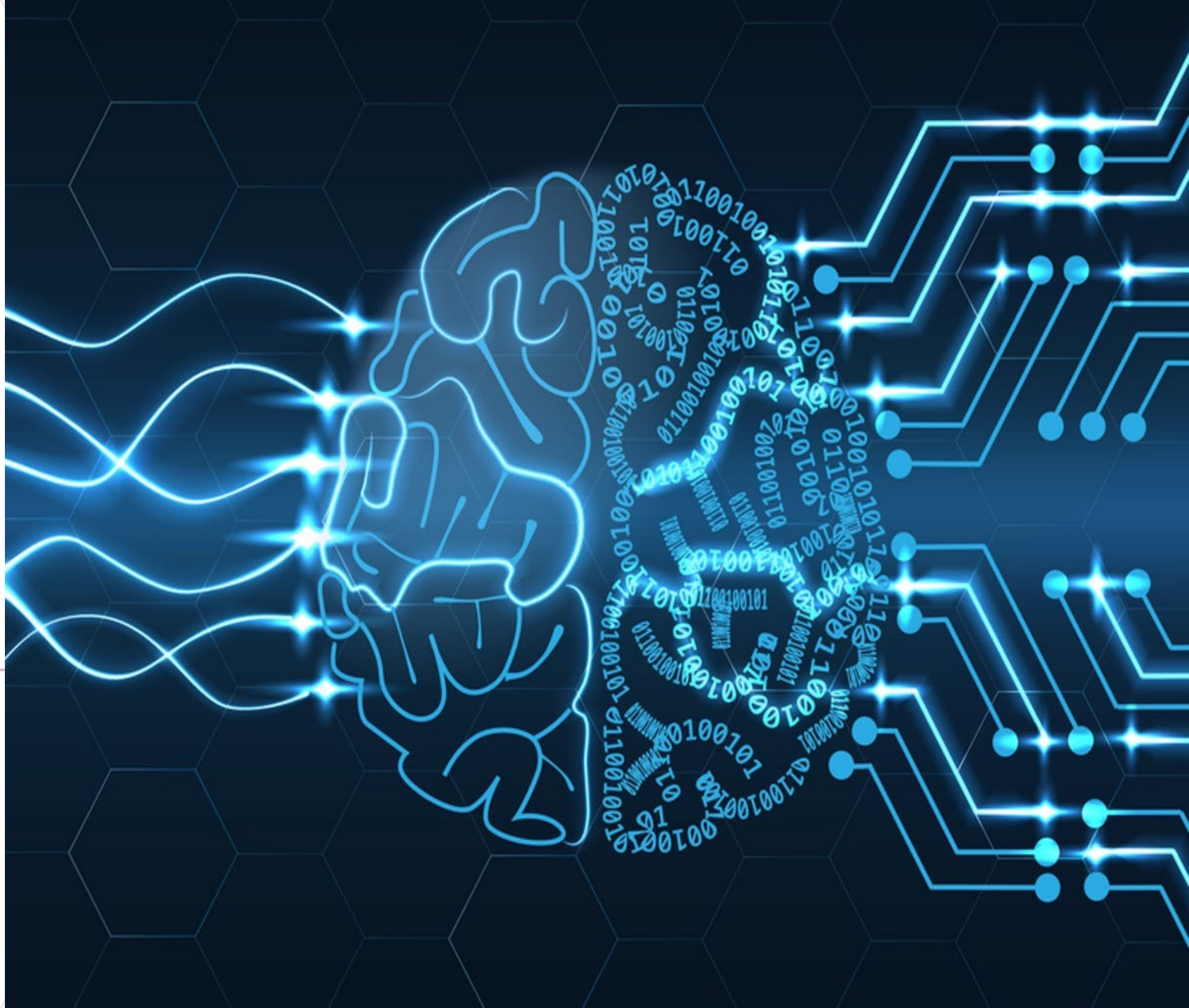


# VAE

SNU SCSC

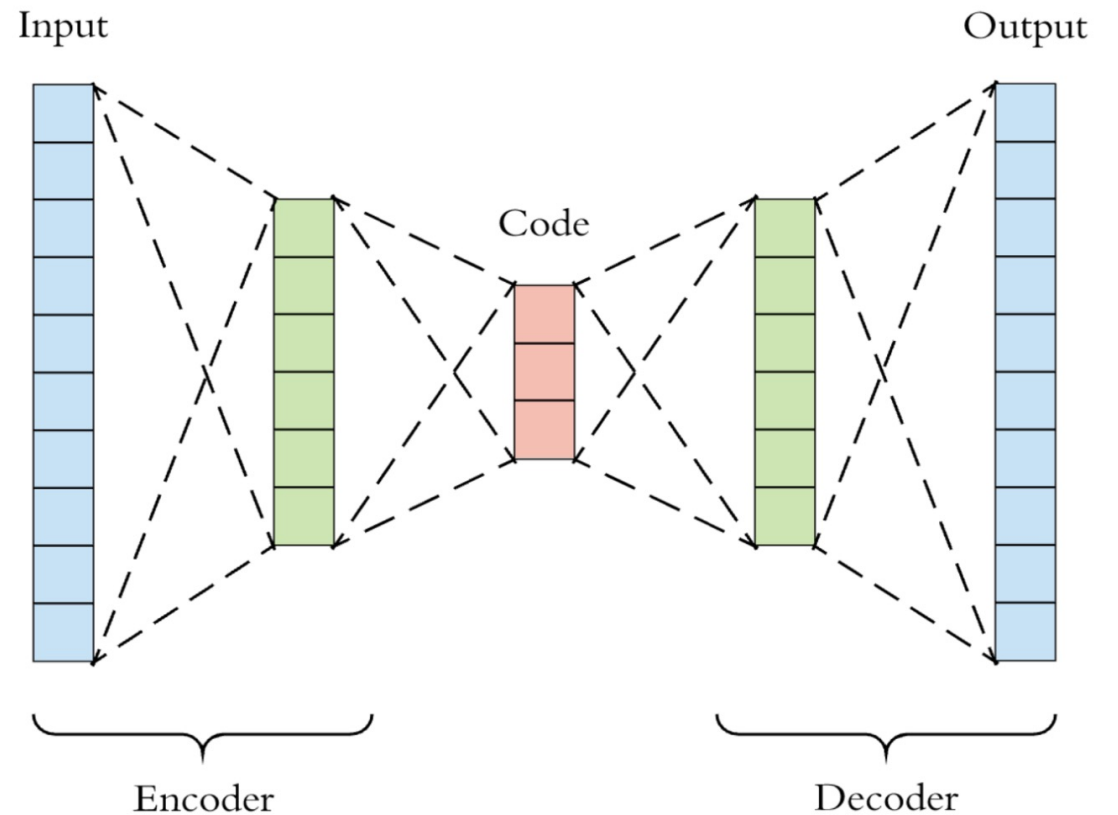
Oct 11, 2022.

Seoyoung Lim

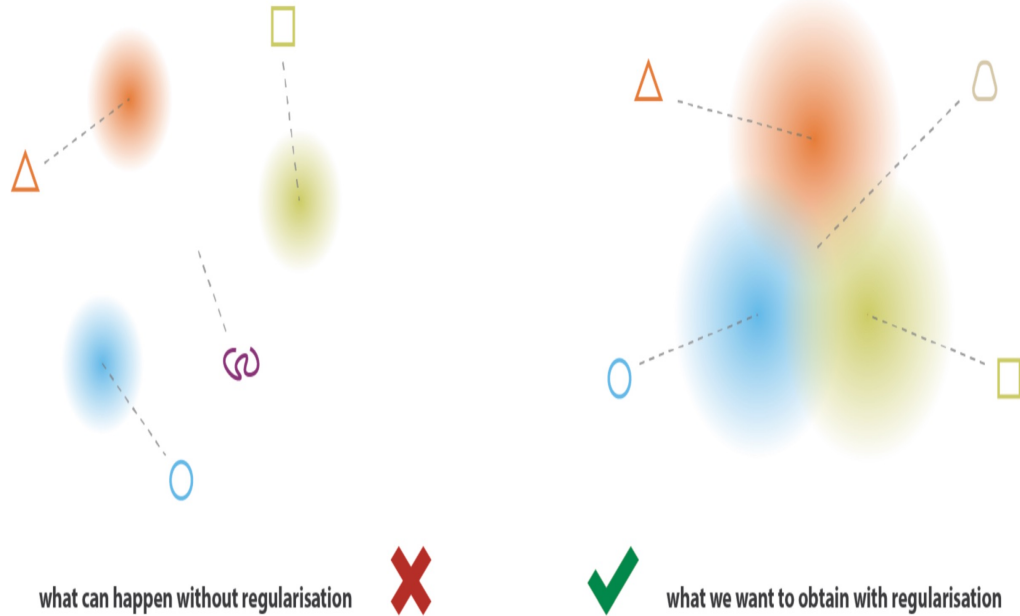


# Autoencoder – Traditional Autoencoder

- Encoder : Compresses the input data a latent – space representation.
- Decoder : Decoded the encoded data back to original dimension.



