Deep Learning & Engineering Applications

12. Variational Autoencoders – Part I

JIDONG J. YANG
COLLEGE OF ENGINEERING
UNIVERSITY OF GEORGIA

Supervised vs. unsupervised learning

Most of the supervised learning algorithms are inherently **discriminative**, which means they learn how to model the conditional probability distribution function, $\boldsymbol{p(y|x)}$.

Although we could make predictions with this probability distribution function, we are not allowed to sample new instances from the input distribution directly.

We need generative models!

Taxonomy of Generative Models

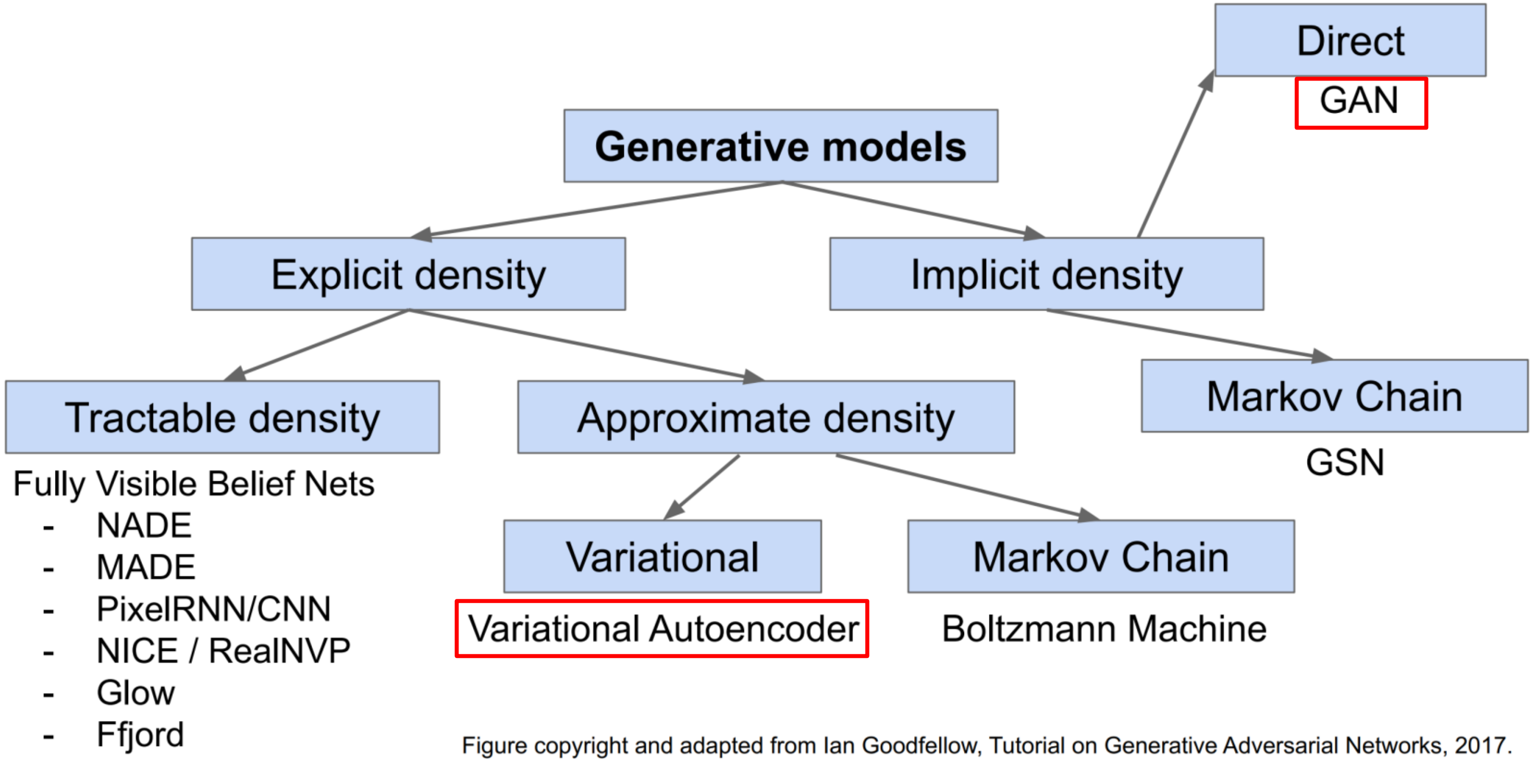
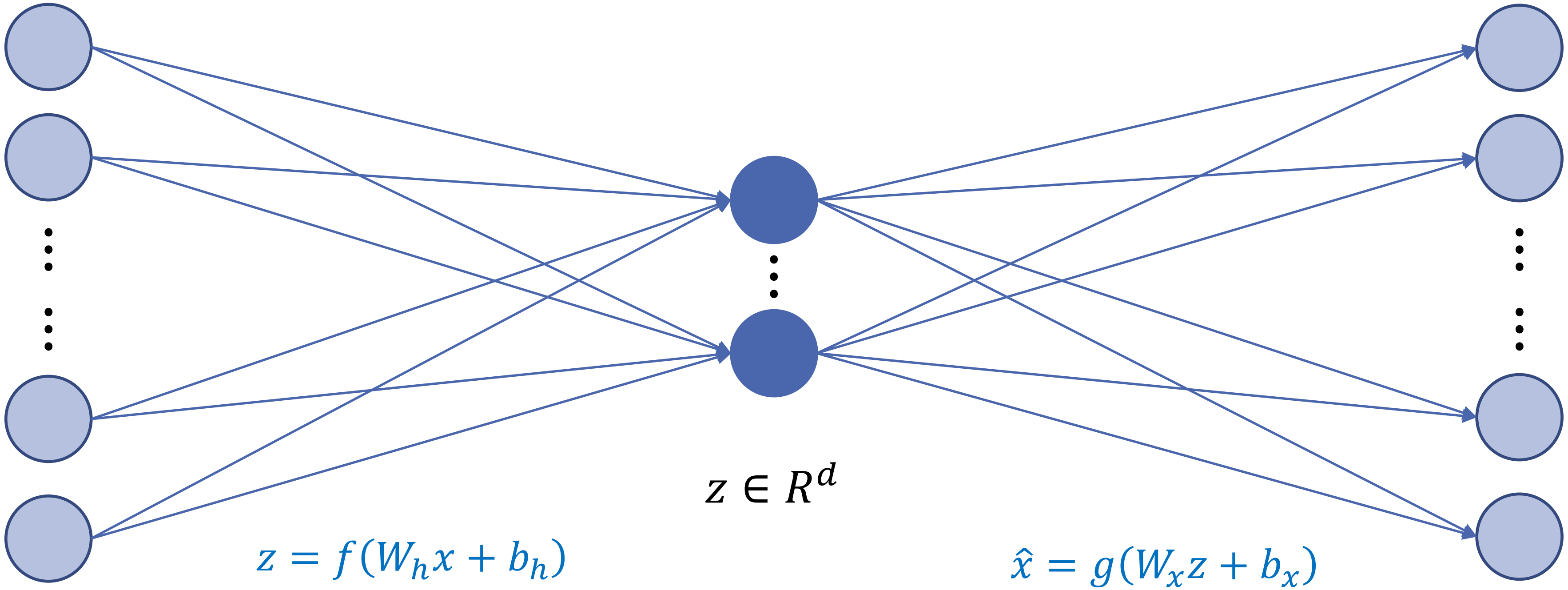


