
Active Learning using Deep Generative Models

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Abstract

Active learning helps to develop label-efficient algorithms by sampling the most *informative* data points to be labeled. Labelling time and cost for large scale datasets hinder the growth of deep learning. Thus, active learning attempts to reduce the cost of acquiring labels by selecting a subset of the training data to be labeled. In this proposal, we utilize the concatenated latent space of Variational Autoencoders (VAEs) and the prediction vector of the classification model for selecting data from the unlabelled pool for labeling. It has been shown that the latent space of VAEs is useful for sampling representative data. In this work, we explore how adding the classifier output to the latent space helps in the selection of samples. Specifically, we exploit the semi-supervised VAE model's latent space for this task. Extensive experiments are conducted on the Fashion-MNIST dataset for analysis of the proposed method.

1 Introduction

Supervised learning has gained great success in recent years. However, it heavily depends on the availability of large amounts of labeled data [1, 2]. In some cases, the labeling process is very expensive and time-consuming, as a result of which, it is impractical to label all available data. To address this issue, semi-supervised learning [3], self-supervised learning [4] and active learning [5] try to make use of unlabelled data in different ways.

Among these approaches, active learning incorporates the label acquisition process in the training pipeline. In each iteration, the algorithm selects a subset of the unlabelled samples based on different criteria and sends these samples to an oracle for labeling. The model is then trained using the pool of labeled data. Since labeling is expensive, active learning tries to be sample-efficient by selecting the most informative samples to be labeled at each step.

There are three scenarios in terms of sampling: (1) *membership query synthesis* [6], where the system learns to generate an instance for the oracle to label; (2) *stream-based sampling* [7], where each sample is provided to the learner one at a time, and the learner determines whether it wants to query its label or not based on its informativeness, and (3) *pool-based sampling* which assumes that there is a large pool of unlabelled data, and samples are selected from this pool according to some informativeness criterion that considers the entire pool simultaneously (unlike stream-based sampling). The current work falls under this category.

All the scenarios above involve the evaluation of the informativeness of unlabelled data. Many strategies have been proposed for this task, such as *uncertainty sampling* [8], where the learner selects the instances for which it is least confident about the class that the instance belongs to; *margin-based*

sampling, which chooses samples that have the smallest difference in confidence between the first and second most probable labels, etc.

In terms of the space in which these acquisition functions operate, certain methods directly consider the input data space, while others look at either the output space of the learner (predictions of the classifier for instance) or the latent space of different models (generative models such as VAEs, for example). As proposed by [9], samples can be selected from the latent space of variational autoencoders (VAE). The VAE is trained using the available data, and informativeness and diversity criteria for the query samples are defined in the latent space. The VAE latent space contains distinctive features of different images, and hence, is more suitable for the finding representative and informative samples compared to the image space.

Based on this idea, several approaches have been proposed, which have been discussed further in Section 2.2. These methods demonstrate the effectiveness of defining acquisition functions on the latent space of VAEs. However, the unlabelled data is not explicitly used for the training of the classifier in any of these proposed approaches, but rather, only the acquisition function gets to observe the unlabelled data pool. Similarly, since the latent space of VAEs is agnostic to the classification task, the acquisition function does not get to benefit from task awareness. In the current proposal, we aim to bridge this gap by exploiting the latent space of the semi-supervised M2 model proposed by Kingma et al. [3]. By using this model and defining acquisition functions on its latent space, we gain on two fronts: (i) the classifier gets to directly utilize unlabelled samples in its training, and (ii) the acquisition function gets to exploit a richer latent space which includes class labels, and hence, provides one latent cluster corresponding to each class.

2 Related Work

2.1 Acquisition Methods

Uncertainty sampling is one of the simplest and most popular strategies for selecting samples, where the learner queries the instance about which it is least confident. For multi-class classification problem, the strategy can be generalized as follows.

$$x_{selected} = \arg \min_x P_{\theta}(\hat{y}|x) \quad (1)$$

where \hat{y} is the label predicted by the classifier parameterized by θ at a given iteration, and $P_{\theta}(\hat{y}|x)$ denotes associated prediction probability.

