SELF-SUPERVISED REPRESENTATION LEARNING WITH MULTI-SEGMENTAL INFORMATIONAL CODING (MUSIC)

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ABSTRACT

Self-supervised representation learning maps high-dimensional data into a meaningful embedding space, where samples of similar semantic contents are close to each other. Most of the recent representation learning methods maximize cosine similarity or minimize the distance between the embedding features of different views from the same sample usually on the $l_2$ normalized unit hypersphere. To prevent the trivial solutions that all samples have the same embedding feature, various techniques have been developed, such as contrastive learning, stop gradient, variance and covariance regularization, etc. In this study, we propose Multi-Segmental Informational Coding (MUSIC) for self-supervised representation learning. MUSIC divides the embedding feature into multiple segments that discriminatively partition samples into different semantic clusters and different segments focus on different partition principles. Information theory measurements are directly used to optimize MUSIC and theoretically guarantee trivial solutions are avoided. MUSIC does not depend on commonly used techniques, such as memory bank or large batches, asymmetry networks, gradient stopping, momentum weight updating, etc, making the training framework flexible. Our experiments demonstrate that MUSIC achieves better results than most related Barlow Twins and VICReg methods on ImageNet classification with linear probing, and requires neither deep projectors nor large feature dimensions. Code will be made available.

1 Introduction

Self-supervised representation learning (SSRL) has been a core task in machine learning and seen rapid progress over past years. Deep neural networks pre-trained on large-scale unlabeled datasets via SSRL have demonstrated desirable characteristics, such as strong robustness and generalizability, and improving various down-stream tasks especially when annotations are scarce. An effective approach for SSRL is to enforce semantically similar samples (i.e., different transformations from the same instance) close to each other in the embedding space. Simply maximizing the similarity or minimizing the Euclidean distance between embedding features of similar semantic samples tends to produce trivial solutions, e.g., all samples have the same embedding. Recently, various excellent methods have been proposed to learn meaningful representations features and avoid trivial solutions. Contrastive learning based methods, such as SimCLR and MoCo, have achieved great successes by additionally minimizing the similarity between embeddings of reference and negative samples, which requires either relatively large batches or a memory bank of negative samples during training. To avoid using negative samples during training, BYOL and SimSiam introduce some clever techniques, such as asymmetry network architecture with additional predictor head and stop gradients, etc. Subsequent theoretical analysis have demonstrated why these techniques can avoid trivial solutions and learn meaningful representations from different aspects. Clustering-based methods DeepCluster, SELA, SwAV alternatively compute the cluster assignment of one view and optimize the network to predict the same assignment from other views of the same sample, where trivial solutions can be avoided via even assignment of samples over different clusters in a non-differentiable manner. In another direction, W-MSE and Barlow Twins propose to drive self- or cross-correlation matrices towards the identity matrix, learning meaningful features without requiring the asymmetry design or a large batch of negative samples. Along the same
Figure 1: Partition of an MUSIC feature vector. An image should be represented by multiple attributes, such as general object parts, textures, shapes, etc. Motivated by this observation, MUSIC divides the embedding feature vector into multiple segments (Seg-1, Seg-2, ..., Seg-S); for example, here we show three different segments colored in red, green, and blue colors respectively to represent different attributes. The general attribute of each segment consists of multiple instantiations, and different instantiated attributes within the same segments are discriminative from each other. For example, Seg-2 represents texture, each unit in Seg-2 represents a specific texture, like dot texture, stripe texture, etc. Here three samples are shown over each unit. The value \( p(s, d) \) in each unit denotes the probability of an image belongs to the \( d^{th} \) instantiated attribute of \( s^{th} \) segment, see Methodology section for more details.
With the empirical joint distribution, two versions of the loss function can be defined. We denote the first version where the probability distribution \( p(s', s'', d', d'') \) gives the dimension of the \( D_S \) instantiated attributes using the softmax function, i.e.,

\[
p_i'(s', d') = \frac{\exp(z_i'(s, d))}{\sum_{k=1}^{D_S} \exp(z_i'(s, k))},
\]

The probability distribution \( p_i'(s, d) \) for the other branch is computed in the same way. Thus, the MUSIC scheme can be interpreted as a combination of multiple classifiers or cluster operators that implement different classification criteria learned in a data-driven fashion.

