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Fundamental Concepts of Generative Machine Learning

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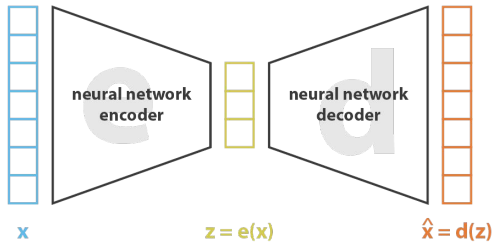
Lesson 3: Auto-Encoding

Welcome to **Part III: “Auto-Encoding”**

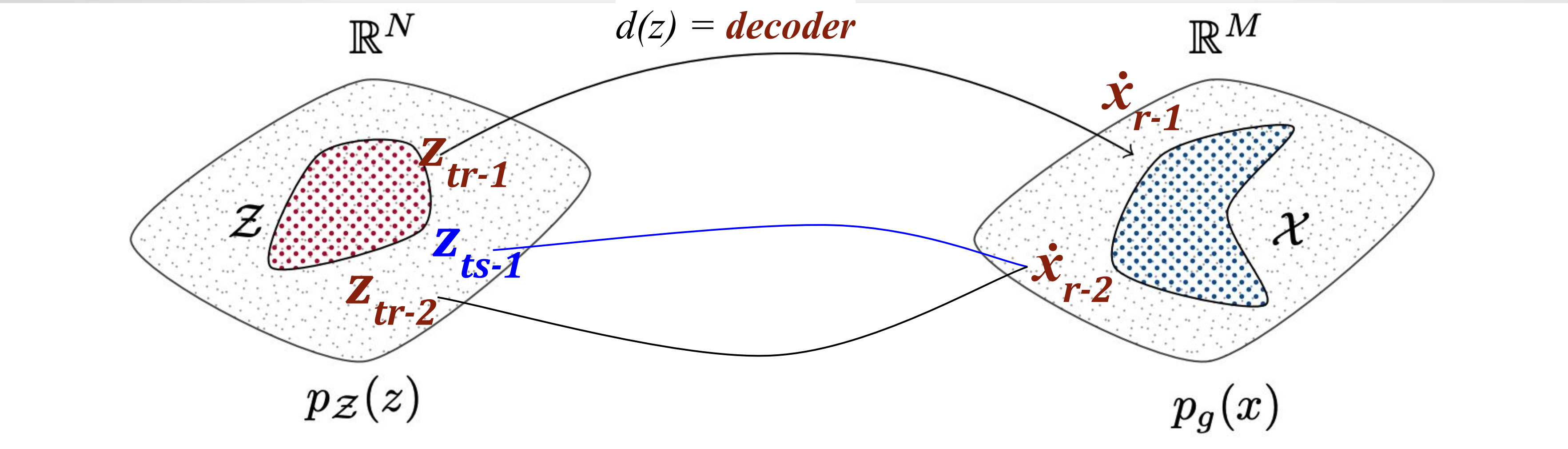
This part includes three subsections:

- Autoencoders and Dimensionality Reduction
- **Variational Inference and VAEs**
- Conclusions

AE problems

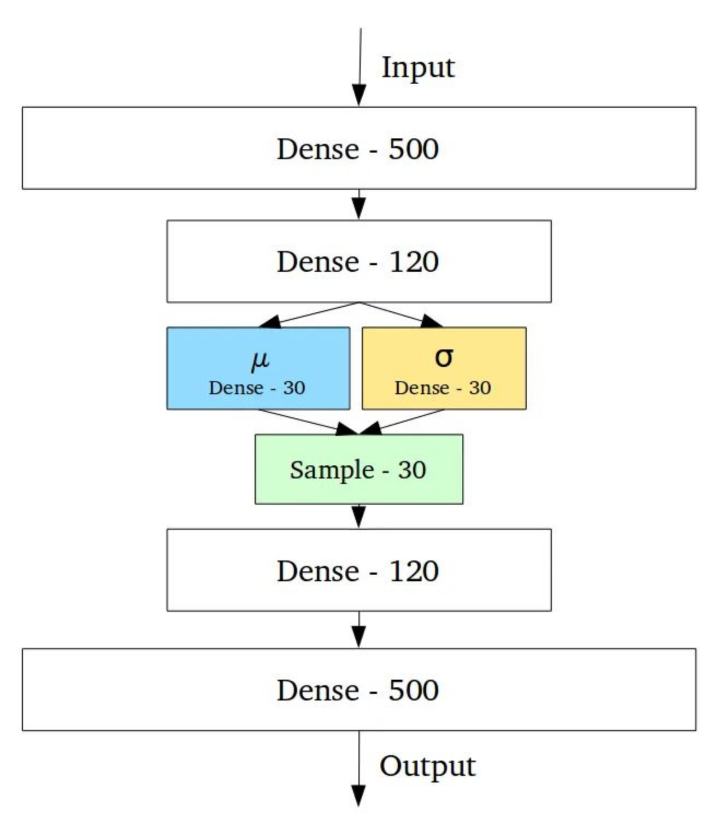


- But when you’re building a generative model, you don’t want to replicate the same input.
- You want to randomly sample from the latent space, or generate variations on an input image, from a continuous latent space.