# Models – Why Variational AutoEncoder



- Traditional AutoEncoder Problem : the latent vectors (encoding) tends to be **irregular, unorganized, uninterpretable**

# Models – VAE(s)

Code

```
def _build_net(self):
    self.x_hat_tfph = tf.placeholder(tf.float32, shape=[None, *self.image_size], name='input_img')
    self.x_tfph = tf.placeholder(tf.float32, shape=[None, *self.image_size], name='target_img')
    self.keep_prob_tfph = tf.placeholder(tf.float32, name='keep_prob')
    self.z_in_tfph = tf.placeholder(tf.float32, shape=[None, self.flags.z_dim], name='latent_variable')

    # encoding
    mu, sigma = self.encoder(self.x_hat_tfph)
    # sampling by re-parameterization technique
    self.z = mu + sigma * tf.random_normal(tf.shape(mu), mean=0., stddev=1., dtype=tf.float32)

    # decoding
    y = self.decoder(self.z)
    self.y = tf.clip_by_value(y, 1e-8, 1 - 1e-8)
    sample_y = self.decoder(self.z_in_tfph, is_reuse=True)
    self.sample_y = tf.clip_by_value(sample_y, 1e-8, 1 - 1e-8)

    # loss
    marginal_likelihood = tf.reduce_sum(self.x_tfph * tf.log(self.y) + (1 - self.x_tfph) * tf.log(1 - self.y),
                                       [1, 2, 3])
    KL_divergence = 0.5 * tf.reduce_sum(tf.square(mu) + tf.square(sigma) - tf.log(1e-8 + tf.square(sigma)) - 1, 1)

    self.marginal_likelihood = tf.reduce_mean(marginal_likelihood)
    self.KL_divergence = tf.reduce_mean(KL_divergence)
    self.ELBO = self.marginal_likelihood - self.KL_divergence
    self.loss = - self.ELBO

    self.train_op = tf.train.AdamOptimizer(self.flags.learning_rate).minimize(self.loss)
```