### 2.2 Multi-Segmental Informational Coding

Here we introduce the MUlti-Segmental Informational Coding (MUSIC) for self-supervised representation learning. The embedding features of the two branches are denoted as: \( z_i'(s, d) \), where \( z_i(s, d) \) is the number of segments, \( D_S \) is the dimension of each segment, and \( D = D_S \times S \) gives the dimension of the whole embedding space. Although the current version of MUSIC scheme evenly splits the embedding vector, it could be in principle extended to uneven configurations. Each segment is normalized to a probability distribution \( p_i'(s', d') \) over \( D_S \) instantiated attributes using the softmax function, i.e.,

\[
p_i'(s', d') = \frac{\exp(z_i'(s, d))}{\sum_{k=1}^{D_S} \exp(z_i'(s, k))},
\]

The probability distribution \( p_i'(s, d) \) for the other branch is computed in the same way. Thus, the MUSIC scheme can be interpreted as a combination of multiple classifiers or cluster operators that implement different classification criteria learned in a data-driven fashion.

### 2.3 Entropy Loss

Based on the probability distributions over multiple segments, we first compute the empirical joint distribution \( p(s', s'', d', d'') \) between the embedding features of two transformations over a batch of samples (similar to [222]):

\[
p(s', s'', d', d'') = \frac{1}{N} \sum_{i=1}^{N} p_i'(s', d') p_i''(s'', d''),
\]

With the empirical joint distribution, two versions of the loss function can be defined. We denote the first version \( L_{ent} \) as a pure entropy-based loss function:

\[
L_{ent} = \frac{1}{S^2} \sum_{s'=1}^{S} \sum_{s''=1}^{S} \sum_{d'=1}^{D_S} \sum_{d''=1}^{D_S} \left(1 - \mathbb{1}(s' = s'', d' \neq d'')\right) p(s', s'', d', d'') \log(p(s', s'', d', d'')), \tag{3}
\]

where \( \mathbb{1}(s' = s'', d' \neq d'') \) is an indicator function that equals to 1 if \( s' = s'' \) and \( d' \neq d'' \), otherwise it is equal to 0. The empirical joint distribution can be denoted by a block matrix in Fig. 2 where \( (1 - \mathbb{1}(s' = s'', d' \neq d'')) \) means...
only keeping diagonal elements and elements of the off-diagonal blocks, as indicated by the orange area. Therefore, minimizing this loss function maximizes the joint entropy over the selected elements. In the next subsection, we show that this single loss function allows to learn meaningful features.

To enhance the transformation invariance of features, we introduce an additional term to maximize the inner product between the embedding features from two transformations. Then, the second version of the loss function is defined as

\[ L = L_{ent} - \lambda \frac{1}{NS} \sum_{i=1}^{N} \sum_{s} \sum_{d=1}^{D_S} \log(p_i(s,d)p_i'(s,d)), \]

where \( \lambda \) is a balancing factor. By default we set \( \lambda = 1 \) and found that \( \lambda \) is not required to be a very small or large number for balancing. Since \( p_i(s,d) \) and \( p_i'(s,d) \) are the probabilities, maximizing their inner product imposes the network to make consistent assignment over all segments between two transformations of the same image. As a result, each segment is encouraged to be a one-hot vector for the maximum inner product. Clearly, this additional term promotes transformation invariance and confident assignments over different attributes. One difference of this term from the entropy loss term is the sample-specific constraint while entropy is a statistical measure.