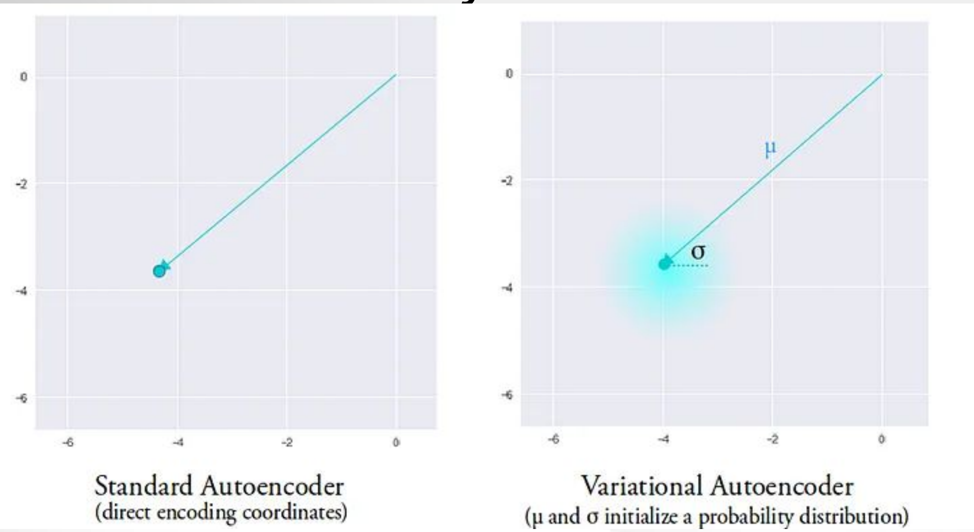
Variational AutoEncoders (VAEs)

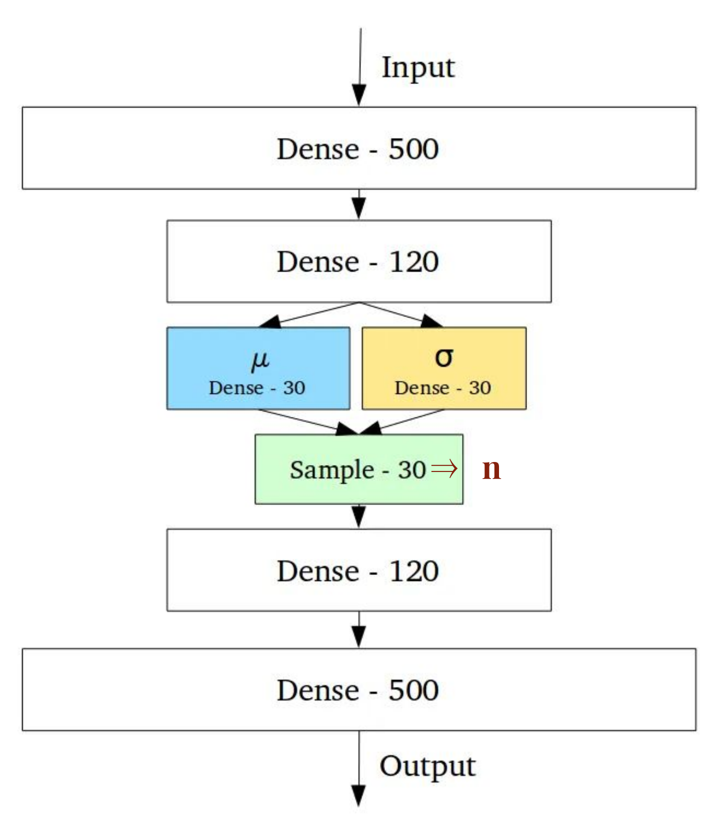
- Variational Autoencoders (VAEs) have one fundamentally unique property that separates them from vanilla autoencoders, and it is this property that makes them so useful for generative modeling:
- their latent spaces are, **by design**, continuous, allowing easy random sampling and interpolation.



Variational AutoEncoders (VAEs)

- Instead of mapping the input to a fixes latent vector, they map it to a distribution!
- What is more, VAEs force the latent variables to be Normal distributed.
- It achieves this by making its encoder :
  *- not output an encoding vector of size **n** (like AEs),*
  *- rather, outputting two vectors of size **n**:*
  - *a vector of means, **μ**,*
  - *and another vector of standard deviations, **σ**.*





