LATENT GAUSSIAN COMPRESSION: DATASET COMPRESSION AND RECONSTRUCTION WITH AUTOENCODERS AND GAUSSIAN MIXTURE MODELS

James Zhao, Blaine Arihara, Emily Tang, and Terrence Weber
University of California, Los Angeles
Los Angeles, CA, USA
jdzhao@ucla.edu, blainearihara@ucla.edu, etangs@ucla.edu, terryjweber@gmail.com

ABSTRACT

This report explores a machine learning-based approach for compressing and reconstructing large-scale image datasets. We combine autoencoders and Gaussian Mixture Models (GMMs) to create a compact, efficient compressed dataset that is able to be effectively decompressed for training models after transport. We evaluate the effectiveness of this Latent Gaussian Compression (LGC) approach on the MNIST dataset. Our evaluation trains a classifier on a decompressed LGC representation of the MNIST training dataset, and the quantifies its accuracy on the original test MNIST dataset. To establish a strong baseline, we compare this approach to a data summarization technique using coreset selection with k-medoids to find representative subset for training. For the LGC autoencoder, we experimented with various autoencoder architectures (vanilla autoencoder, VAE, contrastive VAE, and AE) to optimize performance. We further explore the application of this approach on the SpuCo (spurious correlation) MNIST dataset to assess its robustness to spurious correlations. [1]

1 Introduction

The rapid growth of machine learning has led to the proliferation of massive datasets. While these datasets have enabled significant advancements in various fields, they also present significant challenges related to storage, transmission, and computational costs. As datasets continue to grow in size and complexity, the need for efficient compression techniques becomes increasingly critical. One significant challenge is the transmission of large datasets across networks. Limited bandwidth and high latency can hinder collaborative research and the deployment of machine learning models. Furthermore, privacy concerns often restrict the sharing of sensitive data. To address these issues, researchers have explored various techniques for compressing datasets while preserving their essential information.

1.1 Problem statement

In this paper, we propose an approach to dataset compression called Latent Gaussian Compression (LGC). LGC leverages the power of autoencoders and Gaussian Mixture Models (GMMs) to create a compact, efficient representation of the dataset. By capturing the underlying data distribution and reconstructing the original data from a compressed latent space, LGC enables efficient data transmission and storage while preserving essential features for machine learning tasks.

1.2 Proposed solution

Our approach offers several advantages over traditional compression techniques, including preservation of information, preservation of privacy, efficient transmission, and reduced storage costs. Our LGC algorithm focuses on preserving the information relevant for training the classifier, and anonymizes the training dataset by making sure that specific points in the dataset cannot be fully reconstructed, only general distributions. It is able to achieve a $>$3x compression factor improvement over GZip, and has benefits ranging from more efficient bandwidth utilization to reduced

[1] Code is available at https://github.com/itsjameszhao/260D_Final_Project

storage costs. We evaluate the effectiveness of LGC on the MNIST and SpuCo MNIST databases and compare its performance a data summarization technique. Our results demonstrate that LGC can achieve significant compression ratios while maintaining high levels of accuracy in downstream machine learning tasks.

1.3 Motivations

Autoencoders have been used for dimensionality reduction and feature learning in various applications (1). Variational Autoencoders (VAE) introduce a probabilistic framework for learning latent representations (2). GMMs are employed for density estimation and data modeling (3). Our technique combines these concepts to address this issue.

Our contribution implements several variants of LGC with different autoencoder architectures (vanilla AE, VAE, conditional VAE, with and without contrastive learning). These approaches are then compared against a baseline data summarization approach selecting an optimal coreset in gradient space to represent the dataset. We discover a trade-off between compression factor and classifier accuracy and integrate our empirical findings within the broader Information Bottleneck (IB) theoretical framework.

1.4 Related Work

Submodular maximization techniques have been explored for efficient data selection. These techniques provide a means of representing a large dataset with a subset of relevant examples. Although these technique are commonly used, they often fail to address issues with privacy concerns and can be computationally expensive.

For a baseline comparison, we explore the CRUST algorithm for robust subset selection. CRUST aims to minimize the dissimilarity between a selected subset and the full gradient of the dataset for robust coreset selection in deep learning applications (4). This technique often requires the extraction of the gradients of thousands of parameters per data point. For example, an autoencoder can have on the order of 10^5 trainable parameters, each of which has a corresponding gradient, and it is computationally infeasible to extract and cluster a 10^5-dimensional space for the $60,000$ training points in our MNIST dataset.

In contrast, a LGC algorithm offers a less computationally expensive solution to dataset summarization, mapping individual data points into a simple 64-dimensional latent space on which a small number of GMMs can be fitted. By modeling the distribution using GMMs, LGC can scale up or down the compression factor as the complexity of the dataset dictates simply by changing the number of Gaussian components per GMMs, and can learn a wide variety of non-Gaussian distributions.

2 Methodology

There are three stages to our LGC algorithm: a compression stage, a transport phase, and a decompression phase. The compression phase is analogous to GZip compression, the transport phase is analogous to transportation of the compressed file, and the decompression phase is analogous to decompressing the received GZip file.

2.1 Compression Phase

In the compression phase, an autoencoder, which can be either a vanilla autoencoder or any of the variants we experiment with below, can be used. The encoder portion of the autoencoder maps input images to latent vectors, while the decoder reconstructs the original images from the latent vectors. We divide the MNIST dataset into two parts, train and test. The training dataset is compressed and modeled using GMMs.

A variety of autoencoders were experimented with: a vanilla autoencoder (AE), a variational autoencoder (VAE), a vanilla autoencoder with contrastive learning, a variational autoencoder with contrastive learning, and a conditional autoencoder. Further details about the architecture, motivation, and underlying concepts behind these autoencoders is provided in Appendix A1. The main idea behind all of them is that they are comprised of an encoder and a decoder, where the encoder takes a high-dimensional data input and compresses it down to a lower dimensional latent vector, followed by the decoder that takes the latent vector and dimensionally increases it to reconstruct the

input image. The latent vectors are the compressed image representations that the GMM will find k-number of Gaussian distributions to characterize the latent distribution.

Figure 1 shows the 2-dimensional t-SNE plots for example latent distributions created by the vanilla autoencoder (left) and the variational autoencoder (right). Latent images within classes are color-coded to help give a sense of the 64-dimension latent distributions that the GMM will fit. The AE can be seen to produce irregular and amorphous distributions that would require the GMM to fit multiple Gaussian distributions, while the VAE can be seen to likely need only one Gaussian for every class.

Figure 1: 2D t-SNE Plots For Autoencoder (Left) and Variational Autoencoder (Right)

The GMM models the distribution of latent representations as a mixture of Gaussian components according to the following probability density function:

$$p(z) = \sum k = 1^{K} \pi_k \mathcal{N}(x|\mu_k, \Sigma_k)$$

where K is the number of mixture components, π_k is the mixing coefficient for the k-th component representing the probability of selecting the k-th component, and $N(x|\mu_k, \Sigma_k)$ is the probability density function (PDF) of a Gaussian distribution with mean μ_k and covariance matrix Σ_k.

2.1.1 Interpretation

The GMM PDF represents the probability of observing a data point ‘z‘ given the parameters of the model. It is a weighted sum of Gaussian distributions, where each Gaussian component contributes to the overall probability based on its mixing coefficient. The output of the compression phase are the learned parameters of the fitted GMM (mean vectors, covariance matrices, and component weights) and the decoder part of the autoencoder.