Figure copyright and adapted from Ian Goodfellow, Tutorial on Generative Adversarial Networks, 2017.

Image credit: Fei-Fei Li, Ranjay Krishna, Danfei Xu, Lecture 12: Generative Models, May 11, 2021.
The Original Figure is from Ian Goodfellow, NIPS 2016 Tutorial: Generative Adversarial Networks https://arxiv.org/pdf/1701.00160.pdf

Autoencoder (AE)

Unsupervised approach for learning a lower-dimensional feature representation from unlabeled training data.



$z \in R^d$

$z = f(W_h x + b_h)$

$\hat{x} = g(W_x z + b_x)$

$x \in R^n$

$W_h \in R^{d \times n}$

$W_x \in R^{n \times d}$

$\hat{x} \in R^n$

Under-complete vs. Over-complete Hidden Layer

Does hidden dimension have to be less than the input/output dimension?

What if the hidden dimension is same as or greater than the input dimension?

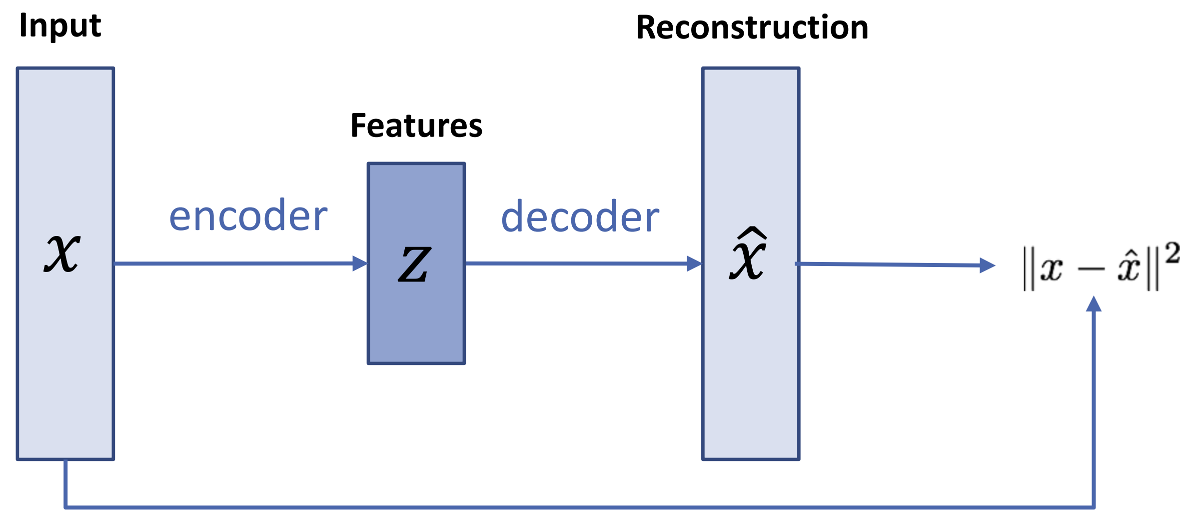
[Ng, lecture note] https://web.stanford.edu/class/cs294a/sparseAutoencoder.pdf
[Rolfe & LeCun, 2013] https://arxiv.org/pdf/1301.3775.pdf

Autoencoder (AE)

Learn representative feature in a lower dimension space.

Train the AE with bottleneck to capture "representative features" in low-dimensional space (compression), which can be used to reconstruct original data.

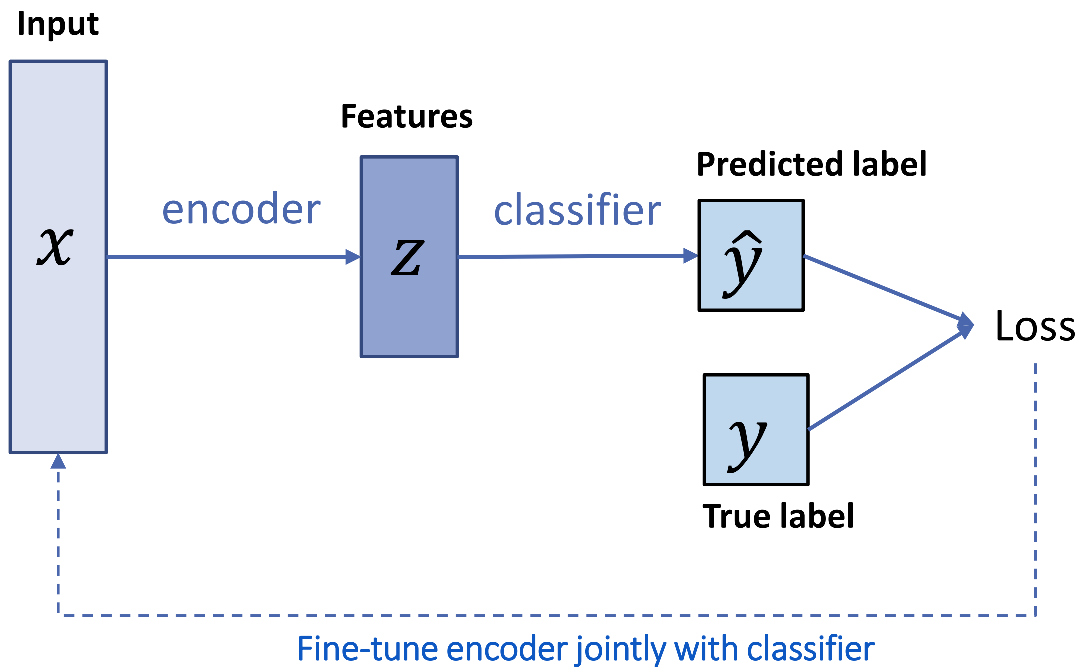
"Autoencoder": Encode input itself.