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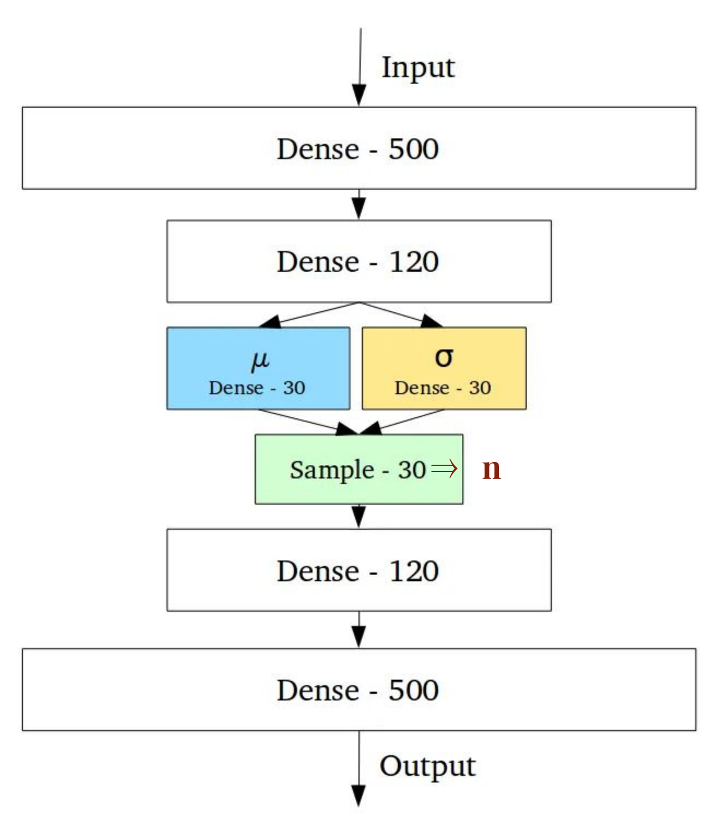
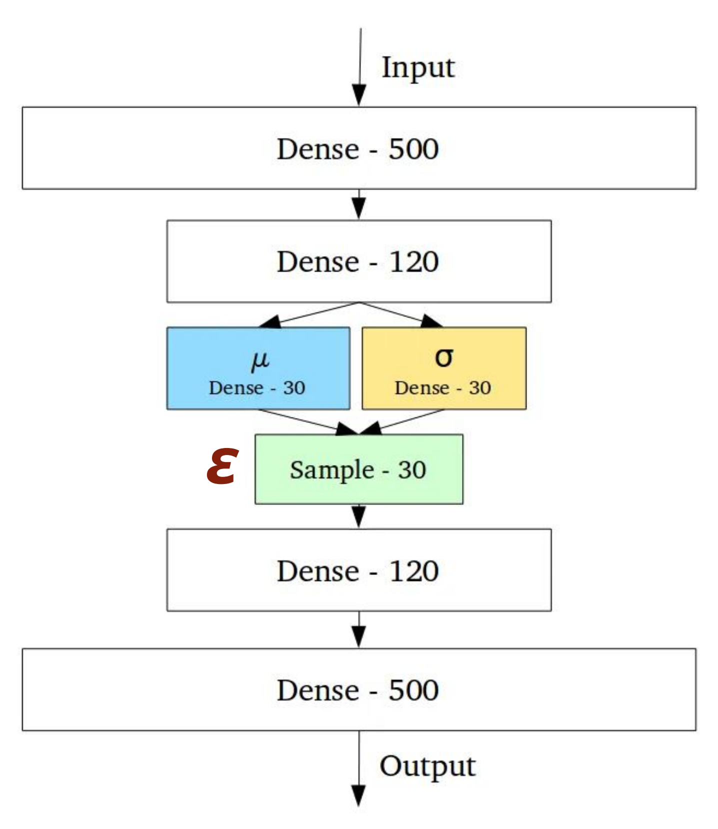


figure from https://towardsdatascien...

Variational AutoEncoders (VAEs)

- To achieve this, VAEs introduce two additional layers in the bottleneck: the mean layer and the standard deviation layer.
- These layers take the output of the previous bottleneck layer and output the mean vector ($\boldsymbol{\mu}$) and the standard deviation vector ($\boldsymbol{\sigma}$) respectively.
- Specifically, we sample a vector $\boldsymbol{\varepsilon}$ from a standard normal distribution (zero-mean, uniti var), and sample **z,** accordingly.

$$\mathbf{z = \mu + \sigma * \varepsilon}$$

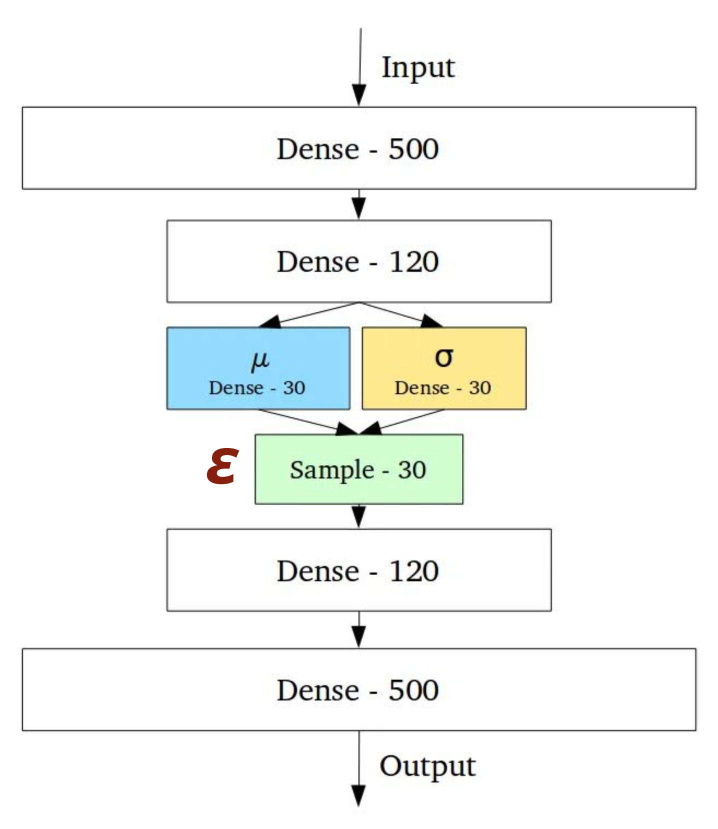


Variational AutoEncoders (VAEs)

