# CSC 412
# Probabilistic Learning and Reasoning
## Week 9: Variational Inference II & VAEs

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# Overview for the first hour

- Variational Inference
- ELBO and its properties
- Estimating gradients of the ELBO
  - Simple Monte Carlo
  - Reparameterization trick

# Recap: Posterior Inference for Latent Variable Models

We encountered a few latent variable models (e.g. the trueskill model).

These models have a factorization $p(x, z) = p(z)p(x|z)$ where:

- $x$ are the observations or data,
- $z$ are the unobserved (latent) variables
- $p(z)$ is usually called the **prior**
- $p(x|z)$ is usually called the **likelihood**
- The conditional distribution of the unobserved variables given the observed variables (aka the **posterior**) is

$$p(z|x) = \frac{p(x, z)}{p(x)} = \frac{p(x, z)}{\int p(x, z)dz}$$

- We assume $p(x) = \int p(x, z)dz$ is hard to compute

# Variational methods

Variational inference works as follows:

- Choose a tractable parametric distribution $q_\phi(z)$ with parameters $\phi$. This distribution will be used to approximate $p(z|x)$.
  - For example, $q_\phi(z) = \mathcal{N}(z|\mu, \Sigma)$ where $\phi = (\mu, \Sigma)$.
- Encode some notion of "distance" between $p(z|x)$ and $q_\phi(z)$ that can be efficiently estimated. Usually we will use the KL divergence.
- Minimize this distance.

# Recall: KL divergence

We will measure the difference between $q$ and $p$ using the **Kullback-Leibler divergence**

$$\begin{aligned} \mathrm{KL}(q_\phi(z) \| p(z|x)) &= \int q_\phi(z) \log \frac{q_\phi(z)}{p(z|x)} dz \\ &= \underset{z \sim q_\phi}{\mathbb{E}} \log \frac{q_\phi(z)}{p(z|x)} \end{aligned}$$

# ELBO: Evidence Lower Bound

- Evaluating $\mathrm{KL}(q_\phi(z) \| p(z|x))$ is intractable because of the integral over $z$ and the term $p(z|x)$, which is intractable to normalize.
- We can still "optimize" this KL without knowing the normalization constant $p(x)$.
- We solve a surrogate optimization problem: maximize the **evidence lower bound (ELBO)**.
- Maximizing the ELBO is equivalent to minimizing

$$\mathrm{KL}(q_\phi(z) \| p(z|x)).$$

# ELBO: Evidence Lower Bound

Maximizing the ELBO is the same as minimizing $\mathrm{KL}(q_\phi(z) \| p(z|x))$.

$$
\begin{aligned}
\mathrm{KL}(q_\phi(z) \| p(z|x)) &= \mathop{\mathbb{E}}_{z \sim q_\phi} \log \frac{q_\phi(z)}{p(z|x)} \\
&= \mathop{\mathbb{E}}_{z \sim q_\phi} \left[ \log \left( q_\phi(z) \cdot \frac{p(x)}{p(z,x)} \right) \right] \\
&= \mathop{\mathbb{E}}_{z \sim q_\phi} \left[ \log \frac{q_\phi(z)}{p(z,x)} \right] + \mathop{\mathbb{E}}_{z \sim q_\phi} \log p(x) \\
&:= -\mathcal{L}(\phi) + \log p(x)
\end{aligned}
$$

Where $\mathcal{L}(\phi)$ is the **ELBO**:

$$
\mathcal{L}(\phi) = \mathop{\mathbb{E}}_{z \sim q_\phi} \left[ \log p(z,x) - \log q_\phi(z) \right]
$$

# ELBO: Evidence Lower Bound

$\mathrm{KL}(q_\phi(z) \| p(z|x)) = -\mathcal{L}(\phi) + \log p(x)$.