2.1.2 Selecting the Optimal Number of Components (K) for GMMs

Determining the optimal number of components (K) in a Gaussian Mixture Model (GMM) is crucial for achieving accurate and robust modeling. Intuitively, if we select too little a number of components, we risk not being able to fully characterize the latent distribution. If we select to large a number of components, we risk overfitting the latent distribution and taking up unneeded space in our compression algorithm. We need to find a criterion to determine when a given K value is enough for our GMM. In this work, we employed the Bayesian Information Criterion (BIC) to select the appropriate number of components for each class in our dataset.

The BIC score is a statistical criterion that balances model fit with model complexity. It is defined as:

$$\text{BIC} = k \ln(n) - 2 \ln(\widehat{L})$$

where $\log$-likelihood is the log-likelihood of the data given the model, k isThe number of parameters in the model, and n is the number of data points. A lower BIC score indicates a better model fit. By comparing BIC scores for different values of K, we can identify the optimal number of components that balances model complexity and predictive accuracy.

For each class in our dataset, we trained GMMs with a varying number of components (K) and calculated their corresponding BIC scores. The optimal number of components for each class was selected as the value of K that minimized the BIC score. This optimal number of K components for each class was then input into a GMM to fit K Gaussian distributions for each class’s latent

distribution. This analysis was performed for each autoencoder architecture. Figure 2 below shows examples of the BIC plots for each class for the vanilla autoencoder (left) and the variational autoencoder (right). The BIC plots for the vanilla autoencoder can be seen to indicate that between 3 and 8 Gaussian distributions are needed to best fit the latent distributions for its classes, while the variational autoencoder clearly indicates that only one Gaussian distribution is needed to best fit its class's latent distributions. BIC plots with more detailed discussion is provided in Appendix A2.

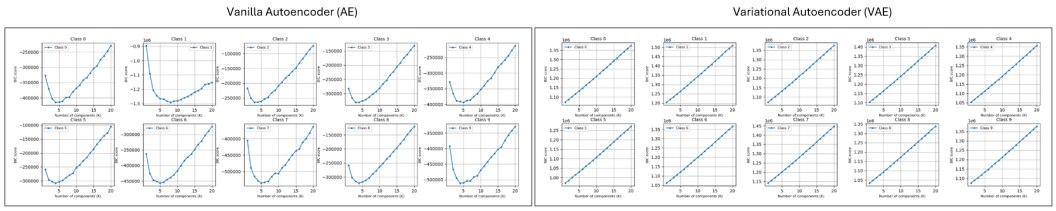


Figure 2: BIC Plots For Autoencoder (Left) and Variational Autoencoder (Right)

Performing this optimal selection of components for each class ensured that our GMMs effectively captured the underlying data distribution without overfitting or underfitting. This optimal model selection is crucial for accurate data compression and reconstruction.

2.2 Transport Phase

In the transport phase, we serialize the parameters of the GMM and the decoder part of the autoencoder using standard serialization libraries, and then compress the serialized file using the standard compression algorithm GZip. The intuition behind extracting the parameters from the GMM is that a each Gaussian component consists of a component weight, a mean vector, and a covariance matrix, which contain far less parameters than the original data itself. For example, if we fit a 5-component GMM on the 64-dimensional latent space consisting of 10,000 64-dimensional vectors, the total number of parameters of the GMM is

$$5 \times (64 + 64 * 64 + 1) = 4161$$

which is far less than the 640,000 parameters of the original latent space data. In practice, the 64x64 covariance matrix of each Gaussian component can be further compressed with matrix compression techniques. The decoder also occupies a modest size when compared to the original data, and can be further compressed using pruning and quantization techniques.

2.3 Decompression Phase

During the decompression phase, the receiver receives a compressed representation of the dataset consisting of GMM paramters and decoder. The receiver then fully reconstructs the GMM using the GMM parameters. Samples are then drawn based on the reconstructed GMM's probability distrbution. Recall that a GMM consists of k Gaussian distributions, each with weight π_i. To draw a sample, the reconstruction algorithm first randomly selects a Gaussian component with probability proportional to its weight π_i. After selecting the Gaussian component, it then randomly draws a sample from the Gaussian distribution based on its μ_i and Σ_i parameters. This sample is a 64-dimensional vector in the latent space. Finally, each sampled latent vector is passed through the decoder to reconstruct the original images. The process is repeated as long as needed to reconstruct a dataset with similar aggregate statistical properties to the original dataset, though the individual points may be different.

3 Experiments and Results

A Convolutional Neural Network (CNN) classifier is used to evaluate the performance of each model. As a baseline comparison, three methods of training this classifier are taken: (1) Training on the full MNIST training set, (2) training on a random subset of equivalent size to the LGC models, and (3) training on a subset selected utilizing a CRUST-like data summarization approach.

3.1 Baseline Comparison

Each autoencoder explored resulted in a compressed representation varying between 1-3 MB in size. In contrast, the amount of disk space taken up by the uncompressed MNIST results in 11.55

GB. Using a GZip compression, the size of the dataset can be reduced by 82.34%. This is still not a scalable solution for addressing even larger datasets. Even with the compression, a linear relationship between compression size and number of examples is inevitable, as demosntrated in Appendix Figure 19. For an equivalent comparison, a subset of 182 examples were extracted from the training data, the equivalent to the size of the LGC retaining 3 MB of data when GZipped. This subset selection method is implemented using a random subset selection, as well as a CRUST-like approach to data summarization.

3.2 CRUST-like Dataset Summarization Approach

To compare the performance of LGC, a CRUST-like data summarization technique was used to find an optimal subset for training. CRUST is a robust coreset selection algorithm for neural networks (4). Selecting a set of medoids from the gradient space eliminates noisy labels, as clean data with similar gradients will cluster together, resulting in a noise robust summarization of the dataset. This algorithm aims to find a coreset that minimizes the following objective:

$$S^*(W) = argmin_{S \subseteq V, |S| \leq k} \sum_{i \in V} \min_{j \in S} d_{ij}(W)$$

To optimize the subset selected, a CRUST-like approach was implemented by training a CNN on the train set, extracting the gradient of the loss from the last layer of the network, and selecting a set of medoids from this gradient loss to minimize the average gradient dissimilarity, d_{ij}. The gradient dissimilarity is calculated as an L2 norm, represented by

$$d_{ij}(W) = ||\nabla \mathcal{L}(W, x_i) - \nabla \mathcal{L}(W, x_j)||_2$$

This dissimilarity can be bounded for submodular maximization, as demonstrated in by CRUST (4). After training the neural network, a greedy k-medoids algorithm was implemented to select an optimal coreset for training. Without a greedy implementation, k-medoids is an NP-hard problem. A Partitioning Around Medoid (PAM) algorithm can be used to approximate an accurate solution, but this can still be very slow. The Alternate approach for solving k-medoids was combined with a k-medoid++ approach (a k-means++ based initialization technique) to increase convergence time (5; 6). The resulting subset is represented in Figure 3, projected onto 2D for visualization using t-SNE. Even after training the CNN on just 1 epoch, the gradients begin to cluster by the classes of images immediately, with just a few noisy examples near the middle.