Common use of AE

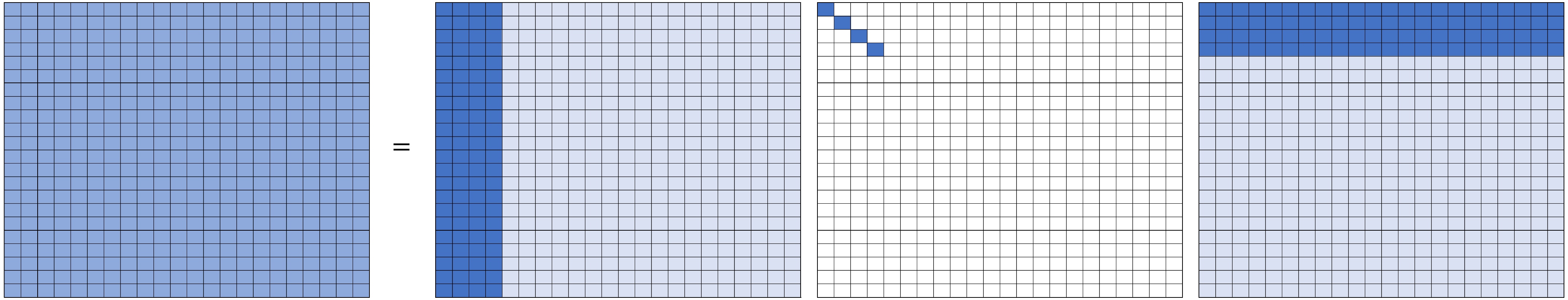
After training, throw away decoder.

Use encoder to initialize a supervised model.

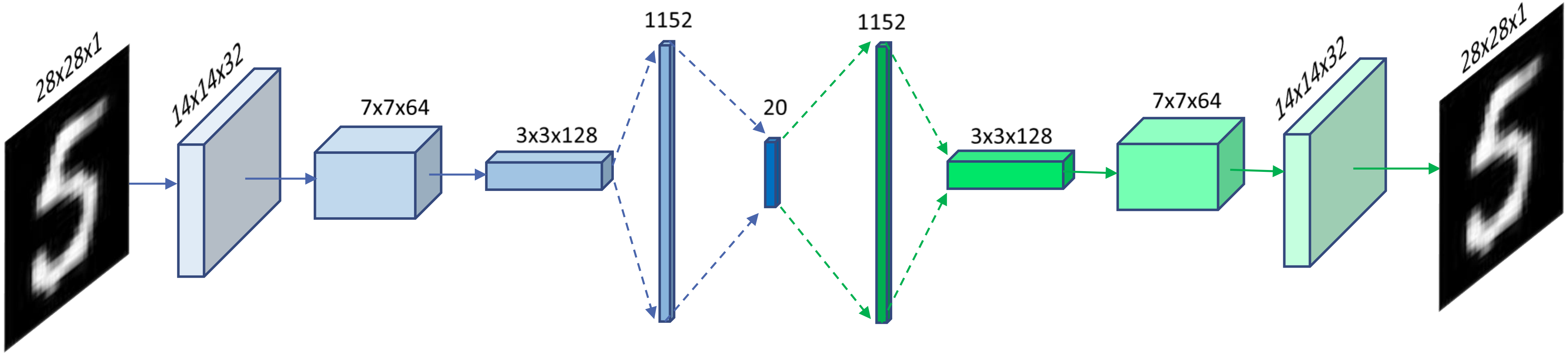


Recall PCA

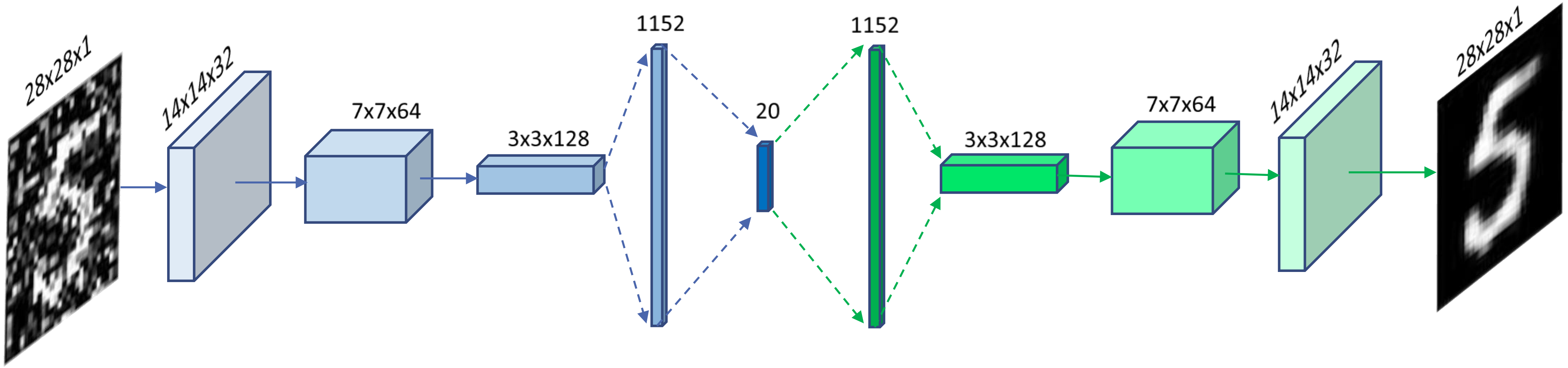
Express the original matrix as a linear combination of k low-rank matrices associated with first k largest singular values.