Our proposed method can be easily implemented, with a PyTorch-style pseudo code in the Appendix. In the following subsection, let us analyze why the entropy loss optimizes meaningful embedding features as illustrated in Fig. [1].

2.4 Analysis

The entropy loss function consists of two parts, including the entropy over diagonal elements and the entropy over the elements of off-diagonal blocks illustrated in Fig. [2] formally denoted as

\[ L_{ent} = \frac{1}{S} \sum_{s',s''} \sum_{d',d''} p(s',s'',d',d'') \log(p(s',s'',d',d'')) + \frac{1}{S(S-1)} \sum_{s',s''} \sum_{d',d''} p(s',s'',d',d'') \log(p(s',s'',d',d'')). \]

For the first part, it can be demonstrated that its optimal solution is \( \forall s, d, p_i(s,d) = p_i'(s,d), p_i'(s,d) \) and \( p''(s,d) \) are one-hot vectors, and \( \frac{1}{N} \sum_{d=1}^{N} p_i(s,d) = \frac{1}{D_S} \). The proof can be found in the Appendix. For the second part, it is intuitive that the optimal solution to maximize the joint entropy over the off-diagonal block items is \( \forall s', s'', d', d'', s' \neq s'', p(s',s'',d',d'') = \frac{1}{(D_S)^2} \); i.e., a batch of samples are evenly assigned over each off-diagonal block.

**Transform Invariance:** The solution that \( p''(s,:) \) and \( p''(s,:) \) are one-hot vectors and equal to each other means that the learned MUSIC embeddings are invariant to transformations, and a sample tends to be confidently represented by a single instantiated attribute within each and every segment.

**Non-trivial Solution:** The solution that \( \frac{1}{N} \sum_{d=1}^{N} p_i(s,d) = \frac{1}{D_S} \) means that each segment evenly partition a batch of samples over \( D_S \) instantiated attributes. Since \( p_i(s,d) \) and \( p''(s,d) \) are one-hot vectors, the trivial solution that all samples have the same embedding features or assigned to the same attribute for each segment can be avoided.

**Minimum Redundancy:** As described in Fig. [1] different segments of the MUSIC embedding vector are expected to focus on complementary attributes. In other words, the redundancy or mutual information between any two segments should be minimized, which is a popular measure for feature selection [23]. Here we can demonstrate the redundancy or mutual information between any two segments is minimized when the optimal solution is obtained. Specifically, the mutual information \( I(s', s'') \) between any segments \( s' \) and \( s'' \) is

\[ I(s', s'') = H(s') + H(s'') - H(s', s'') \]

\[ = - \sum_{d'=1}^{D_S} p'(s',d') \log(p'(s',d')) - \sum_{d''=1}^{D_S} p''(s'',d'') \log(p''(s'',d'')) + \sum_{d'=1}^{D_S} \sum_{d''=1}^{D_S} p(s',s'',d',d'') \log(p(s',s'',d',d'')) \]

\[ = - \log \frac{1}{D_S} - \log \frac{1}{D_S} + \log \frac{1}{(D_S)^2} = 0. \]

Given that the features within each segment are naturally exclusive from each other, MUSIC embedding features are both discriminative and diverse. The redundancy constraint has been studied for W-MSE [19], Barlow Twins [20], and
VICReg \cite{21} by minimizing the covariance in a linear manner. In contrast, our entropy-based loss function reduces the redundancy in a non-linear way. Also, it can be derived that the optimal MUSIC embedding features have zero covariance between any two features in different segments and negative covariance between the features within the same segment. More details can be found in the Appendix.

**Contrastive Learning:** Contrastive learning has proven very effective for representation learning by maximizing the similarity between different transformations of the same instance and minimizing the similarity between the reference and other instances. Here it can be seen that MUSIC is consistent to contrastive learning in a novel way. Specifically, the optimal MUSIC embedding can totally encode \((D_S)^2\) different samples. In our default settings \(D_S = 80, S = 102\) (See the Empirical Analysis below for more details), MUSIC can represent \(80^{102}\) different samples. Maximizing the joint entropy is to evenly assign a batch of samples into all possible embeddings, which means that the embedding features of all instances are enforced to be different from each other like in contrastive learning, given the sufficiently large coding capacity. Therefore, the difference is that contrastive learning differentiates instances by directly enforcing their features to be dissimilar, while MUSIC statistically assigns instances with different assignment codes.