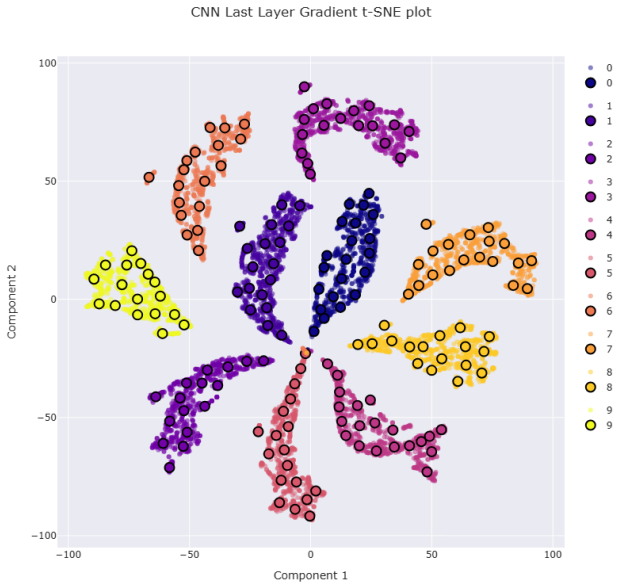


Figure 3: 2D t-SNE Plot Of CNN Classifier Gradient Clusters With K-Medoids

3.3 Results

This LGC approach returns a packaged representation of the dataset fitted GMM (mean vectors, covariance matrices, and component weights) and the decoder part of the autoencoder to be used for image reconstruction and training. Table 1 summarizes the performance of a CNN classifier trained on examples from each model, along with the amount of size reduction the model was able to achieve. Percent reduction is defined the ratio between the disk size of the full MNIST training data (11.55 GB) versus the size of the compressed file. Using a GZip compression, the MNIST dataset can be reduced by 82.34% compared to its original size. The vanilla autoencoder architecture reduced the size by 94.44% while achieving a 95.98% accuracy on the original MNIST test set.

Approach	Percent Reduction	Test Accuracy	Compression Ratio
GZip compression only	82.34	98.36	5.57
Random subset	94.32	82.64	14.55
Gradient subset	94.32	86.65	15.26
Vanilla autoencoder	94.44	95.98	17.26
Contrastive autoencoder	95.51	89.14	19.85
Variational autoencoder	97.77	82.63	37.05
Conditional variational autoencoder	97.36	91.34	34.60
Contrastive variational autoencoder	97.77	91.84	41.18

Table 1: Summary of performance between Compression Techniques

Compression ratios are reported as the following:

$$Compression\ ratio = \frac{Test\ Accuracy}{1 - Percent\ reduction}$$

The goal of this evaluation is to achieve a high test accuracy with a small file size, so a larger compression ratio signifies a ”better” performance. For example, training on the full MNIST data, we’re able to achieve the highest test accuracy, but the amount of compression falls behind, due to the linear relationship between compression size and number of examples. As a result, this technique has the lowest compression ratio. Whereas, the Contrastive-VAE has the largest percent reduction with a fairly high accuracy, resulting in higher compression ratio.

This compression ratio provides a broad comparison of the trade-off between size and accuracy. In application, the amount of compression vs the desired test accuracy is dependent on the use case. Figure 3 draws a convex hull boundary demonstrating the theoretical optimum boundary, highlighting this trade-off. With a higher amount of compression, the trade-off grows rapidly between compression and accuracy. Further optimization of the models could expand this boundary, improving the relationship between accuracy and compression at higher compressions.

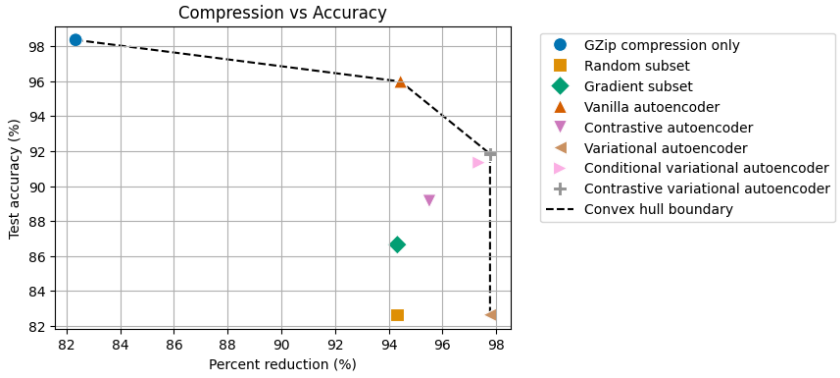


Figure 4: Summary of Compression vs Accuracy

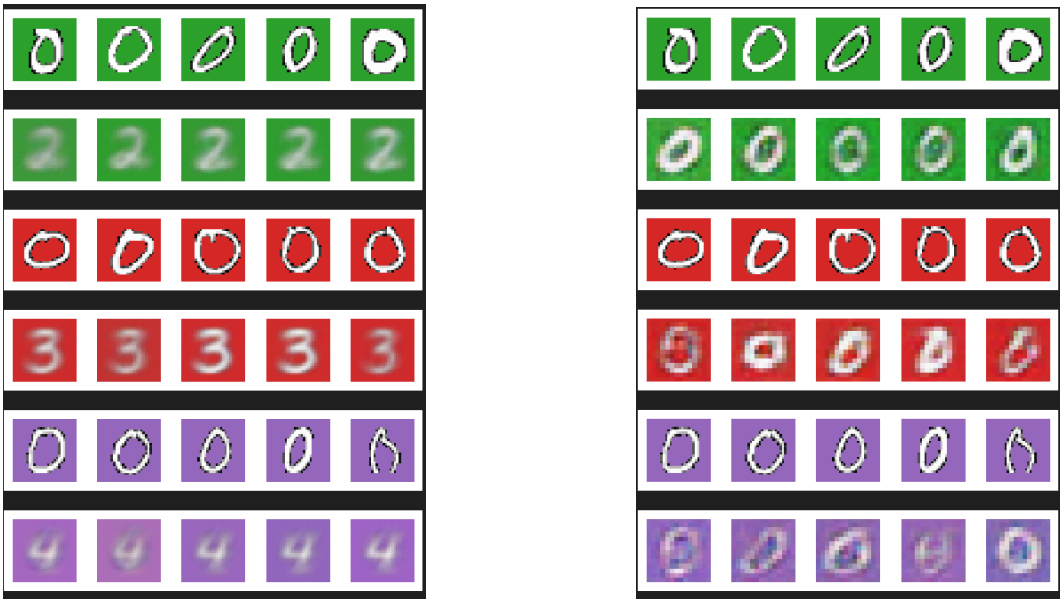
4 Conclusion

This project investigates the feasibility of LGC for dataset compression and reconstruction. We explore various techniques and analyze the trade-off between compression rate and classification performance. We evaluated the performance of our Latent Gaussian Compression (LGC) approach against several baseline methods, including GZip compression, random subsetting, gradient-based subset selection, and coreset selection with k-medoids. We experimented with various autoencoder architectures (vanilla AE, contrastive AE, VAE, conditional VAE, contrastive VAE, and contrastive VAE with convex hull boundary) within the LGC framework. Our results, illustrated in the figure above, demonstrate a compelling trade-off between compression ratio and test accuracy. LGC consistently outperformed baseline methods, especially at higher compression ratios. While coreset selection with k-medoids offered reasonable performance, LGC generally provided superior accuracy, particularly at higher compression levels. However, it's important to note that all methods experienced a significant drop in accuracy at extremely high compression ratios. This highlights the inherent trade-off between compression and performance. In conclusion, our LGC approach offers a promising solution for compressing large-scale datasets while preserving essential information for downstream tasks. Further research can explore more advanced autoencoder architectures and optimization techniques to further improve the performance of LGC.