AE architecture example



Denoising Autoencoder (DAE)



Variational Autoencoder (VAE)

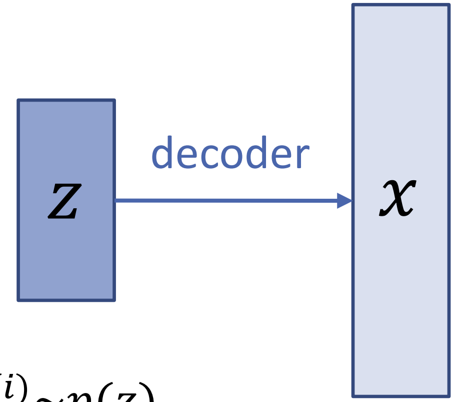
In summary, autoencoders can

- reconstruct data and learn features to initialize a supervised model.
- learned features capture factors of variation in training data.
- use as a denoiser by adding noises to inputs.
- Can we generate new data (e.g., images) from an autoencoder?

Variational Autoencoders

- Probabilistic spin on autoencoders
- Allow to generate data by sampling in the latent space.

Can we generate new x by sampling z?



$z^{(i)} \sim p(z)$

Prior

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

Conditional

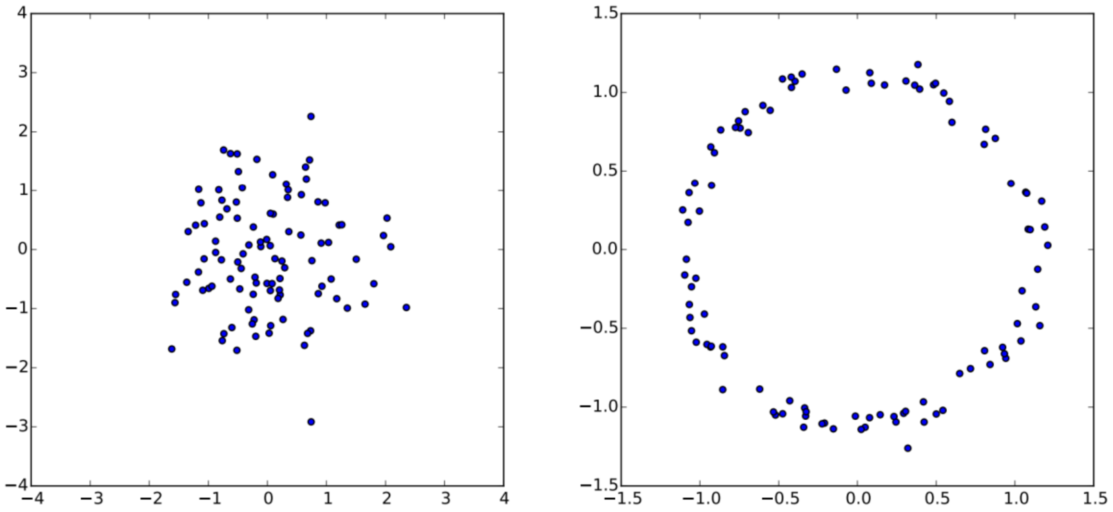
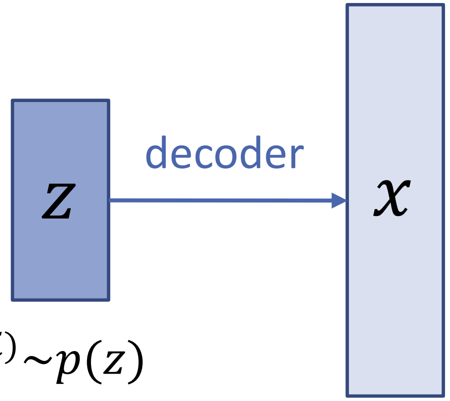


Figure 2: Given a random variable z with one distribution, we can create another random variable $X = g(z)$ with a completely different distribution. Left: samples from a gaussian distribution. Right: those same samples mapped through the function $g(z) = z/10 + z/||z||$ to form a ring. This is the strategy that VAEs use to create arbitrary distributions: the deterministic function g is learned from data.

[Doersch 2016] https://arxiv.org/pdf/1606.05908.pdf

Generate new x by sampling in z



$z^{(i)} \sim p(z)$

Prior

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

Conditional

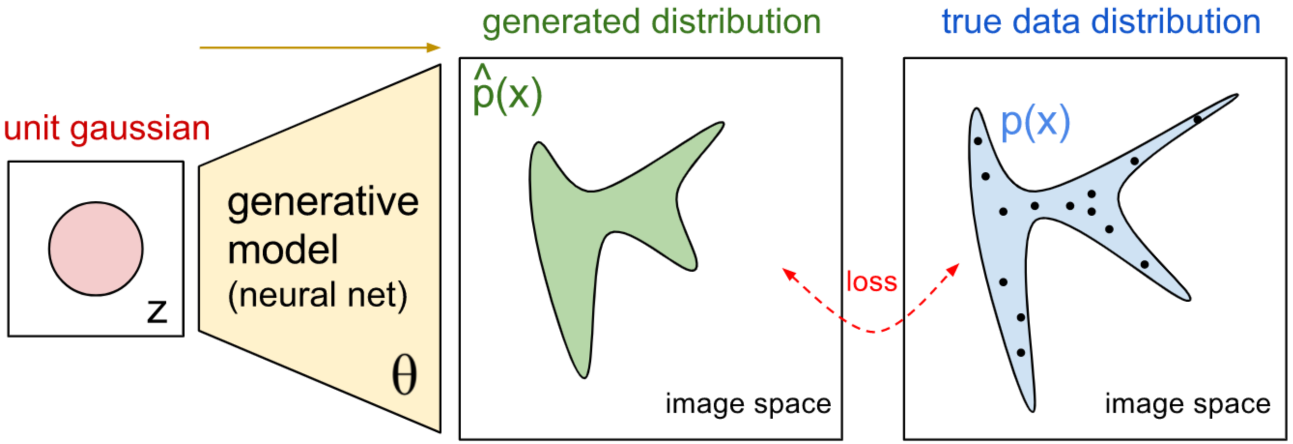
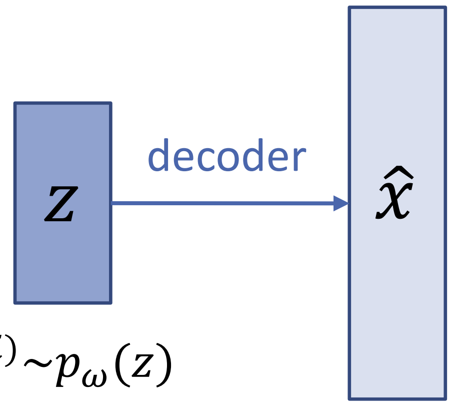


