# Applications


# Of Data Science

# Intro to Autoencoders

## Applications of Data Science - Class 19

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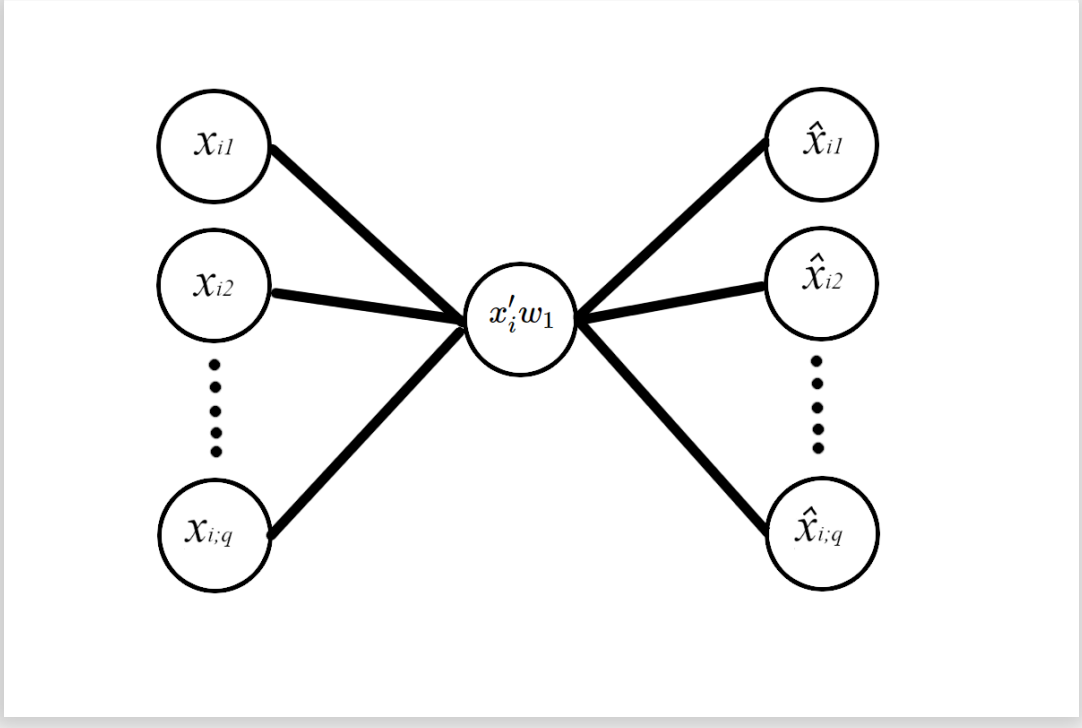
# Stacked Autoencoders (SAE)

(Heavily inspired by Geron 2019)

# Remember me? 😢

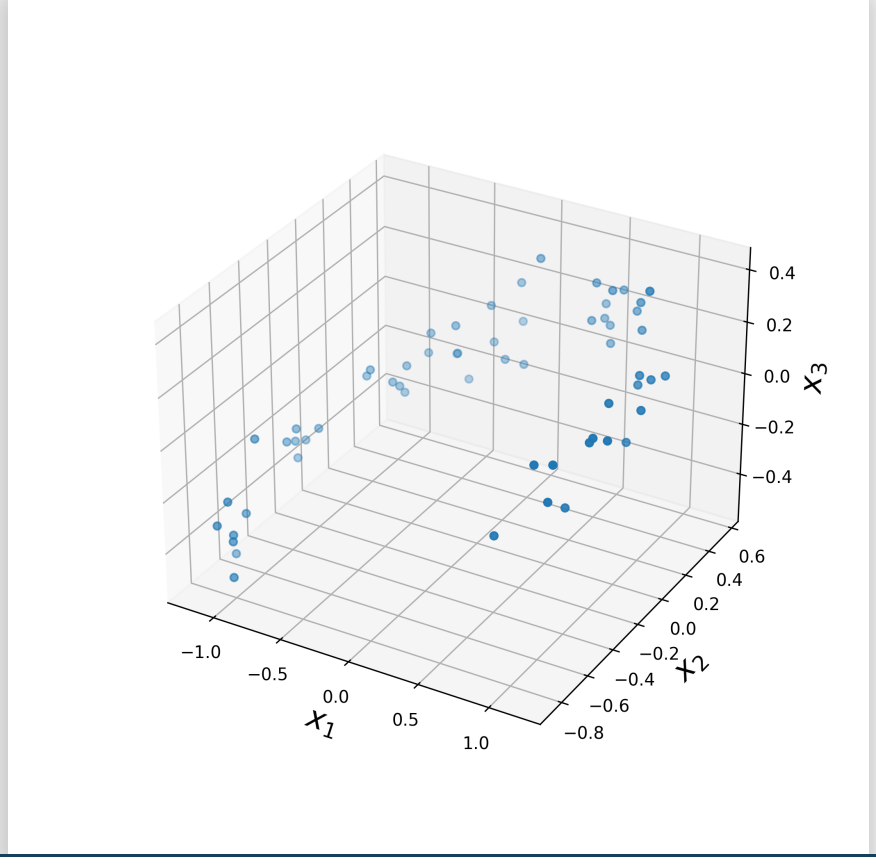
$\max_{w_1} w_1' X' X w_1 \text{ s.t.} ||w_1|| = 1$

PCA is a linear encoder. Sort of.