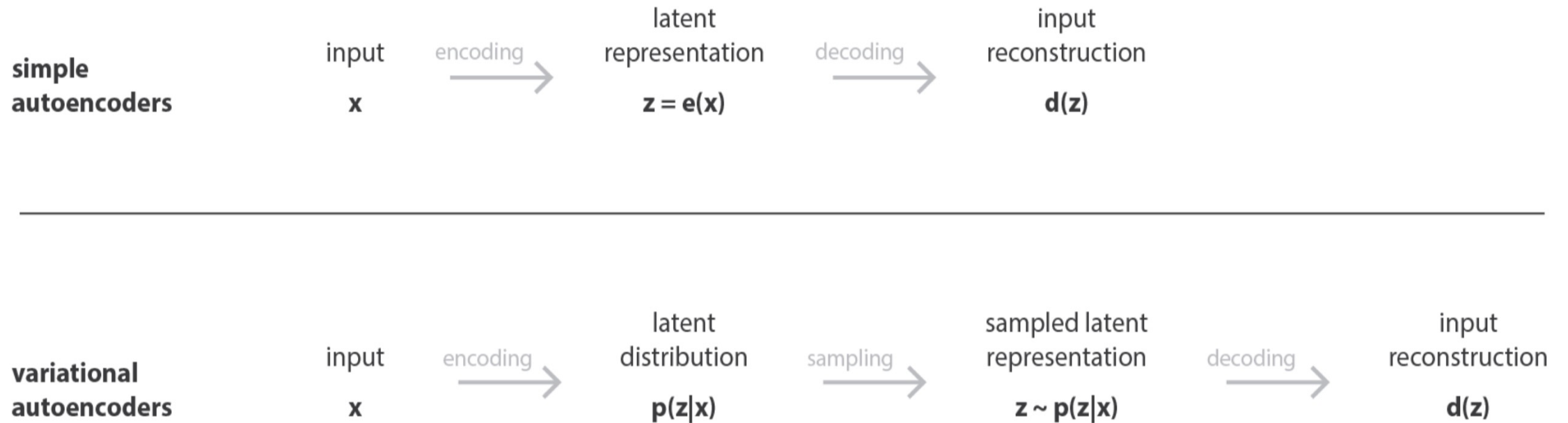
# Models – Loss

## MSE vs Cross Entropy

$$MSE = \frac{1}{n} \sum \left( \underbrace{y - \hat{y}}_{\substack{\text{The square of the difference} \\ \text{between actual and} \\ \text{predicted}}} \right)^2$$

$$E(\mathbf{w}) \equiv \frac{1}{2} \frac{1}{|D|} \sum_{d \in D} (y_d - \hat{y}_d)^2$$

# Models – VAE(s)



# Models – Latent Space

X : 이미지 -> Z : 잠재변수

잠재변수 Z의 예  
: 물체의 형상, 카메라 좌표, 광원의 정보  
( 남자, [10, 2, -4], white)



이미지 X



# Models – Generative Model

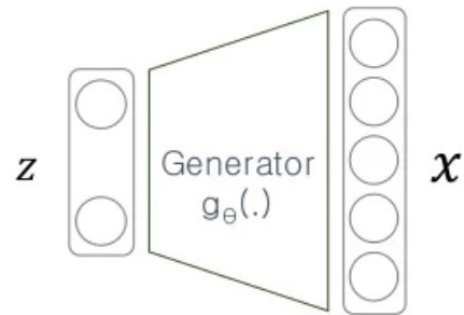


Training Examples



Density Estimation

Sampling



Latent Variable

Target Data

$$z \sim p(z)$$

Random variable

$$g_{\theta}(\cdot)$$

Deterministic function  
parameterized by  $\theta$

$$x = g_{\theta}(z)$$

Random variable

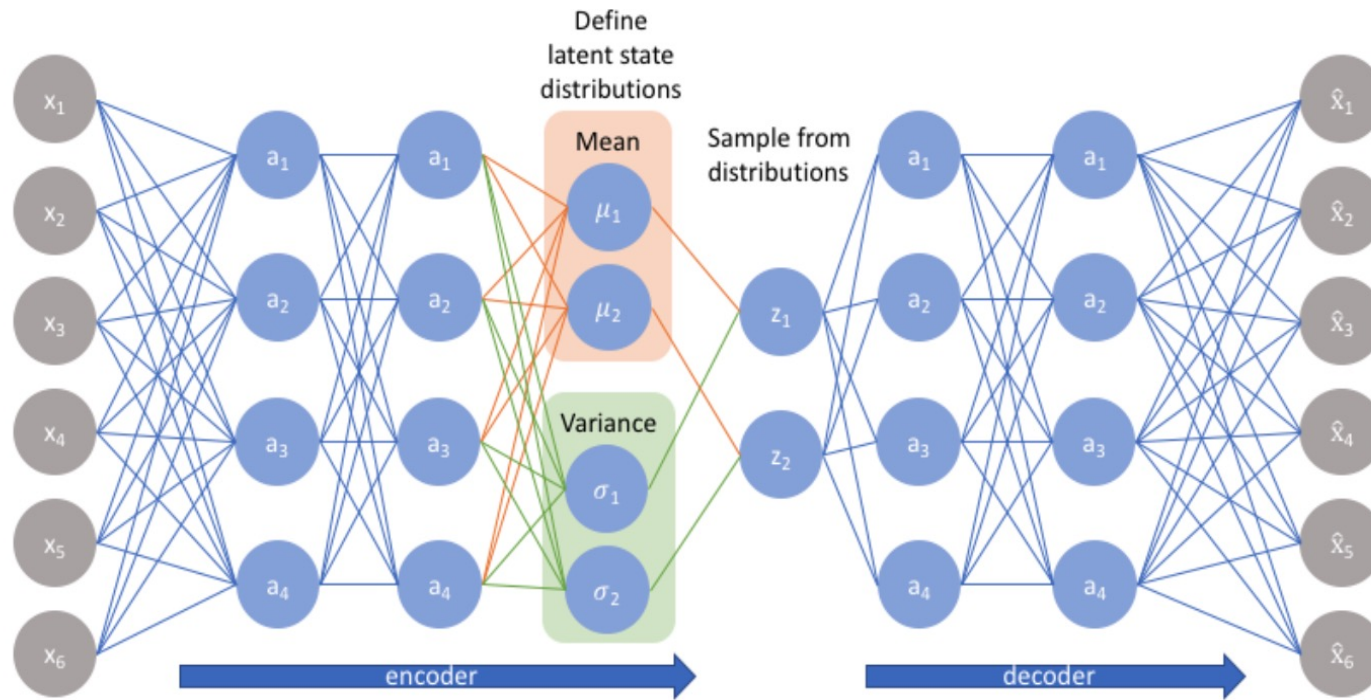
$$p(x|g_{\theta}(z)) = p_{\theta}(x|z)$$