However, the above method only considers the probability of the predicted label, while ignoring the probabilities associated with the other labels. To overcome this, margin-based sampling is proposed to include the second most probable label:

$$x_{selected} = \arg \min_x P_{\theta}(\hat{y}_1|x) - P_{\theta}(\hat{y}_2|x) \quad (2)$$

A more general strategy applies prediction entropy, which often represents the uncertainty of a prediction. The higher the entropy, the closer if the prediction to the uniform probability, implying that the classifier is less confident of its prediction.

$$x_{selected} = \arg \max_x - \sum_i P_{\theta}(y_i|x) \log P_{\theta}(y_i|x) \quad (3)$$

We use the first and third strategies as baselines in our experiments.

2.2 Variational Autoencoders for Active Learning

[10] combines data augmentation with active learning by generating additional training data using VAE-GAN. BALD-VAE [11] considers the uncertainty of labeled data along with unlabelled data when selecting samples for labeling. Pourkamali-Anaraki et al. [12] and Tonnaer [9] have also proposed and studied the effectiveness of using the latent space of variational autoencoders for designing acquisition functions. Tonnaer et. al. studied the use of more traditional acquisition functions (as described earlier) in the latent space of VAEs, whereas Pourkamali-Anaraki et al.

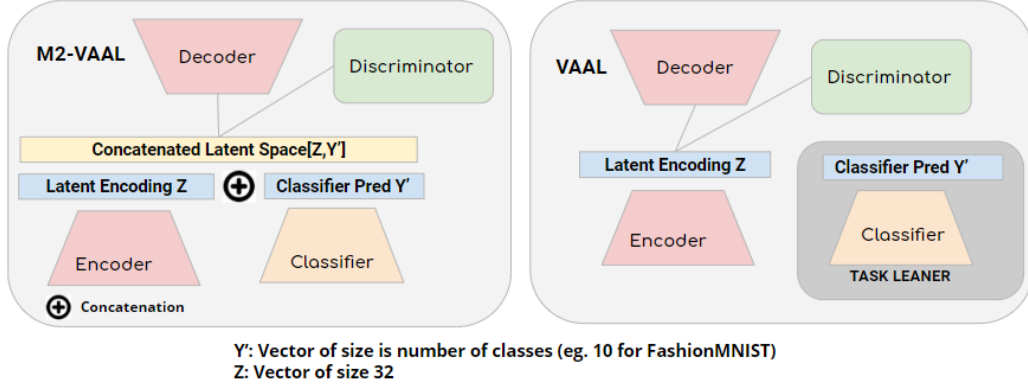


Figure 1: Schematic diagrams of our proposed model M2-VAAL and VAAL: VAAL is effective at picking up representative samples, with the discriminator utilizing the latent space of the VAE. Concatenating the classifier model’s output to the decoder and discriminator makes the latent space task aware.

suggested a geometric technique to select a diverse core-set in this low dimensional space. Both of these lines of work demonstrate that the latent space of VAEs can be exploited to achieve clear gains in the performance of active learning models.

2.3 Semi-Supervised Learning with M2 model

Kingma et al. [3] proposed the semi-supervised VAE model, which can train using both labeled and unlabelled data by incorporating a classifier in the vanilla VAE pipeline. Both the encoder and the classifier take the input image and produce the latent encoding Z and the classifier label Y respectively, which are both fed as inputs to the decoder. The main advantage of this model is that although labels are available for only a subset of the training images, the classifier gets gradients even for the unlabelled pool of samples based on the reconstruction error. This leads to vastly improved semi-supervised learning performance, as demonstrated in [3].

In our work, we propose to exploit the latent space of the M2 semi-supervised VAE model proposed by Kingma et al., as described in the subsequent sections.