- Rearranging, we get

$$\mathcal{L}(\phi) + \mathrm{KL}(q_\phi(z) \| p(z|x)) = \log p(x)$$

- Because $\mathrm{KL}(q_\phi(z) \| p(z|x)) \geq 0$,

$$\mathcal{L}(\phi) \leq \log p(x)$$

- maximizing the ELBO $\Rightarrow$ minimizing $\mathrm{KL}(q_\phi(z) \| p(z|x))$.
- Note: $\mathcal{L}(\phi) = \underset{z \sim q_\phi}{\mathbb{E}}\Big[\log p(z, x)\Big] + \underset{z \sim q_\phi}{\mathbb{E}}\Big[-\log q_\phi(z)\Big]$, so

  ELBO = expected log-joint + entropy

# Maximizing ELBO

Recall: $\nabla \mathcal{L}(\phi)$ gives the direction of the steepest ascent of $\mathcal{L}(\phi)$.

Gradient descent (GD) methods: $\phi_{t+1} = \phi_t + s_t \nabla \mathcal{L}(\phi_t)$.

- We have that $\mathcal{L}(\phi) = \mathop{\mathbb{E}}_{z \sim q_\phi} \Big[ \log p(x, z) - \log q_\phi(z) \Big]$.
- We need $\nabla_\phi \mathcal{L}(\phi)$ or its unbiased estimate (stochastic GD).

Approximating the gradient of some $\mathbb{E}(f(Y, \phi))$:

- If the distribution of $Y$ independent of $\phi$ then

$$\nabla_\phi \mathbb{E}(f(Y, \phi)) = \mathbb{E}(\nabla_\phi f(Y, \phi)).$$

- We then have $\nabla_\phi \mathbb{E}(f(Y, \phi)) \approx \frac{1}{n} \sum_{i=1}^{n} \nabla_\phi f(y_i, \phi)$.
- Problem: In our case the distribution of $z$ depends on $\phi$.

# The reparameterization trick

Problem:

$$\nabla_\phi \mathop{\mathbb{E}}_{z \sim q_\phi} \Big[ \log p(x, z) - \log q_\phi(z) \Big] \neq \mathop{\mathbb{E}}_{z \sim q_\phi} \Big[ \nabla_\phi \left( \log p(x, z) - \log q_\phi(z) \right) \Big].$$

But in some situations there is a trick:

- We break this sampling process into two parts:
  - Sample a random variable $\epsilon$ that has fixed (or no) parameters, such as a uniform distribution or standard normal.
  - Determinsitically compute $z$'s as a function $\phi$ and $\epsilon$, such that:
    - $\epsilon \sim p_0(\epsilon)$
    - $z = T(\epsilon, \phi)$
    - $\implies$
    - $z \sim q_\phi(z)$

# The reparameterization trick

- For example, $z = \mu + \sigma\epsilon = T(\phi, \epsilon)$ (here $\phi = (\mu, \sigma)$).
  - $\epsilon \sim \mathcal{N}(0, 1)$
  - $z = \mu + \epsilon\sigma$
  - $\implies$
  - $z \sim \mathcal{N}(\mu, \sigma)$
- This makes the density independent of the parameter $\phi$, which will let us use simple Monte Carlo: $z = T(\phi, \epsilon)$

$$\begin{aligned}
\nabla_\phi \mathcal{L}(\phi) &= \nabla_\phi \mathbb{E}_{z \sim q_\phi(z)} \Big[ \log p(x, z) - \log q_\phi(z) \Big] \\
&= \nabla_\phi \mathbb{E}_{\epsilon \sim p_0(\epsilon)} \Big[ \log p(x, T(\phi, \epsilon)) - \log q_\phi(T(\phi, \epsilon)) \Big] \\
&= \mathbb{E}_{\epsilon \sim p_0(\epsilon)} \nabla_\phi \Big[ \log p(x, T(\phi, \epsilon)) - \log q_\phi(T(\phi, \epsilon)) \Big]
\end{aligned}$$