In a word, the MUSIC embedding feature optimized with the entropy-based loss is transform-invariant, non-trivial, discriminative, and diverse.

## 3 Implementation Details

For fair comparison, we followed the same settings in VICReg \cite{21}. Specifically, the standard ResNet-50 backbone \cite{24} was used as the encoder that outputs a representation vector of 2,048 units. We used the same training settings including the data augmentation (random cropping, horizontal flip, color jittering, grayscale, Gaussian blur, solarization, with the same parameters in \cite{21}), the optimizer of LARS \cite{25,26} with a weight decay of \(10^{-6}\) and the learning rate of \(lr = \text{batch}_\text{size}/256 \times \text{base}_\text{lr}\), and the cosine decay schedule \cite{27} from 0 with 10 warmup epochs towards the final value of 0.002. Here we set the base learning rate \(\text{base}_\text{lr}\) to 0.6. By default, we used a two-layer MLP projector \((8,192-8,160)\), the number of segments \(S = 102\), the segment dimension \(D_S = 80\), and \(D = D_S \times S = 8,160\) (similar to the feature dimension used by VICReg and Barlow Twins). The results were respectively analyzed for different feature dimensions, depths of projectors, \(\text{batch}_\text{size}\) segment dimension \(D_S\), and training epochs. MUSIC introduces a single extra hyperparameter \(D_S\), its effects on the performance was evaluated. All experiments were conducted on the 1,000-classes ImageNet dataset, where labels were not used for self-supervised representation learning.

## 4 Results

### 4.1 Linear and Semi-Supervised Evaluations on ImageNet

We followed the common evaluation protocol, i.e., linear probing that trains a linear classifier on top of the frozen representations, to evaluate the representations of self-supervised learning methods. Being consistent with Barlow Twins \cite{20} and VICReg \cite{21}, a ResNet-50 backbone was trained with the batch size of 2,048 for 1,000 epochs on the training set of ImageNet, and the linear classification results including Top-1 and Top-5 accuracies of different methods on the evaluation set are reported in Table 1. The difference from Barlow Twins and VICReg is that MIDC used a two-layer MLP projector \((8,192-8,160)\) instead of three layers \((8,192-8,192-8,192)\). We followed exactly the same hyperparameters of VICReg \cite{21} for training the linear classifier. The performance of VICReg is on par with another state of the art method BYOL that uses asymmetric techniques, such as an additional predictor and a momentum encoder. The comparative results show that MUSIC achieves better results than Barlow Twins and VICReg, where all these three methods trained a twin architecture without using negative pairs or any asymmetric techniques. Significantly relaxed constraints on the MUSIC architecture make it adaptable to more applications like multi-modal mapping. The different motivation behind and theoretical framework of MIDC lead to some unique characteristics that the projector depth, feature dimension, and batch size can be smaller than what used in the competing algorithms to obtain similar results. More results are the in Empirical Analysis below.

We also evaluated its effectiveness on semi-supervised learning. Here the pretrained ResNet-50 with MUSIC was fine-tuned on subsets of ImageNet, including 1% and 10% of full ImageNet data respectively. All the comparison methods used the same subset images. Currently, MUSIC is not as good as Barlow Twins and VICReg in the semi-supervised learning settings, while it is better than BYOL and other compared methods. Note that the current results of MUSIC were obtained by simply using the training parameters for Barlow Twins, while different methods usually used different hyperparameters to achieve their best results for this task. The compared methods did a grid search for different learning rates of the backbone and linear head and report the best results. In future, we plan to report more results optimized in a similar way.
Table 1: Comparison of different methods on ImageNet linear classification. Top-1 and Top-5 accuracies (in %) of ResNet50 are reported.