# NN "PCA"

```
X_train = generate_3d_data(60)
X_train = X_train - X_train.mean(axis=0, keepdims=0)
```



```
from sklearn.decomposition import PCA

pca = PCA(n_components=2)
pca.fit(X_train)
```

```
## PCA(n_components=2)
```

```
from tensorflow.keras import Sequential
from tensorflow.keras.layers import Dense, Flatten, Reshape

encoder = Sequential([Dense(2, input_shape=[3])])
decoder = Sequential([Dense(3, input_shape=[2])])
autoencoder = Sequential([encoder, decoder])

autoencoder.compile(loss='mse', optimizer='adam')

history = autoencoder.fit(X_train, X_train, epochs=20, verbose=0)
```

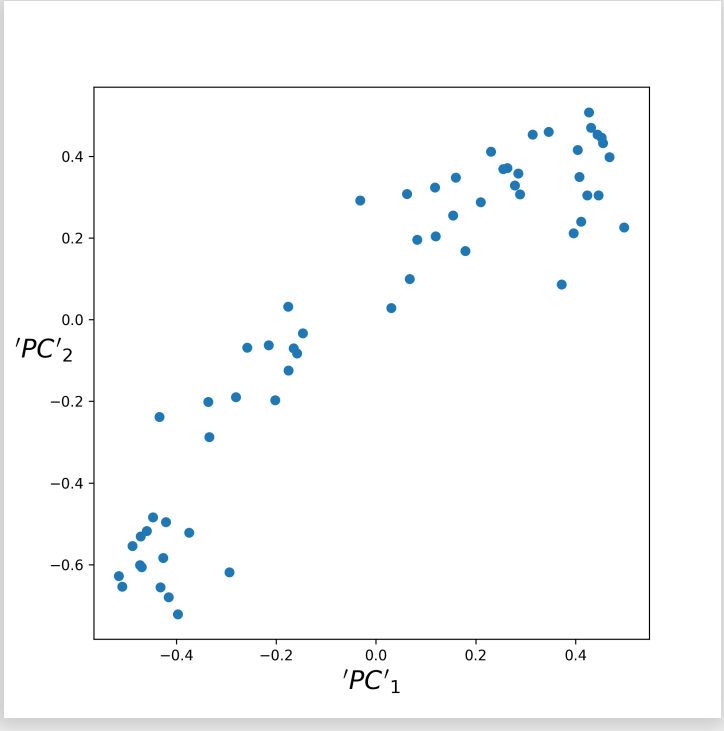
```
codings = encoder.predict(X_train)
pcs = pca.transform(X_train)

print(f'codings shape: {codings.shape}, pcs shape: {pcs.shape}')
```

```
## codings shape: (60, 2), pcs shape: (60, 2)
```

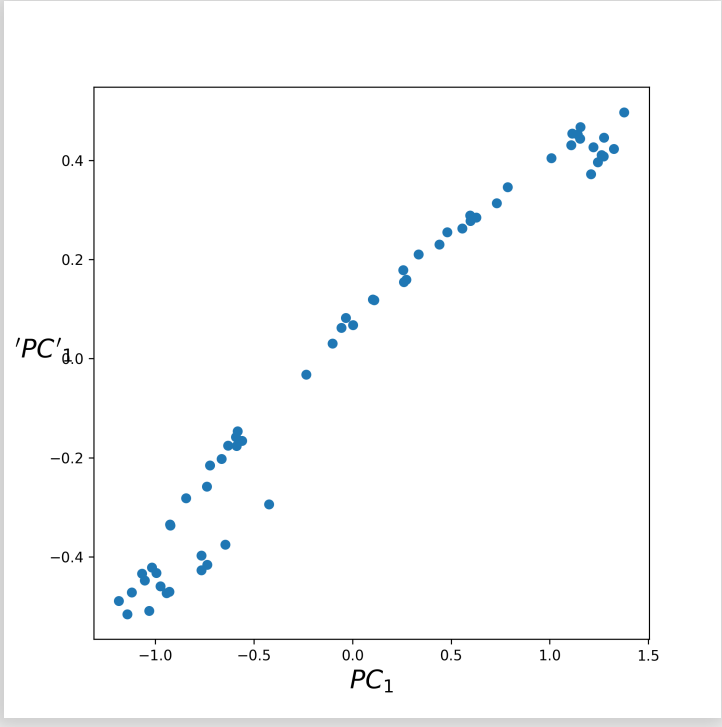
# How did NN "PCA" do?

```
plt.scatter(codings[:,0], codings[:, 1])
plt.xlabel("$'PC'_1$", fontsize=18)
plt.ylabel("$'PC'_2$", fontsize=18, rotation=0)
plt.show()
```



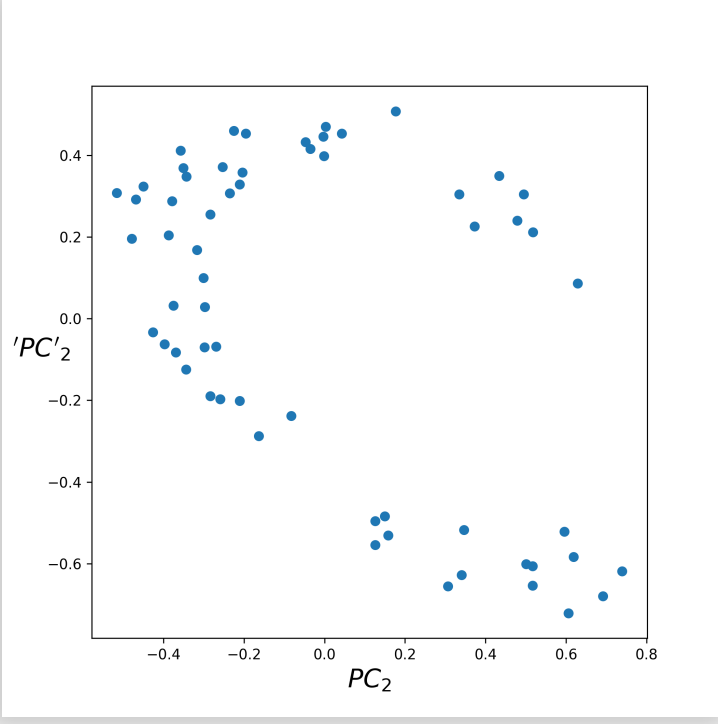
# Is it PCA though?

```
plt.scatter(pcs[:, 0], codings[:, 0])
plt.show()
```



