Gaussian Mixture Variational Autoencoder with Contrastive Learning for Multi-Label Classification

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Abstract

Multi-label classification (MLC) is a prediction task where each sample can have more than one label. We propose a novel contrastive learning boosted multi-label prediction model based on a Gaussian mixture variational autoencoder (C-GMVAE), which learns a multimodal prior space and employs a contrastive loss. Many existing methods introduce extra complex neural modules to capture the label correlations, in addition to the prediction modules. We found that by using contrastive learning in the supervised setting, we can exploit label information effectively, and learn meaningful feature and label embeddings capturing both the label correlations and predictive power, without extra neural modules. Our method also adopts the idea of learning and aligning latent spaces for both features and labels. C-GMVAE imposes a Gaussian mixture structure on the latent space, to alleviate posterior collapse and over-regularization issues, in contrast to previous works based on a unimodal prior. C-GMVAE outperforms existing methods on multiple public datasets and can often match other models’ full performance with only 50% of the training data. Furthermore, we show that the learnt embeddings provide insights into the interpretation of label-label interactions.

Introduction

In many machine learning tasks, an instance can have several labels. The task of predicting multiple labels is known as multi-label classification (MLC). MLC is common in domains like vision (Wang et al. 2016), natural language (Chang et al. 2019), biology (Yu et al. 2013). Unlike the single-label scenario, label correlations are more important in MLC. Early works capture the correlations through classifier chains (Read et al. 2009), bayesian inference (Zhang and Zhou 2007), and dimensionality reduction (Bhatia et al. 2015).

Boosted by the huge capacity of neural networks (NN), many previous methods can be improved by their neural extensions. For example, classifier chains can be naturally enhanced by RNN (Wang et al. 2016). The non-linearity of NN alleviates the design complexity of feature mapping and many deep models can therefore focus on the loss function, feature-label and label-label correlation modeling.

One trending direction is to learn a deep latent space shared by features and labels. The samples from the latent space are then decoded to targets. One typical example is C2AE (Yeh et al. 2017), which learns latent codes for both features and labels. The latent codes are passed through a decoder to obtain target labels. C2AE minimizes an $\ell_2$ distance between feature and label codes, together with a relaxed orthogonality regularization. However, the learnt deterministic latent space lacks smoothness and structures. Small perturbations in this latent space can lead to totally different decoding results. Even if the corresponding feature and label codes are close, we cannot guarantee the decoded targets are similar. To address this concern, MPVAE (Bai, Kong, and Gomes 2020) proposes to replace the deterministic latent space with a probabilistic subspace under a variational autoencoder (VAE) framework. The Gaussian latent spaces are aligned with KL-divergence, and the sampling process enforces smoothness. Similar ideas can be found in (Sundar et al. 2020). However, these methods assume a unimodal Gaussian latent space, which is known to cause over-regularization and posterior collapse (Dilokthanakul et al. 2016; Wu and Goodman 2018). A better strategy would be to learn a multimodal latent space. It is more intuitive to assume the observed data are generated from a multimodal subspace rather than from a unimodal one.

Another popular group of methods targets on better label correlation modeling. Their idea is straightforward: some labels should be more correlated if they co-appear often while others should be less relevant. Existing methods adopt pairwise ranking loss, covariance matrix, conditional random field or even graph neural nets (GNN) (Zhang and Zhou 2013; Bi and Kwok 2014; Belanger and McCallum 2016; Lanchantin, Sekhon, and Qi 2019; Chen et al. 2019b). These methods often either constrain the learning through a predefined structure (which requires larger space), or aren’t powerful enough to capture the correlations (such as pairwise ranking loss).

Our idea is simple: we learn embeddings for each label class and the inner product between embeddings should reflect the similarity. We further learn feature embeddings whose inner products with label embeddings correspond to feature-label similarity and can be used for prediction. We assume these embeddings are generated from a probabilistic multimodal latent space shared by features and labels, where we use KL-divergence to align the feature latent distribution and label latent distribution. On the other hand, one
may concern that embeddings might not be able to capture label-label, label-feature correlations, as what extra GNN and covariance matrix from prior works did (Lanchantin, Sekhon, and Qi 2019; Bai, Kong, and Gomes 2020). To this end, we use pure losses rather than extra structures to capture these correlations. Intuitively, if two labels co-appear often, their embeddings should be close. If two labels seldom co-appear, their embeddings should be distant. A triplet-like loss could be naturally applied in this scenario. Nevertheless, more powerful contrastive loss has shown to be more effective than the triplet loss by introducing more samples rather than just one triplet. We show that contrastive loss can pull together correlated labels, and push away unrelated labels (see Fig. 3), which performs even better than GNN-based or covariance-based methods.

Our new model, the contrastive learning boosted Gaussian mixture variational autoencoder (C-GMVAE) multi-label prediction model, alleviates the over-regularization and posterior collapse concerns, as well as learns useful feature and label embeddings. C-GMVAE is applied to nine datasets and outperforms the existing methods on five metrics. Furthermore, we show that often with only 50% of the data, our results can match the full performance of other state-of-the-art methods. Ablation studies and interpretability of learnt embeddings will also be illustrated in the experiments. Our contributions can be summarized in three aspects: (i) We propose to use contrastive loss instead of triplet or ranking loss to strengthen the label embedding learning. We empirically show that by using a contrastive loss, one can get rid of heavy-duty label correlation modules (e.g. covariance matrix, GNN) while achieving even better performances. (ii) Though contrastive learning is commonly applied in self-supervised learning, our work shows that by properly defining anchor, positive and negative samples, contrastive loss can leverage label information very effectively in the supervised MLC scenario as well. (iii) Unlike prior probabilistic models, C-GMVAE learns a multimodal latent space and associates the probabilistic modeling (VAE module) with embedding learning (contrastive module) synergistically.