5 Future Work

One thing we looked into was how our approach would handle spurious correlations by training the autoencoder component of our pipeline on the SpucoMNIST dataset, setting each digit to be highly correlated to different background colors, as opposed to the black and white MNIST images. What we found was that the fully connected autoencoder in our pipeline did not handle spurious correlations very well, and would associate the background colors more than the features of the digits during reconstruction.

We found using a convolutional VAE architecture helped with mitigating spurious correlations, and reconstructed the images more accurately. Figure 21 shows the convolutional VAE architecture.



(a) Vanilla VAE Reconstruction

(b) Convolutional VAE Reconstruction

Figure 5: VAE vs Convolution VAE Reconstruction Comparison

The usage of convolutional architecture for image recognition is not a new idea and dates back to the Lenet architecture from the 1998 paper, which was used to read zip codes and other digits. It was reported that convolutional networks "ensure some degree of shift, scale, and distortion invariance",

which would have a similar effect to performing augmentations on the data in preprocessing and training on a sequential network (7). From this paper it is known that convolutional networks are not sensitive to "shifts and distortions of the input" and that "once a feature has been detected, its exact location becomes less important" (7). These capabilities contribute to the robustness of convolutional networks for image recognition, and help mitigate spurious correlations in training. For future work, integrating a convolutional VAE could enable this architecture to be generalized and used for different sets of even more complex images, even those containing a high degree of spurious correlations.

Additionally we could have further tuned the hyperparameters of our vanilla VAEs used in the compression pipeline to achieve better accuracy, such as the number of dimensions in the latent space or the nodes within the layers. Our results showed that the non variational autoencoder had a higher test accuracy after compression than the VAE models we tested, but this seems to go against intuition, leading to the conclusion that there was perhaps more we could have done to fine tune those models. A more complex model would take up more bandwidth as well, but it could be worth the trade off.

6 Contributions and Acknowledgements

This project was completed through joint efforts between James Zhao, Blaine Arihara, Emily Tang, and Terry Weber. James spearheaded the concept for this project, diving into methods of representing data in latent spaces, and working with Blaine to implement the autoencoding architecture for this application. Emily worked on evaluating the performance of these architectures by drawing a baseline comparison, while Terry explored improvements for the different architectures and further applications.

Thank you to Professor Baharan Mirzasoleiman and the rest of the teaching staff of CS260D, Yihao Xue, Siddharth Joshi, and Chris Vatt, for their support and guidance throughout the quarter.

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A Appendix

A.1 Problem Statement Explained

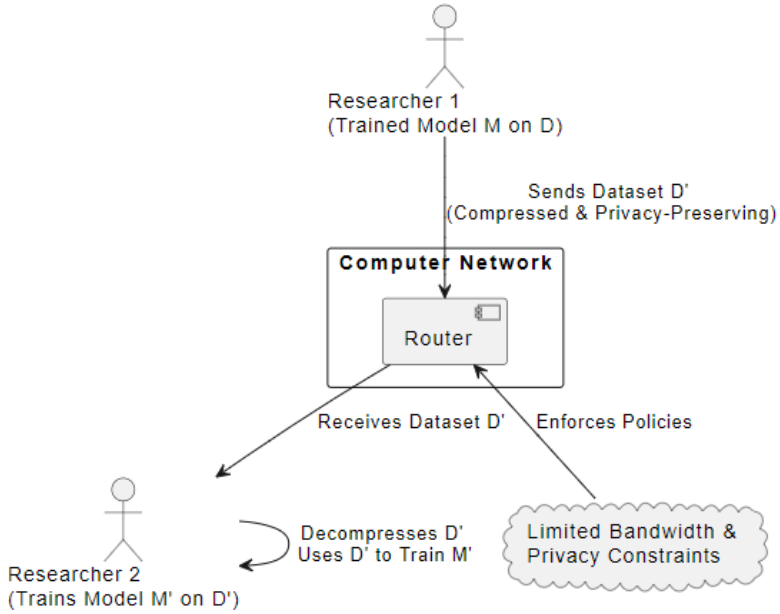


Figure 6: A caption for my image.

Consider a scenario where two researchers, Researcher 1 and Researcher 2, collaborate on a machine learning project. Researcher 1 has trained a model M on a large dataset D. Researcher 2 wants to train a similar model M' on a similar dataset D', but they are constrained by limited bandwidth and privacy concerns.

Using LGC, Researcher 1 can compress their dataset D into a compressed representation D'. This compressed representation can be transmitted over the network to Researcher 2 with minimal bandwidth overhead. Researcher 2 can then decompress D' and use it to train their model M', with the additional benefit that only a similar distribution to the original, but not the exact original data points, can be reconstructed.

A.2 Autoencoder Architectures

This section presents further detail about the architecture and underlying concepts of the autoencoders experimented with in this project.

Vanilla Autoencoder

The vanilla autoencoder is the baseline version of autoencoder that consists of the basic encoder and decoder components that respectively transform the higher-dimensional input images into lower-dimensional representations. Starting with the MNIST dataset, which are 28 by 28 greyscale (single channel dimension) images, the encoder flattens the input into a 784 dimensional vector and then runs the vector through two dimensional reducing linear layers with rectified linear unit (ReLU) activation functions to transform the image into a 64 dimension latent space vector. The decoder reverses the process by taking in the 64 dimensional latent space vectors and dimensionally increases the image back to its 784 dimensional vector before being reshaped back to its 28 by 28 pixel image.

The mean squared error (MSE) reconstruction loss is used to train the model such that the averaged squared errors between the reconstructed image and the original image is minimized. For the autoencoder this is the only loss function that is being minimized.

$$MSE = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2$$

t-Distributed Stochastic Neighbor Embedding (tSNE) is a dimensional reduction technique that attempts to preserve higher dimensional structure in a lower dimension typically for visualization. Figure 7 shows a 2-dimensional t-SNE visualization of the 64-dimensional latent vectors of the 10 classes of the MNIST dataset color-coded by class. It can seen that the encoder is transforming examples of the same class in roughly similar locations in latent space, while placing examples from different classes in different locations in latent space. This plot gives the intution of the latent encodings of different classes that the GMM is attempting to decompose into multiple gaussian distributions.

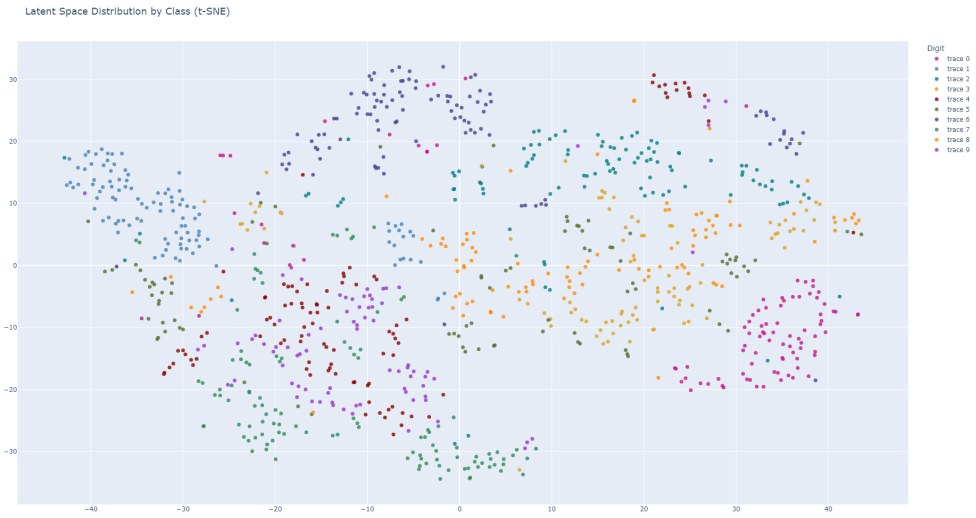


Figure 7: 2D t-SNE Vanilla Autoencoder Latent Distribution

Variational Autoencoder (VAE)