| Methods           | Top-1 | Top-5 |
|-------------------|-------|-------|
| Supervised        | 76.5  | -     |
| MoCo (2020)       | 60.6  | -     |
| PIRL (2020)       | 63.6  | -     |
| CPC v2 (2019)     | 63.8  | -     |
| CMC (2019)        | 66.2  | -     |
| SimCLR (2020)     | 69.3  | 89.0  |
| MoCo v2 (2020)    | 71.1  | 90.1  |
| SimSiam (2020)    | 71.3  | -     |
| SwAV (2020)       | 71.8  | -     |
| BYOL (2020)       | 74.3  | 91.6  |
| Barlow Twins (2021)| 73.2 | 91.0  |
| VICReg (2022)     | 73.2  | 91.1  |
| MUSIC (Ours)      | 73.6  | 91.4  |

Table 2: Semi-Supervised Learning. Top-1 and Top-5 accuracies (in %) of classification on ImageNet. These results were obtained using ResNet50.

| Methods           | Top-1 | Top-5 |
|-------------------|-------|-------|
|                  | 1%    | 10%   | 1%    | 10%   |
| Supervised        | 25.4  | 56.4  | 48.4  | 80.4  |
| MoCo (2020)       | -     | -     | 57.2  | 83.8  |
| SimCLR (2020)     | 48.3  | 65.6  | 75.5  | 87.8  |
| BYOL (2020)       | 53.2  | 68.8  | 78.4  | 89.0  |
| Barlow Twins (2021)| 55.0 | 69.7  | 79.2  | 89.3  |
| VICReg (2022)     | 54.8  | 69.5  | 79.4  | 89.5  |
| MUSIC (Ours)      | 54.0  | 69.0  | 78.9  | 89.1  |

4.2 Empirical Analysis

In this subsection, we evaluated the effects of different hyperparameters on the proposed MUSIC method and compared it with other SSRL methods. All methods were evaluated with linear classification on ImageNet.

4.2.1 Effects of Epoch Number

The SSRL methods in different studies do not always use the same training epochs due to different computational environments. Here MUSIC was evaluated on different training epochs as reported in Table 3. MUSIC is consistently better than most of existing methods on all different training epochs. When the training epochs are small (100 and 200), MUSIC can converge to the best results.

4.2.2 Effect of Batch Size

Here we evaluated the performance of MUSIC on different batch sizes. The results in Table 4 show that MUSIC is consistently better than the compared methods using different batch sizes.
Table 3: **Comparison of different training epochs.** Top-1 accuracy (in %) of linear results for linear classification on ImageNet were obtained using ResNet50.

| Methods    | SimCLR | MoCo v2 | BYOL | SwAV | SimSiam | Barlow Twins | VICReg | MUSIC |
|------------|--------|---------|------|------|---------|--------------|--------|-------|
| 100 epochs | 66.5   | 67.4    | 66.5 | 66.5 | 68.1    | 68.7         | 68.6   | 69.4  |
| 200 epochs | 68.3   | 69.9    | 70.6 | 69.6 | 70.0    | -            | -      | 71.8  |
| 400 epochs | 69.8   | 71.0    | 73.2 | 70.7 | 70.8    | -            | -      | 73.1  |
| 800 epochs | 70.4   | 72.2    | 74.3 | 71.8 | 71.3    | -            | -      | 73.4  |

Table 4: **Batch Size.** Top-1 accuracy (in %) results for linear classification on ImageNet were obtained based on ResNet50 with 100 pretraining epochs.

| Batch Size | 512 | 1024 | 2048 |
|------------|-----|------|------|
| SimSiam    | 68.1| 68.0 | 67.9 |
| VICReg     | 68.2| 68.3 | 68.6 |
| MUSIC      | 68.3| 69.3 | 69.4 |