Methods

In MLC, given the dataset containing \( N \) samples (with labels) \((x, y)\), where \( x \in \mathbb{R}^D \) and \( y \in \{0, 1\}^L \), our goal is to find a mapping from \( x \) to \( y \). \( N, D, L \) are sample number, feature length and label set size respectively. The binary coding indicates the labels associated with the sample \( x \). Labels are correlated with each other.

Preliminaries

Gaussian Mixture VAE A standard VAE (Kingma and Welling 2013) pulls together the posterior distribution and a parameter-free isotropic Gaussian prior. Two losses are optimized together in training: KL-divergence from the prior to the posterior, and the distance between recontracted targets and real targets. One weakness of this formulation is the unimodality of the latent space, inhibiting the learning of more complex representations. Another concern is over-regularization. If the posterior is exactly the same as the prior, the learnt representations would be uninformative of training inputs. Numerous works extend the prior to be more complex (Chung et al. 2015; Eslami et al. 2016; Dilokthanakul et al. 2016). In our work, we adopt the Gaussian mixture prior. The probability density can be depicted as:

\[
p(z) = \frac{1}{k} \sum_{i=1}^{k} \mathcal{N}(z | \mu_i, \sigma_i^2)
\]

where \( i \) is the cluster index of \( k \) Gaussian clusters with mean \( \mu_i \) and covariance \( \sigma_i^2 \) (Shu 2016; Shi et al. 2019). Our intuition is that each label embedding could correlate to a Gaussian subspace. Given a label set, the mixture of the corresponding Gaussians forms a unique multimodal prior distribution. The label embeddings also receive the gradients from the contrastive loss and thus combine the contrastive learning and latent space construction. Our formulation is also related to MVAE (Wu and Goodman 2018; Shi et al. 2020) where the idea of product-of-experts is adopted.

Contrastive Learning

We propose to use contrastive learning to capture the correlations (feature-label, label-label). Contrastive learning (Oord, Li, and Vinyals 2018; Chen et al. 2020; Khosla et al. 2020) is a novel learning style. The core idea is simple: given an anchor sample, it should be close to similar samples (positive) and far from dissimilar samples (negative) in some learnt embedding space. It differs from triplet loss in the number of negative samples and the way of loss estimation. Contrastive loss is largely motivated by the noise contrastive estimation (NCE) (Gutmann and Hyvärinen 2010) and its form is generalizable. The raw contrastive loss formulation only considers the instance-level invariance (multiple views of one instance), but with label information, we can learn category-level invariance (multiple instances per class/category) (Wang et al. 2020). In the multi-label scenario, one can regard the feature embedding as the anchor sample, positive label embeddings as positive samples and negative label embeddings as negative samples. The formulation can fit the contrastive learning framework naturally and is one of our major contributions. Compared to pairwise ranking loss which focuses on the final digits, contrastive loss is defined on the embeddings and thus more expressive. Contrastive loss also includes more samples in estimating the NCE and therefore outperforms triplet loss. In appendix, we show triplet loss is actually a special case of our contrastive loss.

C-GMVAE

C-GMVAE inherits the general variational autoencoder framework, but with a learnable Gaussian mixture prior. During training, the sample’s label set activates and mixes the related Gaussian clusters to derive the prior. Contrastive learning is applied to boost the embedding learning, using a contrastive loss between the feature and label embeddings. Fig. 1 provides a full illustration, and the following subsections will elaborate on the details.

Gaussian Mixture Latent Space

Given a sample \((x, y)\) where feature \( x \in \mathbb{R}^D \) and label \( y \in \{0, 1\}^L \), many previous works take \( y \) as the input and transform it to a dense representation through a fully-connected layer (Yeh et al. 2017; Bai, Kong, and Gomes 2020). This layer essentially maps
each label category to an embedding and sums up all the embeddings using label $y$ as weights (0 or 1). The final embedding is fed into the label encoder to produce a probabilistic space. In C-GMVAE, we directly map each per-category label embedding $w^l_i \in \mathbb{R}^E$ of label class $i$ to an individual Gaussian distribution $\mathcal{N}(\mu, diag(\sigma^2))$, $\mu_i \in \mathbb{R}^d$, $\sigma^2_i \in \mathbb{R}^d$.

The posterior is aligned with the prior via KL-divergence. The decoder takes in a sample from the latent space and produces a feature embedding $w^f_i \in \mathbb{R}^E$. A contrastive loss is designed to pull together the feature embedding and positive label embeddings, while separating the feature embedding from negative label embeddings. Prediction $\hat{y}$ is made by passing the feature-label embedding inner products to the sigmoid functions. In the figure, a sample with label set \{sea, bird\} is provided.