The variational autoencoder (VAE) is a probabilistic extension of the vanilla autoencoder (AE) that replaces the determinstic functionality of the encoder and decoder of an AE with probability distributions. The AE compresses a single image into a latent representation, and then reconstructs an image from that latent. The VAE takes a single image and learns a continuous probability distribution for its latent representation. This probability distribution is modeled as a normal distribution characterized by means and covariances with dimensions that of the latent dimension. Two neural networks comprise the encoder, where one learns how to represent the means of input images and the other learns how to represent the covariances of the input images. Knowing the mean and covariance of a normal distribution allows the distribution to be known entirely, so when an image is encoded by its means and covariances, it is encoded as a latent space probability distribution. To decode the image from its latent, a random sample can be drawn from the distribution that has mean and covariance determined by the neural networks applied to that image. The sample will then get passed through two more sets of neural networks that will map the latent into normal distributions of what the images look like. Similar to the encoder, the decoder is comprised of two neural networks, one which takes the sampled latent representation and determines its means in image space, and the other which determines its covariances in image space. These determined means and covariances describe the image space probability distribution of the latent, from which a random sample can be drawn to return a reconstructed image.

The loss function for the VAE involves defining an Evidence Lower Bound (ELBO) that allows for the probabilistic terms of the image space distribution to be defined as a Kullback-Leibler (KL) divergence. Because the image space distribution is intractable and unable to be written down, it needs to be approximated by the the latent space distribution, such that minimizing the KL divergence term tightens the ELBO, which allows it to more closely approximate the log likelihood, which is equivalent to minimizing the mean squared error of the reconstructed image. This allows an explicit loss function to be derived which can be optimized. A trick is needed to back propagate through the sampling operation, called the Reparameterization trick, which allows for a random sampling of noise from a unit Gaussian to be multiplied by the covariance and added to the mean of the determined latent probability distribution. This allows for the sampling operation to be performed while introducing arithmetic operations into the computational graph needed to compute gradients through the neural networks. Below is the KL divergence term that measures the difference between the approximate posterior $q(z|x)$, which is the conditional distribution of the latents z given an image x, and the prior $p(z)$, which is the assumed unit Gaussian distribution over latents z prior to seeing any data.

$$KL(q(z|x)||p(z)) = \int q(z|x) log \frac{q(z|x)}{p(z)} dz$$

When the approximate posterior $q(z|x)$ is parameterized as a Guassian distribution, $\mathcal{N}(\mu_\phi, \Sigma_\phi)$ with the mean and covariances determined by the encoder, the KL divergence can be represented by the closed-form solution:

$$KL(q(z|x)||p(z)) = \frac{1}{2} \sum_{i=1}^{d} (\Sigma_i + \mu_i^2 - 1 - log\Sigma_i)$$

Figure 8 shows the tSNE plot of the encoding representations of the images of every class as a normal Gaussian distribution, where every image is encoded to have its own unique latent z values. The z values for any image are continuous and can take on any value in latent space, and are defined by the mean and covariances learned for that image by the encoder. The scattered nature of the latents of different classes is the result of the KL divergence term pulling all the latents given an image, $q(z|x)$, closer to the assumed unit Gaussian distribution, $p(z)$.

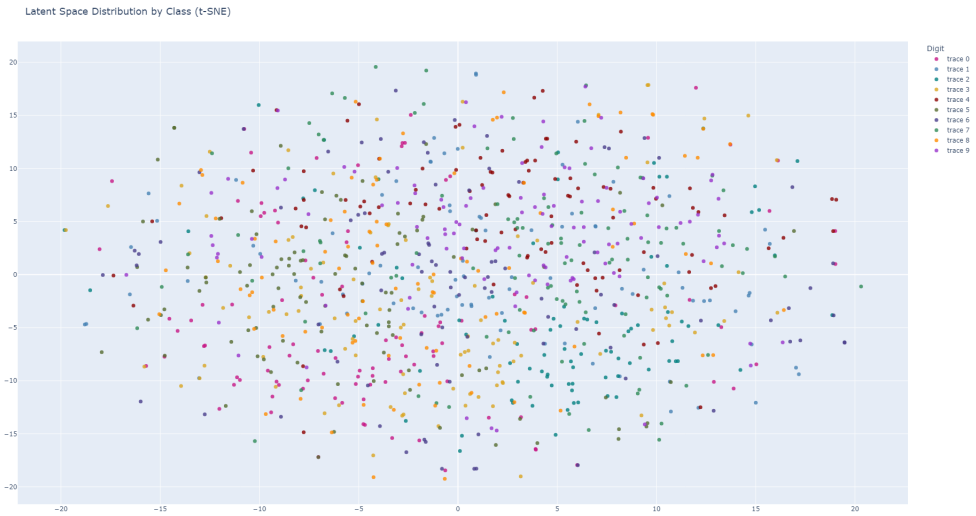


Figure 8: 2D t-SNE Variational Autoencoder Latent Distribution

This scattered distribution of latents across all classes makes it difficult to sample an image reconstruction from a desired class. Sampling random unit Gaussian latent samples results in random reconstruction of images, as seen below in Figure 9, where every reconstructed image started from a random unit Gaussian latent sample. The conditional VAE addresses this.

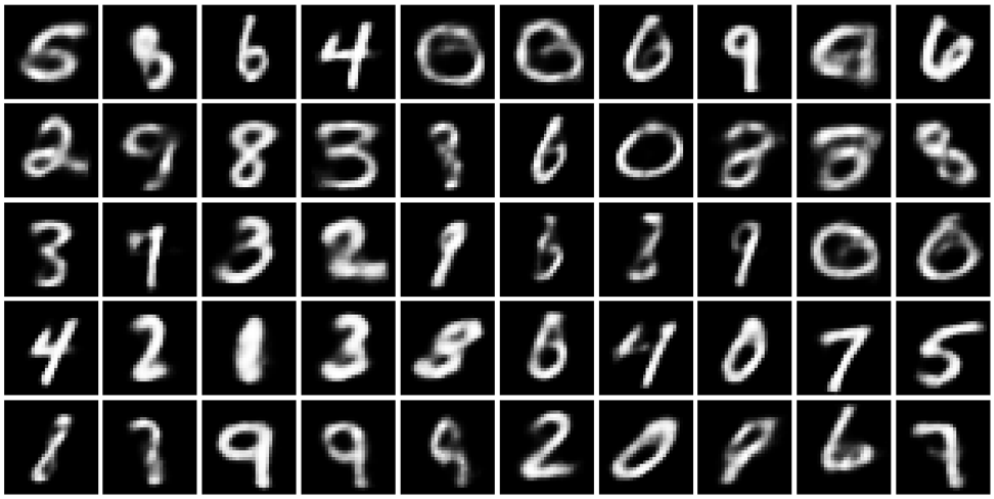


Figure 9: Variational Autoencoder Sampled Reconstructions

Vanilla Autoencoder with Contrastive Learning

Contrastive learning is a technique that can be applied to supervised or self-supervised machine learning. In the self-supervised case, contrastive learning works to pull augmentations of the same example closer together, as well as similar examples with similar augmentations closer together, while pushing dissimilar examples with dissimilar augmentations away, such that different clusterings of examples can be labeled as classes. Supervised contrastive learning does the same thing, but has the advantage of knowing the labels of the examples so that it can effectively pull examples of the same class closer together, while knowing which examples in other classes to push away. The supervised contrastive loss term is defined as below:

$$\mathcal{L}_{SCL} = \frac{1}{|I|} \sum_{i \in I} \frac{-1}{|P(i)|} \sum_{p \in P(i)} \log \frac{\exp(\mathbf{z}_i \cdot \mathbf{z}_p / \tau)}{\sum_{a \in A(i)} \exp(\mathbf{z}_i \cdot \mathbf{z}_a / \tau)}$$