- Here, $\boldsymbol{\varepsilon}$ serves as a source of randomness and allows us to sample different points from the latent space during training or generation.
- Ok. Perfect. Forward run is stochastic! Great! But:

How is this random operation handled during training? Can you backpropagate a layer that creates a random variable?

$$z = \mu + \sigma * \varepsilon$$



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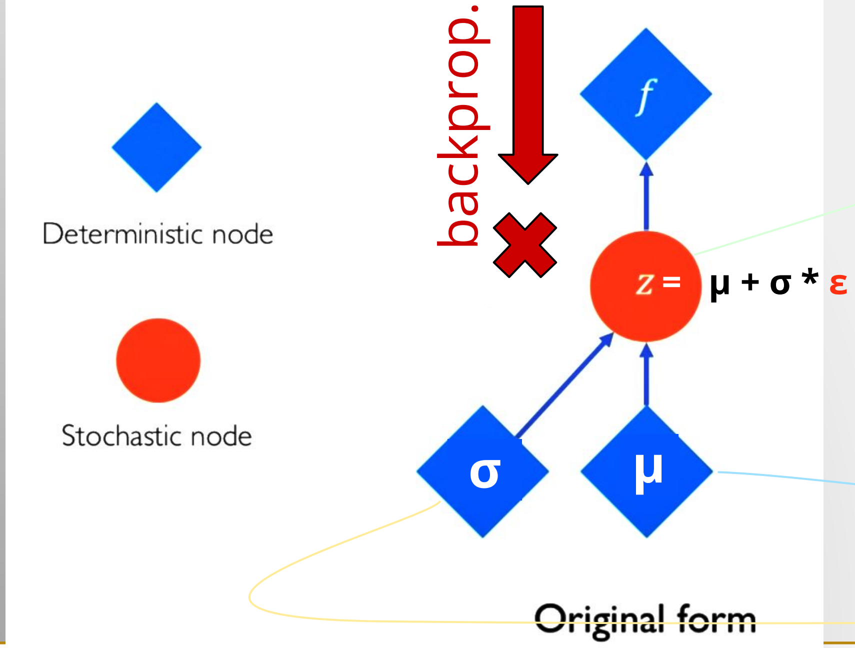
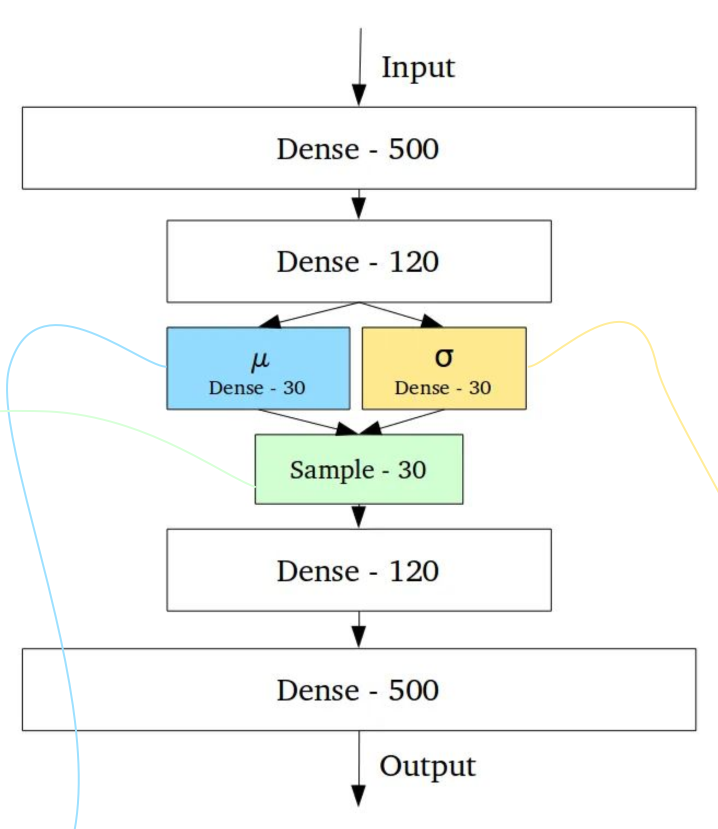
Reparameterization Trick

- The random sampling operation in VAEs, where **ε** is drawn from a standard normal distribution, introduces a challenge for backpropagation since it involves a non-differentiable operation.