We form a standard posterior in our model and match it with the prior. However, unlike vanilla VAE, we cannot analytically compute the KL term. Instead, we use the following estimation:

$$
\mathcal{L}_{KL} \approx \log q_\theta(z_0|x) - \log p_\psi(z_0|y)
= \log \mathcal{N}(z_0|\mu_\phi, diag(\sigma^2_\phi(x))) - \log \mathcal{N}(z_0|\mu, diag(\sigma^2))
$$

where $z_0 \sim q_\theta(z|x)$ denotes a single latent sample. Our formulation follows (Shu 2016), which has been shown to outperform the formulation in (Dilokthanakul et al. 2016).

The reconstruction loss remains to be a standard negative log-likelihood (we add the minus since the objective function is to be minimized. $\theta$ is the decoder parameters.),

$$
\mathcal{L}_{\text{recon}} = -E_{q_\theta(z|x)}[\log p_\theta(x|z)]
$$

Contrastive Learning Module

The decoder function $f_\theta(x)$ decodes the sample from the latent space to a feature embedding $w^f_i \in \mathbb{R}^E$. We train $w^f_i$ together with label embeddings $\{w^l_i\}_{i=1}^L$. The objective function includes contrastive loss and cross-entropy loss terms.

Prior works used to explicitly capture the label-label interactions by GNN or covariance modules, which imposes the structure a priori and might not be the best way. Our contrastive module instead captures the correlation completely driven by data. For example, if in most of the samples, “beach” and “sunshine” appear together, the contrastive learning will implicitly pull their embeddings together (see derivation in appendix). In other words, if two labels do co-appear often, their label embeddings become similar (Fig. 3). On the other hand, if they only co-appear occasionally, their relations are not significant and our module will not optimize for their similarity.
Original contrastive learning (Oord, Li, and Vinyals 2018) augments inputs and learns instance-level invariance, but may not generalize to category-level invariance. In the supervised setting, however, the learning can benefit from labels and discover category-level invariance (Khosla et al. 2020). Let \( A \equiv \{1,...,n\} \). We define \( P(y) \equiv \{ i \in A : y_i = 1 \} \) for sample \( (x,y) \). Suppose we have a batch of samples, \( B \), the contrastive loss can be written as

\[
L_{CL} = \frac{1}{|B|} \sum_{(x,y) \in B} \frac{1}{|P(y)|} \sum_{p \in P(y)} - \log \frac{\text{sim}(w^f_x, w^f_p)}{\sum_{l \in A} \text{sim}(w^f_x, w^l)}
\]

(5)

\( \text{sim}() \) is a function measuring the similarity between two embeddings, and \( w^f_i, w^l_i \) denote the feature and label embeddings respectively. Eq. 5 is built on top of noise-contrastive estimation (Gutmann and Hyvärinen 2010), and the equation is equivalent to a categorical cross-entropy of correctly predicting positive labels. The choice of \( \text{sim}() \) can be a log-bilinear function (Oord, Li, and Vinyals 2018), or a more complicated neural metric function (Chen et al. 2020). In our experiments, we found it is simple and effective to take \( \text{sim}(w_1, w_2) = \exp(w_1 \cdot w_2 / \tau) \) where \( \cdot \) means inner product and \( \tau \) a temperature parameter controlling the scale of the inner products. In SupCon (Khosla et al. 2020), if only 1 class is positive, all other classes are contrastive to it. However, in multi-label, if “beach” is positive in the label while “sea” isn’t for one particular sample, we cannot say these two classes are contrastive. Their correlation will be captured implicitly by all the samples. Therefore, we do not assume contrastive relations between labels and preserve the label correlations. We instead choose the feature embedding to be the anchor and label embeddings to be positive/negative samples. If two label embeddings co-appear often as positive samples, they would implicitly become similar (see Fig. 3). Eq. 5 saves the effort of manually configuring the positive and negative samples, and is totally data-driven. The number of positives or negatives could be greater than one. Note that though \( L \) limits the max samples we can have, this formulation has already used many more samples compared to triplet loss, and we will show in experiments that this formulation is very effective.

The triplet loss often used in multi-label learning (Seymour and Zhang 2018) can be seen as a special case of Eq. 5 with only one positive and one negative. We illustrate the connection in the appendix. Furthermore, one desired property of embedding learning is that when a good positive embedding is already close enough to our anchor embedding, it contributes less to the gradients, while poorly learnt embeddings contribute more to improve the model performance. In appendix, we also show that the contrastive loss can implicitly achieve this goal and a full derivation of the gradients.

Our objective function also includes a supervised cross-entropy loss term to further facilitate the training. With the label embeddings \( w^l_i \) and the feature embedding \( w^f_x \), the cross entropy loss for each \( (x,y) \) is given by

\[
L_{CE} = \sum_{i=1}^{L} y_i \log s(w^f_x w^l_i) + (1 - y_i) \log(1 - s(w^f_x w^l_i))
\]

(6)

where function \( s(\cdot) \) is the sigmoid function. In self-supervised learning, the contrastive loss typically helps the pretraining stage and the learnt representations are applied to downstream tasks. In the supervised setting, though some models (Khosla et al. 2020) stick to the two-stage training process where the model is trained with contrastive loss in the first stage and cross-entropy loss in the second stage, we didn’t observe its superiority to the one-stage scheme where we train the model with an objective function incorporating all losses. This is partly because we also learn a latent space that is closely connected to label embeddings. A joint training strategy reconciles different modules. We show in the experiments that the learnt embeddings are semantically meaningful and can reveal the label correlations.