# Is it PCA though?

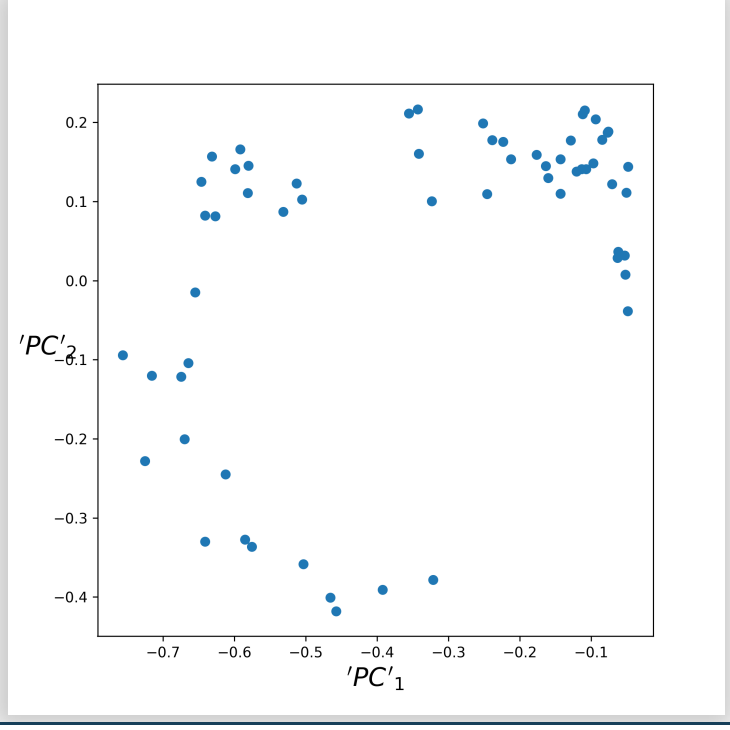
```
plt.scatter(pcs[:, 1], codings[:, 1])
plt.show()
```




Can you make it PCA?

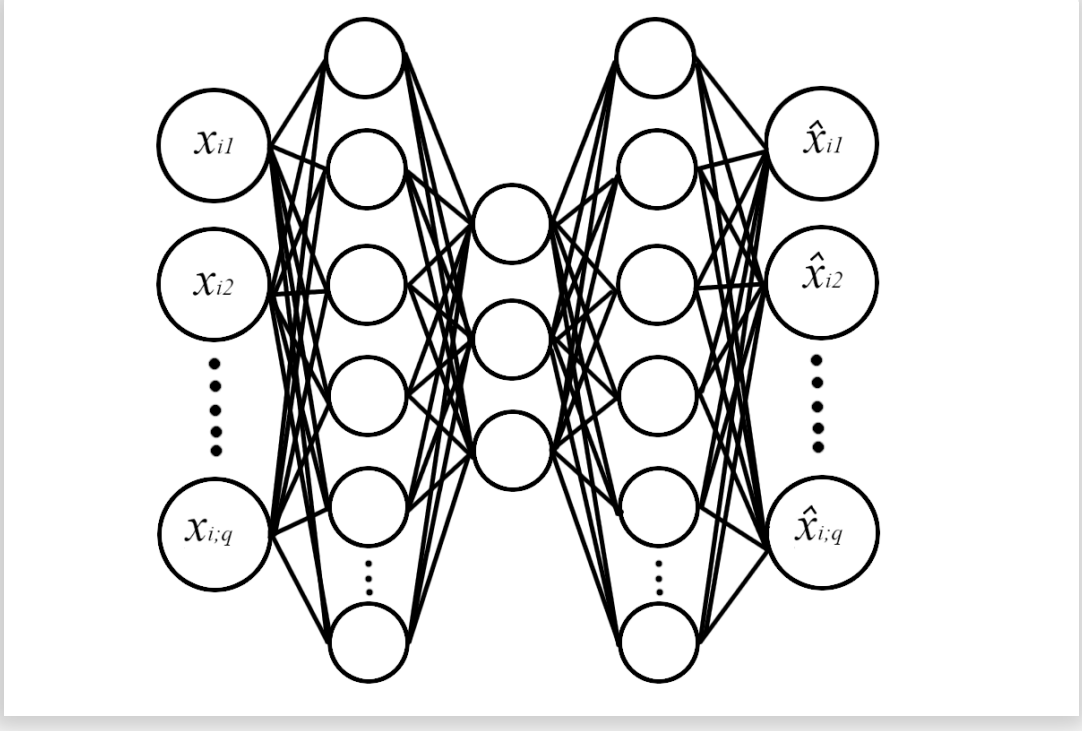
# Will non-linearity help?

```
encoder = Sequential([Dense(20, input_shape=[3], activation='relu'
  Dense(2)])
decoder = Sequential([Dense(20, input_shape=[2], activation='relu'
  Dense(3)])
autoencoder = Sequential([encoder, decoder])
autoencoder.compile(loss='mse', optimizer='adam')
history = autoencoder.fit(X_train, X_train, epochs=20, verbose=0)
```



# Stacked Autoencoders

Stacked autoencoders have been around for NLPCA for over 30 years (see e.g. Kramer 1991).