- I: Set of all indices in the batch.
- $P(i)$: Set of indices of positives for the anchor i (samples from the same class as i).
- $A(i)$: Set of all indices except i itself.
- $\mathbf{z}_i$: Normalized embedding of sample i.
- τ: Temperature scaling parameter.

When taking the vanilla autoencoder architecture and adding a contrastive loss term, the effect that it has on clustering in-class examples is apparent. The tSNE plot below in Figure 10 shows the effect that the contrastive loss has on how the encoder transforms examples to latent space. It is clear that the encoder is learning to place examples of the same class closer together in latent space, while pushing examples in other classes away from each other.

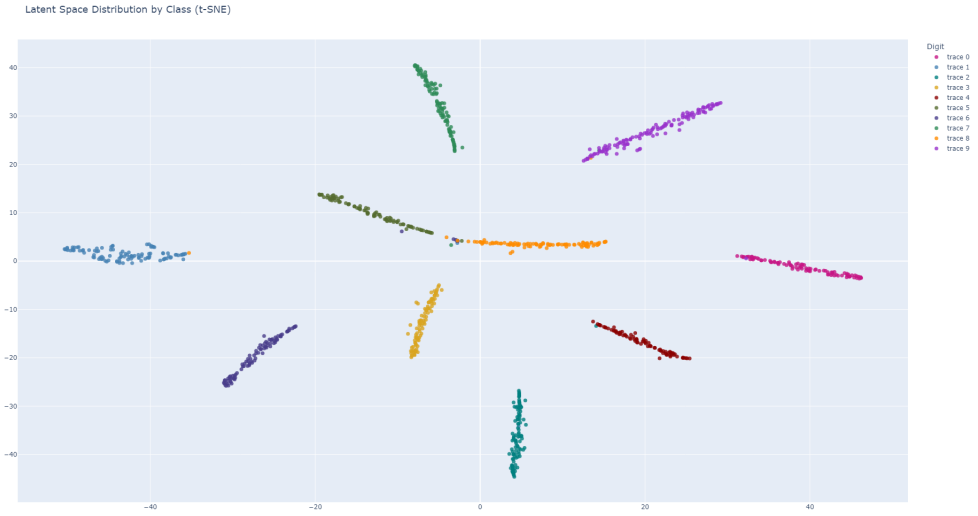


Figure 10: Vanilla Autoencoder with Contrastive Learning Latent Distributions

Variational Autoencoder with Contrastive Learning

Taking the VAE previously described and adding a contrastive loss term produces the tSNE plot below in Figure 11. This VAE with contrastive learning now has three loss terms that are guiding the gradient computations: one for cross entropy image recontrustion, a second for KL divergence, and a third for contrastive learning. It can be seen the interplay of the KL divergence term and the contrastive loss term, as the KL divergence term pulls all examples closer to a unit Gaussian distribution, while the contrastive loss term pulls examples within classes towards each other.

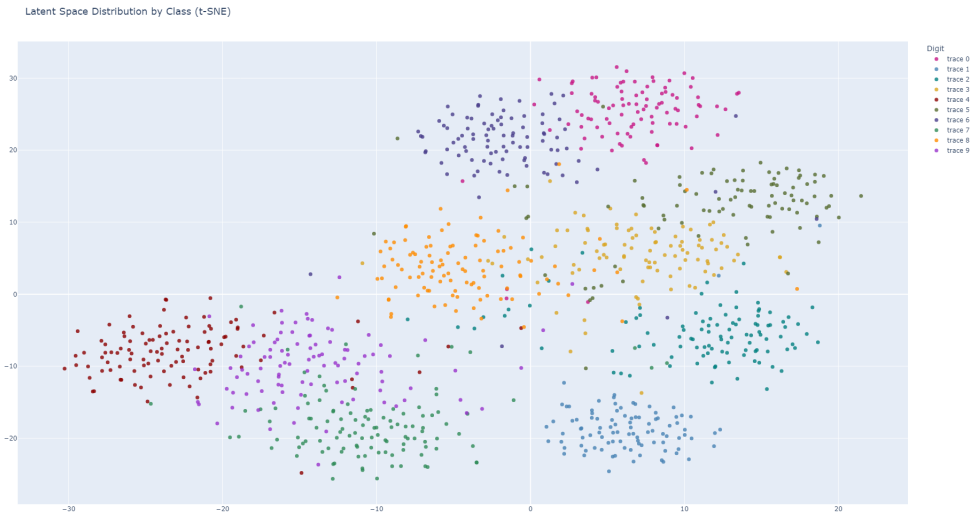


Figure 11: Variational Autoencoder with Contrastive Learning Latent Distributions

Conditional Variational Autoencoder

The conditional variational autoencoder (CVAE) is a variant of the VAE that incorporates conditioning information into the encoding and decoding steps. This conditioning information is implemented

as a one-hot encoding of the images' labels. This one-hot encoding is appended to the flattened image input prior to the encoder, as well as appended to the latent encodings prior to the decoder. This provides conditioning information to the training data for the encoder and decoder to learn associations between examples within a class and their one-hot encodings. This allows for conditioning the random sampling of a latent to reconstruct an image from a desired class. The latent distributions do not show obvious clustering around one-hot encoded groupings, so the tSNE plot for the CVAE looks similar to the VAE, shown below in Figure 12:

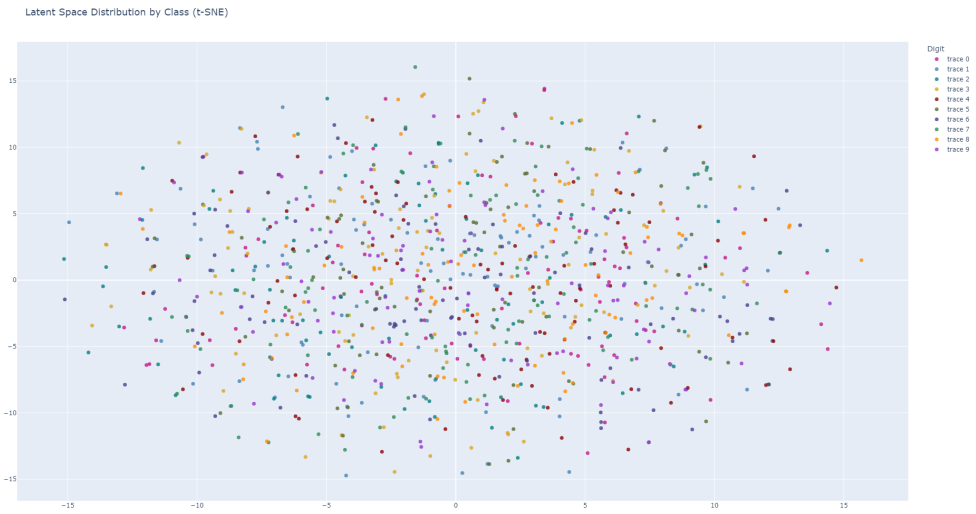


Figure 12: Conditional Variational Autoencoder Latent Distributions

However, the one-hot information is encoded in the latent data such that appending the one-hot encodings to a random sampling of unit Gaussian latent samples allows for images from a desired class to be reconstructed. Figure 13 below show the conditionally-sampled reconstructions from each class, showing that the one-hot encodings allow for the model to learn coded locations in latent space associated with each class.