**Objective Function**

The final objective function to minimize is simply the summation of different losses,

\[
\mathcal{L} = \mathcal{L}_{KL} + \mathcal{L}_{recon} + \alpha \mathcal{L}_{CL} - \beta \mathcal{L}_{CE}
\]

(7)

where \( \alpha, \beta \) are trade-off weights. The model is trained with Adam (Kingma and Ba 2014). Our model is optimized with \( \mathcal{L} \) but will be tested on five different metrics. This is different from the methods that optimize specific metrics (Koyejo et al. 2015; Decubber et al. 2018).

**Prediction**

During the testing phase, the input sample \( x \) will be passed to the feature encoder and decoder to obtain its embedding \( w^f_i \). Label embeddings \( w^l_i \) are fixed during testing. The inner products between \( w^f_i \) and \( w^l_i \) will be passed through a sigmoid function to obtain prediction probability for class \( i \).

**Insights behind C-GMVAE**

C2AE and MPVAE have shown the importance of learning a shared latent space for both features and labels. These methods share the same high-level insight similar to teacher-student regime: we map labels (teacher) to a latent space with some certain structure, which preserves the label information and is easier to be decoded back to labels. Then the features (student) are expected to be mapped to this latent space to facilitate the label prediction. Two general concerns exist for these methods: 1) the uni-Gaussian space previously used is too restrictive to impose sophisticated structures for prior, 2) how to properly capture label correlations with embeddings. For the first, we learn a modality for each label class to form a mixture latent space. For the second, we replace the commonly used ranking and triplet losses with contrastive loss since contrastive loss involves more samples than triplet loss and has a larger capacity than ranking loss.

**Related Work**

Learning a shared latent space for features and labels is a common and useful idea. In single-label prediction tasks, CADA-VAE (Schönfeld et al. 2019) learns and aligns latent label and feature spaces through distribution alignment losses. Similar ideas can be seen in out-of-distribution detection as well (Sundar et al. 2020). In multi-label scenarios, methods adopting this idea typically have a similar module that directly maps the multi-hot labels to embeddings.
Table 1: The example-F1 (ex-F1) and micro-F1 (mi-F1) scores of different methods on all datasets. C-GMVAE’s numbers are averaged over 3 seeds. The standard deviation (std) is also shown. 0.000 means an std < 0.0005.

| Metric              | example-F1 | micro-F1 |
|---------------------|------------|----------|
| Dataset             | C-GMVAE    |          |
| eBird               | 0.576 ± 0.534 | 0.633 ± 0.575 |
| mirflickr           | 0.481 ± 0.481 | 0.510 ± 0.510 |
| nus-vec             | 0.656 ± 0.777 | 0.665 ± 0.762 |
| yeast               | 0.777 ± 0.777 | 0.803 ± 0.803 |
| scene               | 0.917 ± 0.917 | 0.890 ± 0.890 |
| sider               | 0.392 ± 0.392 | 0.377 ± 0.377 |
| reuters             | 0.381 ± 0.381 | 0.377 ± 0.377 |
| bkms                | 0.000 ± 0.000 | 0.000 ± 0.000 |
| delicious           | 0.002 ± 0.002 | 0.000 ± 0.000 |

Table 2: The macro-F1 (ma-F1) and Hamming accuracy (HA) scores of different methods on all datasets. C-GMVAE’s numbers are averaged over 3 seeds.

| Metric              | macro-F1 | Hamming Accuracy |
|---------------------|----------|------------------|
| Dataset             | C-GMVAE  |          |
| eBird               | 0.825 ± 0.732 | 0.847 ± 0.903 |
| mirflickr           | 0.595 ± 0.595 | 0.594 ± 0.796 |
| nus-vec             | 0.751 ± 0.788 | 0.769 ± 0.915 |
| yeast               | 0.962 ± 0.962 | 0.767 ± 0.767 |
| scene               | 0.939 ± 0.939 | 0.997 ± 0.997 |
| sider               | 0.465 ± 0.707 | 0.992 ± 0.992 |
| reuters             | 0.000 ± 0.000 | 0.000 ± 0.000 |
| bkms                | 0.000 ± 0.000 | 0.000 ± 0.000 |
| delicious           | 0.000 ± 0.000 | 0.000 ± 0.000 |

Table 3: The precision@1 scores of different methods on all datasets. “mir.” stands for mirflickr and “del.” means delicious dataset.

| Metric   | Dataset | Metric | Dataset |
|----------|---------|--------|---------|
| precision@1 | eBird   | mirflickr   | nus-vec   |
|          | mirflickr | scene | sider | reuters | bkms | delicious |
| BR       | 0.825 ± 0.732 | 0.595 ± 0.595 | 0.751 ± 0.788 | 0.962 ± 0.962 | 0.465 ± 0.707 |
| MLKNN    | 0.510 ± 0.383 | 0.342 ± 0.618 | 0.691 ± 0.738 | 0.703 ± 0.213 | 0.259 |
| HARAM    | 0.510 ± 0.342 | 0.396 ± 0.629 | 0.717 ± 0.722 | 0.711 ± 0.216 | 0.267 |
| SLEEC    | 0.258 ± 0.416 | 0.431 ± 0.643 | 0.718 ± 0.581 | 0.885 ± 0.363 | 0.308 |
| C2AE     | 0.501 ± 0.501 | 0.435 ± 0.614 | 0.698 ± 0.768 | 0.818 ± 0.309 | 0.326 |
| LaMP     | 0.477 ± 0.492 | 0.376 ± 0.624 | 0.728 ± 0.766 | 0.906 ± 0.389 | 0.372 |
| MPVAE    | 0.551 ± 0.514 | 0.468 ± 0.648 | 0.751 ± 0.769 | 0.893 ± 0.382 | 0.373 |

(Chen et al. 2019a; Bai, Kong, and Gomes 2020). This is a rather difficult learning task. Suppose we have 30 label categories. There could be up to $2^{30}$ label sets. For probabilistic models like MPVAE, that means one latent label space has to represent up to $2^{30}$ label combinations. In contrast, C-GMVAE learns per-category subspace and forms a mixture prior distribution based on the observed samples’ label sets.