# SAE on FNIST

```
from tensorflow.keras.datasets import fashion_mnist

(X_train, y_train), (X_test, y_test) = fashion_mnist.load_data()
X_train = X_train.astype(np.float32) / 255
X_test = X_test.astype(np.float32) / 255

stacked_encoder = Sequential([
    Flatten(input_shape=[28, 28]),
    Dense(100, activation="relu"),
    Dense(30, activation="relu"),
])
stacked_decoder = Sequential([
    Dense(100, activation="relu", input_shape=[30]),
    Dense(28 * 28, activation="sigmoid"), # make output 0-1
    Reshape([28, 28])
])
stacked_ae = Sequential([stacked_encoder, stacked_decoder])

stacked_ae.compile(loss='mse', optimizer='adam')

history = stacked_ae.fit(X_train, X_train, epochs=20, verbose=1)
```

# Can it reconstruct?

```
def show_reconstructions(sae, images, n_images=5):
  reconstructions = sae.predict(images[:n_images])
  fig = plt.figure(figsize=(n_images * 1.5, 3))
  for image_index in range(n_images):
      plt.subplot(2, n_images, 1 + image_index)
      plt.imshow(images[image_index], cmap='binary')
      plt.axis('off')
      plt.subplot(2, n_images, 1 + n_images + image_index)
      plt.imshow(reconstructions[image_index], cmap='binary')
      plt.axis('off')

show_reconstructions(stacked_ae, X_test)
plt.show()
```

## Can it "denoise"?

```
shoe_encoded = stacked_encoder.predict(X_test[np.newaxis, 0,:])
shoe_encoded
```

```
## array([[ 2.92097   , 10.338918  ,  0.        ,  1.4428661 ,  2.6388376 ,
##          2.3139865 ,  2.5651445 ,  3.1734047 ,  3.2220273 ,  4.8254766 ,
##          3.1547084 ,  3.3593066 ,  1.6458672 ,  2.6469245 ,  4.6263247 ,
##          3.5413108 ,  1.239067  ,  9.445068  ,  0.75500596,  5.3597875 ,
##          0.        ,  4.605066  , 10.533057  ,  4.6313896 ,  6.31067   ,
##          3.82158   ,  6.353969  ,  3.82279   ,  3.3340364 ,  0.9221499 ]
##       dtype=float32)
```

```
shoe1 = stacked_decoder.predict(shoe_encoded)[0]
```

```
## WARNING:tensorflow:5 out of the last 7 calls to <function Model.make_pre
```

```
shoe2 = stacked_decoder.predict(shoe_encoded +np.random.normal(sca
shoe3 = stacked_decoder.predict(shoe_encoded +np.random.normal(sca
```

```
fig, axes = plt.subplots(1, 3, figsize=(6, 3))
axes[0].imshow(shoe1, cmap="binary")
axes[1].imshow(shoe2, cmap="binary")
axes[2].imshow(shoe3, cmap="binary")
_ = axes[0].axis('off')
_ = axes[1].axis('off')
_ = axes[2].axis('off')
plt.show()
```

# Can it average?

```
shirt_encoded = stacked_encoder.predict(X_test[np.newaxis, 1,:])
mean_encoded = (shoe_encoded + shirt_encoded) / 2

fig, axes = plt.subplots(1, 3, figsize=(6, 3))
_ = axes[0].imshow(X_test[0,:], cmap="binary")
_ = axes[1].imshow(X_test[1,:], cmap="binary")
_ = axes[2].imshow(stacked_decoder.predict(mean_encoded)[0], cmap=
_ = axes[0].axis('off')
_ = axes[1].axis('off')
_ = axes[2].axis('off')
plt.show()
```

# Can it **generate**?

```
X_test_compressed = stacked_encoder.predict(X_test)
mins = X_test_compressed.min(axis=0)
maxs = X_test_compressed.max(axis=0)

_ = plt.imshow(stacked_decoder.predict(
  np.random.uniform(mins, maxs, size=30)[np.newaxis, :]
  )[0], cmap="binary")
_ = plt.axis('off')
plt.show()
```

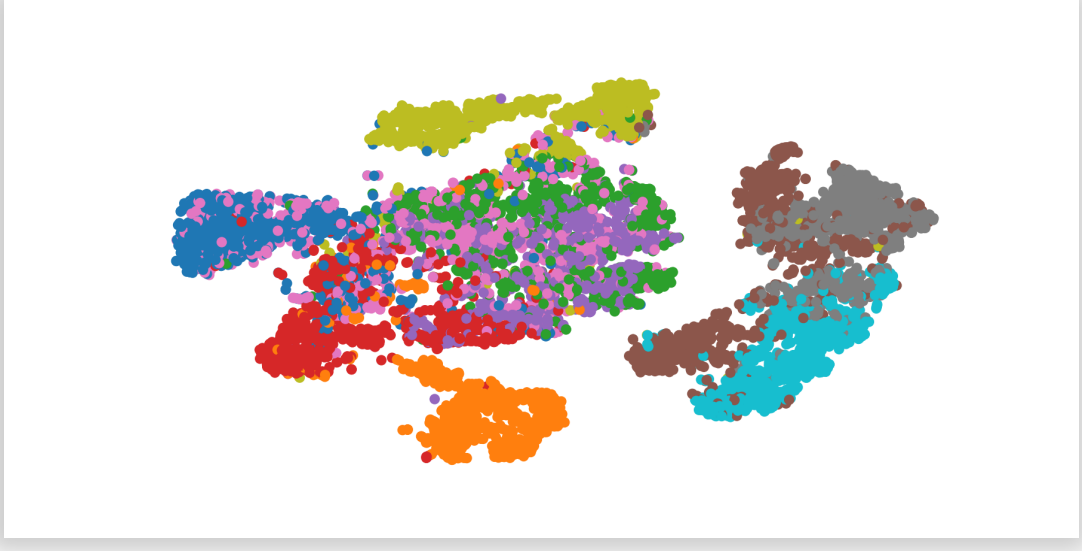
# Variational Autoencoders (VAE)

# How does SAE latent space look like?

```
from sklearn.manifold import TSNE

tsne = TSNE()
X_test_2D = tsne.fit_transform(X_test_compressed)
X_test_2D = (X_test_2D - X_test_2D.min()) / (X_test_2D.max() - X_t

_ = plt.scatter(X_test_2D[:, 0], X_test_2D[:, 1], c=y_test, s=10,
_ = plt.axis('off')
plt.show()
```



# Road to VAE

- The latent space has many "holes", it is "irregular"
- If we sample from these areas and decode, we cannot expect to get a meaningful element in the input space, result would be **unlikely**
- And why should we? Reconstruction loss is "king", it is overfitting! We not to regularize.