Image credit: https://openai.com/blog/generative-models/

We would like to estimate θ given training data x.

How to formulate the problem?



$z^{(i)} \sim p_{\omega}(z)$ $\quad$ $x \sim p_{\theta}(x|z^{(i)})$

Prior

We would like to estimate θ given training data x.

Maximize likelihood of training data, i.e.,

Data likelihood: $p_{\theta}(x) = \int p(z) p_{\theta}(x|z) dz$

Gaussian NN

Monte-Carlo estimation: $\log p_{\theta}(x) \approx log \left[\frac{1}{K} \sum_{i=1}^{K} p_{\theta}\left(x|z^{(i)}\right) \right]$

Posterior density: $p_{\theta}(z|x) = \frac{p_{\theta}(x|z)p(z)}{p_{\theta}(x)}$

Both data likelihood and posterior density are intractable.

$$p_\theta(x) = \int p(z)p_\theta(x|z)dz$$

Solutions?

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

"Decouple" the above two equations by learning $\boldsymbol{q_\phi(z|x)}$ to approximate the posterior $\boldsymbol{p_\theta(z|x)}$

i.e., approximate the unknown posterior distribution from the observed data x (**variational inference**).

We will see this allows us to derive a lower bound on the data likelihood that is tractable and optimizable.

$$\log p_\theta(x^{(i)}) = \boldsymbol{E}_{z\sim q_\phi(z|x^{(i)})}[\log p_\theta(x)]$$

This will be handled by sampling from z parametrized by the encoder network.
We will talk about this shortly.

[Kingma & Welling, 2014] https://arxiv.org/pdf/1312.6114.pdf

Variational Autoencoders (VAE)

$$\log p_\theta(x^{(i)}) = \boldsymbol{E}_{z\sim q_\phi(z|x^{(i)})}[\log p_\theta(x)]$$

$$= \boldsymbol{E}_z\left[\log \frac{p_\theta(x^{(i)}|z)p(z)}{p_\theta(z|x^{(i)})}\right]$$

Bayes' Rule

$$= \boldsymbol{E}_z\left[\log \frac{p_\theta(x^{(i)}|z)p(z)}{p_\theta(z|x^{(i)})}\frac{q_\phi(z|x^{(i)})}{q_\phi(z|x^{(i)})}\right]$$

$$= \boldsymbol{E}_z\left[\log\left(p_\theta(x^{(i)}|z)\frac{p(z)}{q_\phi(z|x^{(i)})}\frac{q_\phi(z|x^{(i)})}{p_\theta(z|x^{(i)})}\right)\right]$$

$$= \boldsymbol{E}_z[\log p_\theta(x^{(i)}|z)] - \boldsymbol{E}_z\left[\log \frac{q_\phi(z|x^{(i)})}{p(z)}\right] + \boldsymbol{E}_z\left[\log \frac{q_\phi(z|x^{(i)})}{p_\theta(z|x^{(i)})}\right]$$

$$= \boldsymbol{E}_z[\log p_\theta(x^{(i)}|z)] - \boldsymbol{D}_{\boldsymbol{KL}}\left(q_\phi(z|x^{(i)})||p(z)\right) + \boldsymbol{D}_{\boldsymbol{KL}}\left(q_\phi(z|x^{(i)})||\, p_\theta(z|x^{(i)})\right)$$

Sampling via decoder

Gaussians
for encoder & z prior

Intractable; KL ≥ 0

Likelihood Lower Bound

$$\log p_\theta(x^{(i)}) = \underbrace{\boldsymbol{E}_z\left[\log p_\theta(x^{(i)}|z)\right] - \boldsymbol{D_{KL}}\left(q_\phi(z|x^{(i)})||p(z)\right)}_{\text{Tractable lower bound, which can be optimized. Both terms are differentiable.}} + \underbrace{\boldsymbol{D_{KL}}\left(q_\phi(z|x^{(i)})||\, p_\theta(z|x^{(i)})\right)}_{\geq 0}$$

We can maximize the loglikelihood lower bound.

$$LL(x^{(i)}, \theta, \phi) = \boldsymbol{E}_z\left[\log p_\theta(x^{(i)}|z)\right] - \boldsymbol{D_{KL}}\left(q_\phi(z|x^{(i)})||p(z)\right)$$

Variational Lower Bound (VLB) or Evidence Lower BOund (ELBO)

This is equivalent to minimize the following loss function:

$$Loss(x^{(i)}, \theta, \phi) = \boldsymbol{E}_z\left[-\log p_\theta(x^{(i)}|z)\right] + \boldsymbol{D_{KL}}\left(q_\phi(z|x^{(i)})||p(z)\right)$$

Reconstruction Loss

$$Loss(x^{(i)}, \theta, \phi) = \boxed{\boldsymbol{E}_z[-\log p_\theta(x^{(i)}|z)]} + \boldsymbol{D_{KL}}\left(q_\phi(z|x^{(i)})||p(z)\right)$$

For continuous data, we could choose Gaussian: $p_\theta(x|z) \sim N\left(f(z), \sigma^2 I\right)$