3 Proposal

Let $(x_L; y_L)$ be a sample pair belonging to the pool of labeled data $(X_L; Y_L)$, and X_U be a much larger pool of unlabelled samples (x_U) . We consider Y'_L to be predictions for labeled data and Y'_U to be predictions for unlabelled data from the classifier T . One thing to note is that even though we do not have Y_U (or true label) for the unlabelled data, we can still predict the classifier output Y'_U for the unlabelled data. The goal of the active learner is to train the most label-efficient model by iteratively querying b (fixed sampling budget) number of the most informative samples from the unlabelled pool using an acquisition function, such that the expected loss is minimized.

3.1 M2 Variational Adversarial Active Learning (M2-VAAL)

We build our M2-VAAL model as an extension to the VAAL [13] model. A schematic diagram of the comparison of VAAL and M2-VAAL is illustrated in Figure 1. VAAL trains the VAE first with both labeled dataset (X_L) and unlabeled dataset (X_U) to learn the representations of both datasets without using any information about the task learner (classifier) T for performing transductive learning. Then, a discriminator for classifying labeled / unlabeled data is connected to the latent space (Z_L, Z_U) of the VAE, and both the VAE and the discriminator are jointly trained in an adversarial manner[14]. Thus, the VAE encodes both the labelled and unlabelled data pools into the same latent space and the discriminator is trained to predict whether a point in the latent space belongs to the labelled or unlabelled data pool. VAAL is a task-agnostic active learner. However, following the

M2 model [3], we add the classifier prediction (Y'_L, Y'_U) to the latent space (Z_L, Z_U) of both the discriminator and the decoder of the VAE as shown in Figure 1. M2-VAAL is trained with the concatenated ($[Z_L, Y'_L], [Z_U, Y'_U]$) with both labelled and unlabelled data to learn representations of both datasets by using the information learned from the classifier T . Then, the discriminator for deciding labelled/unlabelled data uses the same concatenated space ($[Z_L, Y'_L], [Z_U, Y'_U]$) to learn to distinguish between labelled and unlabelled samples. This adds direct task-related information that could be helpful to further improve the overall performance of active learning.

3.1.1 Training loss for M2-VAAL

M2-Classifier The M2-classifier(T) (or task learner) is trained to fit the labelled data pool ($X_L; Y_L$). It is trained to reduce cross-entropy loss $\mathcal{L}_{M2-Classifier}$ for N classes of the dataset.

$$\mathcal{L}_T = \mathbb{E}[-Y_L \cdot \log r_\gamma(X_L)] \quad (4)$$

$$Y'_L = r_\gamma(X_L)$$

$$Y'_U = r_\gamma(X_U)$$

where r_γ is the classifier parameterized by γ . Y'_L and Y'_U are the prediction vectors of size N for labelled data X_L and unlabelled data X_U respectively obtained from the trained classifier.

M2-VAE We use a β -variational autoencoder for representation learning in which the encoder learns a low dimensional space for the underlying distribution using a Gaussian prior and the decoder reconstructs the input data. To capture the features that are missing in the representation learned on the labelled pool, we can benefit from using the unlabelled data and perform transductive learning. The objective function of the M2- β -VAE is minimizing the variational lower bound on the marginal likelihood of a given sample formulated as

$$\begin{aligned} \mathcal{L}_{M2-VAE}^{trd} = & \mathbb{E}[\log D(p_\theta(X_L | [Z_L, Y'_L]))] - \beta D_{KL}(q_\phi(Z_L | X_L) || p(z)) \\ & + \mathbb{E}[\log D(p_\theta(X_U | [Z_U, Y'_U]))] - \beta D_{KL}(q_\phi(Z_U | X_U) || p(z)) \end{aligned} \quad (5)$$

where q_ϕ and p_θ are the encoder and decoder parameterized by ϕ and θ , respectively. $p(z)$ is the prior chosen as a standard normal distribution, and β is the Lagrangian parameter for the optimization problem. The re-parameterization trick is used for computation of the gradient.