우리가 최종적으로 알고자 하는 것은  
 $P(x)$  라는 최종 결과값

$$\int p(x|g_{\theta}(z))p(z)dz = p(x)$$

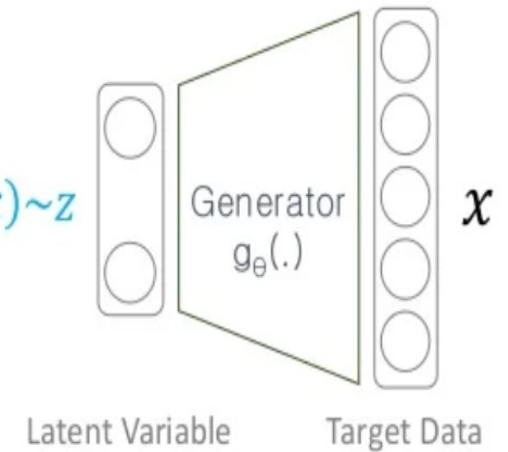


# Models – VAE(s)



[Source: Jeremy Jordan]

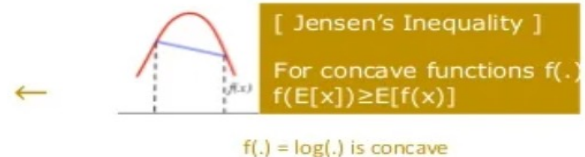
$$p(z|x) \approx q_{\phi}(z|x) \sim z$$



# Models – VAE(s)

## Relationship among $p(x), p(z|x), q_\phi(z|x)$ : Derivation 1

$$\log(p(x)) = \log\left(\int p(x|z)p(z)dz\right) \geq \int \log(p(x|z))p(z)dz$$



$$\log(p(x)) = \log\left(\int p(x|z) \frac{p(z)}{q_\phi(z|x)} q_\phi(z|x) dz\right) \geq \int \log\left(p(x|z) \frac{p(z)}{q_\phi(z|x)}\right) q_\phi(z|x) dz \leftarrow \text{Variational inference}$$

$$\log(p(x)) \geq \int \log(p(x|z)) q_\phi(z|x) dz - \int \log\left(\frac{q_\phi(z|x)}{p(z)}\right) q_\phi(z|x) dz$$

$$= \mathbb{E}_{q_\phi(z|x)}[\log(p(x|z))] - KL(q_\phi(z|x) || p(z))$$

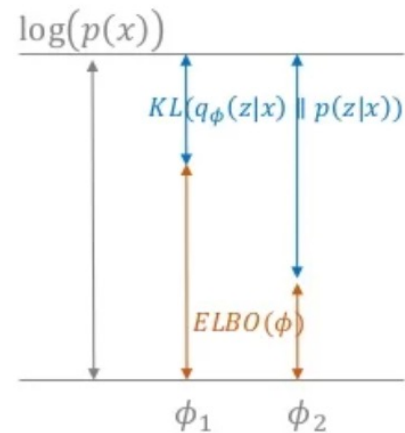
**ELBO**( $\phi$ ) Variational lower bound  
Evidence lower bound (ELBO)