So, we have $\log\ p_\theta(x|z) = C - \frac{1}{2\sigma^2}\|x - f(z)\|^2$

$$l_{recon}(x^{(i)}, \hat{x}^{(i)}) = \boldsymbol{E}_z[-\log p_\theta(x^{(i)}|z)] = \frac{1}{2}\left\|x^{(i)} - f(z)\right\|^2 = \frac{1}{2}\left\|x^{(i)} - \hat{x}^{(i)}\right\|^2$$

For categorical data, we could use cross-entropy:

$$l_{recon}(x^{(i)}, \hat{x}^{(i)}) = \boldsymbol{E}_z[-\log p_\theta(x^{(i)}|z)] = -\sum_{c=1}^{M} x^{(i)} \log p_\theta(x^{(i)}|z)$$

KL divergence of Gaussians

$$Loss(x^{(i)}, \theta, w) = \boldsymbol{E}_z\left[-\log p_\theta\left(x^{(i)}|z\right)\right] + \boxed{\boldsymbol{D_{KL}}\left(q_\phi\left(z|x^{(i)}\right)||p(z)\right)}$$

KL-divergence between two multivariate Gaussian distributions can be computed in closed form:

$$\boldsymbol{D_{KL}}[N(\mu_0, \Sigma_0)||N(\mu_1, \Sigma_1)] = \frac{1}{2}\left(tr\left(\Sigma_1^{-1}\Sigma_0\right) + (\mu_1 - \mu_0)^T \Sigma_1^{-1}(\mu_1 - \mu_0) - k + log\left(\frac{det\Sigma_1}{det\Sigma_0}\right)\right)$$

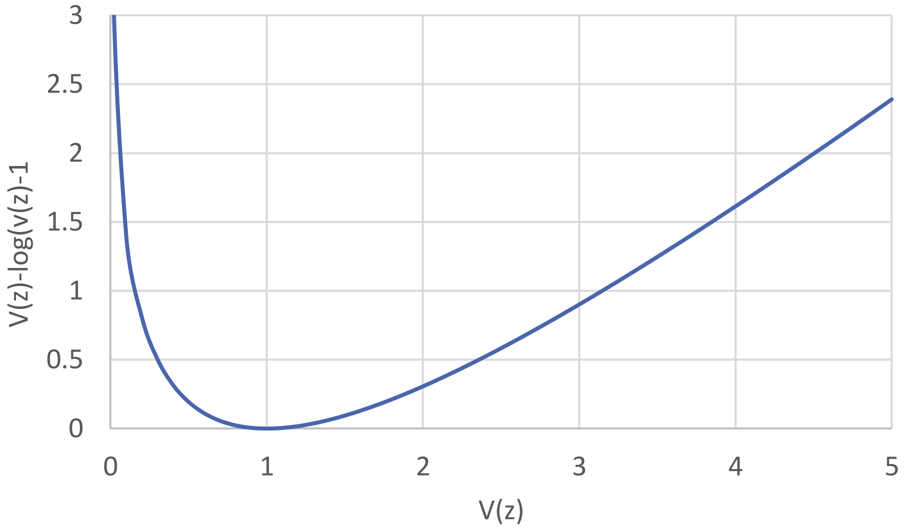
$$\boldsymbol{D_{KL}}[N(\mu(z), \Sigma(z))||N(0, I)] = \frac{1}{2}\left(tr\left(\Sigma(z)\right) + \mu(z)^T\mu(z) - k - logdet\left(\Sigma(z)\right)\right)$$

$q_\phi\left(z|x^{(i)}\right)$ $\quad$ $p(z)$

$$l_{KL}(z, N(0, I_k)) = \frac{1}{2}\sum_{i=1}^{k}\left(V(z_i) + E(z_i)^2 - 1 - \log V(z_i)\right)$$

$$= \frac{1}{2}\sum_{i=1}^{k}\left(V(z_i) - \log V(z_i) - 1 + E(z_i)^2\right)$$

$V(z_i) \rightarrow 1$ $\quad$ $E(z_i) \rightarrow 0$



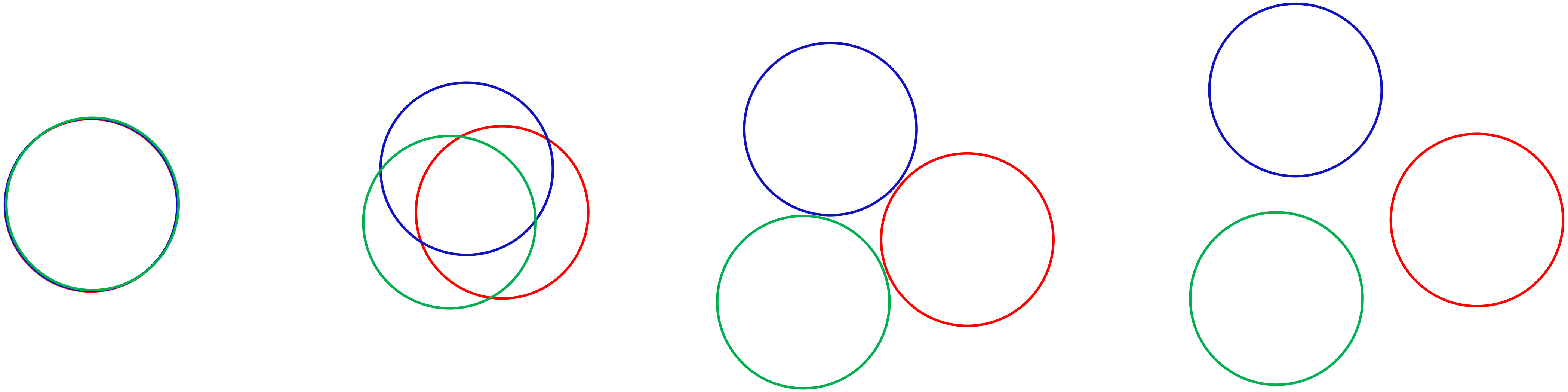
Loss Function

$$Loss\left(x^{(i)}, \theta, w\right) = \boldsymbol{E}_z\left[-\log p_\theta\left(x^{(i)}|z\right)\right] + \boldsymbol{D_{KL}}\left(q_\phi\left(z|x^{(i)}\right)||p(z)\right)$$

$$Loss\left(x^{(i)}, \theta, w\right) = l_{recon}(x^{(i)}, \hat{x}^{(i)}) + \beta l_{KL}(z, N(0, I_k))$$

$$= l_{recon}(x^{(i)}, \hat{x}^{(i)}) + \frac{\beta}{2}\sum_{i=1}^{k}\left(V(z_i) - \log V(z_i) - 1 + E(z_i)^2\right)$$