Source: Rocca 2019

# Road to VAE

In a landmark paper, Kingma & Welling (2013) suggest:

- Suppose there's a latent variable (LV) $z$
- The **probabilistic** encoder is defined by $p(z|x)$
- The **probabilistic** decoder is defined by $p(x|z)$
- Make $p(z)$, the prior of the LV, $N(0, I)$ - so the posterior encoder $p(z|x)$ cannot "run away"
- Make $p(x|z)$ be $N(f_\theta(z), \sigma^2 I)$ where $f$ would be modeled by DNN
- Goal: make the $x$'s produced by the decoder **likely**, i.e. maximize the marginal likelihood: $p(x) = \int p(x|z)p(z)dz$

But what is the posterior $p(z|x)$?

# Variational Inference (VI)

- A technique to approximate complex distributions (posteriors)
- Set a parametrised family of distribution $q(z)$ (for example the family of Gaussians)
- Look for the best approximation of our target distribution among this family: $q(z) \approx p(z|x)$
- The best element in the family is one that minimizes: $D_{KL}(q(z)||p(z|x)) = \int q(z) \log \frac{q(z)}{p(z|x)}$
- Mark $q$ as $q(z|x)$, so that this "family" would be $N(g_\eta(x), h_\psi(x))$
- This is how it will depend on the data $x$, and $g$, $h$ will be found with the encoder network, minimizing the KL loss

💡 Our encoder finds means and variances for a distribution! When we have them we would sample from that distribution.

Now dig this:

$$
\begin{aligned}
D_{KL}(q(z|x)||p(z|x)) &= \int q(z|x) \log \frac{q(z|x)}{p(z|x)} \\
&= E_q[\log(q(z|x)) - \log(p(z|x))] \\
&= E_q[\log(q(z|x)) - \log \frac{p(z)p(x|z)}{p(x)}] \\
&= E_q[\log(q(z|x)) - \log(p(z))] \\
&- E_q[\log(p(x|z))] + \log(p(x)) \\
&= D_{KL}(q(z|x)||p(z)) - E_q[\log(p(x|z))] + \log(p(x)
\end{aligned}
$$

But we want to maximize $p(x)$!

When writing:

$$\log(p(x)) - D_{KL}(q(z|x)||p(z|x)) = E_q[\log(p(x|z))] - D_{KL}(q(z|x)||p(z)$$

we see that maximizing log-likelihood $\log(p(x))$ combined with minimizing KL-divergence $D_{KL}(q(z|x)||p(z|x))$ boils down to maximizing the RHS or maximizing the **Evidence Lower BOund**:

$$ELBO(\theta, \eta, \psi|X) = E_q[\log(p(x|z))] - D_{KL}(q(z|x)||p(z))$$

Which is called like this since $D_{KL} \geq 0$ always, so $log(p(x)) \geq ELBO$.

Turning this to a loss function we need to minimize:

$$-ELBO(\theta_f, \theta_g, \theta_h|X) = -E_q[\log(p(x|z))] + D_{KL}(q(z|x)||p(z))$$

## Almost there (I)

Fortunately $D_{KL}$ for two Gaussians has closed form:

For $p_1 = N(\mu_1, \Sigma_1)$ and $p_2 = N(\mu_2, \Sigma_2)$:

$$D_{KL}(p_1 \,||\, p_2) = \frac{1}{2}\left[\log\frac{|\Sigma_2|}{|\Sigma_1|} - n + \mathrm{tr}\Sigma_2^{-1}\Sigma_1 + (\mu_2 - \mu_1)^T\Sigma_2^{-1}(\mu_2 - \mu_1\right.$$

In our case $\mu_1 = g_\eta(x) = \mu, \Sigma_1 = h_\psi(x) = \Sigma$, where $\Sigma$ is diagonal with $\sigma_i^2$ on its diagonal, $\mu_2 = \vec{0}, \Sigma_2 = I$, so:

$$D_{KL}(q(z|x)||p(z)) = -\frac{1}{2}\sum_i \left[1 + \gamma_i - \exp(\gamma_i) - \mu_i^2\right]$$

where $\gamma_i = \log\sigma_i^2$ for better stability. See here for a full proof.

**Here $i$ goes over number of neurons in the latent layer, $D$.**

## Almost there (II)

Since we assumed $p(x|z)$ is $N(f_\theta(z), \sigma^2 I)$:

$$-E_q[\log(p(x|z))] = C \cdot E_q[||x - f_\theta(z)||^2] = C \cdot E_q[||x - \hat{x}||^2],$$

where $C$ is some constant depndent on $\sigma^2$.

We use standard mini-batch SGD for approximation that expectation.