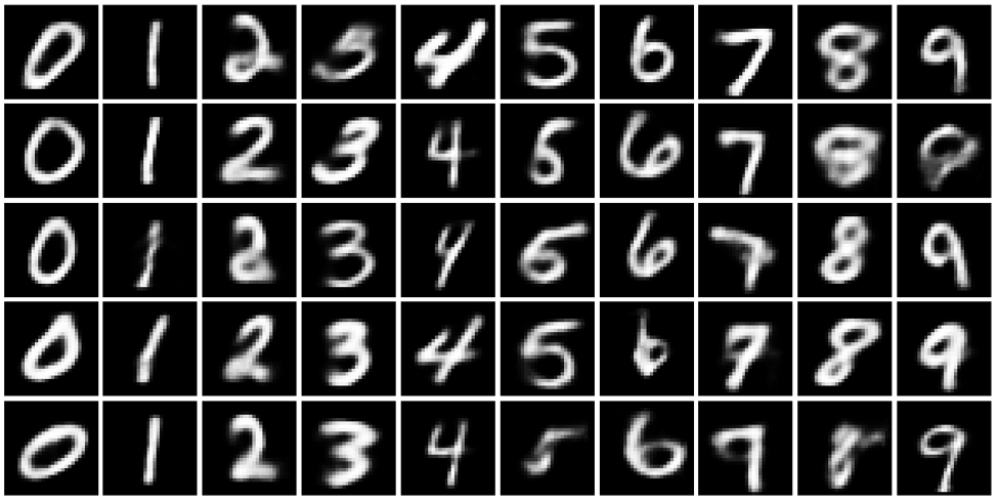


Figure 13: Conditional Variational Autoencoder Sampled Reconstructions

A.3 Bayesian Information Criterion (BIC) Plots

This section presents the Bayesian Information Criterion plots that illustrate the method used to determine the optimal number of components or Gaussian mixture distributions needed to characterize the latent distributions for every class.

Vanilla Autoencoder

For the vanilla autoencoder, it can be seen in Figure 14 that for most of the classes, around 3 to 8 Gaussian distributions minimized the BIC criterion. The variability across classes reaffirms the already known fact that the latent space distributions generated by the vanilla autoencoder are amorphous, irregular, and unpredictable in their characteristics. Thus the latent space distributions require multiple Gaussian distributions, or multiple GMM components to best characterize them.

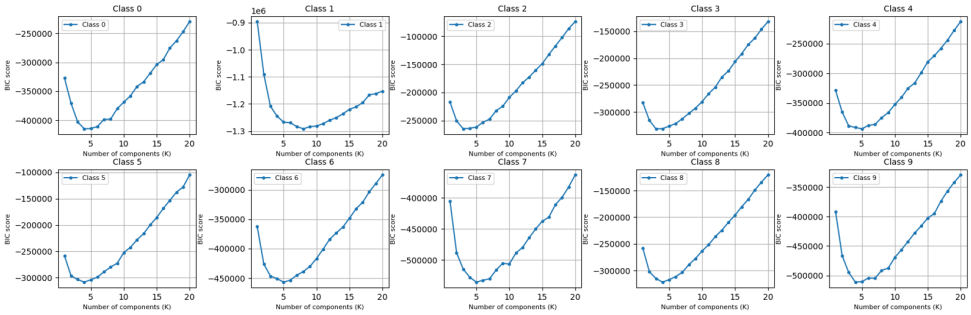


Figure 14: Vanilla Autoencoder BIC Plots

Variational Autoencoder (VAE)

For the variational autoencoder, the BIC plots in Figure 15 clearly indicate that a single Gaussian distribution is needed to characterize the latent space distribution for all classes. This makes sense because by definition of how the VAE operates, it transforms the inputs into probability distributions characterized by drawing unit Gaussian samples and reparameterizing them to determine their latent encodings. This transformation defines the latent space distributions as multi-dimensional unit Gaussian distributions, so a GMM would require only a one Guassian distrbution to characterize the latent space distribution.

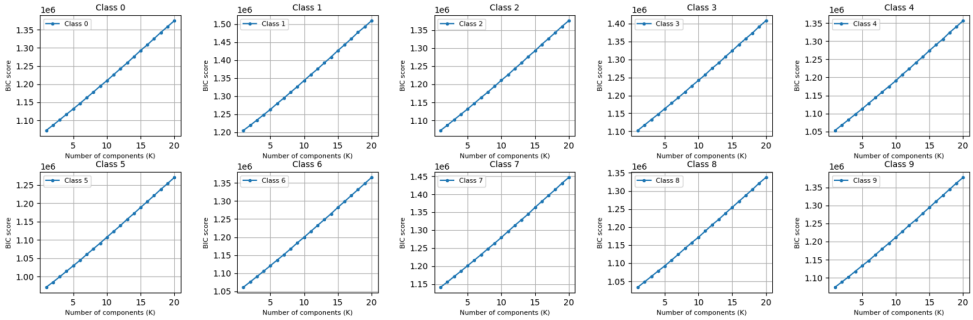


Figure 15: Variational Autoencoder BIC Plots

Vanilla Autoencoder with Contrastive Learning

Similar to the vanilla autoencoder, the AE with contrastive learning indicates that around 3 to 6 components are optimal to characterize the latent space distributions, seen in Figure 16. Due to the contrastive loss term, the encoder was incentivized to position examples within classes closer together, which likely caused the examples within a class to be more consolidated. This may have allowed the GMMs to require on average less components to characterize the latent distributions, but still comparable to the vanilla autoencoder.

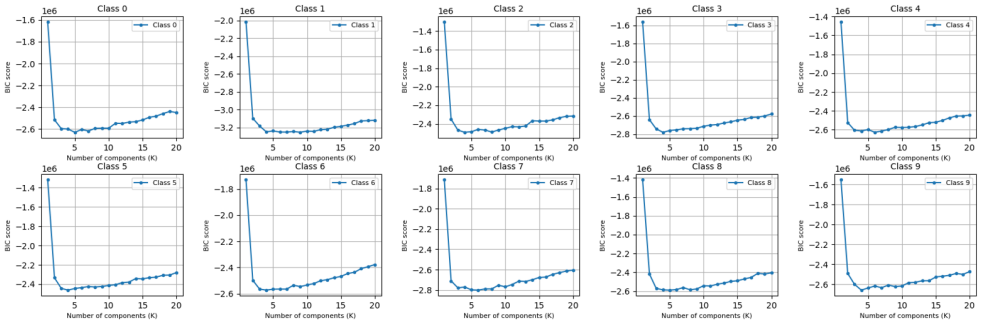


Figure 16: Vanilla Autoencoder with Contrastive Learning BIC Plots

Variational Autoencoder with Contrastive Learning

The VAE with contrastive learning demonstrated to only need a single Gaussian distribution to characterize the latent distributions for all classes, similar to the VAE without contrastive learning, Figure 17. Although the contrastive loss term pulls examples closer together, the KL divergence loss term still forces the encoder to learn to reparameterize the inputs to unit Gaussian distributions.