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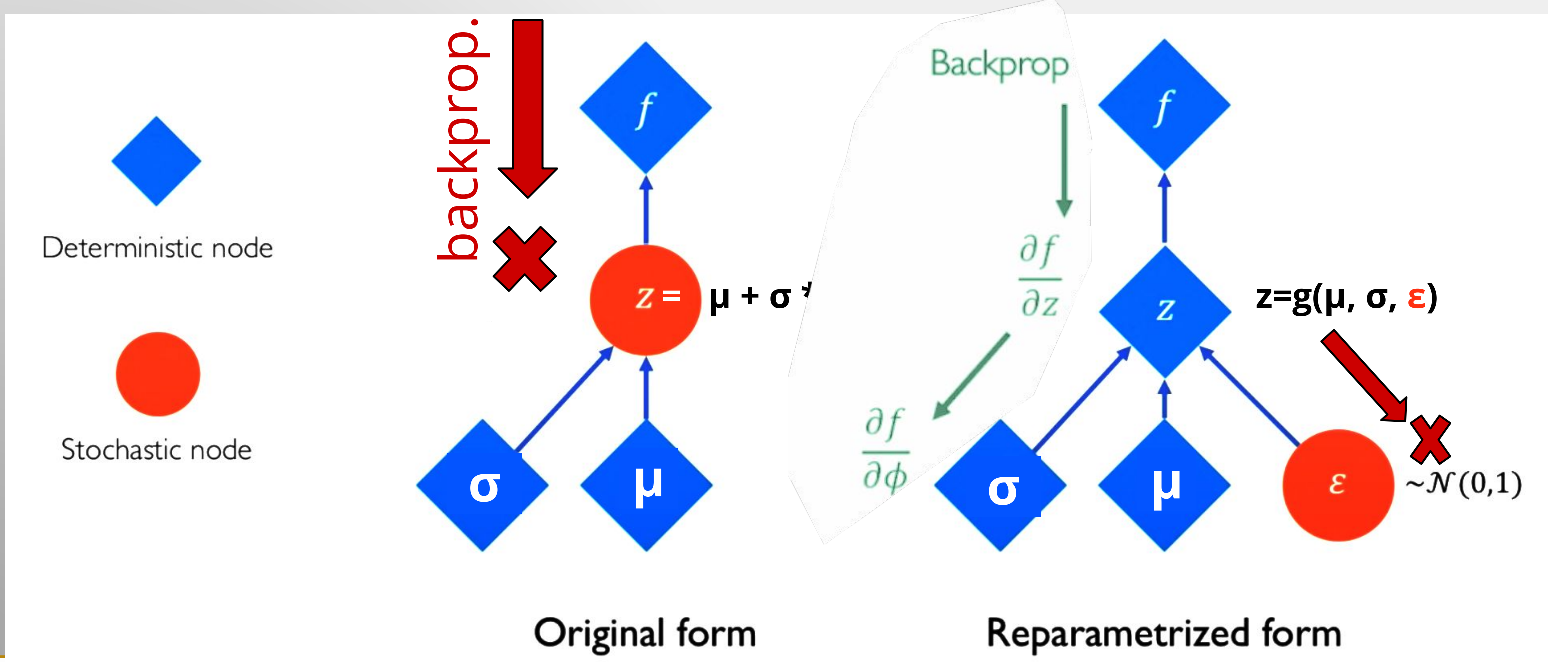