# SVI: Stochastic Variational Inference

- Instead of computing the full gradient (which is in general not possible), we compute a simple Monte Carlo estimate of it.
- For example, instead of

$$\mathbb{E}_{\epsilon \sim p_0(\epsilon)} \nabla_\phi \Big[ \log p(x, T(\phi, \epsilon)) - \log q_\phi(T(\phi, \epsilon)) \Big]$$

we work with a mini-batch of size $m$

$$\begin{aligned} &\widehat{\mathbb{E}}_{\epsilon \sim p_0(\epsilon)} \nabla_\phi \Big[ \log p(x, T(\phi, \epsilon)) - \log q_\phi(T(\phi, \epsilon)) \Big] \\ &\approx \frac{1}{m} \sum_{i=1}^{m} \nabla_\phi \Big[ \log p(x, T(\phi, \epsilon_i)) - \log q_\phi(T(\phi, \epsilon_i)) \Big] \end{aligned}$$

# MCMC: Pros & Cons

Pros of MCMC:

- Accurate results (at least asymptotically)
- Flexibility
- No approximation
- Handles multimodal distributions

Cons of MCMC:

- High computational cost
- Requires tuning of hyperparameters
- Convergence issues
- Inefficient in sampling complex dependencies

# SVI: Pros & Cons

Pros of SVI:

- Faster convergence
- Scalability
- Ease of use

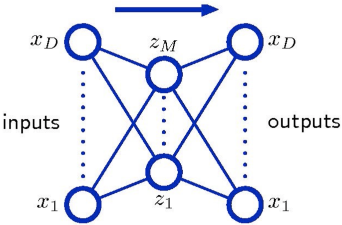
Cons of SVI:

- Approximate results
- Limited flexibility
- Mode seeking
- Sensitive to choice of hyperparameters

# Overview of the second hour

- Autoencoders
- Variational Autoencoders

# Non-linear Dimension Reduction




- Neural networks can be used for nonlinear dimensionality reduction.
- This is achieved by having the same number of outputs as inputs. These models are called autoencoders.
- Consider a multilayer perceptron that has $D$ inputs, $D$ outputs, and $M$ hidden units, with $M < D$.
- We can squeeze the information through some kind of bottleneck.
- If we use a linear network (linear activation) this is very similar to Principal Components Analysis.

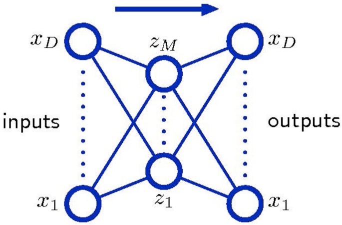
# Autoencoders and PCA

- Given an input $\boldsymbol{x}$, its corresponding reconstruction is given by:

$$y_k(\boldsymbol{x}, \boldsymbol{w}) = \sum_{j=1}^{M} w_{kj}^{(2)} \sigma\Big(\sum_{i=1}^{D} w_{ji}^{(1)} x_i\Big), \quad k = 1, ..., D.$$

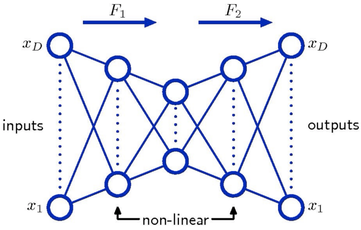
- We can determine the network parameters $\boldsymbol{w}$ by minimizing the reconstruction error:

$$E(\boldsymbol{w}) = \frac{1}{2} \sum_{n=1}^{N} \|y(\boldsymbol{x}_n, \boldsymbol{w}) - \boldsymbol{x}_n\|^2$$




- If the hidden and output layers are linear, it will learn hidden units that are linear functions of the data and minimize squared error.
- $M$ hidden units will span the same space as the first $M$ principal components.