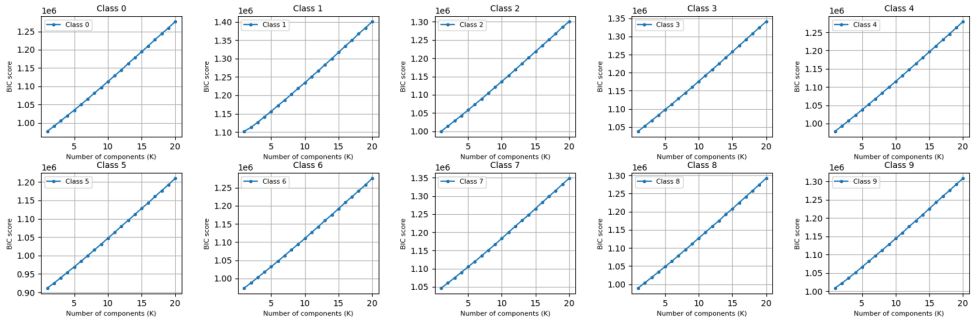


Figure 17: Variational Autoencoder with Contrastive Learning BIC Plots

Conditional Variational Autoencoder (CVAE)

The conditional VAE expectedly also indicates that only one Gaussian distribution is needed to characterize the latent distributions, Figure 18, similar to the VAE. The CVAE is only different than the VAE in that it appends the one-hot encodings of the images to the inputs of the encoder and decoder, but it would not significantly affect the characteristics of the spread in latent space that the encoder learns to transform images into. So similar to the VAE, the BIC plots suggest one component to be sufficient to characterize the latent distributions.

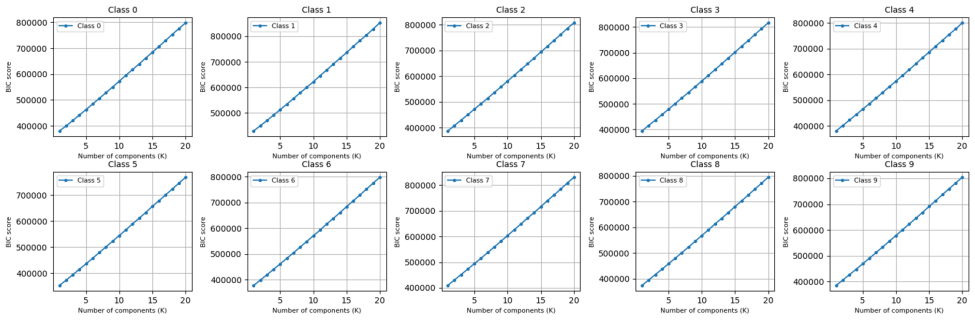


Figure 18: Conditional Variational Autoencoder BIC Plots

A.4 Subset selection further explored

The size of the MNIST dataset can be compressed, however the relationship between the number of examples and the size of the compressed representation is still linear. Because of this, scaling subset selection techniques can still be heavily budget contrained, demonstrated in Figure 19

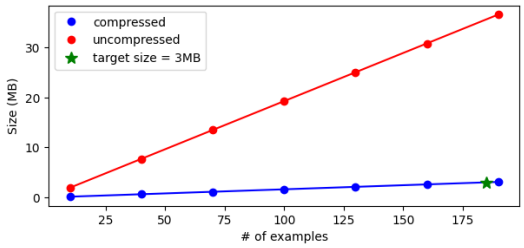
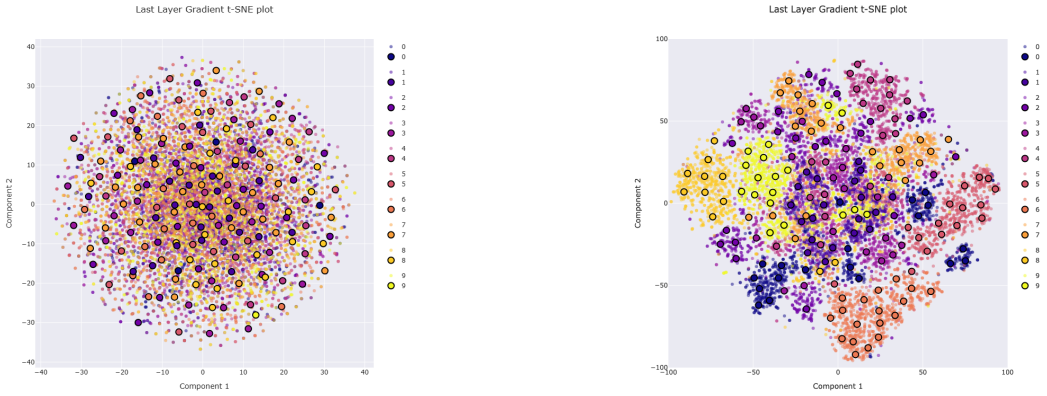


Figure 19: Size of MNIST subsets

Different neural network architectures was also explored for selecting an optimal subset. Visualizing the gradient space for the AE and VAE (Figure 20) was interesting because it mirrored what was observed in the latent space projections, where the AE had classes begin to separate, while the VAE did not cluster by class without the addition of the contrastive element.



(a) AE Gradient Space Representation

(b) VAE Gradient Space Representation

Figure 20: AE vs VAE Gradient Space t-SNE projections

The CNN was ultimately selected, as the goal of this study was to compare the performance of the CNN alone.

A.5 Convolution AE Model Used For SPUCO Experiment

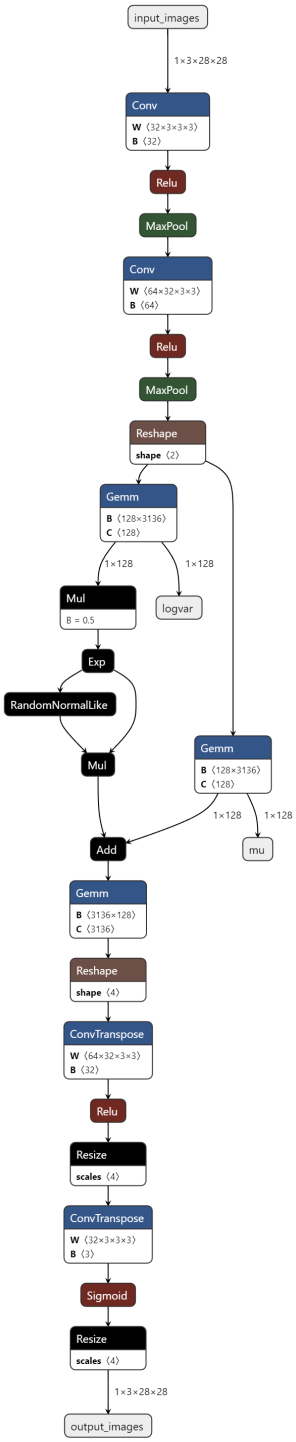


Figure 21: Convolution AE Model Used For SPUCO Experiment