Adversarial Discriminator There are two components to the discriminator (D), adversarial and discriminative components. The adversarial component is trained to make the latent space $[Z_L, Y'_L]$ of labelled data close to the latent space $[Z_U, Y'_U]$ of unlabelled data. This adversarial network is analogous to discriminator in GANs, where their role is to discriminate between real and fake images created by the generator. We can formulate the objective function for the adversarial role of the VAE as a binary cross-entropy loss as below

$$\mathcal{L}_{M2-VAE}^{adv} = -\mathbb{E}[\log D(q_\phi(Z_L|X_L))] - \mathbb{E}[\log D(q_\phi(Z_U|X_U))] \quad (6)$$

While the M2-VAE maps the labelled and unlabelled data into the same latent space with similar probability distributions $q_\phi(Z_L|X_L)$ and $q_\phi(Z_U|X_U)$, it fools the discriminator into classifying all the inputs as labelled. On the other hand, the discriminator attempts to effectively estimate the probability that the data comes from the unlabelled data. The objective function to train the discriminator is given as below

$$\mathcal{L}_D = -\mathbb{E}[\log D(q_\phi(Z_L|X_L))] - \mathbb{E}[1 - \log D(q_\phi(Z_U|X_U))] \quad (7)$$

Overall Objective of M2-VAAL By combining Eq 4, Eq 5 and Eq 6, we get the full objective of M2-VAAL as follows.

$$\mathcal{L}_{M2-VAAL}^1 = \mathcal{L}_T + \mathcal{L}_{M2-VAE}^{trd} + \mathcal{L}_{M2-VAE}^{adv} \quad (8)$$

Though the adversarial loss $\mathcal{L}_{M2-VAE}^{adv}$ is seen to perform well for VAAL [13], it has orthogonal objective to task learner classifier loss objective \mathcal{L}_T . So we also consider the objective of M2-VAAL without using the adversarial loss as follows.

$$\mathcal{L}_{M2-VAAL}^2 = \mathcal{L}_T + \mathcal{L}_{M2-VAE}^{trd} \quad (9)$$

Selection through Trained Discriminator We use the probability associated with the discriminator’s predictions as a score to collect b samples in every batch. The samples whose latent encodings are labelled as “unlabelled” with the lowest confidence by the discriminator are sent to the oracle. Note that the closer the probability is to zero, the more likely it is that it comes from the unlabelled pool.

3.2 Alternative Acquisition Functions

We note that to select a batch of samples at every iteration of active learning, we must incorporate a notion of *diversity* among the selected samples for labeling. We experiment only in the batch setting, since selecting a single sample in every iteration is much more computationally expensive. Since the notion of diversity is not explicitly incorporated in the earlier method, we propose the following alternatives.

3.2.1 Algorithm 1

We propose selecting b/N samples from the cluster for each class in the latent space of the M2 model, to promote diversity in terms of sample selection from all classes. Further, to select diverse samples within each cluster, we select unlabelled samples that maximize the total distance (Euclidean distance in the latent space) from the labeled samples in the corresponding cluster (called *anchor points*). Once a sample is selected for labeling, it is added to the set of anchor points, and subsequent sample selections account for the distance from this point as well. Essentially, by following this method, we try to distribute the selected samples across each cluster in the latent space, rather than allowing them to be concentrated in a particular region. Thus, we hope to reduce the labeling requirement and improve the model’s performance.

3.2.2 Algorithm 2

We note that Algorithm 1, despite promoting diversity, forces the model to select samples from all classes even if the model is less confident about predictions from only a subset of the classes. Hence, we propose a different version of the earlier algorithm, which keeps the distance-based selection criteria the same but does not force the class distribution among the selected samples. Hence, it maximizes the distance of the selected points across clusters in the latent space of the M2 model. Further, we take into account the prediction probabilities for each sample and weight them by the normalized distance scores as computed earlier. By doing this, we hope to allow the model to select more samples that it is less confident about, while still maintaining diversity in the selected batch of samples.