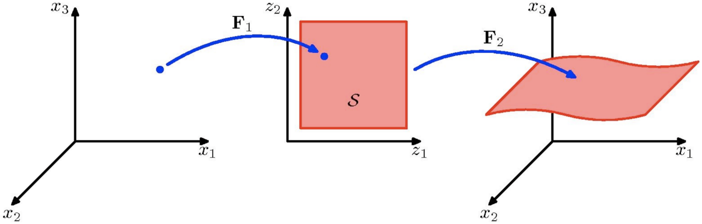
# Deep Autoencoders




- We can put extra nonlinear hidden layers between the input and the bottleneck and between the bottleneck and the output.
- This gives nonlinear generalization of PCA, providing non-linear dimensionality reduction.
- The network can be trained by the minimization of the reconstruction error function.
- Much harder to train.

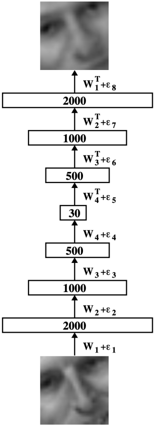
# Geometrical Interpretation

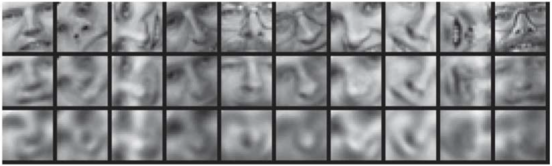
- Geometrical interpretation of the mappings performed by the network with 2 hidden layers for the case of $D = 3$ and $M = 2$ units in the middle layer.




- The mapping $F_1$ defines a nonlinear projection of points in the original $D$-space into the $M$-dimensional subspace.
- The mapping $F_2$ maps from an $M$-dimensional space into $D$-dimensional space.

# Deep Autoencoders

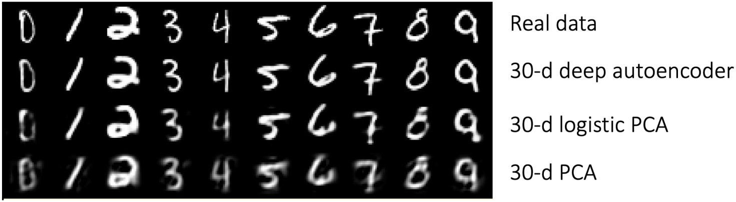


- We can consider very deep autoencoders.
- By row: Real data, Deep autoencoder with a bottleneck of 30 linear units, and 30-d PCA.

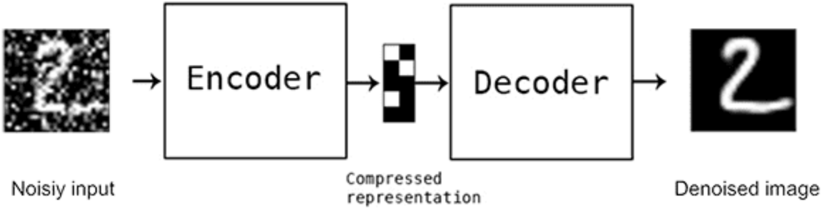
# Deep Autoencoders

- Similar model for MNIST handwritten digits:



- Deep autoencoders produce much better reconstructions.

# Application: Image Denoising




- We can train a **denoising autoencoder**.
- We feed noisy image as an input to the encoder
- Minimize the reconstruction error between the decoder output and original image.
- This method requires training and knowledge of the noise structure (fully supervised).
- In contrast, loopy BP works for a single noisy image and doesn't require the knowledge of noise structure (unsupervised).

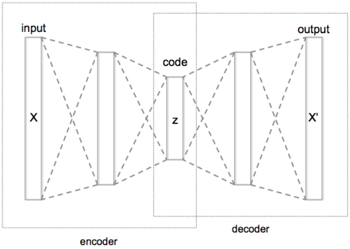
# Autoencoders: Summary

Autoencoders reconstruct their input via an encoder and a decoder.

- **Encoder**: $g(x) = z \in F, \quad x \in X$
- **Decoder**: $f(z) = \tilde{x} \in X$
- where $X$ is the data space, and $F$ is the feature (latent) space.
- $z$ is the code, compressed representation of the input, $x$. It is important that this code is a bottleneck, i.e. that

$$\dim F \ll \dim X$$

- Goal: $\tilde{x} = f(g(x)) \approx x$.