Table 5: **Projector Depth.** Top-1 and Top-5 accuracies (in %) of linear classification on ImageNet were obtained based on ResNet50 with 100 pretraining epochs.

| Projector Depth | 2 (8192-8160) | 3 (8192-8192-8160) | 4 (8192-8192-8192-8160) |
|-----------------|---------------|--------------------|--------------------------|
| Top-1           | 69.4          | 68.5               | 67.9                     |
| Top-5           | 89.3          | 88.3               | 87.9                     |

Table 6: **Enhanced Transform Invariance Loss.** Top-1 and Top-5 accuracies (in %) of linear classification on ImageNet were obtained based on ResNet50 with 100 pretraining epochs.

| Loss                  | Entropy       | Entropy + Transform Invariance |
|-----------------------|---------------|--------------------------------|
| Top-1                 | 65.4          | 69.4                           |
| Top-5                 | 86.9          | 89.3                           |

Table 7: **Segment Dimension.** Top-1 and Top-5 accuracies (in %) of linear classification on ImageNet were obtained based on ResNet50 with 100 pretraining epochs.

| DS | 32 | 64 | 80 | 96 | 128 |
|----|----|----|----|----|-----|
| Top-1 | 67.8 | 69.1 | 69.4 | 69.2 | 68.4 |
| Top-5 | 88.5 | 89.1 | 89.3 | 89.1 | 88.5 |
Table 8: **Feature Dimension**. Top-1 accuracy (in %) results for linear classification on ImageNet were obtained based on ResNet50 with 100 pretraining epochs.

| Feature Dimension | 1024 (960) | 2048 (2000) | 4096 (4080) | 8192 (8160) | 16384 (16320) |
|-------------------|------------|-------------|-------------|-------------|---------------|
| VICReg            | 62.4       | 65.1        | 67.3        | 68.6        | 68.8          |
| MUSIC             | 64.1       | 66.6        | 69.2        | 69.4        | 69.1          |

4.2.3 **Effect of Projector Depth**

The existing methods [20] require at least 3 layers of MLP as the projector for the best results. However, MUSIC has a different behavior that a two-layer MLP achieves the best results as shown in Table 5. These results may be due to the discriminability and diversity of MUSIC embeddings, making it easy to meaningfull representations.

4.2.4 **Effects of Loss Function**

As described in the Methodology section, optimizing the entropy loss only can avoid trivial solutions and learn meaningful representations. This theoretical analysis is consistent with the empirical results in Table 5 that 65.4% Top-1 was achieved using the entropy loss only, comparable to some methods reported in Table 1. Adding the enhanced transform invariance term can significantly improve the performance, as also discussed in the Methodology section, the transform invariance can be further enhanced with this image-level constraint.

4.2.5 **Effect of Segment Dimension**

The effect of our unique hyperparameter, i.e., segment dimension, was underlined. Our experimental results of different segment dimensions in Table 7 indicate that $D_s = 80$ achieved the best results, where the dimension of the whole embedding feature was kept the same. It can be seen that the performance is not sensitive to this hyperparameter.

4.2.6 **Effects of Feature Dimension**

In the previous studies for Barlow Twins and VICReg, it was found that increasing the feature dimension is very effective to improve the representation learning performance. It was also found that the feature dimension plays an important role in MUSIC. The results of different feature dimensions for VICReg and MUSIC are reported in Table 8. It can be seen that MUSIC achieves consistently better results than VICReg on different embedding feature dimensions. Importantly, when the embedding feature dimension is reasonably large (4,096 and 8,192), MUSIC achieves the best results and better than the best results of VICReg using the large dimension of 16,384. In practice, we found that the large embedding feature dimension (i.e., 16,384) significantly increases the computational and memory cost for Barlow Twins, VICReg, and MUSIC that compute the covariance or joint entropy matrix, which was also discussed in the Barlow Twins study [20]. Therefore, MUSIC seems both efficient and effective.

