From PCA To VAE:
A Comprehensive Survey

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CS 229 Final Project

Introduction

Dimensionality reduction is a fundamental tool in machine learning.

Transform high-dimensional data into a lower-dimensional representation

PCA -> Autoencoder

Generative modeling is an unsupervised form of machine learning where the model learns to discover the patterns in input data.

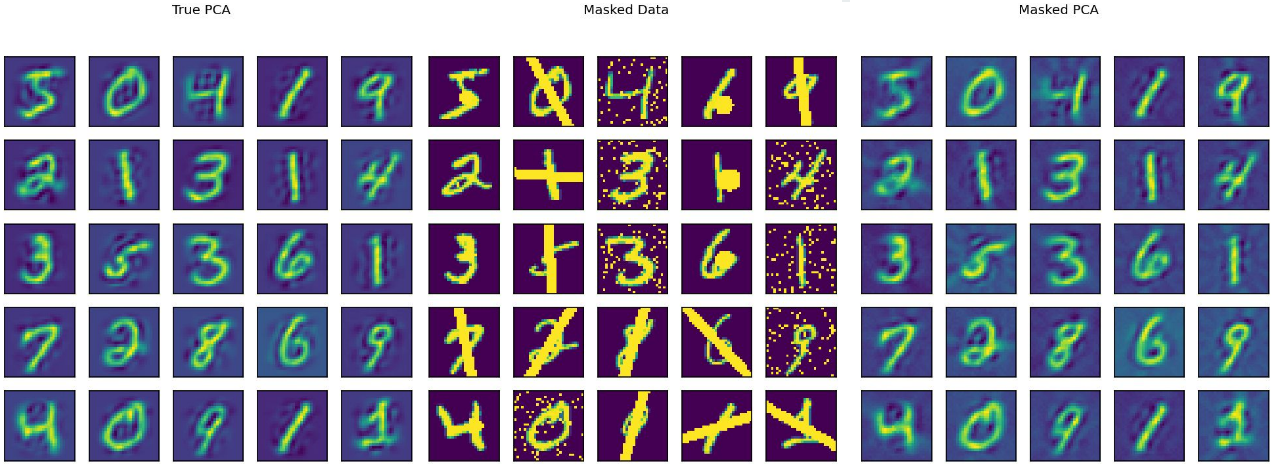
Can generate new data on its own, which is relatable to the original training dataset.

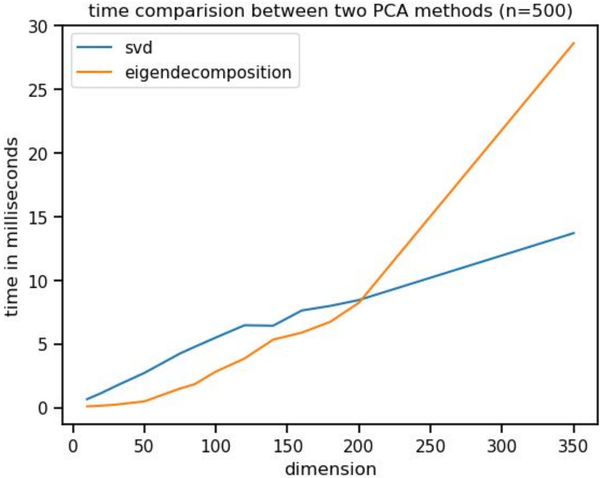
-> Factor Analysis -> Variational Autoencoders !

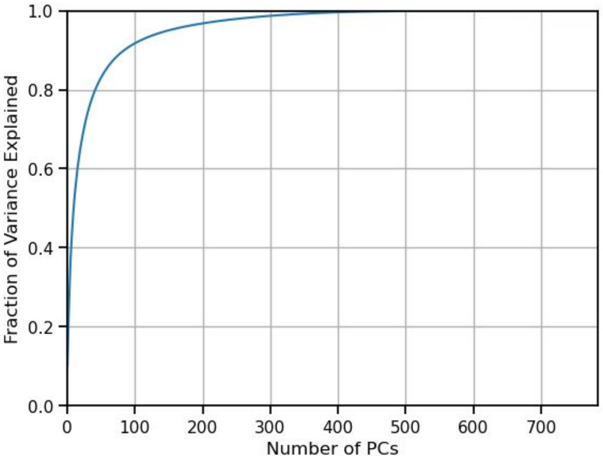
Dataset: MNIST   Reproducible   image dimension: 28*28=784