4 Experiments

4.1 Setup

Dataset Used We have used Fashion-MNIST [15] dataset, which consists of grayscale fashion images of shape (28, 28). It consists of images from 10 classes. There are 60K training and 10K test images. Out of 60K samples, 5K samples were reserved for validation, and the remaining 55K were used as an unlabelled pool from which samples were selected.

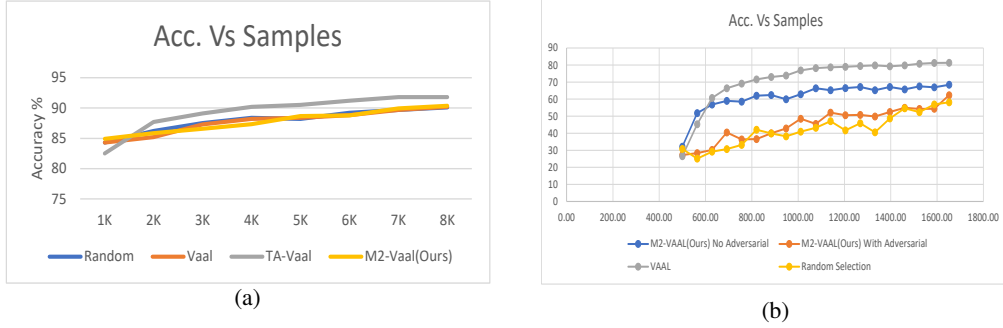


Figure 2: (2a) Results for our proposed method M2-VAAL compared to VAAL [13], TA-VAAL [17] and Random, starting with 1K samples and accuracy ($> 80\%$). (2b) Results for our proposed method M2-VAAL compared to VAAL [13] and Random, when starting 500 samples and accuracy $< 30\%$

We also tried experimenting with the MNIST [16] dataset, but it produced more than 95% accuracy with just 100 labeled samples. Hence, it was not ideal for showing improvements with active learning since the accuracy increments with strategic sample selection were comparable with that for random sample selection. We also tried training with CIFAR-10, but it required larger models for the encoder, decoder, and classifier networks, so time/compute resources required to train the model was out of our scope since active learning requires retraining of the model after every acquisition step. Hence, we kept the experiments limited to the Fashion-MNIST dataset.

Architecture of Encoder, Decoder, and Discriminator (M2-VAAL) The encoder network maps images of shape $(28, 28)$ to a latent space of dimension 32. We use two convolutions, two fully-connected linear layers for the encoder, with the final layer of encoder mapping to a latent dimension of size 32. For the decoder, we use the reverse encoder architecture with latent space of dimension 32 mapped to image dimension of $(28, 28)$, with two fully-connected linear layers, followed by two deconvolution layers. For the classifier, we use a similar architecture as the encoder, except for the final linear layer which is mapped to size $N = 10$ classes. Discriminator maps the concatenated output of encoder and classifier of size 42 to a single output node with sigmoid activation. We project the 42 dimensional latent space vector to size 512 with a fully connected linear layer and add another fully-connected linear layer before the final sigmoid output.

For the other two algorithms, we experiment with a larger model with 3M parameters, to study how far the accuracy values can be pushed.

Hyperparameters Initial pool of (X_L, Y_L) consists of 500 samples of the Fashion-MNIST dataset. At every iteration, we add $b = 64$ samples from the unlabelled pool to the labeled pool for the M2-VAAL model, and 50 samples in each iteration for the other two algorithms. We train the M2-VAAL, discriminator from scratch every time a new set of labeled data is added to the existing labeled pool.

Performance measurement We evaluate the performance of M2-VAAL for image classification by measuring the accuracy achieved by the classifier (T) trained with 500, 564, 628, 692 . . . , 2000 images of Fashion-MNIST dataset, as the labeled data get added after selection by the discriminator. We had initially experimented with 1K, 2K, 3K, . . . , 8K images, following the setup by [17], results, and analysis for which are also included in the experiments section.