# Models – VAE(s)

Relationship among  $p(x), p(z|x), q_\phi(z|x)$  : Derivation 2

$$\begin{aligned}
 \log(p(x)) &= \int \log(p(x)) q_\phi(z|x) dz \quad \leftarrow \int q_\phi(z|x) dz = 1 \\
 &= \int \log\left(\frac{p(x, z)}{p(z|x)}\right) q_\phi(z|x) dz \quad \leftarrow p(x) = \frac{p(x, z)}{p(z|x)} \\
 &= \int \log\left(\frac{p(x, z)}{q_\phi(z|x)} \cdot \frac{q_\phi(z|x)}{p(z|x)}\right) q_\phi(z|x) dz \\
 &= \underbrace{\int \log\left(\frac{p(x, z)}{q_\phi(z|x)}\right) q_\phi(z|x) dz}_{ELBO(\phi)} + \underbrace{\int \log\left(\frac{q_\phi(z|x)}{p(z|x)}\right) q_\phi(z|x) dz}_{KL(q_\phi(z|x) \parallel p(z|x))}
 \end{aligned}$$

두 확률분포 간의 거리  $\geq 0$



# Models – VAE(s)

Code

```
def _build_net(self):
    self.x_hat_tfph = tf.placeholder(tf.float32, shape=[None, *self.image_size], name='input_img')
    self.x_tfph = tf.placeholder(tf.float32, shape=[None, *self.image_size], name='target_img')
    self.keep_prob_tfph = tf.placeholder(tf.float32, name='keep_prob')
    self.z_in_tfph = tf.placeholder(tf.float32, shape=[None, self.flags.z_dim], name='latent_variable')

    # encoding
    mu, sigma = self.encoder(self.x_hat_tfph)
    # sampling by re-parameterization technique
    self.z = mu + sigma * tf.random_normal(tf.shape(mu), mean=0., stddev=1., dtype=tf.float32)

    # decoding
    y = self.decoder(self.z)
    self.y = tf.clip_by_value(y, 1e-8, 1 - 1e-8)
    sample_y = self.decoder(self.z_in_tfph, is_reuse=True)
    self.sample_y = tf.clip_by_value(sample_y, 1e-8, 1 - 1e-8)

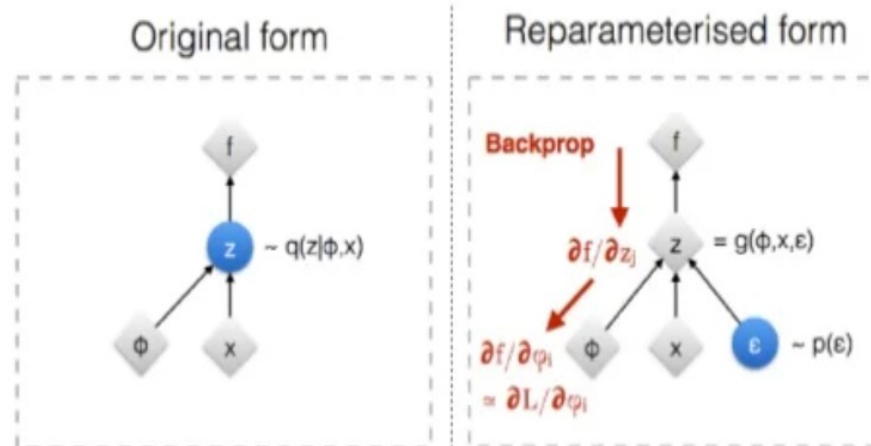
    # loss
    marginal_likelihood = tf.reduce_sum(self.x_tfph * tf.log(self.y) + (1 - self.x_tfph) * tf.log(1 - self.y),
                                         [1, 2, 3])
    KL_divergence = 0.5 * tf.reduce_sum(tf.square(mu) + tf.square(sigma) - tf.log(1e-8 + tf.square(sigma)) - 1, 1)

    self.marginal_likelihood = tf.reduce_mean(marginal_likelihood)
    self.KL_divergence = tf.reduce_mean(KL_divergence)
    self.ELBO = self.marginal_likelihood - self.KL_divergence
    self.loss = - self.ELBO

    self.train_op = tf.train.AdamOptimizer(self.flags.learning_rate).minimize(self.loss)
```