Illustration of the trade-off between reconstruction loss and KL loss



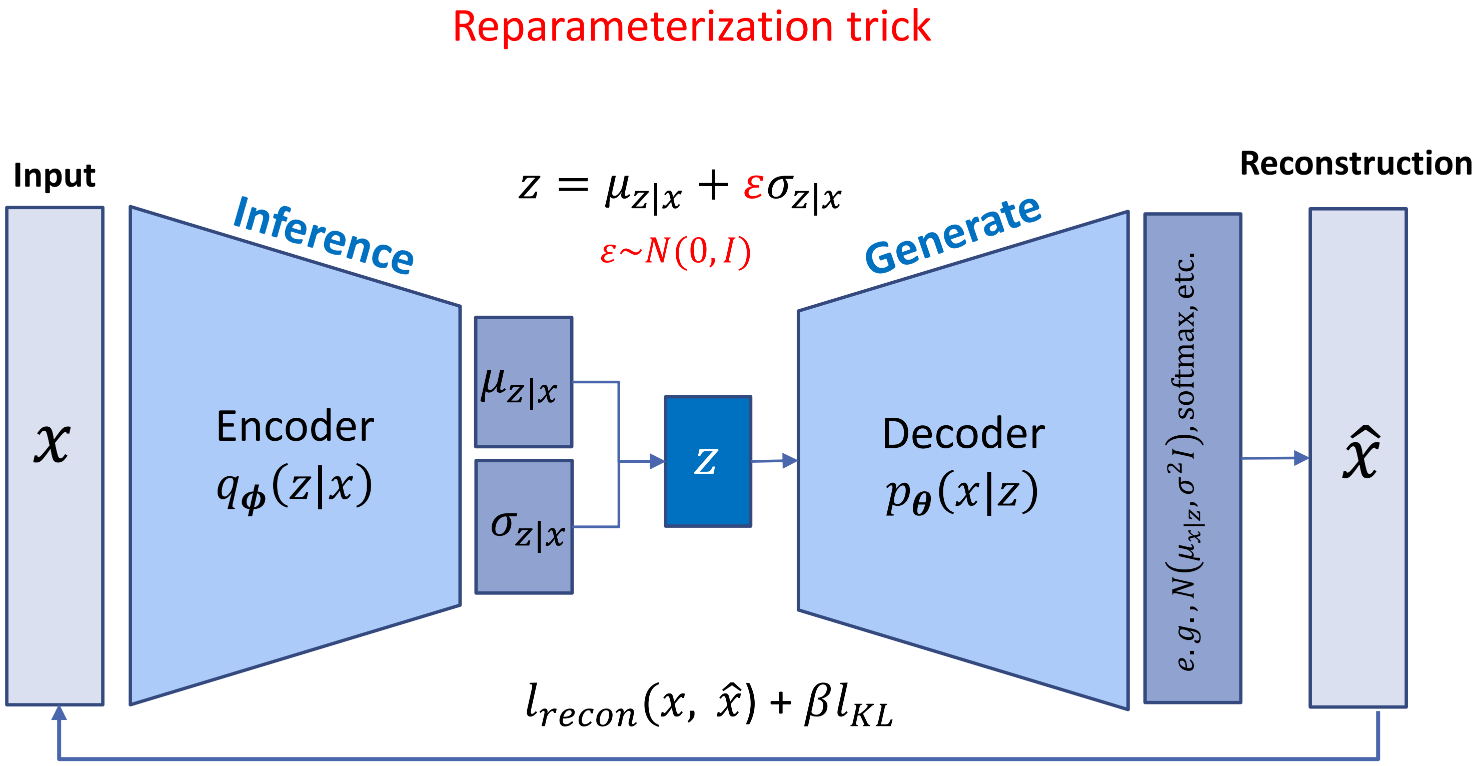
Lowest l_{KL}
Highest l_{recon}

Lower l_{KL}
Higher l_{recon}

Low l_{KL}
Low l_{recon}

Higher l_{KL}
Lower l_{recon}

Train a VAE



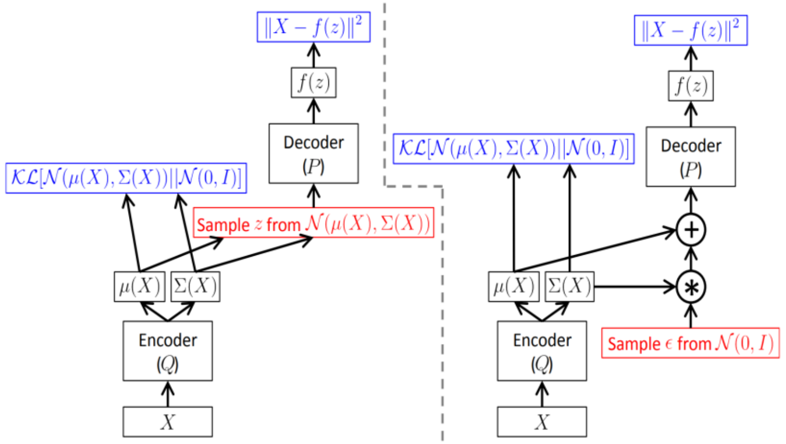


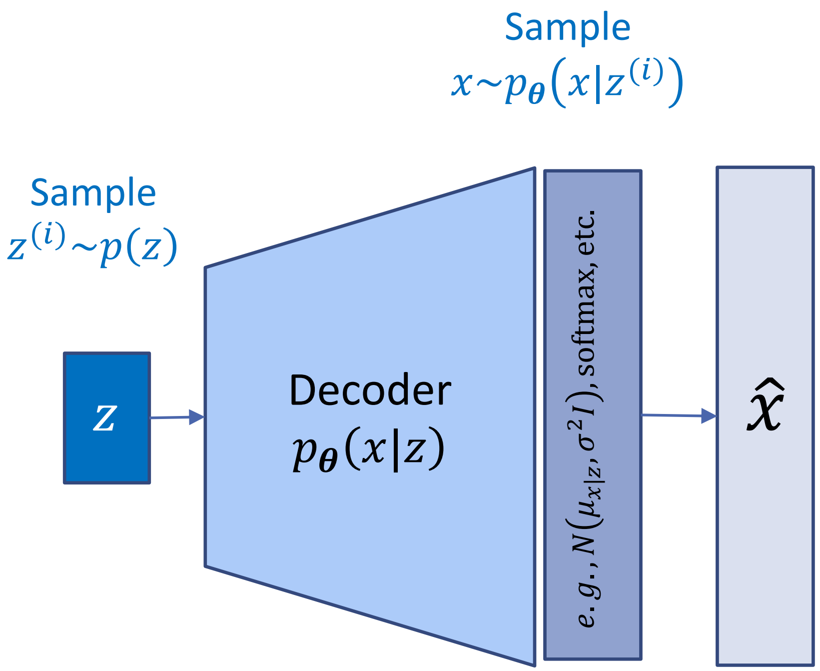
Figure 4: A training-time variational autoencoder implemented as a feed-forward neural network, where $P(X|z)$ is Gaussian. Left is without the "reparameterization trick", and right is with it. Red shows sampling operations that are non-differentiable. Blue shows loss layers. The feedforward behavior of these networks is identical, but backpropagation can be applied only to the right network.