Contrastive learning has become one of the most popular self-supervised learning techniques. It has also drawn attention in supervised tasks. SupCon (Khosla et al. 2020) first demonstrated the effectiveness of supervised contrastive loss in image classification. It was soon generalized to other domains like visual reasoning (Malinowski and Madzio2020). Nevertheless, these methods depend on vision-specific augmentation techniques. Another related work is multi-label contrastive learning (Song and Ermon 2020). But the work does not deal with MLC. Instead, it extends the contrastive learning to identifying more than 1 positive sample, which resembles a multi-label scenario.

Some earlier works also attempted metric learning or triplet loss in MLC (Annarumma and Montana 2017). Triplet loss typically only takes one pair of positive and negative samples for one anchor, while contrastive loss uses many more negative/positive samples. Recent papers found that more samples can greatly boost the performance (Chen et al. 2020; Wang et al. 2020). Note that though our contrastive module is constrained by the maximum number of label classes, it has already used many more samples than triplet loss, and our observations support that more samples help with the performance.

**Experiments**

We have various setups to validate the performance of C-GMVAE. First, we compare the example-F1, micro-F1 and macro-F1 scores, Hamming accuracies and precision@1 of different methods. Second, we compare their performances when fewer training data are available. Third, an ablation study shows the importance of the proposed modules. Finally, we demonstrate the interpretability of label embeddings on an eBird dataset. Our code is available in appendix.

**Setup**

For the main evaluation experiments, we use nine datasets, including image datasets mirflickr, nuswide, scene (Huiskes...
| variations          | eb-F1 | mi-F1 | ma-F1 |
|---------------------|-------|-------|-------|
| **ebird**           |       |       |       |
| uni-Gaussian        | 0.545 | 0.583 | 0.490 |
| GM only             | 0.561 | 0.603 | 0.511 |
| contrastive only    | 0.558 | 0.594 | 0.515 |
| GM+contrastive      | 0.576 | 0.633 | 0.538 |
| **mirflickr**       |       |       |       |
| uni-Gaussian        | 0.510 | 0.541 | 0.413 |
| GM only             | 0.521 | 0.561 | 0.429 |
| contrastive only    | 0.526 | 0.565 | 0.428 |
| GM+contrastive      | 0.534 | 0.575 | 0.440 |
| **nus-vec**         |       |       |       |
| uni-Gaussian        | 0.461 | 0.479 | 0.203 |
| GM only             | 0.472 | 0.505 | 0.218 |
| contrastive only    | 0.470 | 0.501 | 0.213 |
| GM+contrastive      | 0.481 | 0.510 | 0.226 |

Table 4: Ablation study on the contrastive learning module and Gaussian mixture module. Note that both contrastive learning module and mixture Gaussian space are contributions in this work. GM can bring improvements consistently. Contrastive module can further boost the performance.

| method (data %) | HA | ex-F1 | mi-F1 | ma-F1 |
|-----------------|----|-------|-------|-------|
| **ebird**       |    |       |       |       |
| MPVAE (100%)    | 0.829 | 0.551 | 0.593 | 0.494 |
| C-GMVAE (50%)   | 0.842 | 0.557 | 0.615 | 0.521 |
| **mirflickr**   |    |       |       |       |
| MPVAE (100%)    | 0.898 | 0.514 | 0.552 | 0.422 |
| C-GMVAE (50%)   | 0.890 | 0.512 | 0.553 | 0.412 |
| **nus-vec**     |    |       |       |       |
| MPVAE (100%)    | 0.980 | 0.468 | 0.492 | 0.211 |
| C-GMVAE (50%)   | 0.975 | 0.465 | 0.494 | 0.201 |

Table 5: Comparisons between MPVAE and C-GMVAE using 100% and 50% respectively.

Table of contents

1. **Table 4**: Ablation study on the contrastive learning module and Gaussian mixture module.
2. **Table 5**: Comparisons between MPVAE and C-GMVAE using 100% and 50% respectively.
3. **Metrics**: We evaluate our method trained with objective Eq. 7 on several commonly used multi-label metrics. Suppose the ground-truth label is $y$ and the predicted label is $\hat{y}$. We denote true positives, false positives, false negatives by $tp_j, fp_j, fn_j$ respectively for the $j$-th of $L$ label categories. (i) HA: $\frac{1}{L} \sum_{j=1}^{L} \mathbb{1}[y_j = \hat{y}_j]$ (ii) example-F1: $\frac{2 \sum_{j=1}^{L} y_j \hat{y}_j}{\sum_{j=1}^{L} y_j + \sum_{j=1}^{L} \hat{y}_j}$ (iii) micro-F1: $\frac{\sum_{j=1}^{L} tp_j}{2 \sum_{j=1}^{L} tp_j + \sum_{j=1}^{L} fp_j + \sum_{j=1}^{L} fn_j}$ (iv) macro-F1: $\frac{1}{L} \sum_{j=1}^{L} \frac{2 tp_j}{2 tp_j + fp_j + fn_j}$

Furthermore, precision@1 is the proportion of correctly predicted labels in the top-1 predictions.