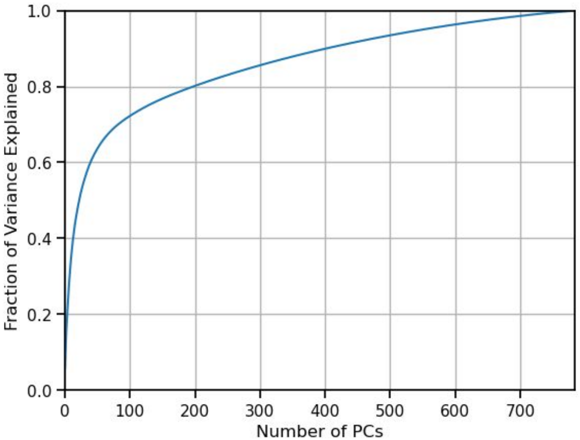
PCA

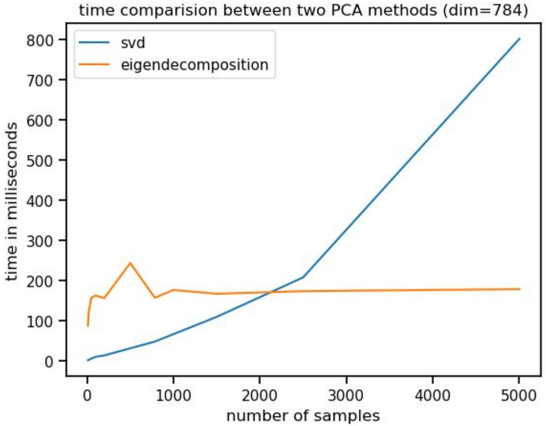
latent dim = 50









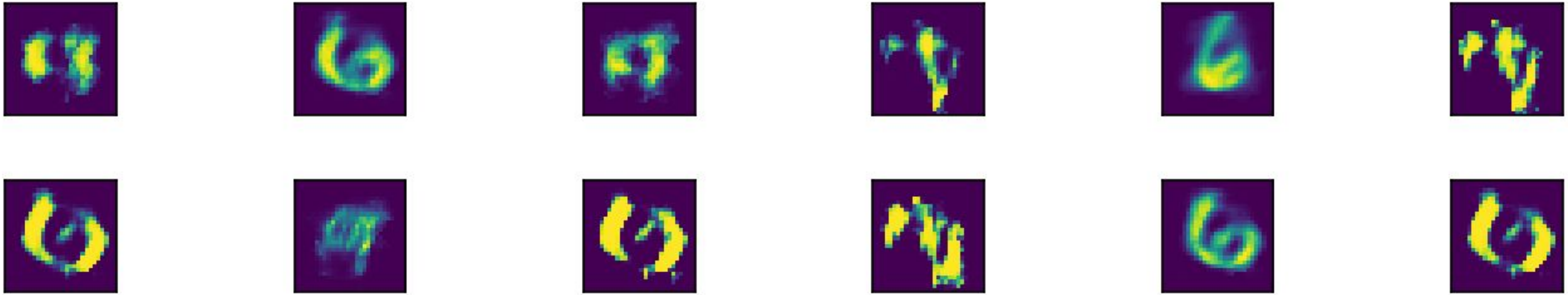


Autoencoder latent dim = 3

True Images

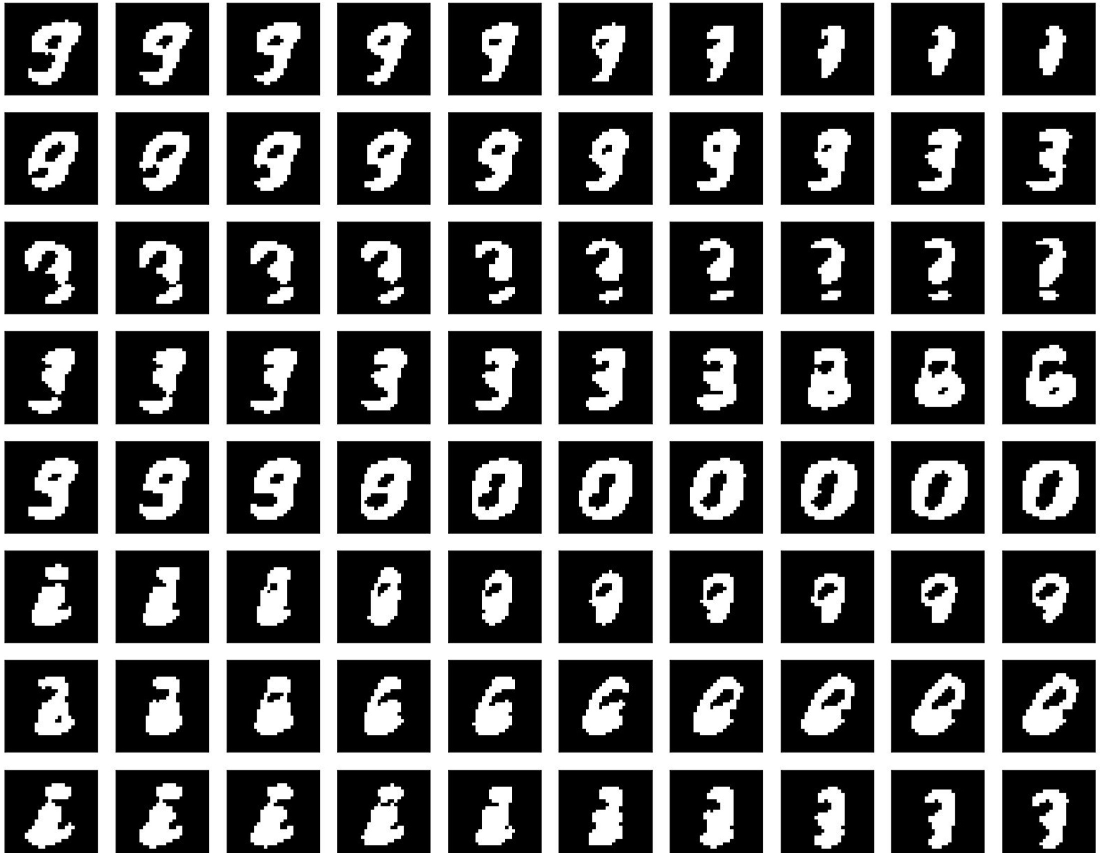
Reconstructed Images

Generated Images



Factor Analysis latent dim = 4