5 **Conclusion**

We have presented the multi-segment informational coding (MUSIC) optimized with an entropy-based loss function for self-supervised representation learning. Experimental results show that MUSIC achieves equivalent or better representation learning results compared with the state of the art methods in terms of linear classification. The presented new framework ensures that MUSIC can avoid trivial solutions and learn discriminative and diverse features. Interestingly, MUSIC has shown some unique characteristics that the projector can be a shallower MLP, the batch size and the embedding feature dimension can be smaller than that used in existing methods while achieving comparable or better results. In the future, we will adapt and evaluate MUSIC to more downstream tasks, such as multi-modality tasks and medical applications.
Appendix A  PyTorch Pseudocode

An example of PyTorch-style implementation for MUSIC is described in Algorithm 1.

Algorithm 1: PyTorch-style pseudocode for MUSIC

for i in loader:  # load a batch with N samples
    # two randomly augmented versions of x
    x', x'' = augment(x)

    # compute embeddings
    z' = augment(x')
    z'' = augment(x'')

    # multi-segment discriminative coding
    x' = torch.reshape(x', [N, -1, D_S])  # N × S × D_S
    x'' = torch.reshape(x'', [N, -1, D_S])  # N × S × D_S
    p' = torch.softmax(x', dim=2)  # transform to probability
    p'' = torch.softmax(x'', dim=2)  # transform to probability

    # compute transform invariance loss
    loss_TI = -torch.log((p'*p'').sum(dim=2)).mean()

    # compute entropy loss
    p' = torch.reshape(p', [N, D])  # N × D
    p'' = torch.reshape(p'', [N, D])  # N × D
    p = torch.einsum('np,nq->pq', [p', p'']) / N  # compute empirical joint distribution
    p_s = select(p)
    loss_ent = (p_s * torch.log(p_s)).sum() / (S × S)

    # final loss
    loss = loss_ent + lambda * loss_TI  # lambda=1 by default

    # optimization step
    loss.backward()
    optimizer.step()
Since every diagonal block has the same optimal solution, here we can only consider the $s^{th}$ diagonal block, and the object function can be simplified as

$$L_{ent}(s, s) = \sum_{d=1}^{D_S} p(s, s, d, d) \log(p(s, s, d, d))$$  \hfill (B-8)

where $0 \leq p(s, s, d, d) \leq 1$, $0 \leq \sum_{d=1}^{D_S} p(s, s, d, d) \leq 1$. Then, it is easy to find the solution that minimizes this objective function, i.e., $\forall s, d, p(s, s, d, d) = \frac{1}{D_S}$, or $\forall s', s''$, $s' = s''$, $d', d'' = d''$, $p(s', s'', d', d'') = \frac{1}{D_S}$.

As defined in Eqs. (1) and (2), we have $\forall s', s'', s' = s''$, if $d', d'' = d''$, either $0 < p_i'(s', d') < 1$ or $0 < p_i''(s'', d'') < 1$, then we have either $p_i'(s', d') < \sum_{d''=1}^{D_S} p_i(s', d') = 1$ or $p_i''(s'', d'') < \sum_{d''=1}^{D_S} p_i(s'', d'') = 1$. When $p_i'(s', d') < \sum_{d''=1}^{D_S} p_i(s', d'') = 1$, then we have

$$\sum_{d', d'', d''=d''} p(s', s'', d', d'') = \sum_{d', d'', d''=d''} \frac{1}{D_S} = \frac{D_S}{D_S} = 1$$  \hfill (B-9)

Given the above derived results, let us next prove that for $\forall s', s''$, $s' = s''$, $\exists d', d'', d' = d''$, $p_i'(s', d) = p_i''(s'', d) = 1$ by contradiction.