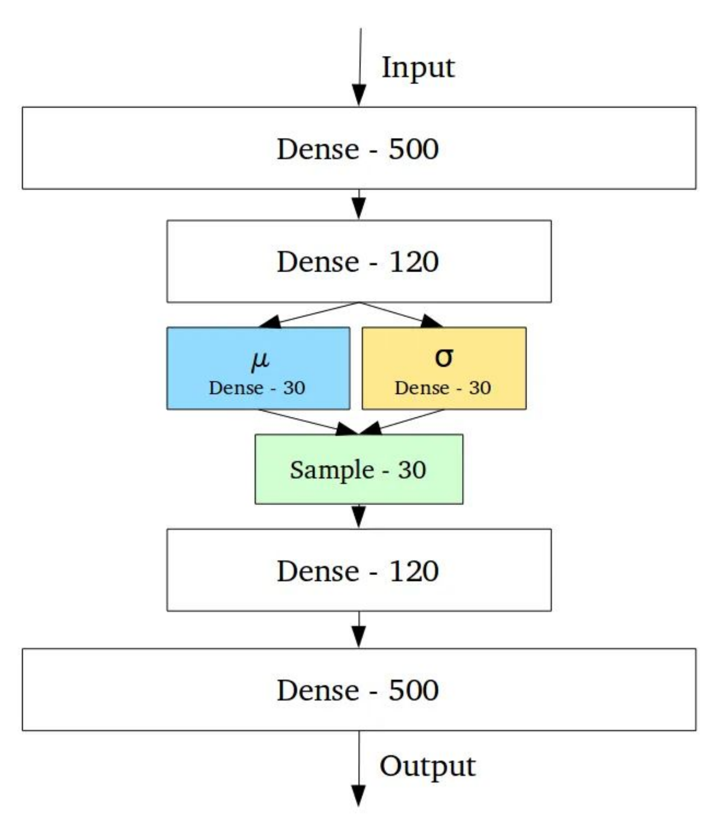

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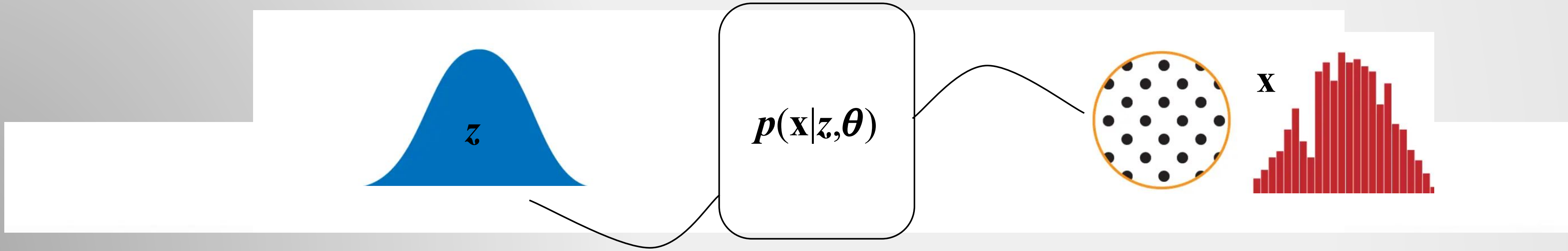
VAE Loss as ELBO

- To train a VAE, we need to maximize the likelihood of the observed data 'x' given the model parameters 'θ'. However, directly computing p(x | z, θ) is not feasible because we do not have access to the “true” latent variables 'z', and the encoding process is not perfectly reversible.
- Instead, VAEs use the Evidence Lower Bound (ELBO) as an approximation to the log-likelihood. The ELBO involves two terms: the expected log-likelihood of the data given the latent space (decoder part) and the negative KL divergence between the approximate posterior (encoded distribution) and the prior distribution over the latent space.

$$\mathcal{L}(\phi, \theta, x) = \boxed{\text{(reconstruction loss)}} + \text{(regularization term)}$$

VAE Loss as ELBO

- By maximizing the ELBO, the VAE effectively encourages the latent space to be structured and follow the prior distribution (usually a standard normal distribution), and it encourages the decoder to generate data that is similar to the observed data.
- The inability to directly calculate p(x|z, θ) due to the non-invertibility of the encoder is the reason why VAEs use ELBO for training instead of maximum likelihood.



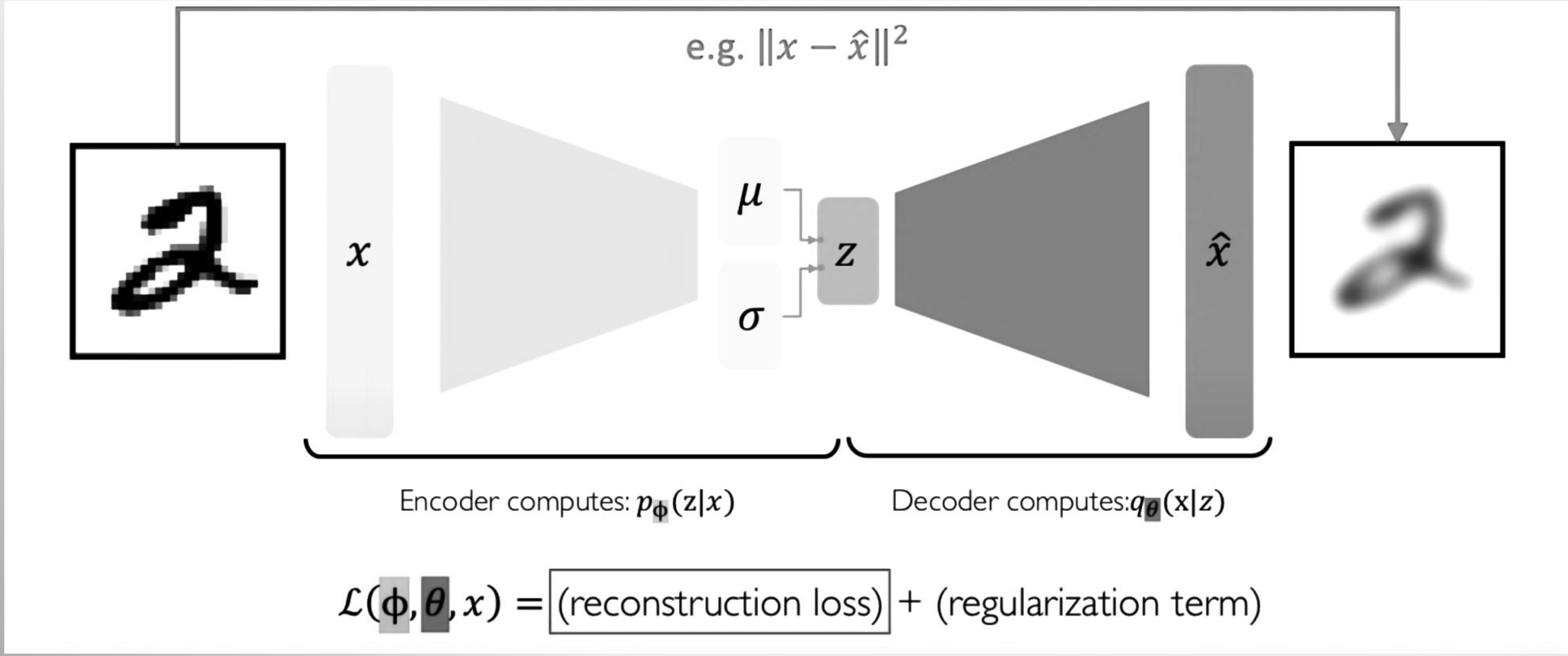
VAE Loss

- So we know how to backprop a VAE. Ready for training then!
- During training, VAEs has two optimization goals:
  - minimize the reconstruction error (similar to traditional autoencoders)
  - and to ensure that the generated latent vectors follow the desired probability distribution.
- The first component is the reconstruction loss and it is trivial.