factor analysis interpolated images

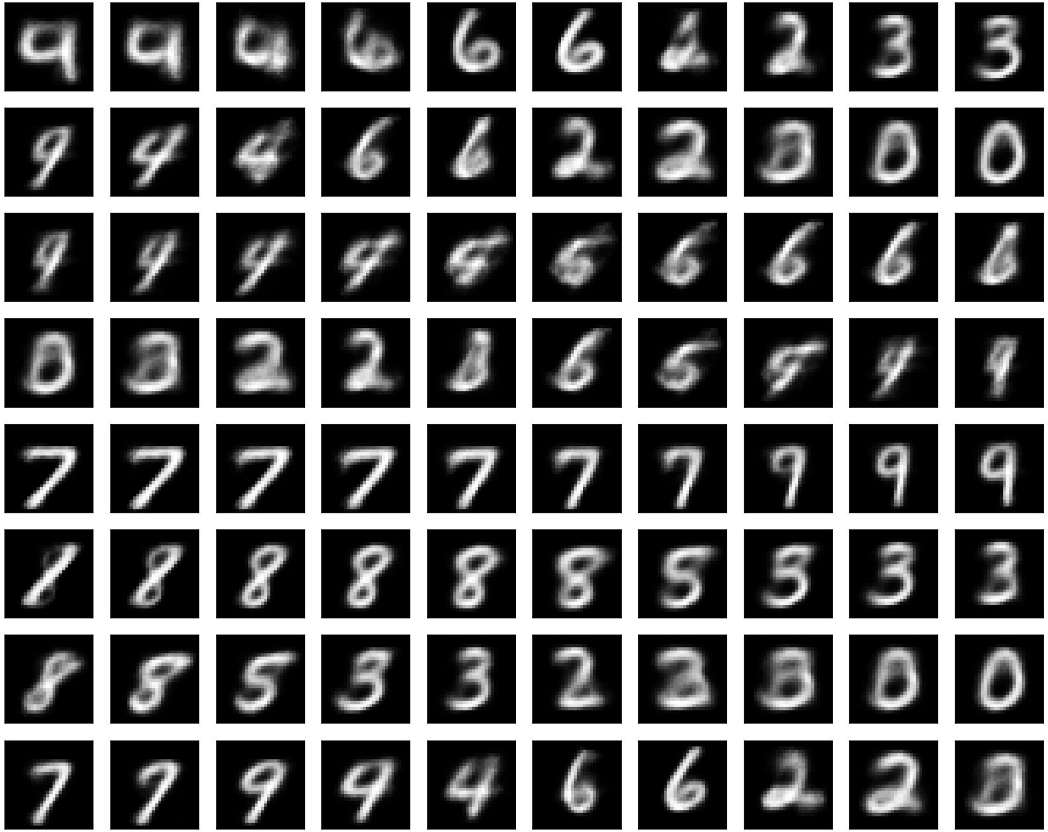


Problem:

Cannot capture non-linear features!

Variational Autoencoder (VAE)

VAE



Much Better!

Still a little bit blurred….

Disentanglement Problem

factor analysis generated images

Factor Analysis On Each Digit

Difficulty in Inference