[Doersch 2016] https://arxiv.org/pdf/1606.05908.pdf

Generate data

Given a trained VAE, we can generate data by:

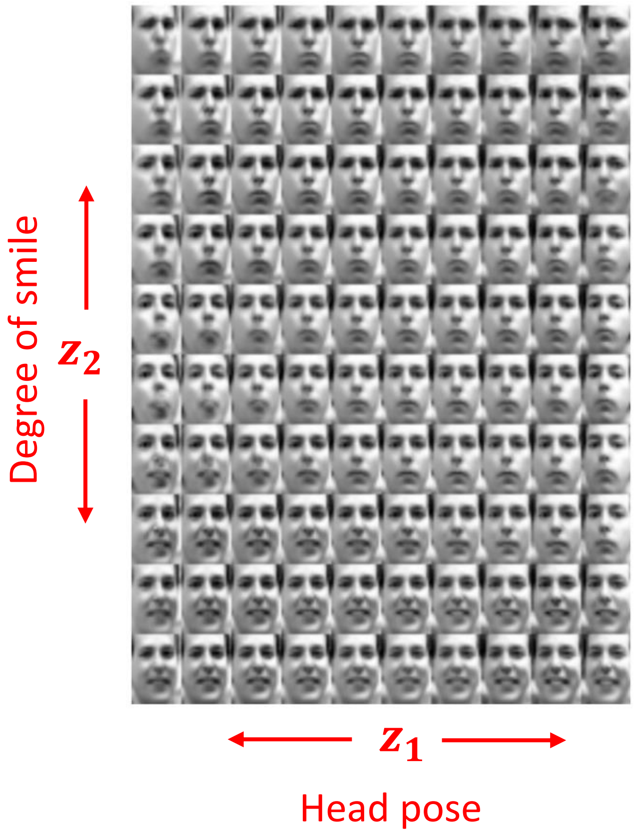
- Sampling z from the prior, $p(z)$
- Sampling x from conditional probability, $p_{\boldsymbol{\theta}}(x|z)$.

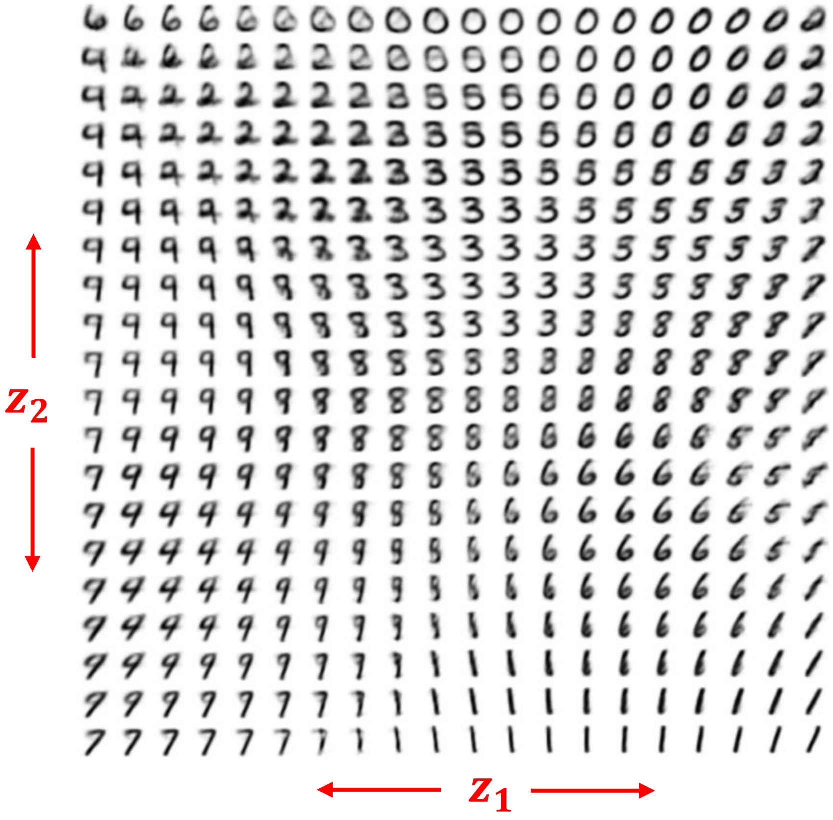


VAE

Learn the low-dimensional data manifold in latent space.

The diagonal prior on z [i.e., $p(\mathrm{z}) \sim N(0, I_k)$] $\rightarrow$ independent latent variables.





[Kingma & Welling, 2013] https://arxiv.org/pdf/1312.6114v10.pdf