$$\mathcal{L}(\phi, \theta, x) = \boxed{\text{(reconstruction loss)}} + \text{(regularization term)}$$

VAE Reconstruction Loss

- Reconstruction loss is straightforward.



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VAE Regularization Loss

- So we know how to backprop a VAE. Ready for training then!
- During training, VAEs has two optimization goals:
  - minimize the reconstruction error (similar to traditional autoencoders)
  - and to ensure that the generated latent vectors follow the desired probability distribution.
- The second is done by including a regularization term in the loss function called the Kullback-Leibler (KL) divergence.
  - The KL divergence measures how different the distribution of the generated latent vectors is from the desired distribution (in this case, a standard normal distribution).

$$\mathcal{L}(\phi, \theta, x) = (\text{reconstruction loss}) + \boxed{(\text{regularization term})}$$

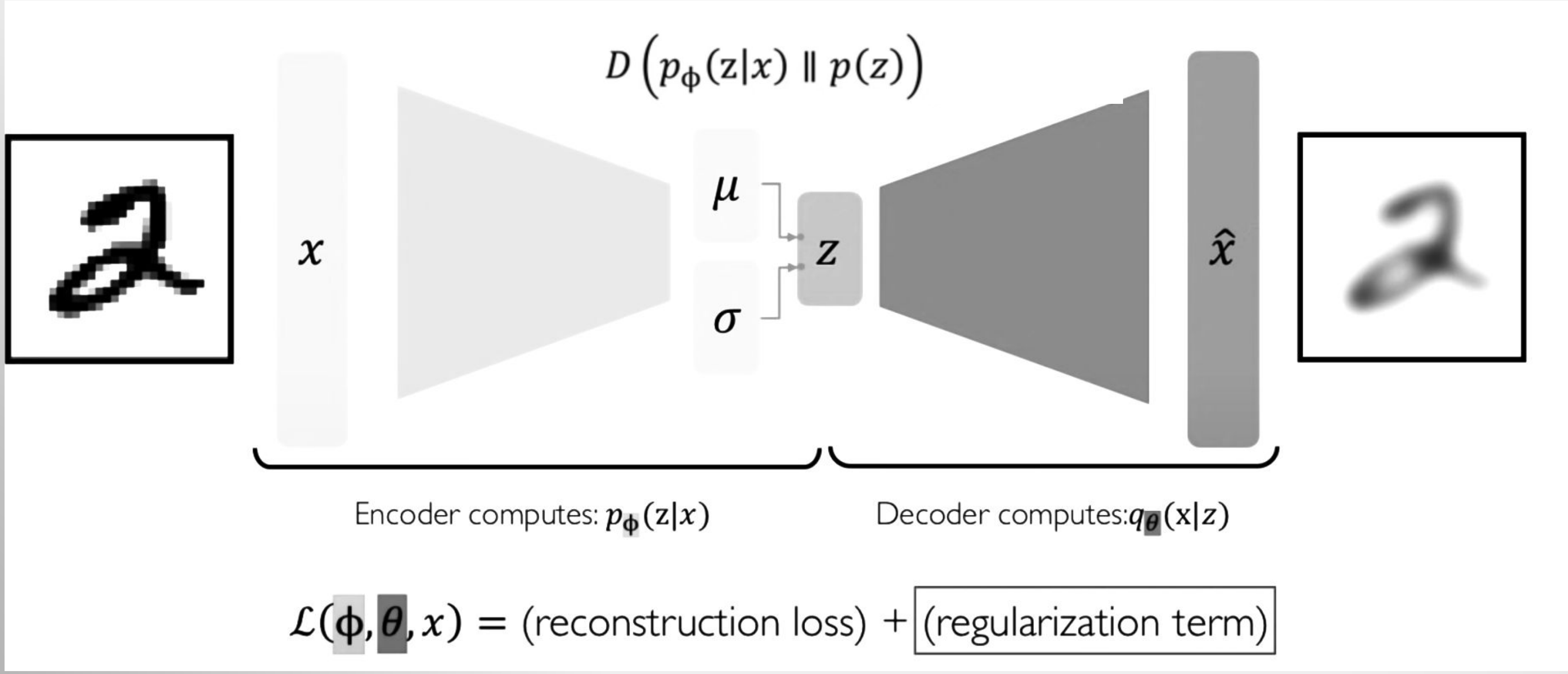
Kullback-Leibler (KL) Divergence

- The KL divergence is a measure of the difference between two probability distributions, P and Q.
- It is defined as the expected value of the logarithmic difference between P and Q, where <u>the expectation is taken with respect to P</u>. The KL divergence is denoted as D(P||Q).

$$D_{KL}(P||Q) = \sum_i P(i) \log \frac{P(i)}{Q(i)}$$

VAE Regularization Loss

- Regularization loss shapes the distributions.