Hard to Change VAE architecture

Reparametrization Only Works for Certain Distributions:

$$z \in \mathcal{N}(\mu, \sigma^2) \longrightarrow z = \mu + \sigma \odot \epsilon, \text{ where } \epsilon \in \mathcal{N}(0,1)$$

Generally Does Not Work For Discrete Variables!

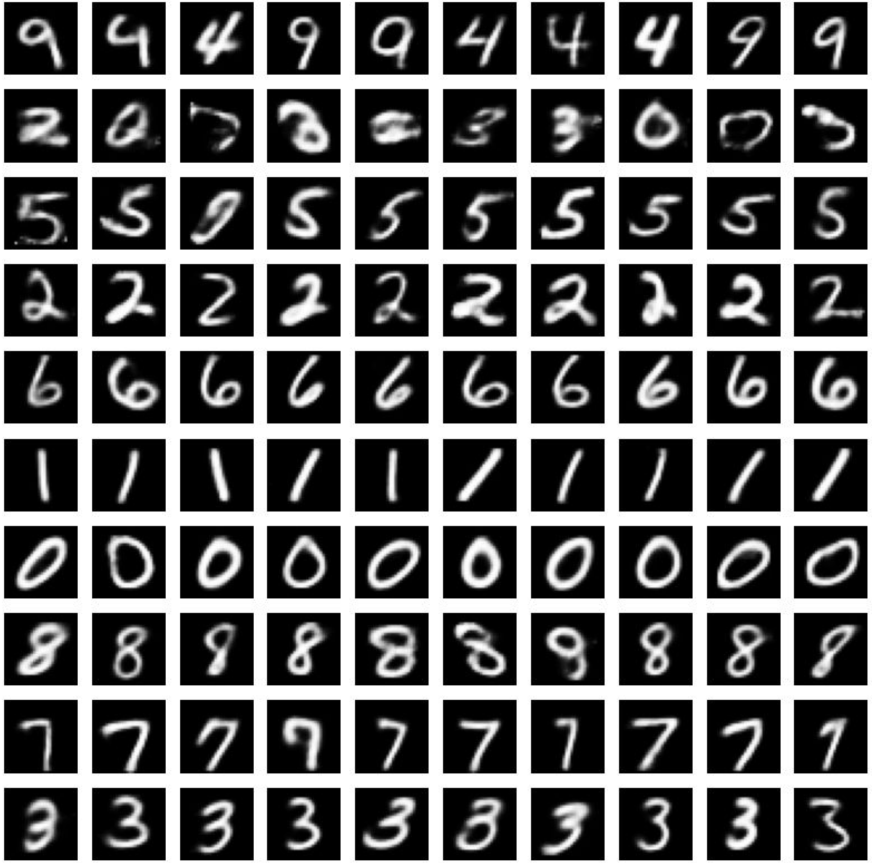
My Naive Attempt:

$$\begin{aligned} \omega &\sim \mathcal{N}(0, I) \\ \pi &\sim \text{Dirichlet}(\alpha) \\ z &\sim \text{Categorical}(\pi) \\ x|z,\omega &\sim \mathcal{N}(\mu_z(x;\theta), \text{diag}(\sigma_z^2(x;\theta))) \\ y|x &\sim \text{Bernoulli}(\sigma(D_\theta(x))) \end{aligned}$$

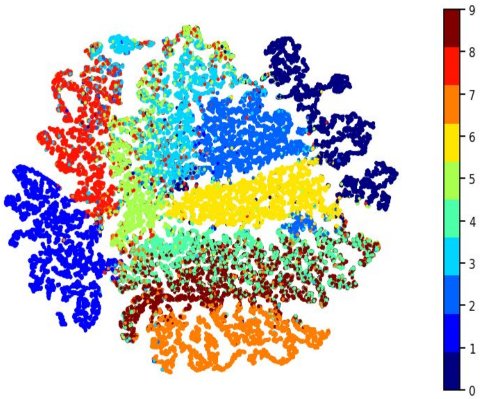
Solution: Add a Gaussian Mixture Prior! (GMVAE)

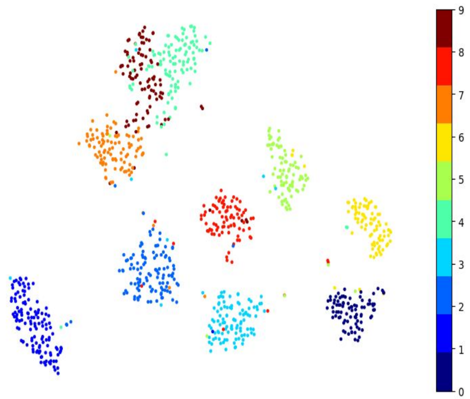
Dilokthanakul et al. (2017)

Gaussian Mixture VAE generated digits (with random interpolation)



$$
\begin{aligned}
\omega &\sim \mathcal{N}(0, I) \\
z &\sim \mathrm{Multinomial}(\pi) \\
x|z,\omega &\sim \prod_{k=1}^{K} \mathcal{N}\left(\mu_{z_k}(\omega;\beta), \mathrm{diag}(\sigma^2_{z_k}(\omega;\beta))\right)^{z_k} \\
y|x &\sim \mathcal{N}(\mu(x;\theta), \mathrm{diag}(\sigma^2(x;\theta)))
\end{aligned}
$$





Conclusion

$$
\begin{tikzcd}
\text{PCA} \arrow[r, "Randomness"] \arrow[d, "Non\!-\!Linearity"'] & \text{Factor Analysis} \arrow[d, "Non\!-\!Linearity"] \\
\text{AE} \arrow[r, "Randomness"] & \text{Variational AE}
\end{tikzcd}
$$

PCA: $\text{Minimize} \sum_{i=1} \|y_i - \hat{y}_i\|_2$ $\quad$ $\text{Maximize Var}(\{\hat{y}_i\}_{i=1}^{N})$

VAE: $\text{ELBO}(x;q) = \mathbb{E}_{z\sim q} \log p(x|z) - D_{KL}(q \| p_z)$

Thank You For Listening!