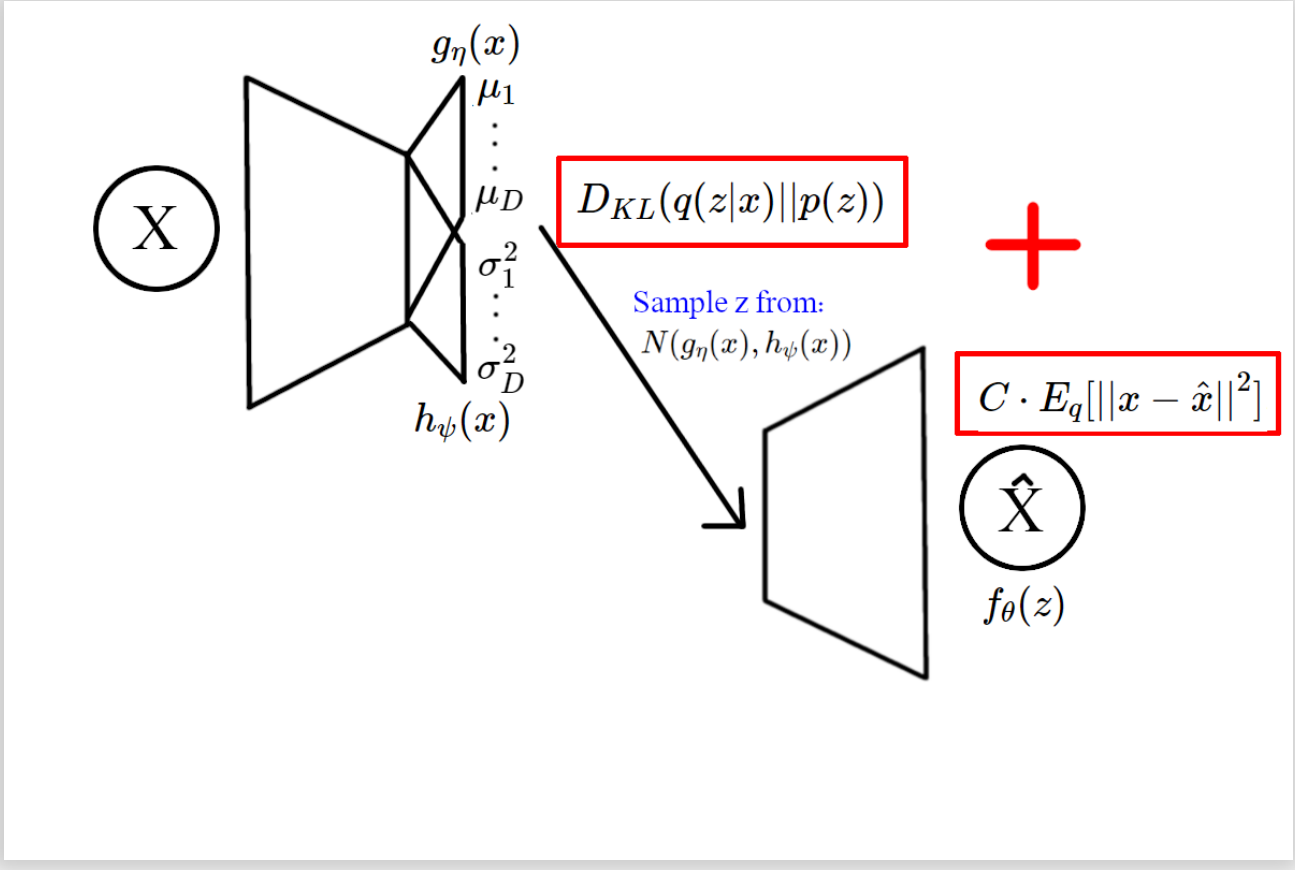
So our final loss optimized with SGD, is the sum of MSE and KL:

$$\text{VAE-Loss}(\theta, \eta, \psi|X)$$

$$= C \cdot \sum_{batch}(x_{batch} - \hat{x}_{batch})^2 - \frac{1}{2}\sum_i \left[1 + \gamma_i - \exp(\gamma_i) - \mu_i^2\right]$$

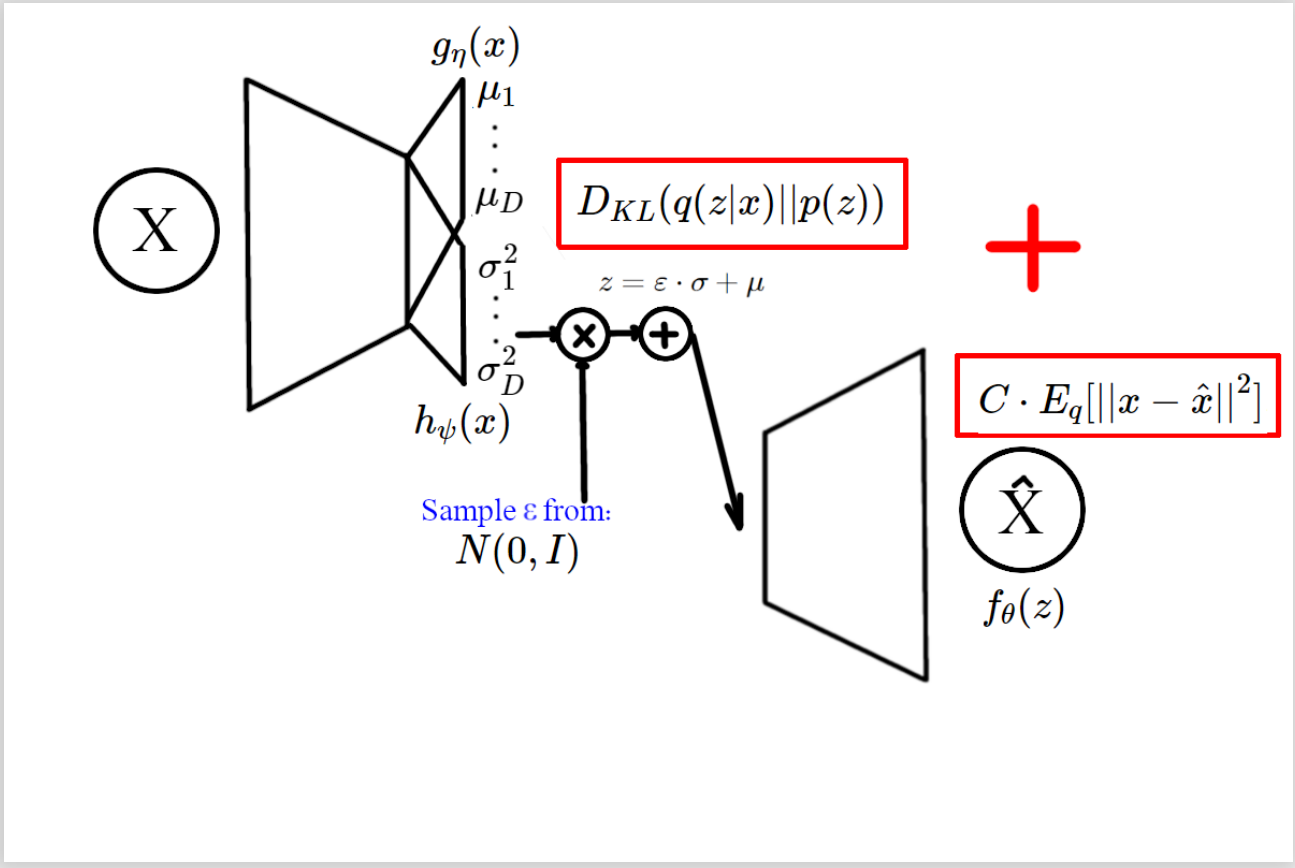
Reconstruction loss + Regularization!