**Architecture and Hyperparameters**: As we state in the introduction, we do not require very sophisticated neural architectures in C-GMVAE. All the neural layers are fully connected. The feature encoder is a fully connected neural network with 3 hidden layers and the activation function is ReLU. The label encoder is also fully connected comprising two hidden layers and the decoder has two hidden layers as well. More details of the model can be found in the appendix. We set $\alpha = 1, \beta = 0.5, E = 2048$ from tuning for most runs. Grid search is applied to find the best learning rate, dropout ratio, weight decay ratio for each dataset. We use one V100 GPU for all experiments. More architecture, hyper-parameter tuning and final selection (Tab. 7 in Appx), and implementation details can be found in the appendix.

**Evaluations**

**Full supervision**: In the full supervision scenario which is commonly adopted by the methods we compare against, we evaluate four metrics: example-F1 (ex-F1), micro-F1 (mi-F1), macro-F1 (ma-F1), Hamming accuracy (HA) and precision@1. ex-F1 score is the averaged F1-score over all the samples. mi-F1 score measures the aggregated contributions of all classes. ma-F1 treats each class equally and takes the class-wise average. HA counts the correctly predicted labels regardless of samples or classes. The full definitions of these metrics can be found in the appendix.
Tab. 1, 2 and 3 present the performance of all the methods w.r.t. the metrics. We abbreviate nuswide-vector to nus-vec, and bookmarks to bkms. C-GMV AE outperforms the existing state-of-the-art methods on all the datasets. The best numbers are marked in bold. All the numbers for C-GMV AE are averaged over 3 seeds for stability and the standard deviations are included in the table. On ex-F1, C-GMV AE improves over MPVAE by 2.5%, and LaMP by 8.8% on average across all the datasets. Similarly, on mi-F1, C-GMV AE improves over MPVAE by 2.4% and LaMP 6.1% on average. On ma-F1, the improvements are as large as 4.1% and 11% respectively. C-GMV AE outperforms other methods consistently.

Ablation study To demonstrate the strength of our C-GMV AE, we compare it with a uni-Gaussian latent model, a Gaussian mixture (GM) only latent model (without contrastive module), and a contrastive only model (without KL term) in Tab. 4. Our C-GMV AE (GM+contrastive) consistently outperforms other models by a margin. For instance, on ma-F1, C-GMV AE improves over uni-Gaussian model by 7%.

Training on fewer data Contrastive learning learns contrastive views and thus requires less information compared to generative learning which demands a more complete representation for reconstruction. Contrastive learning has the potential to discover the intrinsic structures present in the data, and therefore is widely used in self-supervised learning since it generalizes well. We observe this with C-GMV AE as well. To demonstrate this, we shrink the size of training data by 50% or 90% and train methods on them. Surprisingly, we found C-GMV AE can often match the performance of other methods with only 50% of the training data. Tab. 5 compares MPVAE trained on full data and C-GMV AE trained on 50% of data. Their performances approximately match. We further compare several major state-of-the-art methods including ours all trained on the same randomly selected 10%, 50% and 100% of the data and show their performance over C2AE. Fig. 2 shows the improvements over C2AE on ma-F1. Ours clearly outperforms others on fewer data. More plots on other datasets and metrics are in appendix.

Interpretability Our work is also motivated by ecological applications (Gomes, Dietterich et al. 2019), where it is important to understand species interactions. Fig. 3 shows a map of label-label embedding inner-product weights for the eBird dataset. The bird species on the x-axis and the y-axis are the same. The first 3 bird species are water birds, the following 4 bird species are forest birds. The last 3 bird species are residential birds. The darker the grid is, the closer two birds will be. We subtract the diagonal to exclude the self correlation. The heatmap matrix clearly form three blocks. The first block contains Black-backed Gull, Rough-winged Swallow and Great Blue Heron. These three birds are water birds living near sea or lake. The second block has Tufted Titmouse, Northern Flicker, Northern Mockingbird, and Cedar Waxwing. These birds typically live in the forest with a lot of trees. The remaining birds are commonly seen residential birds, Mourning Dove, House Sparrow and Common Starling. They live inside or near human residences. Since human activities are wide-spread, the distribution of these birds are therefore quite broad. For example, Mourning Dove also has some correlations with forest birds in Fig. 3. But one can observe that for each group of birds, their intra-group correlations are always stronger than inter-group correlations. Therefore, the learnt embeddings do encompass semantic meanings. The derived correlations could also help the study of wildlife protection (Johnston et al. 2019).

Conclusion In this work, we propose a contrastive learning boosted Gaussian mixture variational autoencoder (C-GMV AE) multi-label predictor, a novel method for MLC. C-GMV AE combines the learning of a Gaussian mixture latent space with the contrastive learning of feature and label embeddings. Not only does C-GMV AE achieve the state-of-the-art
performance, it also provides insights into semi-supervised learning and model interpretability. Interesting future directions include the exploration of various contrastive learning mechanisms, model architecture improvements, and other latent space structures.