If its negation is true, i.e., $\forall s', s'', s' = s''$, if $\exists d', d'', d' = d''$, either $0 < p_i'(s', d') < 1$ or $0 < p_i''(s'', d'') < 1$, then we have either $p_i'(s', d') < \sum_{d''=1}^{D_S} p_i(s', d') = 1$ or $p_i''(s'', d'') < \sum_{d''=1}^{D_S} p_i(s'', d'') = 1$. When $p_i'(s', d') < \sum_{d''=1}^{D_S} p_i(s', d'') = 1$, then we have

$$\sum_{d', d'', d''=d''} p(s', s'', d', d'') = \sum_{d', d'', d''=d''} \frac{1}{N} \sum_{i=1}^{N} p_i'(s', d') p_i''(s'', d'')$$

$$= \frac{1}{N} \sum_{i=1}^{N} \sum_{d', d'', d''=d''} p_i'(s', d') p_i''(s'', d'')$$

$$= \frac{1}{N} \sum_{i=1}^{N} \sum_{d'=1}^{D_S} p_i'(s', d') p_i''(s'', d')$$

$$< \frac{1}{N} \sum_{i=1}^{N} \sum_{d'=1}^{D_S} p_i'(s', d') \sum_{d''=1}^{D_S} p_i''(s'', d'')$$

$$= 1$$

That is, $\sum_{d', d'', d''=d''} p(s', s'', d', d'') < 1$, which leads to a contradiction with Eq. (B-9). Similarly, when $p_i''(s'', d'') < \sum_{d''=1}^{D_S} p_i(s'', d'') = 1$, we have the same conclusion. Therefore, the statement that $\forall s', s'', s' = s''$, if $d' = d''$, then $p_i'(s', d') = p_i''(s'', d'') = 1$ is true. It means that for $\forall s$, $p_i'(s, :)$ and $p_i''(s, :)$ are one-hot vectors and equals to each other.

Because $\forall s, d, p(s, s, d, d) = \frac{1}{D_S}, p'(s, d) = p''(S, d)$, and $p'(S, d)$ and $p''(S, d)$ are one-hot vectors, then $p'(s, d) = \frac{1}{D_S} \sum_{i=1}^{D_S} p_i'(s, d) p_i''(s, d) = \frac{1}{N} \sum_{i=1}^{N} p_i'(s, d) = \frac{1}{D_S}$. This each segment evenly assigns samples into each unit.

**Covariance of the optimal solution.** The optimal solution to maximize the joint entropy over the off-diagonal blocks for the second part is $p(s', s'', d', d'') = \frac{1}{(D_S)^2}$, $\forall s' \neq s''$. According to the above proof that each segment evenly assigns samples into each unit, then $\mathbb{E}[p(s', d')] = \frac{1}{D_S}$. We can theoretically demonstrate the covariance between any two bins from different segments is zero. Specifically, $\forall s', s'', s' \neq s'', d', d''$, we have

$$\text{cov}[p(s', d'), p(s'', d'')] = \mathbb{E}[p(s', d') p(s'', d'')] - \mathbb{E}[p(s', d')] \mathbb{E}[p(s'', d'')]$$

$$= p(s', d', s'', d'') - \frac{1}{D_S} \times \frac{1}{D_S}$$

$$= \frac{1}{(D_S)^2} - \frac{1}{D_S} \times \frac{1}{D_S} = 0.$$  \hfill (B-11)
Furthermore, any two units within the same segment are negatively correlated. Formally, \( \forall s, d' \neq d'' \), we have
\[
\text{cov}[p(s, d'), p(s, d'')] = \mathbb{E}[p(s, d')p(s, d'')] - \mathbb{E}[p(s, d')]\mathbb{E}[p(s, d'')]
\]
\[
= p(s, d', s, d'') - \frac{1}{D_S} \times \frac{1}{D_S}
\]
\[
= 0 - \frac{1}{D_S} \times \frac{1}{D_S} = -\frac{1}{D_S^2}.
\]
That is, the unit within each segment encodes discriminative features, while the units from different segments encode unrelated and diverse features.

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