For the other algorithms, we start with a budget of 50 labeled samples, and set $b = 50$, i.e., 50 unlabelled samples are selected for labeling and added to the set of labeled samples at each iteration.

4.2 Results

4.2.1 Comparison to State of the Art

Initial Budget 1K comparisons We followed the same experimental setup from the TA-VAAL paper [17] to start experimenting with Fashion-MNIST dataset. Results of our method (M2-VAAL)

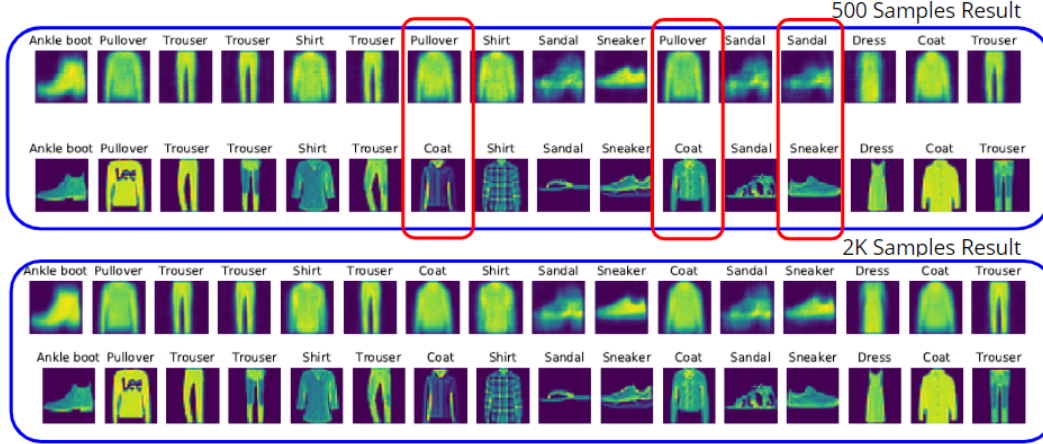


Figure 3: Qualitative examples showing reconstruction output of M2-VAE along with Task Learner predicted output. 1st and 3rd row represents reconstructed output and predicted label. 2nd and 4th row represent the original image and ground truth label. We can see better-reconstructed images and correct task predictions when labeled training samples reaches 2K.

compared to random selection, VAAL and TA-VAAL are shown in Figure 2a. TA-VAAL is another method that adds task aware sample selection through the addition of ranking loss. We perform poorly than the TA-VAAL and equivalent to VAAL [13] and random selection method. To analyze these results, we conducted further experiments to find that the discriminator for our method does not work with high classifier accuracy ($> 80\%$ in our case). It is unable to learn to distinguish between labeled and unlabeled samples at such high accuracy. Also, because the purpose of active learning is to select samples for training, it is more practical to start active learning with lower accuracy. So we move on to a new setup with less number of samples and lower accuracy to test our proposed method. Another thing to note here is that random selection is an important baseline for comparison of active learning acquisition functions, as the Fashion-MNIST has an equivalent number of images for each class, and picking up random samples at each iteration provides a diverse set of class labels.

Initial Budget 500 comparison Next, we experiment with 500 samples containing labeled samples from **only 3 classes** $\{2 : \text{PullOver}, 4 : \text{Coat}, 7 : \text{Sneaker}\}$. Initial accuracy with these 500 labeled samples is $< 30\%$. Results of the comparison of our proposed model with VAAL and random selection are shown in Figure 2b. Even though M2 VAE is shown to perform better than VAE in [3], our model (M2-VAAL) is seen to be performing worse than VAAL. After experimentation and analysis, we found that the adversarial discriminator loss objective $\mathcal{L}_{M2-VAE}^{adv}$ performs orthogonal to the task learner objective \mathcal{L}_T . So, we have M2-VAAL trained for the objective function defined in equation 8, which is M2-VAAL with adversarial loss. Second version is for objective function defined in equation 9, which is M2-VAAL without adversarial loss. M2-VAAL without adversarial loss is shown to perform better than with an adversarial loss. It is shown to perform better than random uniform sampling, which shows selection based on active learning is important. But it is not able to reach the state of art VAAL accuracy, because removing adversarial loss makes the selection of samples skewed to few classes only.