# Models – VAE(s) : Backpropagation

## Reparameterization Trick



◊ : Deterministic node  
● : Random node

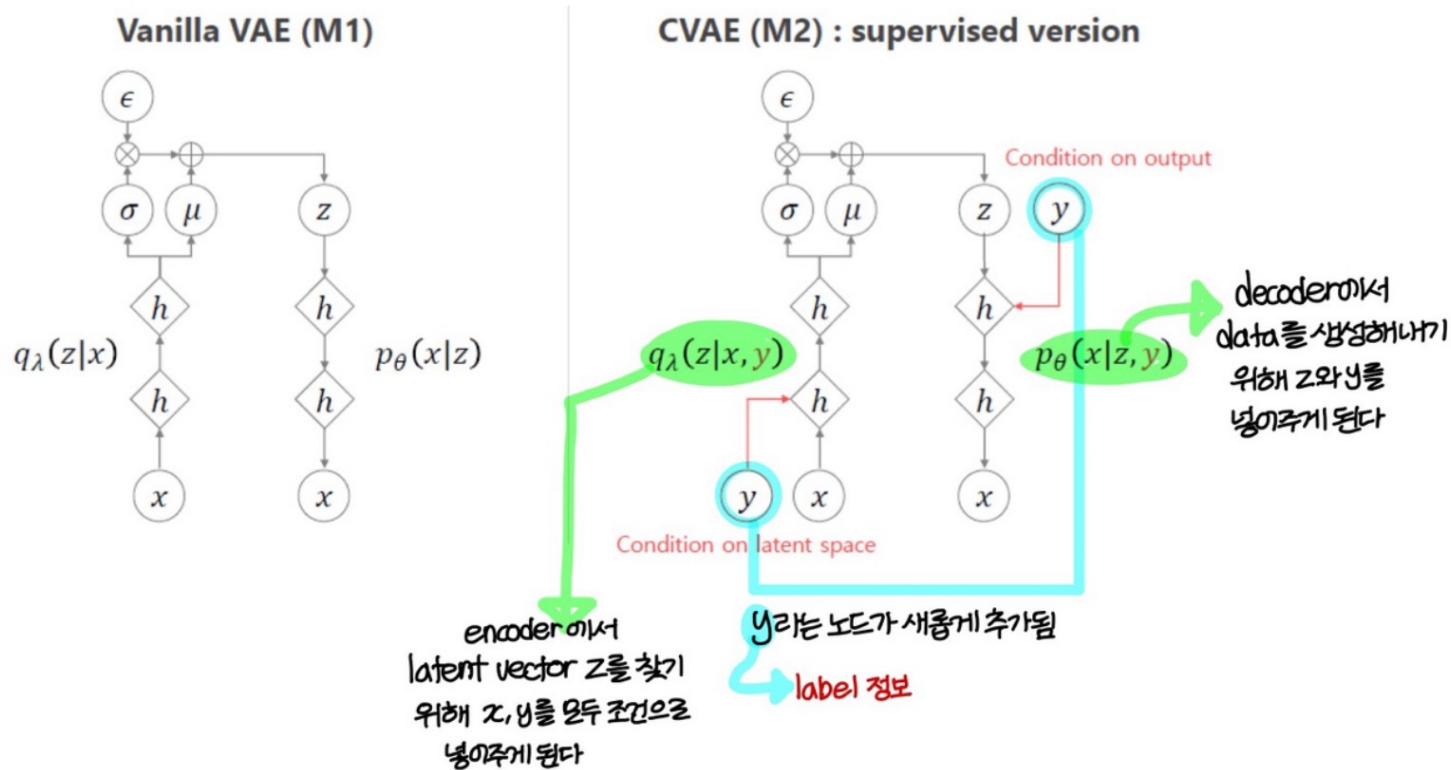
[Kingma, 2013]  
[Bengio, 2013]  
[Kingma and Welling 2014]  
[Rezende et al 2014]