# Issues with (deterministic) Autoencoders

- **Issue 1**: Proximity in data space does not mean proximity in feature space
  - The codes learned by the model are deterministic, i.e.

$$g(x_1) = z_1 \Rightarrow f(z_1) = \tilde{x}_1$$
$$g(x_2) = z_2 \Rightarrow f(z_2) = \tilde{x}_2$$

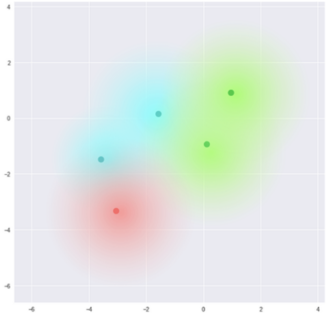
  - but proximity in feature space is not "directly" enforced for inputs in close proximity in data space, i.e.

$$x_1 \approx x_2 \not\Rightarrow z_1 \approx z_2$$

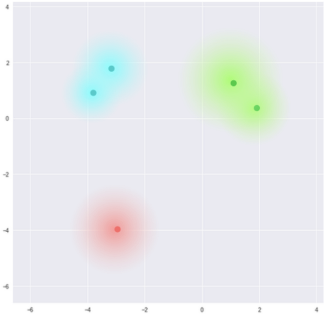
  - The latent space may not be continuous, or allow easy interpolation.

# Issues with (deterministic) Autoencoders

- **Issue 1**: Proximity in data space does not mean proximity in feature space
  - If the space has discontinuities (eg. gaps between clusters) and you sample/generate a variation from there, the decoder will simply generate an unrealistic output.



What we require

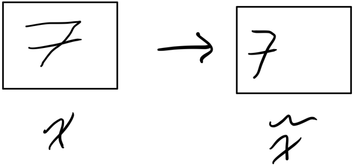


What we may inadvertently end up with

Image credit: I. Shafkat

# Issues with (deterministic) Autoencoders

- **Issue 2**: How to measure the goodness of a reconstruction?



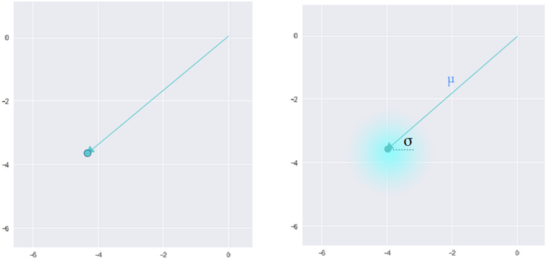
  - The reconstruction looks quite good. However, if we chose a simple distance metric between inputs and reconstructions, we would heavily penalize the left-shift in the reconstruction $\tilde{x}$.
  - Choosing an appropriate metric for evaluating model performance can be difficult, and that a miss-aligned objective can be disastrous.

# Variational Autoencoders

- Variational autoencoders (VAEs) encode inputs with uncertainty.
- Unlike standard autoencoders, the encoder of a VAE outputs a probability distribution, $q_\phi(z)$ to approximate $p(z|x)$.
- Instead of the encoder learning an encoding vector, it learns two vectors: vector of means, $\mu$, and another vector of standard deviations, $\sigma$.

# Variational Autoencoders

- The mean $\mu$ controls where encoding of input is centered while the standard deviation controls how much can the encoding vary.




Standard Autoencoder
(direct encoding coordinates)

Variational Autoencoder
(μ and σ initialize a probability distribution)

- Encodings are generated at random from the "circle", the decoder learns that all nearby points refer to the same input.