# Still not there




Why wouldn't this work?

# Reparametrisation trick




In terms of $\gamma = \log \sigma^2$, this means: $z = \varepsilon \cdot \frac{\exp(\gamma)}{2} + \mu$

# VAE in Keras

```
from tensorflow.keras.layers import Layer, Input
from tensorflow.keras.losses import mean_squared_error as mse
from tensorflow.keras import Model
import tensorflow.keras.backend as K

# need a sampling layer which takes \mu and \gamma, samples \varep
# and turns it to N(\mu, "\gamma")
class Sampling(Layer):
  def call(self, inputs):
      mean, log_var = inputs
      return K.random_normal(tf.shape(log_var)) * K.exp(log_var /

D = 30

inputs = Input(shape=[28, 28])
z = Flatten()(inputs)
z = Dense(150, activation='relu')(z)
z = Dense(100, activation='relu')(z)
codings_mean = Dense(D)(z)
codings_log_var = Dense(D)(z)
codings = Sampling()([codings_mean, codings_log_var])
variational_encoder = Model(
    inputs=[inputs], outputs=[codings_mean, codings_log_var, codir
)
```

```
decoder_inputs = Input(shape=[D])
x = Dense(100, activation='relu')(decoder_inputs)
x = Dense(150, activation='relu')(x)
x = Dense(28 * 28, activation='sigmoid')(x) # make output 0-1
outputs = Reshape([28, 28])(x)
variational_decoder = Model(inputs=[decoder_inputs], outputs=[outp

_, _, codings = variational_encoder(inputs)
reconstructions = variational_decoder(codings)
variational_ae = Model(inputs=[inputs], outputs=[reconstructions])

kl_loss = -0.5 * K.sum(
  1 + codings_log_var - K.exp(codings_log_var) - K.square(codings_
  axis=-1)

# if inputs/outputs were flat I think it would work
# reconstruction_loss = mse(inputs, outputs) * 784
# vae_loss = K.mean(reconstruction_loss + kl_loss)
# variational_ae.add_loss(vae_loss)

variational_ae.add_loss(K.mean(kl_loss) / 784.)
variational_ae.compile(loss='mse', optimizer='adam')

history = variational_ae.fit(X_train, X_train, epochs=10, verbose=
```

## Can it reconstruct?

```
show_reconstructions(variational_ae, X_test)
plt.show()
```

So you see the difference in comparison to SAE?

## Can it "denoise"?

```
shoe_encoded = variational_encoder.predict(X_test[np.newaxis, 0,:]
shoe1 = variational_decoder.predict(shoe_encoded)[0]
shoe2 = variational_decoder.predict(shoe_encoded +np.random.normal
shoe3 = variational_decoder.predict(shoe_encoded +np.random.normal

fig, axes = plt.subplots(1, 3, figsize=(6, 3))
_ = axes[0].imshow(shoe1, cmap='binary')
_ = axes[1].imshow(shoe2, cmap='binary')
_ = axes[2].imshow(shoe3, cmap='binary')
_ = axes[0].axis('off')
_ = axes[1].axis('off')
_ = axes[2].axis('off')
plt.show()
```

# Can it average?

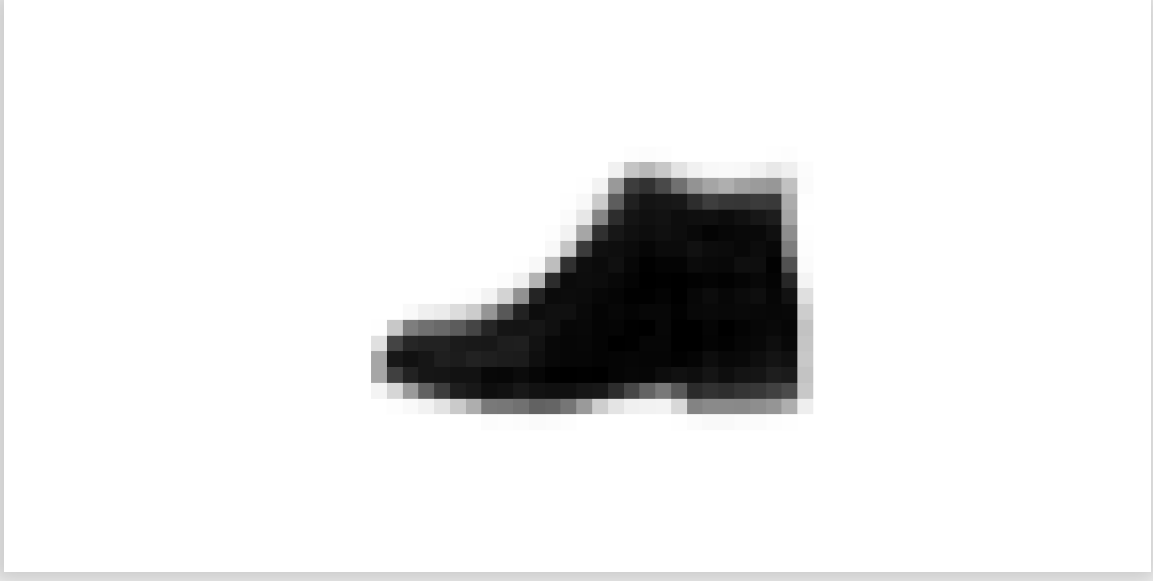
```
shirt_encoded = variational_encoder.predict(X_test[np.newaxis, 1,:
mean_encoded = (shoe_encoded + shirt_encoded) / 2

fig, axes = plt.subplots(1, 3, figsize=(6, 3))
_ = axes[0].imshow(X_test[0,:], cmap='binary')
_ = axes[1].imshow(X_test[1,:], cmap='binary')
_ = axes[2].imshow(variational_decoder.predict(mean_encoded)[0], c
_ = axes[0].axis('off')
_ = axes[1].axis('off')
_ = axes[2].axis('off')
plt.show()
```