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Contrastive Learning Module

Connection with Triplet Loss

Triplet loss (Wang et al. 2014) is one of the popular ranking losses used in multi-label learning (Seymour and Zhang 2018).

Given an anchor embedding \( v^f_\mathbf{a} \), a positive embedding \( v^f_+ \), and a negative embedding \( v_- \), they form a triplet \((v^f_\mathbf{a}, v^f_+, v_-)\). A triplet loss is defined as

\[
\mathcal{L}_{\text{trip}}(v^f_\mathbf{a}, v^f_+, v_-) = \max\{0, g + \text{dist}(v^f_\mathbf{a}, v^f_+) - \text{dist}(v^f_\mathbf{a}, v_-)\} \tag{8}
\]

where \( g \) is a gap parameter measuring the distance between \((v^f_\mathbf{a}, v^f_+)\) and \((v^f_\mathbf{a}, v_-)\), and \( \text{dist}(\cdot, \cdot) \) is a distance function. This hinge loss \( \mathcal{L}_{\text{trip}} \) encourages fewer violations to “positive > negative” ranking order. Let \( \tau = 1/2 \). With the same triplet, we can write down a contrastive loss

\[
\begin{align*}
\mathcal{L}_{\text{CL}}(v^f_\mathbf{a}, v^f_+, v^-) &= -\log \frac{\exp(2 \cdot v^f_\mathbf{a} \cdot v^f_+)}{\sum_{t \in \{+, -\}} \exp(2 \cdot v^f_t \cdot v^f_t)} \\
&= \log(1 + \frac{\exp(2 \cdot v^f_\mathbf{a} \cdot v^f_-)}{\exp(2 \cdot v^f_t \cdot v^f_t)}) \\
&\approx 1 + (2 \cdot v^f_\mathbf{a} \cdot v^f_- - 2 \cdot v^f_\mathbf{a} \cdot v^f_+) \\
&= 1 + (v^f_\mathbf{a} \cdot v^f_- + 2v^f_\mathbf{a} \cdot v_- - v^f_\mathbf{a} \cdot v_+ + v^f_+ \cdot v_+) \\
&= ||v^f_- - v^f_+||^2 + ||v^f_- - v^f_-||^2 + 1 \tag{9}
\end{align*}
\]

Note that in the second to the last equation, \( v^f_+ \) and \( v^- \) have the same norm due to the normalization in our contrastive learning module.

By setting \( \text{dist}(\cdot, \cdot) \) to commonly used \( \ell_2 \) distance and \( g = 1 \), Eq. 9 is a fair approximation of Eq. 8. Therefore, triplet loss can be viewed as a special case of our contrastive loss. But in contrastive losses, embeddings are normalized and more positives/negatives are available. As shown in (Chen et al. 2020), contrastive loss generally outperforms triplet loss.

Gradients of Contrastive Loss

Recall our contrastive loss:

\[
\mathcal{L}_{\text{CL}} = \sum_{(x, y) \in B} \frac{1}{|P(y)|} \sum_{p \in P(y)} -\log \frac{\exp(v^f_x \cdot v^f_{y} / \tau)}{\sum_{t \in A} \exp(v^f_x \cdot v^f_t / \tau)} \tag{10}
\]

For the illustration purpose, we only consider one sample \((x, y)\) instead of one batch:

\[
\mathcal{L}_{\text{CL}} = \frac{1}{|P(y)|} \sum_{p \in P(y)} -\log \frac{\exp(v^f_x \cdot v^f_{y} / \tau)}{\sum_{t \in A} \exp(v^f_x \cdot v^f_t / \tau)} \tag{11}
\]

Define \( N(y) = A \setminus P(y) \). We now derive the gradients w.r.t. \( v^f_x \).

\[
\frac{\partial \mathcal{L}_{\text{CL}}}{\partial v^f_x} = \frac{1}{\tau|P(y)|} \sum_{p \in P(y)} \left( \sum_{t \in A} v^f_t \exp(v^f_t \cdot v^f_x / \tau) - v^f_x \right) \\
= \frac{1}{\tau|P(y)|} \sum_{p \in P(y)} \left( \sum_{t \in A} v^f_t \exp(v^f_t \cdot v^f_x / \tau) + \sum_{t \in N(y)} v^f_t \exp(v^f_t \cdot v^f_x / \tau) - v^f_x \right) \\
= \frac{1}{\tau} \sum_{t \in A} \exp(v^f_x \cdot v^f_t / \tau) + \frac{1}{\tau} \sum_{t \in N(y)} \exp(v^f_x \cdot v^f_t / \tau) - \frac{1}{\tau|P(y)|} \sum_{p \in P(y)} v^f_t \\
= \frac{1}{\tau|P(y)|} \sum_{p \in P(y)} \left( \sum_{t \in A} \exp(v^f_t \cdot v^f_x / \tau) - \frac{1}{|P(y)|} \right) + \frac{1}{\tau} \sum_{t \in N(y)} \exp(v^f_x \cdot v^f_t / \tau) \\
\]

Further, we have the unnormalized feature embedding \( w^f_x, v^f_x = \frac{w^f_x}{||w^f_x||} \).

\[
\frac{\partial v^f_x}{\partial w^f_x} = \frac{1}{||w^f_x||}(I - w^f_x w^f_x^T) \frac{1}{||w^f_x||^2} \\
= \frac{1}{||w^f_x||}(I - w^f_x w^f_x^T) \tag{13}
\]

where \( I \) is an \( E \times E \) identity matrix.