Image credit: I. Shafkat

# VAE: Specifics

- Our model is generated by the joint distribution over the latent codes and the input data $p(x, z)$. Decomposing

$$p(x, z) = \text{prior} \times \text{likelihood} = p(z)p(x|z)$$

- The encoder is $p(z|x) = p(x, z)/p(x)$.
- However, learning $p(x) = \int p(x|z)p(z)dz$ is intractable.
- We introduce an approximation with its own set of parameters, $q_\phi$, and learn these parameters such that

$$q_\phi(z) \approx p(z|x).$$

# VAE: Specifics

- VI idea:

$$\begin{aligned}\mathcal{L}(\theta,\phi;x) =& \text{ELBO}\\ =& \mathbb{E}_{z\sim q_\phi}\Big[\log p_\theta(x|z)\Big] - KL(q_\phi(z)||p(z))\end{aligned}$$

  which is the (negative) loss function we use when training VAEs.
- First term is the expected log-likelihood and the second is the divergence of $q_\phi$ from the true prior.
- The encoder and decoder in a VAE become:
  - **Encoder**: $q_{\phi_i}(z) = q_{\phi_i}(z|x_i) = \mathcal{N}(\mu_i, \sigma_i^2)$ where $\phi_i = (\mu_i, \log \sigma_i)$
  - **Decoder**: $f(z_i) = \theta_i$ typically a neural network

# VAE Pipeline

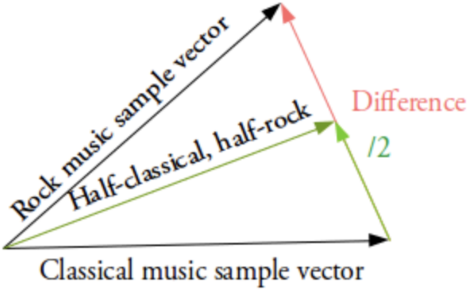
- For a given input (or minibatch) $x_i$,
  - Sample $z_i \sim q_{\phi_i}(z|x_i)$. This is the code in our feature space $F$.
  - Run the code through decoder and write the likelihood: $p_\theta(x|z)$.
  - Compute the loss function:
    $\mathcal{L}(x;\theta,\phi) = -E_{z_\phi \sim q_\phi}\Big[\log p_\theta(x|z)\Big] + KL(q_\phi(z|x)||p(z))$
- Use gradient-based optimization to backpropogate $\nabla_\theta L$, $\nabla_\phi L$

# After VAE is trained

- Once a VAE is trained, we can sample new inputs

$$z \sim p(z) \qquad \tilde{x} \sim p_\theta(x|z)$$

- We can also interpolate between inputs, using simple vector arithmetic.




Interpolating between samples

# Example: MNIST

- We choose the prior on $z$ to be the standard Gaussian

$$p(z) \sim \mathcal{N}(0, I)$$

- our likelihood function to be

$$p_\theta(x|z) = \text{Bernoulli}(\theta)$$

- and our approximate posterior is

$$q_{\phi_i}(z|x_i) = \mathcal{N}(\mu_i, \sigma_i^2 I)$$

- To get our reconstructed input, we simply evaluate

$$\tilde{x} \sim p_\theta(x|z)$$

- We will use neural networks as our encoder and decoder!

# The Reparametrization Trick

- Encoder generates a code by sampling from $q_\phi(z|x)$.
- This sampling process introduces a major problem: gradients are blocked from flowing into the encoder, and hence it will not train.
- To solve this problem, we use the **reparameterization trick**.
  - Instead of sampling $z$ directly from its distribution (e.g. $z_i \sim \mathcal{N}(\mu_i, \sigma_i^2)$) we express $z_i$ as

$$z_i = \mu_i + \sigma_i \times \varepsilon_i \quad \text{where } \varepsilon_i \sim \mathcal{N}(0, I)$$

    with this, gradients can now flow through the entire network.

# Amortized Inference

- Instead of doing VI from scratch every time we see a new datapoint, we learn a function that can look at the data for a point $x_i$, and then output an approximate posterior $q_\phi(z_i|x_i)$. We'll call this a "recognition model"
- Instead of a separate $\phi_i$ for each data example, we'll just have a single global $\phi$ that specifies the parameters of the recognition model.
- Because the relationship between data and posteriors is complex and hard to specify by hand, we'll do this with a neural network!