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VAE Regularization Loss

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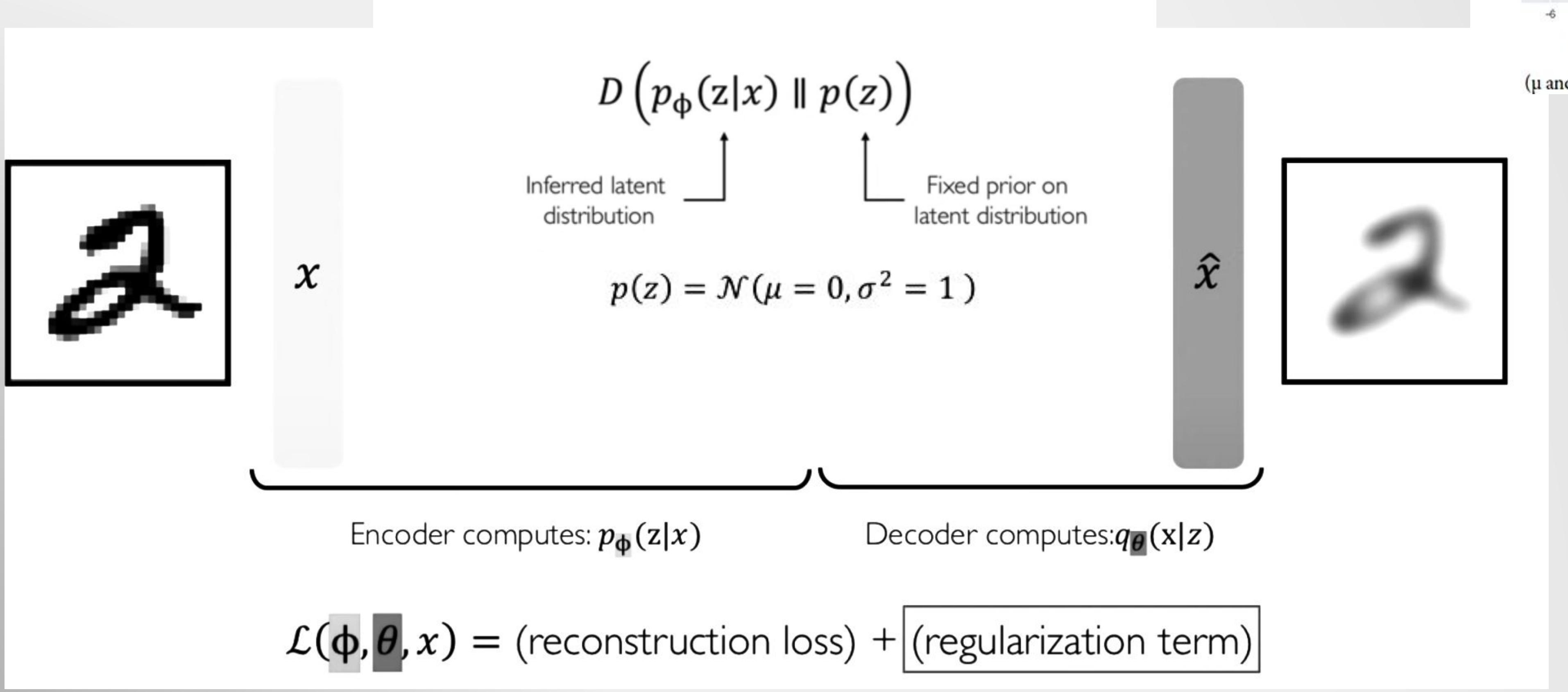

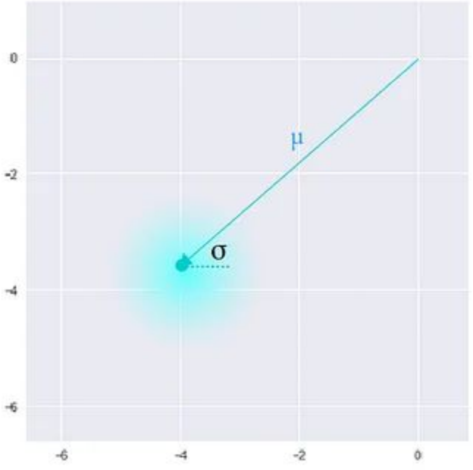

Variational Autoencoder
(μ and σ initialize a probability distribution)

figure from http://introtodeeplearning...

VAE Regularization Loss

- Regularization loss shapes the distributions.

$$D\left(p_{\phi}(z|x) \parallel p(z)\right)$$

Inferred latent distribution

Fixed prior on latent distribution

$$p(z) = \mathcal{N}(\mu = 0, \sigma^2 = 1)$$

- The KL divergence mea ent the distribution of the generated latent vectors is from the desired distribution (in this case, a standard normal distribution).

Next lecture:

- PART III: Auto-Encoding

- Autoencoders and Dimensionality Reduction
- Variational Inference and VAEs
- **Conclusions**

Thanks

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