The gradient of \( \mathcal{L}_{\text{CL}} \) w.r.t. \( w^f_x \) can be derived using chain rule,

\[
\frac{\partial \mathcal{L}_{\text{CL}}}{\partial w^f_x} = \frac{\partial v^f_x}{\partial w^f_x} \frac{\partial \mathcal{L}_{\text{CL}}}{\partial v^f_x} \\
= \frac{1}{\tau|P(y)|} \sum_{p \in P(y)} \left( \sum_{t \in A} \exp(v^f_t \cdot v^f_x / \tau) \right) - \frac{1}{\tau} \sum_{t \in N(y)} \exp(v^f_x \cdot v^f_t / \tau) \\
= \frac{1}{\tau} \left( \sum_{t \in A} \exp(v^f_t \cdot v^f_x / \tau) \right) - \frac{1}{\tau} \sum_{t \in N(y)} \exp(v^f_x \cdot v^f_t / \tau) \tag{14}
\]

We can then observe that if \( v^f_x \) and \( v^f_t \) are orthogonal \((v^f_x v^f_t \to 0)\), \( ||v^f_x - (v^f_x v^f_t) v^f_t|| \) will be close to 1 and the gradients would be large. Otherwise, for weak positives or negatives \((||v^f_x v^f_t|| \to 1)\), the gradients would be small.
Figure 4: Relative performances w.r.t. HA, ex-F1, mi-F1 and ma-F1 on *mirflickr* dataset.

Figure 5: Relative performances w.r.t. HA, ex-F1, mi-F1 and ma-F1 on *nus-vec* dataset.
Supplementary Experimental Results

Implementation Details

We use one Tesla V100 GPU on CentOS for every experiment. The batch size is set to 128. The latent dimensionality is 64. The feature encoder is an MLP with 3 hidden layers of sizes [256, 512, 256]. The label encoder has 2 hidden layers of sizes [512, 256]. The decoder contains 2 hidden layers of sizes [512, 512]. On reuters and bookmarks, we add one more hidden layer with 512 units to the decoder. The embedding size E is 2048 (tuned within the range [512, 1024, 2048, 3072]). We set α = 1 (tuned within [0.1, 0.5, 1, 1.5, 2]), β = 0.5 (tuned within [0.1, 0.5, 1, 1.5, 2.0]) for most runs. We tune learning rates from 0.0001 to 0.004 with interval 0.0002, dropout ratio from [0.3, 0.5, 0.7], and weight decay from [0, 0.01, 0.0001]. Grid search is adopted for tuning. The final hyper-parameter selections are shown in Tab. 7. Every batch in our experiments requires less than 16GB memory. The number of epochs is 100 by default.

Training on Fewer Data

We provide relative performances of several major state-of-the-art methods including ours to C2AE, on HA, ex-F1, mi-F1, ma-F1 scores. All methods are trained on 10% or 50% of the data, including C2AE. The compared results have the

![Figure 7: Label-label embedding inner-products by MP-VAE.](image)

| # Samples | # Labels /Sample | Mean Labels /Sample | Median Labels /Sample | Max Labels /Sample |
|-----------|-----------------|---------------------|-----------------------|-------------------|
| eBird     | 41778           | 100                 | 20.69                 | 18                | 96                |
| bookmarks | 87856           | 208                 | 2.03                  | 1                 | 44                | 584.67            |
| nus-vec   | 269648          | 85                  | 1.86                  | 1                 | 12                | 372.17            |
| mirflickr | 25000           | 38                  | 4.80                  | 5                 | 17                | 1247.34           |
| reuters   | 10789           | 90                  | 1.23                  | 1                 | 15                | 106.50            |
| scene     | 2407            | 6                   | 1.07                  | 1                 | 3                 | 170.83            |
| sider     | 1427            | 27                  | 15.3                  | 16                | 26                | 731.07            |
| yeast     | 2417            | 14                  | 4.24                  | 4                 | 11                | 363.14            |
| delicious | 16105           | 983                 | 19.06                 | 20                | 25                | 250.15            |

Table 6: Dataset Statistics.
Table 7: Major hyperparameters used in training. “lr” stands for learning rate.

| Dataset   | lr   | α  | β  | E    | dropout | bs  |
|-----------|------|----|----|------|---------|-----|
| eBird     | 0.001| 1  | 0.5| 2048 | 0.5     | 128 |
| bookmarks | 0.002| 1  | 1  | 2048 | 0.5     | 128 |
| nus-vec   | 0.004| 1  | 0.5| 1024 | 0.5     | 256 |
| mirflickr | 0.001| 2  | 0.5| 2048 | 0.5     | 128 |
| reuters   | 0.005| 2  | 1  | 2048 | 0.5     | 128 |
| scene     | 0.003| 1  | 0.5| 512  | 0.3     | 128 |
| sider     | 0.002| 1  | 0.5| 512  | 0.5     | 128 |
| yeast     | 0.002| 1  | 0.5| 512  | 0.5     | 128 |
| delicious | 0.001| 1  | 0.5| 2048 | 0.5     | 128 |

same amount of data for training and thus the comparison is fair.

Fig. 4, Fig. 5, Fig. 6 show the relative performance of various state-of-the-art methods over C2AE, on mirflickr, nus-vec, eBird respectively.