# Amortized Inference

- We can simply have a network take in $x_i$, and output the mean and variance vector for a Gaussian:
- Then the approximate posterior is given by

$$q_\phi(z_i|x_i) = \mathcal{N}(z_i|\mu_\phi(x_i), \Sigma_\phi(x_i))$$

# VAE vs Amortized VAE Pipeline

- For a given input (or minibatch) $x_i$,
  - **Standard VAE**
  - Sample $z_i \sim q_{\phi_i}(z|x_i) = \mathcal{N}(\mu_i, \sigma_i^2 I)$.
  - **Amortized VAE**
  - Sample $z_i \sim q_{\phi}(z|x_i) = \mathcal{N}(\mu_{\phi}(x_i), \Sigma_{\phi}(x_i))$
- Run the code through decoder and get likelihood: $p_\theta(x|z)$.
- Compute the loss function:
  $L(x;\theta,\phi) = -E_{z_\phi \sim q_\phi}\Big[\log p_\theta(x|z)\Big] + KL(q_\phi(z|x)||p(z))$
- Use gradient-based optimization to backpropogate $\nabla_\theta L$, $\nabla_\phi L$

# Standard vs Amortized VAE

- This allows us to use the share parameters for all data points, and reduce the number of parameter for the encoder to that of the encoding NN.
- Standard VAE encoder is more expressive since no parameters are shared across different data points.

# Example: MNIST

- We choose the prior on $z$ to be the standard Gaussian

$$p(z) \sim \mathcal{N}(0, I)$$

- our likelihood function to be

$$p_\theta(x|z) = \text{Bernoulli}(\theta)$$

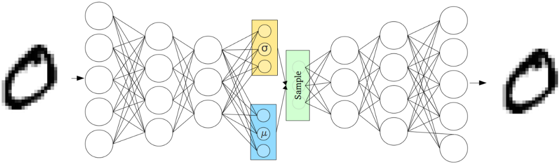
- and our approximate posterior is

$$q_\phi(z|x_i) = \mathcal{N}(\mu_\phi(x_i), \Sigma_\phi(x_i))$$

- Finally, we use neural networks as our encoder and decoder
  - **Encoder**: $g_\phi(x_i) = [\mu(x_i), \log \Sigma(x_i)]$
  - **Decoder**: $f_\theta(z_i) = \theta(z_i)$
  - where $\theta_i$ are parameters of a Bernoulli rv for each input pixel.
- To get our reconstructed input, we simply evaluate

$$\tilde{x} \sim p_\theta(x|z)$$

# Example: MNIST




- We use neural networks for both the encoder and the decoder.
- We compute the loss function $-\mathcal{L}(\theta, \phi; x)$ and propagate its derivative with respect to $\theta$ and $\phi$, $\nabla_\theta L$, $\nabla_\phi L$, through the network during training.
- We need reparametrization trick as before!

# MNIST: Autoencoder vs VAE

Codes generated by L: AE R: VAE


Image credit: I. Shafkat

# VAE loss interpretation

- The VAE maximization objective can be written as

$$\begin{aligned}\mathcal{L}(x;\theta,\phi) =& E_{z_\phi \sim q_\phi}\Big[\log p_\theta(x|z)\Big] - KL(q_\phi(z|x)||p(z)) \\ =& E_{z_\phi \sim q_\phi}\Big[\log p_\theta(x,z)\Big] + H(q_\phi)\end{aligned}$$

- **Interpretation 1:** Maximize expected complete data log-likelihood while penalizing low entropy solutions.
- **Interpretation 2:** Maximize expected log-likelihood while penalizing solutions that are different from the prior.

# Summary

- This lecture covered the basics of variational inference:
  - Elbo
  - Autoencoders
  - VAEs