## Sampling Process

$$z^{i,l} \sim N(\mu_i, \sigma_i^2 I)$$

$$z^{i,l} = \mu_i + \sigma_i^2 \odot \epsilon$$
$$\epsilon \sim N(0, I)$$

# Models – Contrastive Autoencoder



Ex) Encoder, Decoder 에 레이블의 정보를 입력해주는것

# Models – CVAE (CODE)

```
# Gaussian MLP as conditional encoder
def gaussian_MLP_conditional_encoder(x, y, n_hidden, n_output, keep_prob):
    with tf.variable_scope("gaussian_MLP_encoder"):
        # concatenate condition and image
        dim_y = int(y.get_shape()[1])
        input = tf.concat(axis=1, values=[x, y])

        # initializers
        w_init = tf.contrib.layers.variance_scaling_initializer()
        b_init = tf.constant_initializer(0.)

        # 1st hidden layer
        w0 = tf.get_variable('w0', [input.get_shape()[1], n_hidden+dim_y], initializer=w_init)
        b0 = tf.get_variable('b0', [n_hidden+dim_y], initializer=b_init)
        h0 = tf.matmul(input, w0) + b0
        h0 = tf.nn.elu(h0)
        h0 = tf.nn.dropout(h0, keep_prob)

        # 2nd hidden layer
        w1 = tf.get_variable('w1', [h0.get_shape()[1], n_hidden], initializer=w_init)
        b1 = tf.get_variable('b1', [n_hidden], initializer=b_init)
        h1 = tf.matmul(h0, w1) + b1
        h1 = tf.nn.tanh(h1)
        h1 = tf.nn.dropout(h1, keep_prob)
```



# CVAE – Result



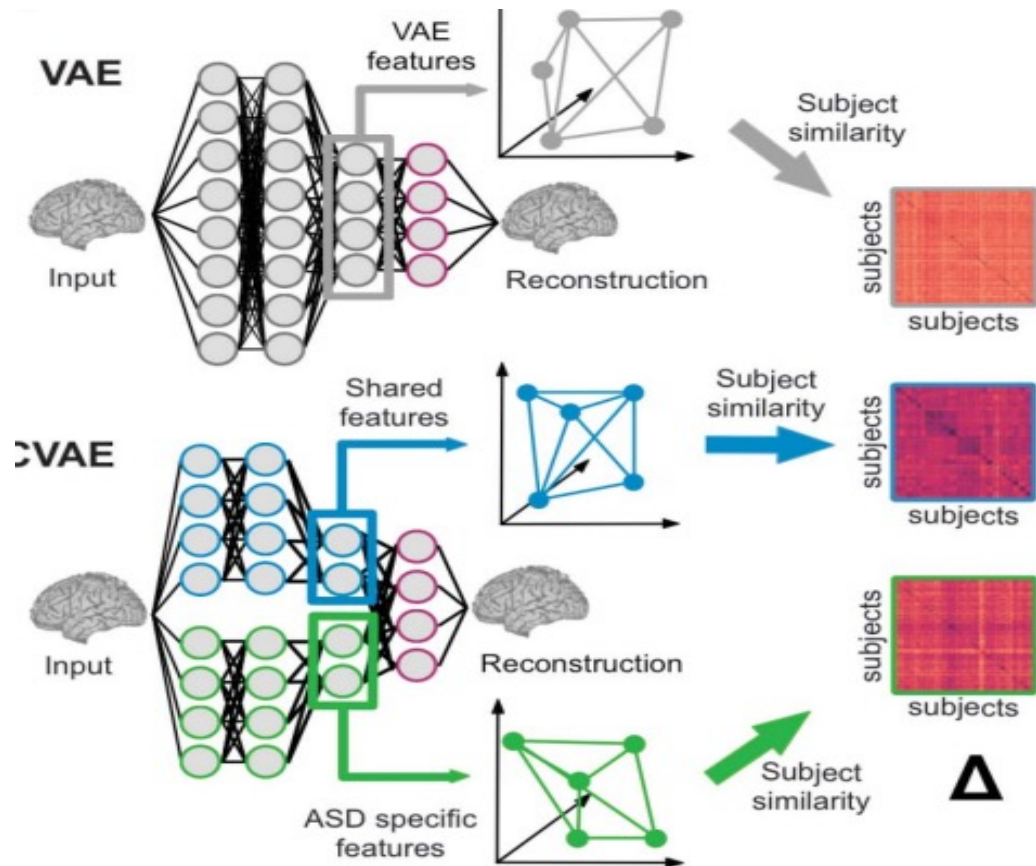
Z-sampling

$|z| = 2$



Handwriting style for a given  $z$  must be preserved for all labels

# Models – Application



## VAE

(1) Purpose - to test whether association between neuroanatomy and ASD symptoms can be identified using VAE

(2) Used Representational Similarity Analysis(RSA) - to correlated with individual variation in the ASD patients' characteristics (Scanner type, age etc.)