# Can it **generate**?

```
X_test_compressed = variational_encoder.predict(X_test)[0]
mins = X_test_compressed.min(axis=0)
maxs = X_test_compressed.max(axis=0)

_ = plt.imshow(variational_decoder.predict(
  np.random.uniform(mins, maxs, size=D)[np.newaxis, :]
  )[0], cmap='binary')
_ = plt.axis('off')
plt.show()
```

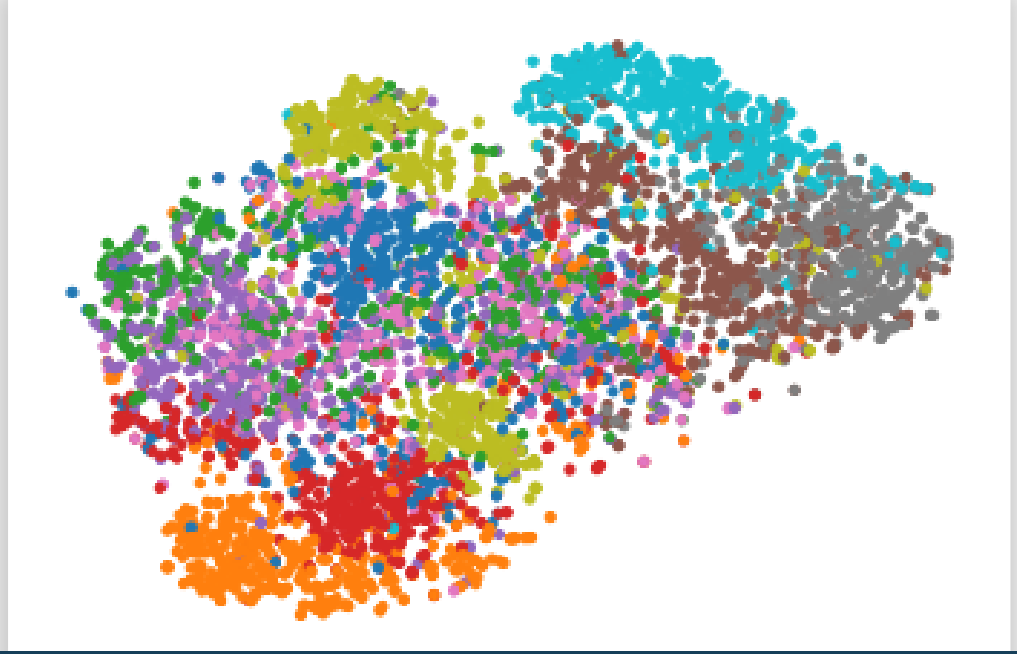


# Latent space slightly more regular

```
from sklearn.manifold import TSNE

tsne = TSNE()
X_test_2D = tsne.fit_transform(X_test_compressed)
X_test_2D = (X_test_2D - X_test_2D.min()) / (X_test_2D.max() - X_t

_ = plt.scatter(X_test_2D[:, 0], X_test_2D[:, 1], c=y_test, s=10,
_ = plt.axis('off')
plt.show()
```

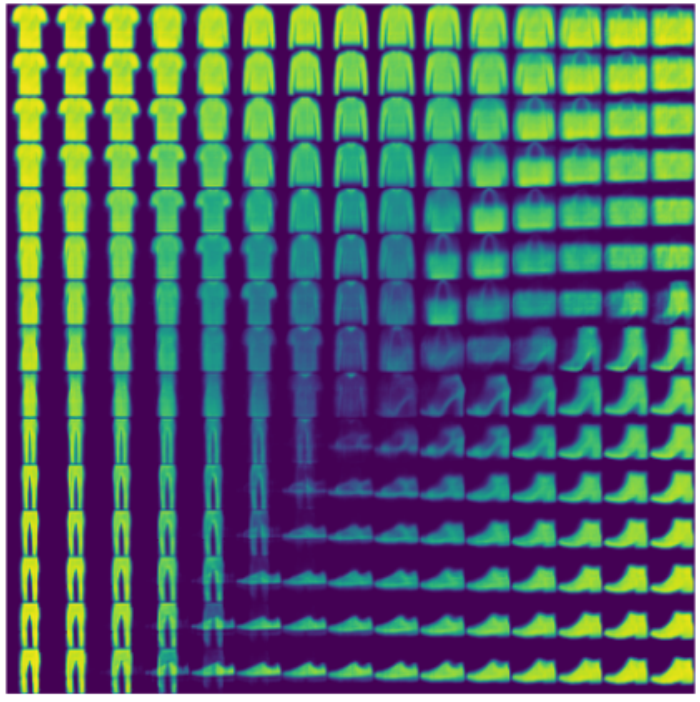


For a 2D latent space we could actual "travel" within the space:

```
n = 15  # figure with 15x15 items
item_size = 28
figure = np.zeros((item_size * n, item_size * n))
# We will sample n points within [-2, 2]
grid_x = np.linspace(-2, 2, n)
grid_y = np.linspace(-2, 2, n)

for i, yi in enumerate(grid_x):
    for j, xi in enumerate(grid_y):
        z_sample = np.array([[xi, yi]])
        x_decoded = variational_decoder.predict(z_sample)
        item = x_decoded[0]#.reshape(item_size, item_size)
        figure[i * item_size: (i + 1) * item_size,
               j * item_size: (j + 1) * item_size] = item

plt.figure(figsize=(10, 10))
plt.imshow(figure)
plt.axis('off')
plt.show()
```



# What's next?

GANs!


Source: [Karras, ICLR 2018]