4.2.2 Qualitative Reconstruction Examples

In Figure 3 we show some reconstructed output of M2-VAE and predicted labels from the task learner. We see that the reconstructed output and the task predictions improve with an increase in the number of labeled samples.

4.2.3 Alternative Algorithms Results

In Figure 4, we compare the performance of the proposed algorithms with common baselines, such as random selection, least confidence based selection, and entropy-based selection. As can be observed from the figure, the methods perform quite similarly, and it cannot be concluded that any particular method outperforms the others.

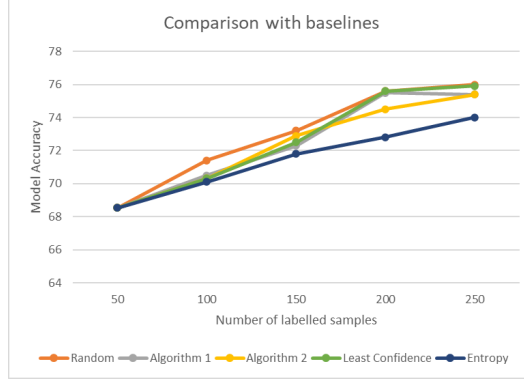


Figure 4: Comparison of the performance of Algorithm 1 and Algorithm 2 with random sampling based selection, least confident prediction based selection, and predictive entropy based selection.

Further analysis of the performance of Algorithm 1 shows that at each iteration, the algorithm forces selection of an equal number of samples from each class even if the model is confident of the predictions for particular classes. This hampers the selection of samples from classes where labeling is more important, leading to a comparable performance with baselines.

We next analyze the performance of Algorithm 2, where we take into account the prediction confidence of the classifier along with the distance-based diversity measure. Even in this case, the performance achieved is comparable to that of the baselines. However, we do note that the selected samples show a good mix of samples from different classes, as well as samples that are mostly incorrectly labeled by the classifier at a particular iteration.

Based on the above results, we feel that the proposed methods can be expected to outperform more traditional active learning schemes if the classifier accuracy is not as high as that obtained by using the M2 model. E.g., when the classifier test accuracy obtained by training with 50 labeled samples is around 70%, random sampling can be expected to select around 30% samples which are incorrectly labeled by the classifier. However, our method selects more than 60% samples with incorrect labels, showing the effectiveness of the proposed approach. Hence, as a possible future line of work, we intend to study the effect of the proposed algorithms in the scenarios where classifier accuracy is much lower, either due to lower labeled data size or due to lower capacity models.

5 Conclusion

We use the semi-supervised VAE model in the active learning pipeline. For the selection of diverse, representative samples from entire semi-supervised VAE space, we have tried the deep learning based discriminator both with and without adversarial loss in M2-VAE. One important observation we analyzed is using discriminator at very high test accuracy makes the discriminator behave randomly and it is unable to learn the difference between labeled and unlabeled samples. Also, we find it is more practical to show active learning usage when starting with lower accuracy. Semi-supervised VAE space (of M2-VAE) works well without adversarial loss. It performs much better than random uniform selection, showing selection based on active learning is important. But it was not able to reach accuracy of standard VAE space(VAAL). Considering this, we proposed two different methods to exploit the richer latent structure provided by M2-VAE. Based on the experimental results, we conclude that although the accuracy increments obtained by sample selection using the proposed methods are comparable to existing methods, the selected samples do not represent intra-batch diversity, as well as informativeness. As future work, we aim to study the effect of the proposed methods in lower labeled data size regimes with lower capacity models, such that the difference in performance can be observed.

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